



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 05:58 PM EST

PDB ID : 7KW9
BMRB ID : 30820
Title : NMR Structure of a tRNA 2'-phosphotransferase from *Runella slithyformis* in complex with NAD⁺
Authors : Alphonse, S.; Dantuluri, S.; Banerjee, A.; Shuman, S.; Ghose, R.
Deposited on : 2020-11-30

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

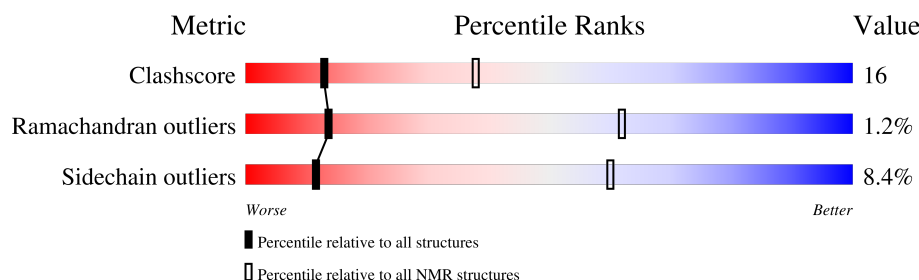
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	178	

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:77 (74)	0.53	9
2	A:91-A:115, A:121-A:178 (83)	0.75	19

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 5 single-model clusters were found.

Cluster number	Models
1	2, 3, 11, 13, 15, 19
2	12, 16, 17, 20
3	8, 9, 14
4	4, 6
Single-model clusters	1; 5; 7; 10; 18

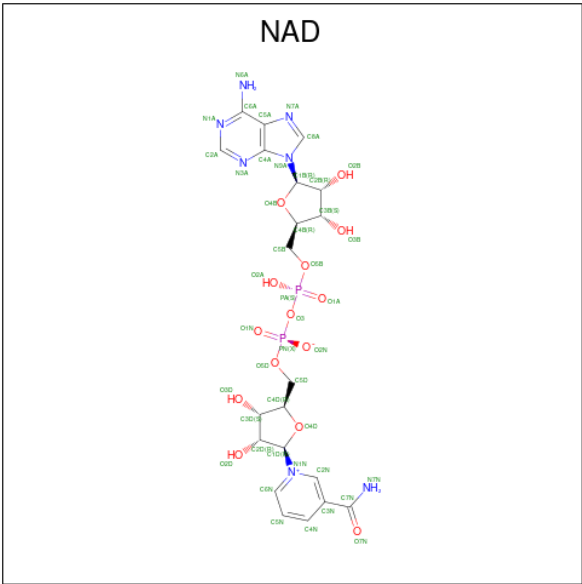
3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 2902 atoms, of which 1461 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called tRNA 2'-phosphotransferase.

Mol	Chain	Residues	Atoms						Trace
1	A	178	Total	C	H	N	O	S	0
			2832	896	1435	248	247	6	

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



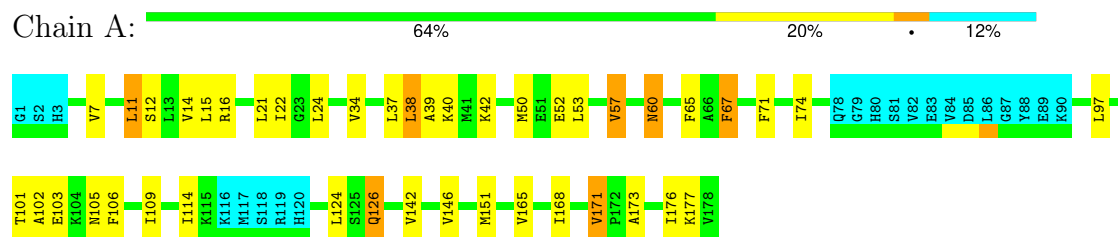
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			70	21	26	7	14	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: tRNA 2'-phosphotransferase

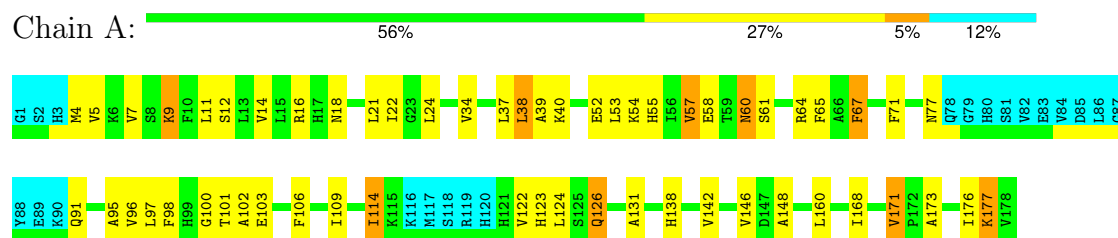


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

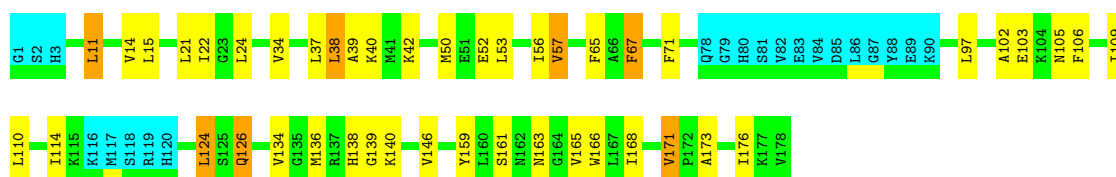
- Molecule 1: tRNA 2'-phosphotransferase



4.2.2 Score per residue for model 2

- Molecule 1: tRNA 2'-phosphotransferase





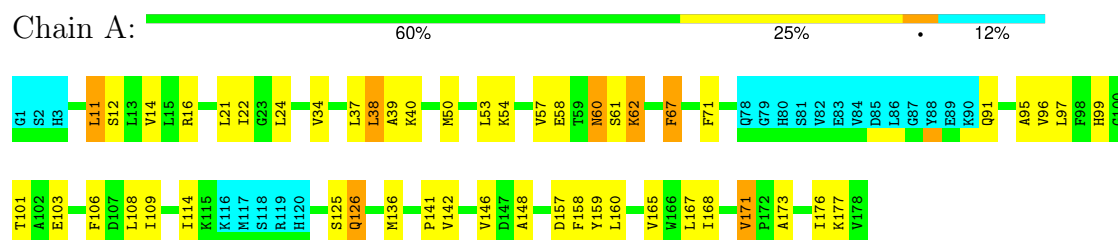
4.2.3 Score per residue for model 3

- Molecule 1: tRNA 2'-phosphotransferase



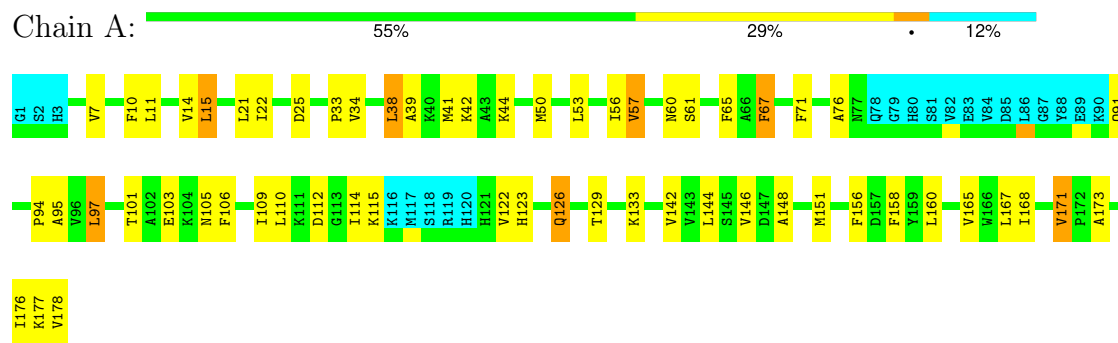
4.2.4 Score per residue for model 4

- Molecule 1: tRNA 2'-phosphotransferase



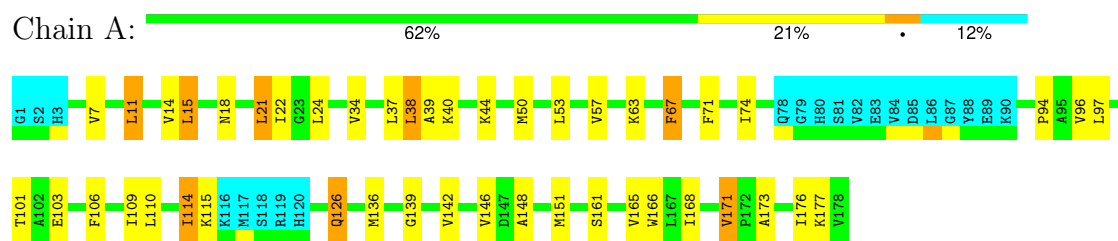
4.2.5 Score per residue for model 5

- Molecule 1: tRNA 2'-phosphotransferase



4.2.10 Score per residue for model 10

- Molecule 1: tRNA 2'-phosphotransferase



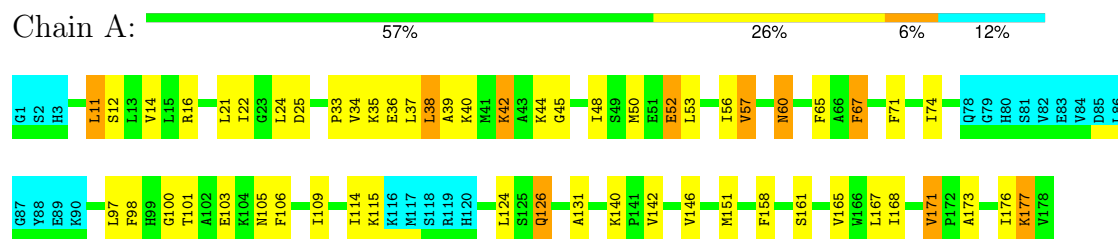
4.2.11 Score per residue for model 11

- Molecule 1: tRNA 2'-phosphotransferase



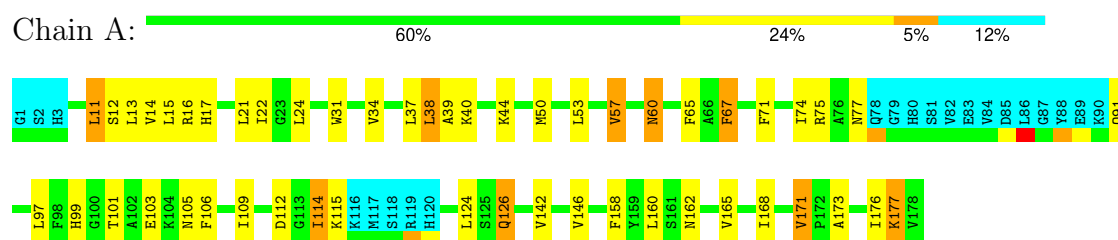
4.2.12 Score per residue for model 12

- Molecule 1: tRNA 2'-phosphotransferase



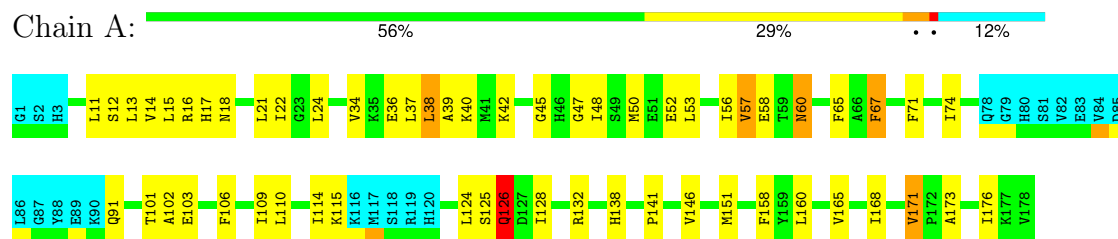
4.2.13 Score per residue for model 13

- Molecule 1: tRNA 2'-phosphotransferase



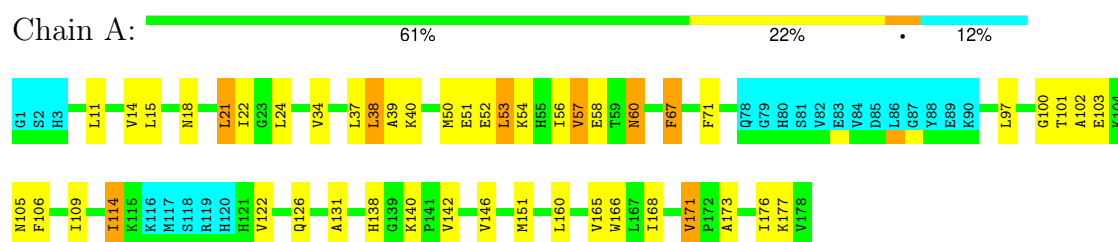
4.2.14 Score per residue for model 14

- Molecule 1: tRNA 2'-phosphotransferase



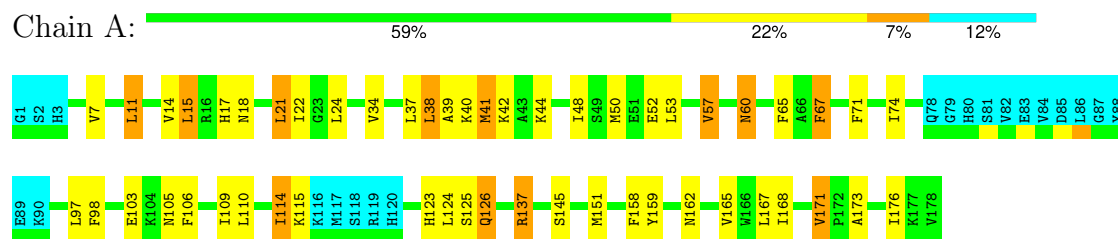
4.2.15 Score per residue for model 15

- Molecule 1: tRNA 2'-phosphotransferase



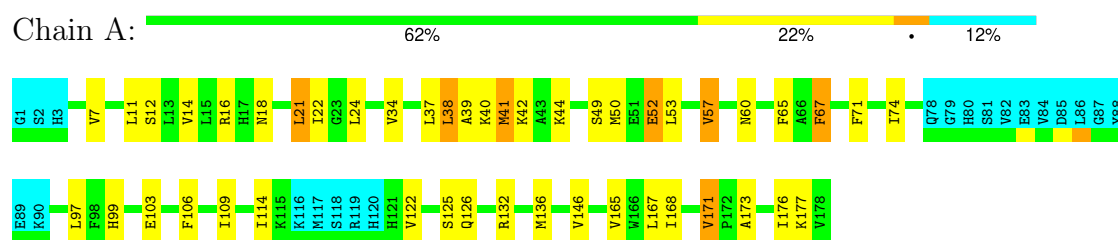
4.2.16 Score per residue for model 16

- Molecule 1: tRNA 2'-phosphotransferase



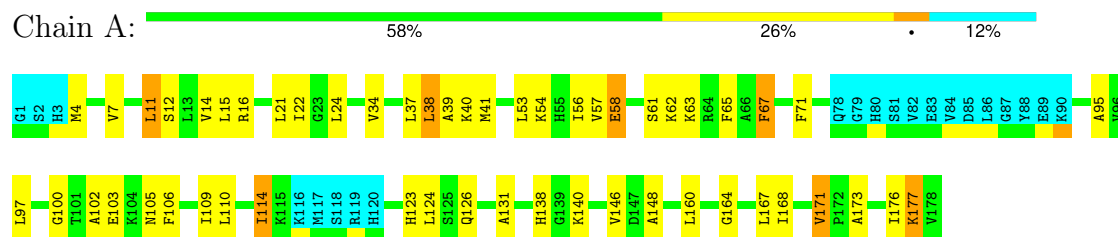
4.2.17 Score per residue for model 17

- Molecule 1: tRNA 2'-phosphotransferase



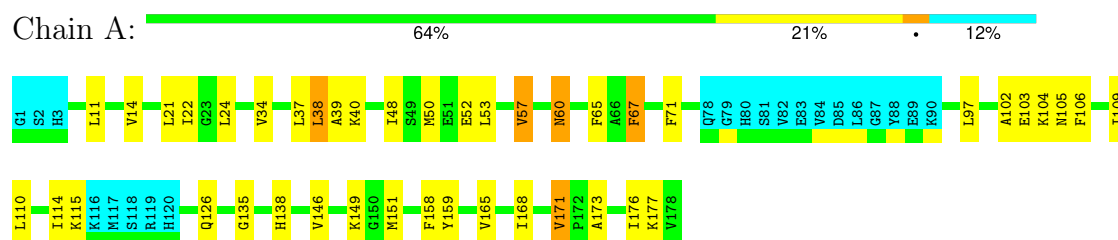
4.2.18 Score per residue for model 18

- Molecule 1: tRNA 2'-phosphotransferase



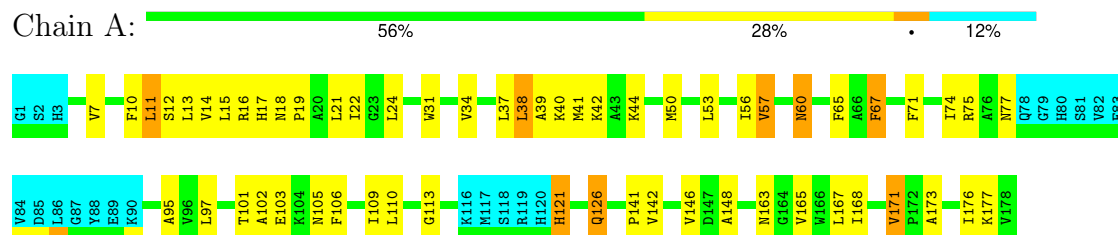
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: tRNA 2'-phosphotransferase



4.2.20 Score per residue for model 20

- Molecule 1: tRNA 2'-phosphotransferase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
ARIA	structure calculation	2.3.2
X-PLOR NIH	refinement	2.52

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1986
Number of shifts mapped to atoms	1986
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
NAD

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1231	1275	1268	42±5
2	A	44	26	26	1±1
All	All	25500	26020	25880	834

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG23	1:A:21:LEU:HD21	0.80	1.52	5	17
1:A:38:LEU:HG	1:A:39:ALA:N	0.76	1.95	16	20
1:A:168:ILE:HD13	1:A:171:VAL:HG13	0.76	1.58	4	20
1:A:165:VAL:HG11	2:A:201:NAD:C6N	0.70	2.17	7	11
1:A:106:PHE:HA	1:A:109:ILE:HG22	0.68	1.66	4	20
1:A:34:VAL:HG13	1:A:53:LEU:HD13	0.68	1.66	5	4
1:A:67:PHE:CE2	1:A:71:PHE:HB3	0.67	2.23	4	20
1:A:146:VAL:HG11	1:A:171:VAL:HG11	0.67	1.67	3	15
1:A:11:LEU:HA	1:A:14:VAL:HG12	0.65	1.66	12	17
1:A:126:GLN:HE21	1:A:126:GLN:N	0.65	1.90	10	1
1:A:57:VAL:HG11	1:A:67:PHE:CG	0.65	2.28	16	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HG	1:A:53:LEU:HD11	0.63	1.68	6	19
1:A:67:PHE:CD2	1:A:71:PHE:HB3	0.62	2.29	13	7
1:A:12:SER:O	1:A:16:ARG:HB3	0.62	1.94	12	10
1:A:14:VAL:HG23	1:A:21:LEU:CD2	0.62	2.24	5	17
1:A:37:LEU:O	1:A:41:MET:HB3	0.62	1.94	16	2
1:A:34:VAL:O	1:A:38:LEU:HD23	0.61	1.94	18	20
1:A:10:PHE:HZ	1:A:22:ILE:HG21	0.61	1.56	5	1
1:A:21:LEU:HG	1:A:22:ILE:HG23	0.61	1.72	5	3
1:A:163:ASN:HB2	1:A:165:VAL:HG13	0.61	1.72	2	1
1:A:126:GLN:NE2	1:A:126:GLN:H	0.60	1.93	1	4
1:A:21:LEU:O	1:A:44:LYS:HE3	0.60	1.95	16	9
1:A:101:THR:HG23	1:A:142:VAL:HG13	0.60	1.73	12	12
1:A:126:GLN:HE21	1:A:165:VAL:HG12	0.60	1.56	2	5
1:A:57:VAL:HG11	1:A:67:PHE:CD1	0.59	2.32	18	20
1:A:39:ALA:O	1:A:42:LYS:HB3	0.58	1.98	12	9
1:A:14:VAL:HA	1:A:21:LEU:HD21	0.58	1.73	12	5
1:A:151:MET:HE3	1:A:171:VAL:HG12	0.58	1.74	7	3
1:A:22:ILE:O	1:A:40:LYS:HB3	0.58	1.98	12	17
1:A:102:ALA:HA	1:A:140:LYS:O	0.58	1.99	15	2
1:A:10:PHE:CZ	1:A:22:ILE:HG21	0.57	2.34	5	1
1:A:115:LYS:O	1:A:121:HIS:HA	0.57	1.99	6	1
1:A:7:VAL:HG13	1:A:41:MET:SD	0.56	2.39	6	4
1:A:21:LEU:HG	1:A:22:ILE:N	0.56	2.16	18	17
1:A:173:ALA:HA	1:A:176:ILE:HD12	0.56	1.78	14	20
1:A:103:GLU:O	1:A:106:PHE:HB3	0.56	2.01	1	19
1:A:53:LEU:HA	1:A:56:ILE:HD13	0.56	1.78	2	10
1:A:146:VAL:HB	1:A:151:MET:SD	0.55	2.42	11	1
1:A:38:LEU:HD13	1:A:50:MET:N	0.55	2.16	16	15
1:A:106:PHE:CZ	1:A:110:LEU:HD22	0.55	2.36	16	9
1:A:168:ILE:HD13	1:A:171:VAL:CG1	0.55	2.32	6	15
1:A:100:GLY:HA3	1:A:131:ALA:O	0.54	2.02	1	3
1:A:97:LEU:HD12	1:A:124:LEU:HB2	0.54	1.78	6	1
1:A:126:GLN:H	1:A:126:GLN:CD	0.54	2.06	11	4
1:A:24:LEU:HD22	1:A:37:LEU:HD13	0.54	1.80	9	19
1:A:151:MET:SD	1:A:175:PHE:HB3	0.53	2.43	6	3
1:A:91:GLN:HG2	1:A:160:LEU:HD13	0.53	1.78	5	1
1:A:96:VAL:HB	1:A:148:ALA:HB2	0.53	1.79	1	3
1:A:126:GLN:HA	1:A:166:TRP:CE3	0.53	2.39	15	2
1:A:146:VAL:HG11	1:A:171:VAL:CG1	0.52	2.34	3	12
1:A:10:PHE:CD2	1:A:11:LEU:HD12	0.52	2.39	5	1
1:A:37:LEU:O	1:A:41:MET:HG2	0.52	2.04	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:VAL:HG21	1:A:67:PHE:CE1	0.52	2.40	18	17
1:A:101:THR:O	1:A:141:PRO:HA	0.52	2.04	20	2
1:A:136:MET:HA	1:A:139:GLY:O	0.52	2.05	2	2
1:A:109:ILE:HD11	1:A:114:ILE:HD12	0.52	1.80	6	1
1:A:15:LEU:HD21	1:A:76:ALA:HB2	0.51	1.81	5	1
1:A:57:VAL:HG11	1:A:67:PHE:CD2	0.51	2.41	15	12
1:A:62:LYS:HA	1:A:157:ASP:OD2	0.51	2.05	4	1
1:A:14:VAL:HB	1:A:21:LEU:HD12	0.51	1.83	20	2
1:A:7:VAL:O	1:A:11:LEU:HB2	0.51	2.04	20	4
1:A:50:MET:CE	1:A:71:PHE:HB2	0.51	2.35	16	6
1:A:12:SER:O	1:A:16:ARG:HG2	0.51	2.04	20	1
1:A:57:VAL:HG23	1:A:65:PHE:HB3	0.51	1.82	3	16
1:A:54:LYS:O	1:A:58:GLU:HG3	0.51	2.05	15	1
1:A:97:LEU:HD12	1:A:124:LEU:HD21	0.51	1.80	2	1
1:A:91:GLN:NE2	1:A:160:LEU:HB2	0.50	2.21	13	4
1:A:52:GLU:O	1:A:55:HIS:HB3	0.50	2.06	1	1
1:A:11:LEU:O	1:A:15:LEU:HD22	0.50	2.07	5	1
1:A:18:ASN:O	1:A:21:LEU:HD23	0.50	2.06	17	5
1:A:114:ILE:HG12	1:A:176:ILE:HD11	0.50	1.84	17	5
1:A:14:VAL:HA	1:A:18:ASN:O	0.50	2.07	3	1
1:A:102:ALA:HB3	1:A:105:ASN:HB3	0.50	1.84	3	2
1:A:64:ARG:HA	1:A:77:ASN:O	0.50	2.06	1	1
1:A:103:GLU:CD	1:A:140:LYS:HD2	0.50	2.27	11	1
1:A:102:ALA:HB2	1:A:138:HIS:HB2	0.50	1.82	3	2
1:A:98:PHE:O	1:A:124:LEU:HB3	0.49	2.07	3	3
1:A:163:ASN:CB	1:A:165:VAL:HG13	0.49	2.36	9	3
1:A:95:ALA:O	1:A:148:ALA:HA	0.49	2.07	6	7
1:A:54:LYS:O	1:A:58:GLU:HB2	0.49	2.07	4	3
1:A:134:VAL:HG11	2:A:201:NAD:H51N	0.49	1.83	6	2
1:A:168:ILE:HG21	1:A:171:VAL:HG13	0.49	1.85	10	5
1:A:126:GLN:OE1	1:A:165:VAL:HA	0.49	2.07	17	1
1:A:91:GLN:HE21	1:A:160:LEU:HB2	0.49	1.67	5	1
1:A:176:ILE:O	1:A:177:LYS:HD3	0.49	2.07	1	3
1:A:95:ALA:C	1:A:148:ALA:HB3	0.49	2.29	5	1
1:A:10:PHE:HD2	1:A:11:LEU:HD12	0.48	1.67	5	1
1:A:10:PHE:CZ	1:A:21:LEU:HD13	0.48	2.42	20	1
1:A:109:ILE:CG1	1:A:114:ILE:HD13	0.48	2.38	19	8
1:A:136:MET:SD	1:A:141:PRO:HG3	0.48	2.49	4	1
1:A:57:VAL:O	1:A:60:ASN:HB3	0.48	2.08	8	15
1:A:102:ALA:CB	1:A:138:HIS:HB2	0.48	2.39	7	8
1:A:124:LEU:HD13	1:A:168:ILE:HG22	0.48	1.86	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ASP:O	1:A:33:PRO:HD3	0.48	2.09	5	2
1:A:168:ILE:CD1	1:A:171:VAL:HG13	0.48	2.37	5	1
1:A:124:LEU:O	1:A:165:VAL:HB	0.48	2.08	13	1
1:A:36:GLU:O	1:A:40:LYS:HB2	0.48	2.09	8	3
1:A:114:ILE:O	1:A:171:VAL:HG23	0.48	2.09	16	1
1:A:124:LEU:CD2	1:A:166:TRP:HB2	0.48	2.38	2	2
1:A:158:PHE:CE1	1:A:168:ILE:HD12	0.48	2.44	14	1
1:A:99:HIS:HA	1:A:125:SER:OG	0.48	2.08	17	2
1:A:35:LYS:HA	1:A:38:LEU:CD2	0.48	2.39	8	1
1:A:160:LEU:HD11	1:A:164:GLY:HA2	0.48	1.85	18	1
1:A:147:ASP:OD2	1:A:149:LYS:HG2	0.47	2.09	8	1
1:A:134:VAL:HG11	2:A:201:NAD:H4D	0.47	1.86	7	1
1:A:11:LEU:O	1:A:15:LEU:HD23	0.47	2.09	13	1
1:A:123:HIS:CE1	1:A:167:LEU:HD12	0.47	2.44	18	1
1:A:57:VAL:HG21	1:A:67:PHE:CD1	0.47	2.44	17	4
1:A:126:GLN:HA	1:A:166:TRP:CD2	0.47	2.44	15	1
1:A:122:VAL:O	1:A:167:LEU:HG	0.47	2.10	11	2
1:A:37:LEU:CD2	1:A:74:ILE:HG21	0.47	2.40	20	11
1:A:112:ASP:OD2	1:A:115:LYS:HD3	0.47	2.10	13	1
1:A:22:ILE:O	1:A:40:LYS:HE3	0.47	2.10	1	2
1:A:62:LYS:N	1:A:62:LYS:HE2	0.47	2.24	4	1
1:A:103:GLU:HA	1:A:106:PHE:HB3	0.47	1.87	13	4
1:A:114:ILE:HB	1:A:171:VAL:HG23	0.47	1.86	15	4
1:A:42:LYS:HG3	1:A:47:GLY:HA2	0.47	1.86	14	1
1:A:13:LEU:O	1:A:17:HIS:HB2	0.46	2.10	20	2
1:A:159:TYR:CE1	1:A:167:LEU:HD22	0.46	2.44	4	1
1:A:165:VAL:HG23	1:A:167:LEU:CD1	0.46	2.41	20	1
1:A:103:GLU:HA	1:A:106:PHE:CB	0.46	2.40	9	8
1:A:18:ASN:ND2	1:A:21:LEU:HD21	0.46	2.26	20	1
1:A:94:PRO:HG3	1:A:166:TRP:CD1	0.46	2.46	10	1
1:A:11:LEU:HD21	1:A:53:LEU:HD21	0.46	1.88	14	1
1:A:137:ARG:NE	1:A:137:ARG:HA	0.46	2.26	16	1
1:A:48:ILE:HB	1:A:52:GLU:CB	0.45	2.41	16	2
1:A:134:VAL:HG11	2:A:201:NAD:H3D	0.45	1.88	2	1
1:A:54:LYS:O	1:A:57:VAL:HG12	0.45	2.11	15	1
1:A:13:LEU:HA	1:A:17:HIS:CD2	0.45	2.46	14	1
1:A:148:ALA:HA	1:A:151:MET:HB3	0.45	1.87	5	1
1:A:49:SER:HB3	1:A:52:GLU:OE2	0.45	2.12	17	1
1:A:106:PHE:HB2	1:A:142:VAL:HG11	0.45	1.89	4	2
1:A:161:SER:HB2	1:A:165:VAL:CG2	0.45	2.41	2	1
1:A:105:ASN:ND2	2:A:201:NAD:H1B	0.45	2.27	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:THR:O	1:A:133:LYS:HB2	0.45	2.11	5	1
1:A:108:LEU:HB2	2:A:201:NAD:H2A	0.45	1.89	4	1
1:A:176:ILE:C	1:A:177:LYS:HD3	0.45	2.32	12	1
1:A:31:TRP:CE3	1:A:75:ARG:HB2	0.44	2.48	20	2
1:A:21:LEU:HG	1:A:22:ILE:H	0.44	1.72	14	5
1:A:17:HIS:CE1	1:A:162:ASN:HB2	0.44	2.47	16	1
1:A:97:LEU:O	1:A:145:SER:HA	0.44	2.11	16	3
1:A:15:LEU:H	1:A:15:LEU:HD23	0.44	1.73	16	5
1:A:165:VAL:HG21	2:A:201:NAD:C5N	0.44	2.42	19	1
1:A:48:ILE:HB	1:A:52:GLU:HB2	0.43	1.90	3	7
1:A:94:PRO:HD2	1:A:158:PHE:CE2	0.43	2.48	9	1
2:A:201:NAD:H3B	2:A:201:NAD:O3	0.43	2.12	17	1
1:A:144:LEU:HD23	1:A:178:VAL:HA	0.43	1.90	5	2
1:A:151:MET:CE	1:A:171:VAL:HG12	0.43	2.43	15	4
1:A:103:GLU:OE2	1:A:140:LYS:HG2	0.43	2.13	2	1
1:A:115:LYS:O	1:A:122:VAL:HB	0.43	2.13	5	1
1:A:98:PHE:O	1:A:125:SER:HB2	0.43	2.13	16	1
1:A:173:ALA:O	1:A:176:ILE:HB	0.43	2.13	20	2
1:A:114:ILE:HG22	1:A:122:VAL:HG21	0.43	1.90	5	2
1:A:91:GLN:NE2	1:A:160:LEU:HD22	0.43	2.28	5	1
1:A:49:SER:HB2	1:A:52:GLU:OE1	0.43	2.13	8	1
1:A:160:LEU:HA	1:A:165:VAL:O	0.43	2.14	8	2
1:A:91:GLN:HB2	1:A:160:LEU:HD13	0.43	1.91	1	1
1:A:7:VAL:HG13	1:A:41:MET:CE	0.43	2.43	5	1
1:A:126:GLN:NE2	1:A:165:VAL:HG12	0.43	2.25	2	2
1:A:70:ASN:HD22	1:A:72:GLU:HB2	0.43	1.74	3	1
1:A:38:LEU:O	1:A:42:LYS:HB2	0.43	2.14	17	2
1:A:114:ILE:C	1:A:122:VAL:HG11	0.42	2.34	1	1
1:A:53:LEU:O	1:A:53:LEU:HD23	0.42	2.14	5	3
1:A:31:TRP:CD2	1:A:75:ARG:HB2	0.42	2.50	9	1
1:A:113:GLY:HA2	1:A:173:ALA:HB2	0.42	1.91	20	1
1:A:114:ILE:HG12	1:A:171:VAL:CG2	0.42	2.44	6	1
1:A:151:MET:HB3	1:A:158:PHE:CZ	0.42	2.49	12	2
1:A:114:ILE:HB	1:A:171:VAL:CG2	0.42	2.44	15	1
1:A:11:LEU:HD23	1:A:65:PHE:CE1	0.42	2.50	18	3
1:A:105:ASN:O	1:A:109:ILE:HB	0.42	2.15	15	1
1:A:106:PHE:HA	1:A:109:ILE:CG2	0.42	2.42	6	3
1:A:21:LEU:HD23	1:A:21:LEU:H	0.42	1.74	7	1
1:A:159:TYR:CE2	1:A:167:LEU:HD22	0.42	2.50	16	1
1:A:106:PHE:CA	1:A:109:ILE:HG22	0.41	2.42	7	4
1:A:161:SER:HB2	1:A:167:LEU:HD11	0.41	1.91	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG22	1:A:19:PRO:HA	0.41	1.92	20	1
1:A:114:ILE:HD13	1:A:176:ILE:HD11	0.41	1.91	6	1
1:A:115:LYS:HG3	1:A:169:ASP:O	0.41	2.15	6	1
1:A:99:HIS:HB2	1:A:124:LEU:HG	0.41	1.92	13	1
1:A:5:VAL:O	1:A:9:LYS:HG2	0.41	2.14	1	1
1:A:95:ALA:HB1	1:A:148:ALA:HB1	0.41	1.92	4	1
1:A:100:GLY:N	1:A:131:ALA:HB1	0.41	2.30	18	1
1:A:146:VAL:HG12	1:A:176:ILE:HA	0.41	1.93	15	1
1:A:94:PRO:HD2	1:A:158:PHE:CD2	0.41	2.50	5	1
1:A:109:ILE:HG12	1:A:114:ILE:HD13	0.41	1.91	19	1
1:A:96:VAL:HG23	1:A:146:VAL:O	0.41	2.15	4	1
1:A:91:GLN:NE2	1:A:160:LEU:HD12	0.41	2.30	6	1
1:A:99:HIS:HB2	1:A:124:LEU:HA	0.41	1.93	6	1
1:A:15:LEU:HD23	1:A:15:LEU:H	0.41	1.76	10	1
1:A:128:ILE:O	1:A:132:ARG:HG3	0.40	2.16	14	1
1:A:51:GLU:O	1:A:54:LYS:HB3	0.40	2.16	15	2
1:A:124:LEU:HD11	1:A:168:ILE:HG22	0.40	1.94	11	1
1:A:151:MET:SD	1:A:168:ILE:HD11	0.40	2.56	16	1
1:A:97:LEU:HG	1:A:146:VAL:CG2	0.40	2.46	5	1
1:A:109:ILE:HG13	1:A:114:ILE:HG23	0.40	1.93	6	1
1:A:132:ARG:O	1:A:136:MET:HG3	0.40	2.16	17	1
1:A:14:VAL:CG2	1:A:21:LEU:HD21	0.40	2.34	5	1
1:A:112:ASP:CG	1:A:115:LYS:HD3	0.40	2.37	13	1
1:A:102:ALA:HB2	1:A:135:GLY:O	0.40	2.17	19	1
1:A:112:ASP:O	1:A:115:LYS:HE3	0.40	2.15	5	1
1:A:102:ALA:HB3	1:A:105:ASN:OD1	0.40	2.17	15	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/178 (88%)	145±3 (93±2%)	9±2 (6±1%)	2±1 (1±1%)	14	62
All	All	3120/3560 (88%)	2901 (93%)	181 (6%)	38 (1%)	14	62

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	60	ASN	17
1	A	61	SER	6
1	A	115	LYS	6
1	A	125	SER	2
1	A	63	LYS	2
1	A	45	GLY	2
1	A	126	GLN	1
1	A	62	LYS	1
1	A	121	HIS	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/150 (88%)	121±2 (92±2%)	11±2 (8±2%)	11	60
All	All	2640/3000 (88%)	2418 (92%)	222 (8%)	11	60

All 43 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	38	LEU	20
1	A	67	PHE	20
1	A	171	VAL	20
1	A	57	VAL	15
1	A	126	GLN	15
1	A	97	LEU	14
1	A	177	LYS	14
1	A	114	ILE	13
1	A	11	LEU	12
1	A	52	GLU	8
1	A	105	ASN	7
1	A	15	LEU	7
1	A	124	LEU	6
1	A	36	GLU	4
1	A	21	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	123	HIS	3
1	A	158	PHE	3
1	A	41	MET	3
1	A	4	MET	2
1	A	18	ASN	2
1	A	159	TYR	2
1	A	101	THR	2
1	A	122	VAL	2
1	A	137	ARG	2
1	A	156	PHE	2
1	A	35	LYS	2
1	A	58	GLU	2
1	A	9	LYS	1
1	A	62	LYS	1
1	A	165	VAL	1
1	A	64	ARG	1
1	A	42	LYS	1
1	A	140	LYS	1
1	A	151	MET	1
1	A	53	LEU	1
1	A	167	LEU	1
1	A	104	LYS	1
1	A	115	LYS	1
1	A	149	LYS	1
1	A	44	LYS	1
1	A	77	ASN	1
1	A	121	HIS	1
1	A	163	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	NAD	A	201	-	42,48,48	1.75±0.10	9±1 (20±2%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	NAD	A	201	-	50,73,73	1.42±0.05	6±1 (12±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	201	-	-	0±0,26,62,62	0±0,5,5,5

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	201	NAD	O4D-C1D	6.32	1.49	1.40	5	20
2	A	201	NAD	C2N-N1N	6.03	1.41	1.35	18	20
2	A	201	NAD	O4B-C1B	4.98	1.47	1.40	10	20
2	A	201	NAD	C3N-C7N	3.77	1.56	1.50	11	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	201	NAD	C2N-C3N	3.64	1.44	1.39	12	16
2	A	201	NAD	C5A-N7A	3.18	1.28	1.39	19	20
2	A	201	NAD	C2A-N3A	3.17	1.37	1.32	7	17
2	A	201	NAD	C2D-C3D	2.86	1.45	1.53	3	10
2	A	201	NAD	C2A-N1A	2.76	1.38	1.33	2	9
2	A	201	NAD	O3B-C3B	2.41	1.48	1.43	3	8
2	A	201	NAD	C3D-C4D	2.38	1.46	1.53	2	1
2	A	201	NAD	C2B-C3B	2.31	1.47	1.53	7	9
2	A	201	NAD	C8A-N7A	2.10	1.38	1.34	16	1
2	A	201	NAD	PA-O3	2.04	1.61	1.59	7	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

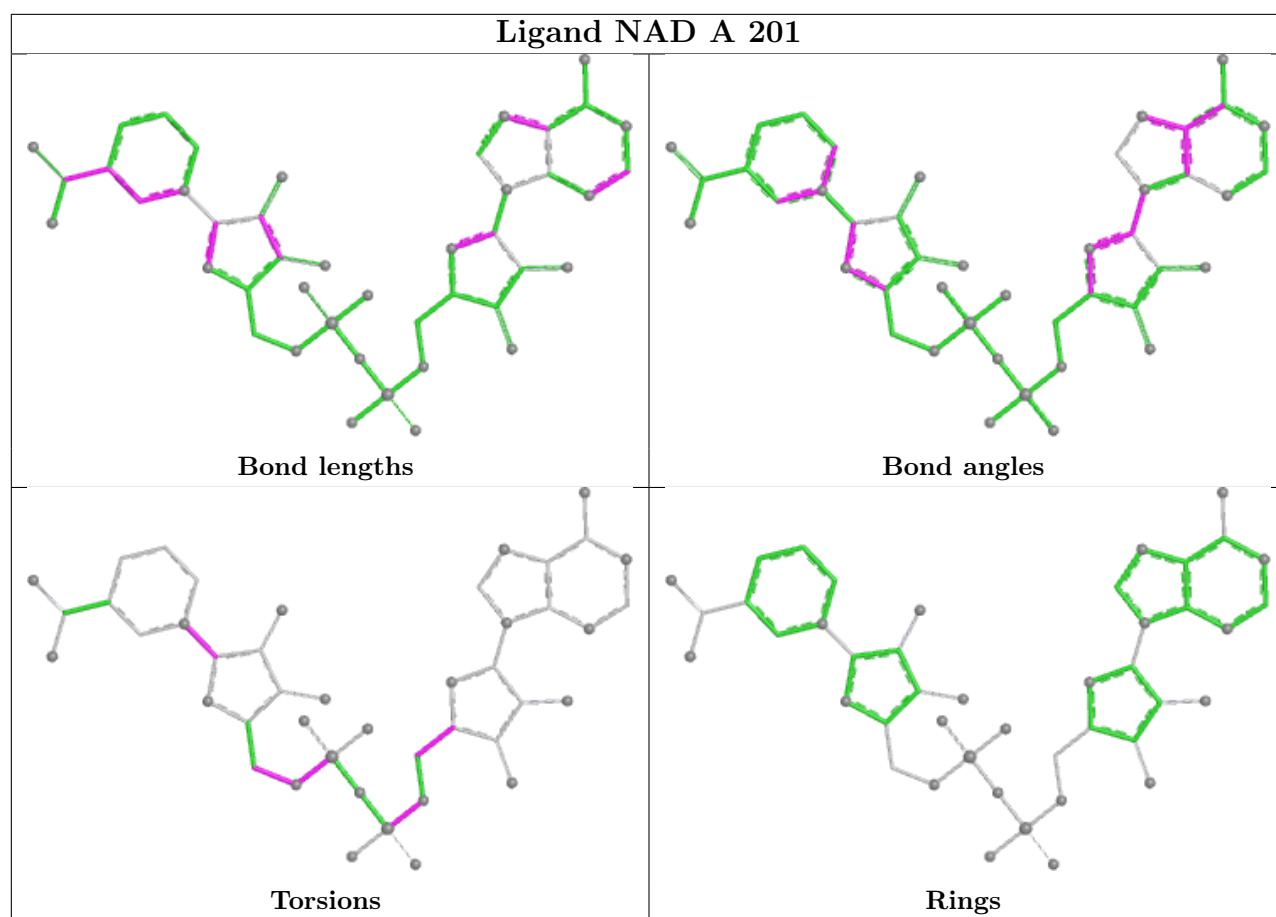
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	201	NAD	C4A-C5A-N7A	4.70	114.30	109.34	19	20
2	A	201	NAD	C4B-O4B-C1B	4.33	105.96	109.92	1	20
2	A	201	NAD	C4D-O4D-C1D	4.17	106.11	109.92	11	20
2	A	201	NAD	C6A-C5A-C4A	3.60	124.90	117.90	19	20
2	A	201	NAD	C6N-N1N-C2N	3.42	118.97	121.88	15	20
2	A	201	NAD	O4B-C1B-N9A	2.76	112.40	108.75	3	4
2	A	201	NAD	N3A-C2A-N1A	2.74	124.95	128.67	20	19
2	A	201	NAD	C1B-N9A-C4A	2.37	122.48	126.64	3	3
2	A	201	NAD	C2N-N1N-C1D	2.04	123.65	119.13	2	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1986
Number of shifts mapped to atoms	1986
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	161	-0.09 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	137	0.09 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	146	-0.00 ± 0.14	None needed (< 0.5 ppm)
^{15}N	159	0.41 ± 0.30	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 1773 atoms were assigned a chemical shift out of a possible 2192. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	718/785 (91%)	295/320 (92%)	279/314 (89%)	144/151 (95%)
Sidechain	969/1218 (80%)	652/797 (82%)	307/379 (81%)	10/42 (24%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	86/189 (46%)	45/94 (48%)	39/79 (49%)	2/16 (12%)
Overall	1773/2192 (81%)	992/1211 (82%)	625/772 (81%)	156/209 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1950 atoms were assigned a chemical shift out of a possible 2469. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	793/893 (89%)	327/365 (90%)	307/356 (86%)	159/172 (92%)
Sidechain	1057/1354 (78%)	712/884 (81%)	334/422 (79%)	11/48 (23%)
Aromatic	100/222 (45%)	52/110 (47%)	46/90 (51%)	2/22 (9%)
Overall	1950/2469 (79%)	1091/1359 (80%)	687/868 (79%)	172/242 (71%)

7.1.4 Statistically unusual chemical shifts [i](#)

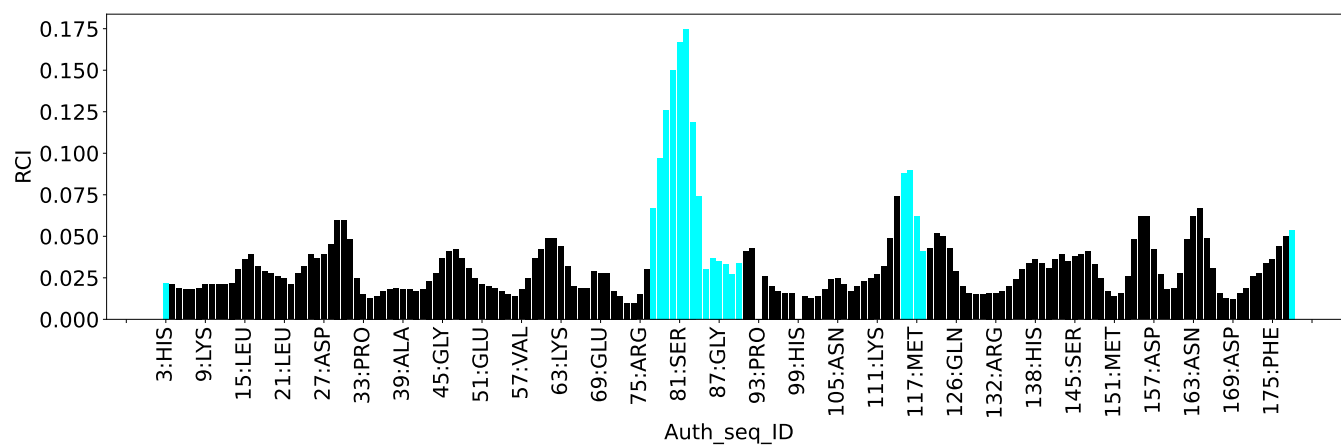
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	123	HIS	CD2	137.98	103.95 – 136.66	5.4

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	4573
Intra-residue ($ i-j =0$)	1606
Sequential ($ i-j =1$)	1068
Medium range ($ i-j >1$ and $ i-j <5$)	684
Long range ($ i-j \geq 5$)	990
Inter-chain	99
Hydrogen bond restraints	126
Disulfide bond restraints	0
Total dihedral-angle restraints	269
Number of unmapped restraints	0
Number of restraints per residue	27.1
Number of long range restraints per residue ¹	5.7

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	176.6	0.2
0.2-0.5 (Medium)	281.5	0.5
>0.5 (Large)	183.4	6.05

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	17.0	4.91
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

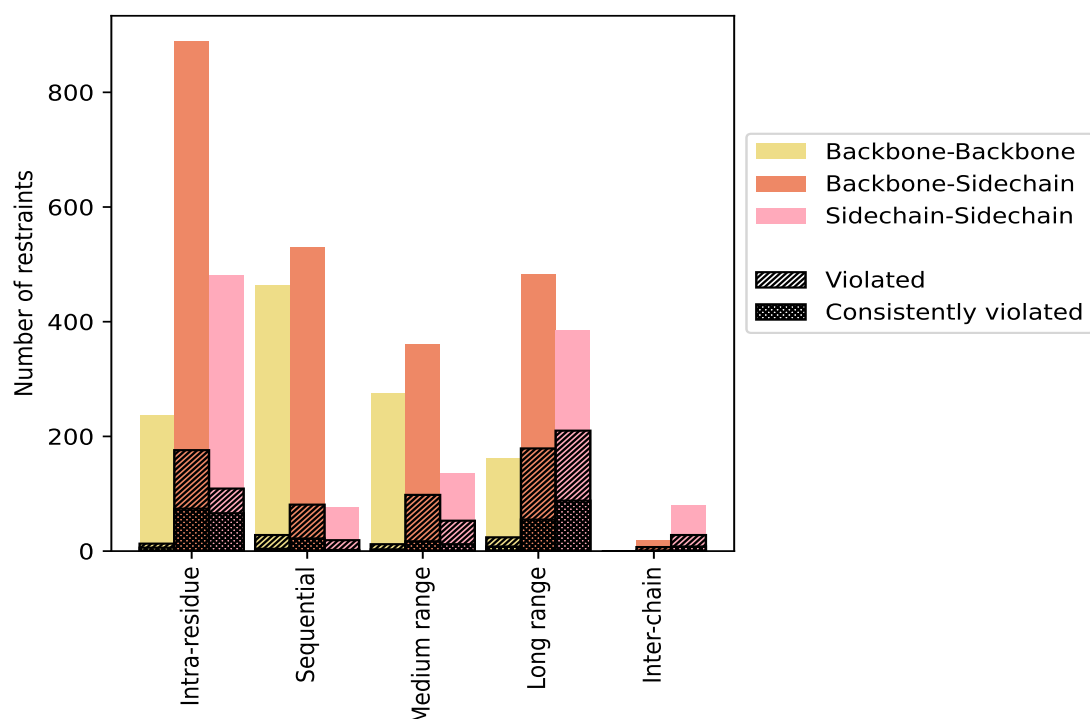
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	1606	35.1	298	18.6	6.5	146	9.1	3.2
Backbone-Backbone	237	5.2	13	5.5	0.3	6	2.5	0.1
Backbone-Sidechain	889	19.4	176	19.8	3.8	74	8.3	1.6
Sidechain-Sidechain	480	10.5	109	22.7	2.4	66	13.8	1.4
Sequential (i-j =1)	1068	23.4	128	12.0	2.8	28	2.6	0.6
Backbone-Backbone	463	10.1	28	6.0	0.6	4	0.9	0.1
Backbone-Sidechain	529	11.6	81	15.3	1.8	22	4.2	0.5
Sidechain-Sidechain	76	1.7	19	25.0	0.4	2	2.6	0.0
Medium range (i-j >1 & i-j <5)	684	15.0	116	17.0	2.5	28	4.1	0.6
Backbone-Backbone	275	6.0	12	4.4	0.3	3	1.1	0.1
Backbone-Sidechain	273	6.0	51	18.7	1.1	13	4.8	0.3
Sidechain-Sidechain	136	3.0	53	39.0	1.2	12	8.8	0.3
Long range (i-j ≥5)	990	21.6	386	39.0	8.4	146	14.7	3.2
Backbone-Backbone	162	3.5	24	14.8	0.5	8	4.9	0.2
Backbone-Sidechain	444	9.7	152	34.2	3.3	50	11.3	1.1
Sidechain-Sidechain	384	8.4	210	54.7	4.6	88	22.9	1.9
Inter-chain	99	2.2	35	35.4	0.8	9	9.1	0.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	19	0.4	7	36.8	0.2	1	5.3	0.0
Sidechain-Sidechain	80	1.7	28	35.0	0.6	8	10.0	0.2
Hydrogen bond	126	2.8	74	58.7	1.6	9	7.1	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4573	100.0	1037	22.7	22.7	366	8.0	8.0
Backbone-Backbone	1137	24.9	77	6.8	1.7	21	1.8	0.5
Backbone-Sidechain	2280	49.9	541	23.7	11.8	169	7.4	3.7
Sidechain-Sidechain	1156	25.3	419	36.2	9.2	176	15.2	3.8

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	199	73	85	253	16	626	0.45	3.67	0.42	0.3
2	218	81	95	270	16	680	0.46	6.05	0.46	0.32
3	207	72	88	250	16	633	0.46	3.38	0.43	0.32
4	213	75	89	259	16	652	0.45	3.55	0.41	0.31
5	212	75	89	272	13	661	0.45	3.73	0.4	0.31
6	208	76	84	257	20	645	0.46	4.35	0.43	0.31
7	214	74	87	255	19	649	0.47	3.62	0.43	0.33
8	206	69	88	253	16	632	0.46	3.49	0.42	0.32
9	216	82	84	270	16	668	0.46	5.03	0.45	0.32
10	218	73	90	248	16	645	0.45	4.05	0.41	0.31

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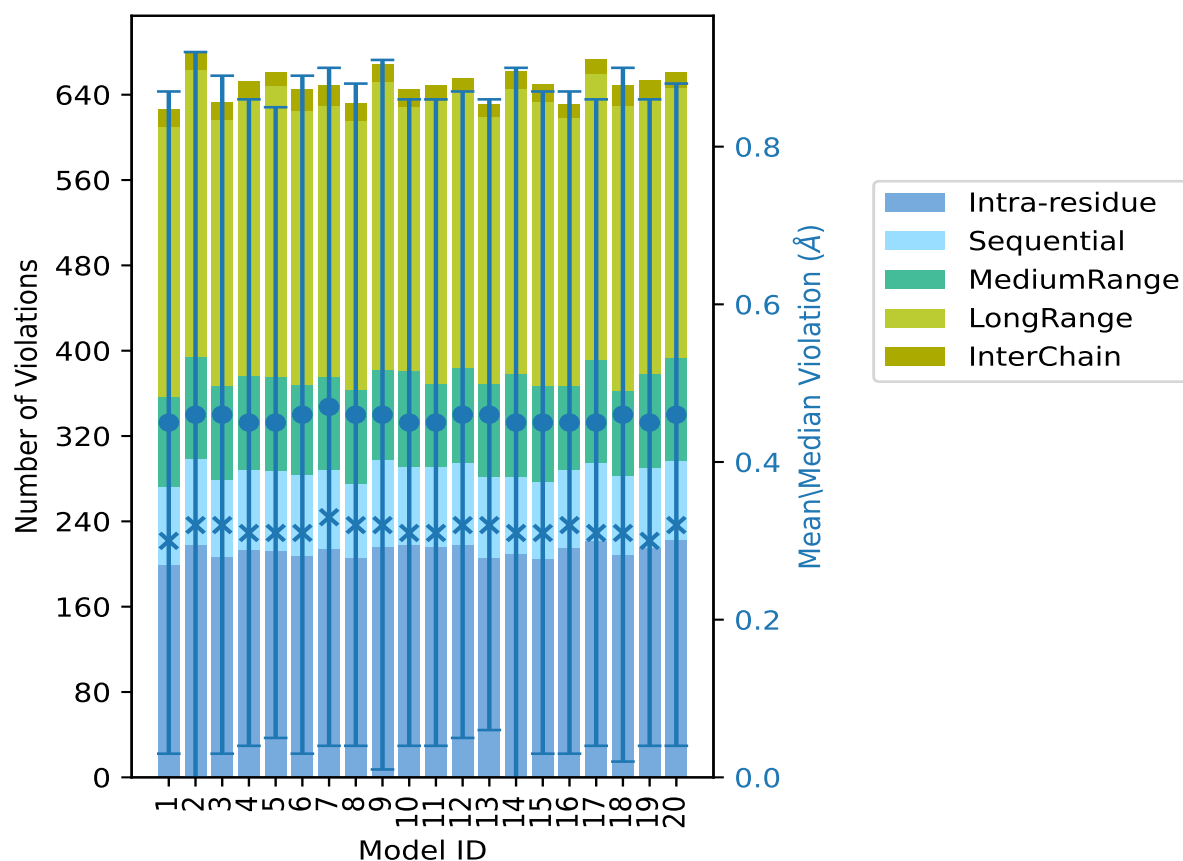
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	216	75	78	265	15	649	0.45	3.78	0.41	0.31
12	218	77	89	260	12	656	0.46	4.02	0.41	0.32
13	206	76	87	250	12	631	0.46	2.77	0.4	0.32
14	209	73	96	268	16	662	0.45	5.97	0.45	0.31
15	205	72	90	267	16	650	0.45	3.24	0.42	0.31
16	215	74	78	251	13	631	0.45	4.57	0.42	0.32
17	222	73	96	268	14	673	0.45	3.66	0.41	0.31
18	208	75	79	268	19	649	0.46	3.83	0.44	0.31
19	215	75	89	257	17	653	0.45	3.54	0.41	0.3
20	223	74	96	253	15	661	0.46	4.4	0.42	0.32

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

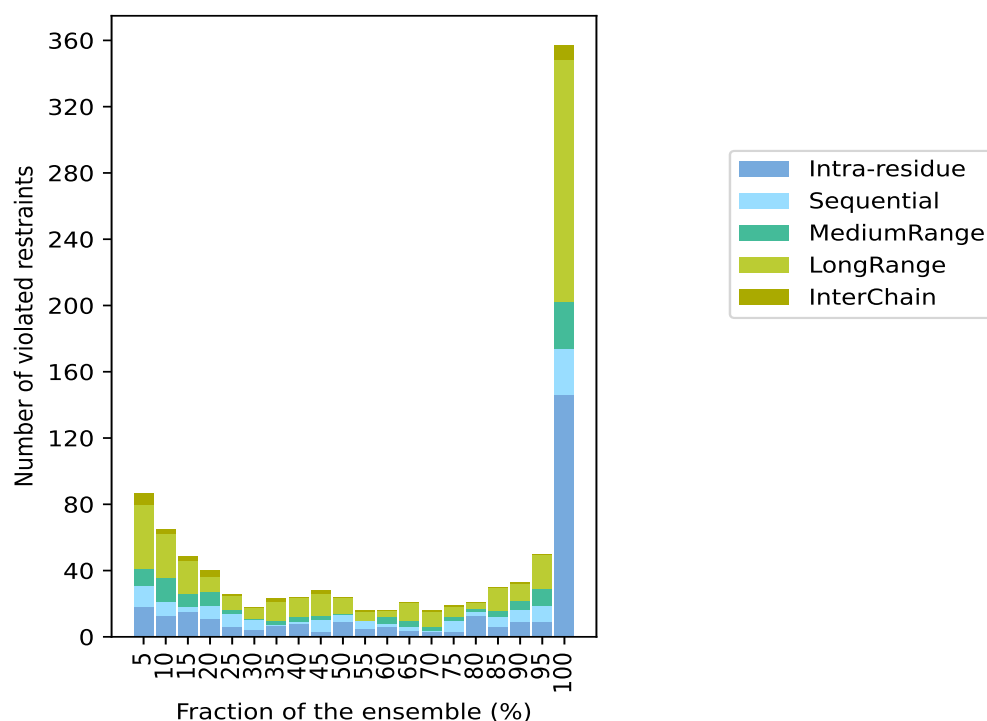
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3484(IR:1308, SQ:940, MR:568, LR:604, IC:64) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
18	13	10	39	7	87	1	5.0
13	8	15	26	3	65	2	10.0
15	3	8	20	3	49	3	15.0
11	8	8	9	4	40	4	20.0
6	8	2	9	1	26	5	25.0
4	6	1	7	0	18	6	30.0
7	0	3	11	2	23	7	35.0
8	1	3	12	0	24	8	40.0
3	7	3	13	2	28	9	45.0
9	4	1	10	0	24	10	50.0
5	5	0	5	1	16	11	55.0
6	2	4	4	0	16	12	60.0
4	2	4	11	0	21	13	65.0
3	1	2	9	1	16	14	70.0
3	7	2	6	1	19	15	75.0
13	2	2	4	0	21	16	80.0
6	6	4	14	0	30	17	85.0
9	7	6	10	1	33	18	90.0
9	10	10	21	0	50	19	95.0
146	28	28	146	9	357	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

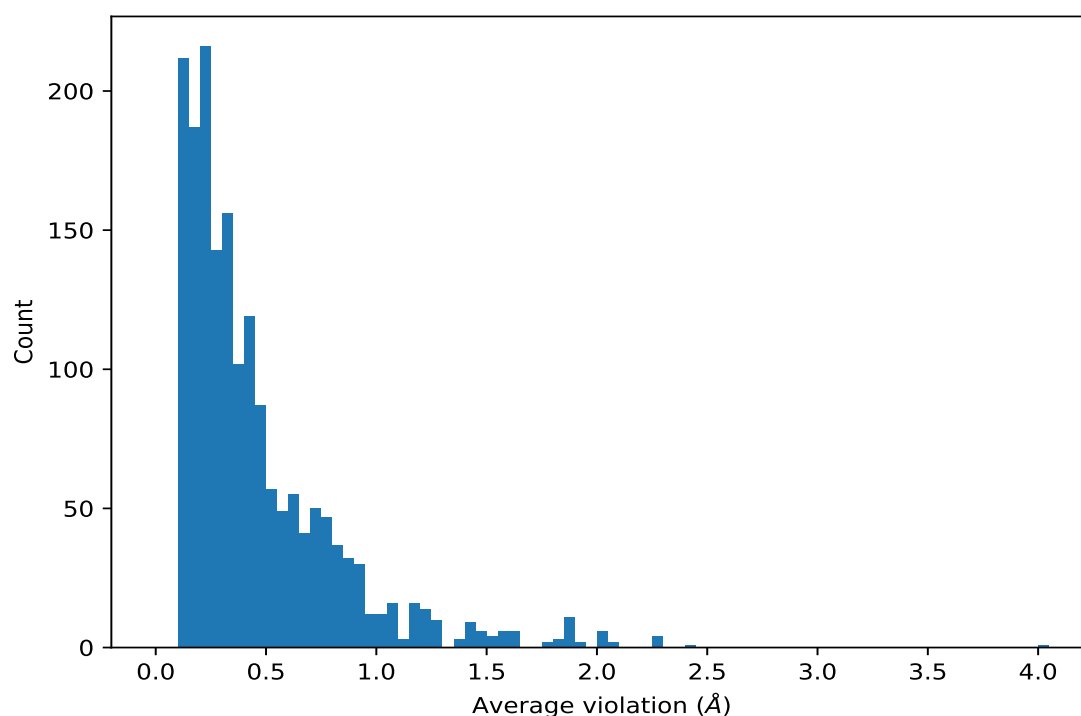
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	20	4.0	0.85	3.76
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	20	2.4	0.53	2.17
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	20	2.26	0.04	2.26
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	20	2.26	0.04	2.26
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	20	2.25	0.11	2.26
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD13	20	2.25	0.11	2.26
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	20	2.09	0.38	2.13
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	20	2.05	1.11	2.06
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	20	2.03	0.14	2.02
(4,315)	1:56:A:ILE:HG21	1:6:A:LYS:HA	20	2.03	0.14	2.02
(4,315)	1:56:A:ILE:HG22	1:6:A:LYS:HA	20	2.03	0.14	2.02
(4,315)	1:56:A:ILE:HG22	1:38:A:LEU:HA	20	2.03	0.14	2.02
(2,1527)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	20	2.01	0.42	2.17
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	20	2.01	0.42	2.17
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	20	1.94	0.36	1.94
(4,186)	1:175:A:PHE:H	2:201:A:NAD:H2A	20	1.94	0.36	1.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	20	1.88	0.97	1.72
(4,326)	1:124:A:LEU:HD21	1:177:A:LYS:HE2	20	1.86	0.21	1.96
(4,326)	1:124:A:LEU:HD22	1:163:A:ASN:HB2	20	1.86	0.21	1.96
(4,326)	1:124:A:LEU:HD22	1:177:A:LYS:HE2	20	1.86	0.21	1.96
(4,326)	1:124:A:LEU:HD23	1:177:A:LYS:HE2	20	1.86	0.21	1.96
(4,326)	1:124:A:LEU:HD21	1:163:A:ASN:HB2	20	1.86	0.21	1.96
(4,326)	1:124:A:LEU:HD23	1:163:A:ASN:HB2	20	1.86	0.21	1.96
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	20	1.85	0.15	1.85
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG22	20	1.85	0.15	1.85
(2,1802)	1:53:A:LEU:HD13	1:74:A:ILE:HG23	20	1.85	0.15	1.85
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG21	20	1.85	0.15	1.85
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	20	1.79	0.06	1.8
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD13	20	1.79	0.06	1.8
(4,441)	1:56:A:ILE:HD11	1:38:A:LEU:HB2	20	1.58	0.16	1.59
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	20	1.58	0.16	1.59
(4,441)	1:56:A:ILE:HD11	1:6:A:LYS:HB3	20	1.58	0.16	1.59
(4,441)	1:56:A:ILE:HD12	1:38:A:LEU:HB2	20	1.58	0.16	1.59
(4,441)	1:56:A:ILE:HD12	1:6:A:LYS:HB3	20	1.58	0.16	1.59
(4,441)	1:56:A:ILE:HD13	1:6:A:LYS:HB3	20	1.58	0.16	1.59
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	20	1.5	0.23	1.53
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	20	1.5	0.23	1.53
(2,3454)	1:168:A:ILE:HD13	1:149:A:LYS:H	20	1.5	0.23	1.53
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD11	20	1.48	0.04	1.48
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	20	1.48	0.04	1.48
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD12	20	1.48	0.04	1.48
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	20	1.46	0.05	1.45
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	20	1.46	0.05	1.45
(2,1421)	1:21:A:LEU:HD21	1:10:A:PHE:HE1	20	1.46	0.05	1.45
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	20	1.43	0.07	1.42
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG22	20	1.43	0.07	1.42
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	20	1.42	0.56	1.66
(4,316)	1:37:A:LEU:HD22	1:8:A:SER:HB2	20	1.42	0.56	1.66
(4,316)	1:37:A:LEU:HD23	1:23:A:GLY:HA3	20	1.42	0.56	1.66
(4,316)	1:37:A:LEU:HD21	1:8:A:SER:HB2	20	1.42	0.56	1.66
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	20	1.42	0.7	1.86
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	20	1.41	0.34	1.48
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	20	1.37	0.03	1.37
(2,1530)	1:178:A:VAL:HG21	1:109:A:ILE:HA	20	1.37	0.03	1.37
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	20	1.28	0.07	1.29
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	20	1.28	0.07	1.29
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	20	1.28	0.23	1.31
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	20	1.28	0.23	1.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1487)	1:168:A:ILE:HD13	1:149:A:LYS:H	20	1.28	0.23	1.31
(2,3498)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	20	1.26	0.42	1.42
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	20	1.26	0.42	1.42
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	20	1.25	0.3	1.14
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	20	1.25	0.3	1.14
(2,1559)	1:21:A:LEU:HD21	1:41:A:MET:HB2	20	1.25	0.3	1.14
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	20	1.24	0.04	1.25
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB1	20	1.24	0.13	1.21
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	20	1.24	0.13	1.21
(2,3830)	1:97:A:LEU:HD22	1:95:A:ALA:HB2	20	1.24	0.13	1.21
(2,3830)	1:97:A:LEU:HD23	1:95:A:ALA:HB2	20	1.24	0.13	1.21
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB3	20	1.24	0.13	1.21
(2,3830)	1:97:A:LEU:HD22	1:95:A:ALA:HB1	20	1.24	0.13	1.21
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	20	1.21	0.27	1.3
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	20	1.21	0.25	1.28
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	20	1.21	0.25	1.28
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD21	20	1.21	0.25	1.28
(2,1783)	1:44:A:LYS:HG3	1:21:A:LEU:HD22	20	1.21	0.25	1.28
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	20	1.2	0.07	1.18
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG22	20	1.2	0.07	1.18
(2,1452)	1:38:A:LEU:HD12	1:38:A:LEU:H	20	1.19	0.02	1.19
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	20	1.19	0.02	1.19
(2,1452)	1:38:A:LEU:HD11	1:38:A:LEU:H	20	1.19	0.02	1.19
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	20	1.18	0.2	1.18
(4,414)	1:133:A:LYS:HB2	1:128:A:ILE:HG21	20	1.18	0.2	1.18
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	20	1.17	0.14	1.16
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG12	20	1.17	0.14	1.16
(2,1260)	1:142:A:VAL:HG23	1:178:A:VAL:HG11	20	1.17	0.14	1.16
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	20	1.15	0.09	1.2
(2,1843)	1:110:A:LEU:HD13	1:110:A:LEU:HB3	20	1.15	0.09	1.2
(2,1843)	1:110:A:LEU:HD12	1:110:A:LEU:HB3	20	1.15	0.09	1.2
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	20	1.15	0.03	1.15
(2,1806)	1:13:A:LEU:HD21	1:13:A:LEU:HB2	20	1.15	0.03	1.15
(2,1806)	1:13:A:LEU:HD23	1:13:A:LEU:HB2	20	1.15	0.03	1.15
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	20	1.11	0.03	1.11
(2,3501)	1:178:A:VAL:HG21	1:109:A:ILE:HA	20	1.11	0.03	1.11
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB1	20	1.09	0.13	1.06
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	20	1.09	0.13	1.06
(2,1868)	1:97:A:LEU:HD22	1:95:A:ALA:HB2	20	1.09	0.13	1.06
(2,1868)	1:97:A:LEU:HD23	1:95:A:ALA:HB2	20	1.09	0.13	1.06
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB3	20	1.09	0.13	1.06
(2,1868)	1:97:A:LEU:HD22	1:95:A:ALA:HB1	20	1.09	0.13	1.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	20	1.08	0.27	1.17
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	20	1.07	0.02	1.07
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	20	1.07	0.02	1.07
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	20	1.07	0.08	1.12
(2,3807)	1:110:A:LEU:HD13	1:110:A:LEU:HB3	20	1.07	0.08	1.12
(2,3807)	1:110:A:LEU:HD12	1:110:A:LEU:HB3	20	1.07	0.08	1.12
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	20	1.04	0.25	1.07
(4,184)	1:105:A:ASN:H	1:136:A:MET:H	20	1.04	0.25	1.07
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	20	1.04	0.25	1.08
(4,202)	1:173:A:ALA:HA	1:145:A:SER:HB2	20	1.04	0.25	1.08
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	20	1.02	0.13	1.1
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	20	1.02	0.13	1.1
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG13	20	1.02	0.13	1.1
(4,378)	1:24:A:LEU:HA	1:15:A:LEU:HB2	20	1.01	0.12	0.98
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	20	1.01	0.12	0.98
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	20	0.99	0.02	1.0
(2,1444)	1:56:A:ILE:HG23	1:56:A:ILE:H	20	0.99	0.02	1.0
(2,1444)	1:56:A:ILE:HG21	1:56:A:ILE:H	20	0.99	0.02	1.0
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	20	0.99	0.08	1.0
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	20	0.99	0.57	0.76
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	20	0.94	0.25	1.02
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	20	0.94	0.25	1.02
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD21	20	0.94	0.25	1.02
(2,3749)	1:44:A:LYS:HG3	1:21:A:LEU:HD22	20	0.94	0.25	1.02
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	20	0.94	0.04	0.94
(2,816)	1:53:A:LEU:HD21	1:53:A:LEU:H	20	0.94	0.04	0.94
(2,816)	1:53:A:LEU:HD22	1:53:A:LEU:H	20	0.94	0.04	0.94
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	20	0.93	0.21	1.01
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	20	0.92	0.03	0.92
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD21	20	0.92	0.03	0.92
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	20	0.92	0.03	0.92
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD23	20	0.92	0.03	0.92
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD21	20	0.92	0.1	0.93
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD22	20	0.92	0.1	0.93
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD12	20	0.92	0.1	0.93
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD13	20	0.92	0.1	0.93
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD23	20	0.92	0.1	0.93
(2,1851)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	20	0.9	0.19	0.93
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	20	0.9	0.19	0.93
(2,1851)	1:56:A:ILE:HD12	1:11:A:LEU:HD11	20	0.9	0.19	0.93
(2,1851)	1:56:A:ILE:HD12	1:11:A:LEU:HD13	20	0.9	0.19	0.93
(2,1851)	1:56:A:ILE:HD11	1:11:A:LEU:HD13	20	0.9	0.19	0.93

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD13	20	0.9	0.19	0.93
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	20	0.9	0.03	0.9
(2,3771)	1:13:A:LEU:HD21	1:13:A:LEU:HB2	20	0.9	0.03	0.9
(2,3771)	1:13:A:LEU:HD23	1:13:A:LEU:HB2	20	0.9	0.03	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	20	0.89	0.03	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD22	20	0.89	0.03	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD21	20	0.89	0.03	0.9
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	20	0.88	0.06	0.9
(2,1830)	1:34:A:VAL:HG12	1:50:A:MET:HE2	20	0.88	0.22	0.94
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	20	0.88	0.22	0.94
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE2	20	0.88	0.22	0.94
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE1	20	0.88	0.22	0.94
(2,1830)	1:34:A:VAL:HG12	1:50:A:MET:HE1	20	0.88	0.22	0.94
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	20	0.87	0.17	0.89
(2,1500)	1:11:A:LEU:HD12	1:38:A:LEU:HA	20	0.87	0.17	0.89
(2,1495)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	20	0.85	0.1	0.86
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	20	0.85	0.1	0.86
(2,1495)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	20	0.85	0.1	0.86
(2,3421)	1:38:A:LEU:HD12	1:38:A:LEU:H	20	0.85	0.02	0.85
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	20	0.85	0.02	0.85
(2,3421)	1:38:A:LEU:HD11	1:38:A:LEU:H	20	0.85	0.02	0.85
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD23	20	0.85	0.24	0.9
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	20	0.85	0.24	0.9
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD22	20	0.85	0.24	0.9
(4,36)	1:76:A:ALA:H	1:57:A:VAL:HG23	20	0.85	0.24	0.9
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	20	0.85	0.09	0.84
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD13	20	0.85	0.09	0.84
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD11	20	0.85	0.09	0.84
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	20	0.84	0.1	0.84
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD13	20	0.84	0.1	0.84
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD12	20	0.84	0.1	0.84
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	20	0.84	0.17	0.88
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD22	20	0.84	0.17	0.88
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD21	20	0.84	0.17	0.88
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	20	0.84	0.24	0.82
(4,103)	1:114:A:ILE:H	1:123:A:HIS:HA	20	0.84	0.24	0.82
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	20	0.83	0.16	0.9
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	20	0.83	0.08	0.83
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	20	0.83	0.05	0.82
(2,1845)	1:176:A:ILE:HB	1:110:A:LEU:HD11	20	0.83	0.05	0.82
(2,1845)	1:110:A:LEU:HD13	1:176:A:ILE:HB	20	0.83	0.05	0.82
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	20	0.82	0.02	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1856)	1:22:A:ILE:HD12	1:14:A:VAL:HG23	20	0.82	0.23	0.76
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	20	0.82	0.23	0.76
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG23	20	0.82	0.23	0.76
(2,1856)	1:22:A:ILE:HD12	1:14:A:VAL:HG22	20	0.82	0.23	0.76
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG21	20	0.82	0.23	0.76
(2,1856)	1:22:A:ILE:HD13	1:14:A:VAL:HG21	20	0.82	0.23	0.76
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	20	0.81	0.12	0.81
(4,329)	1:142:A:VAL:HG21	1:106:A:PHE:HA	20	0.81	0.12	0.81
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	20	0.81	0.02	0.81
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG12	20	0.81	0.02	0.81
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	20	0.81	0.17	0.87
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG22	20	0.81	0.17	0.87
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	20	0.8	0.09	0.81
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	20	0.79	0.11	0.84
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	20	0.79	0.11	0.84
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	20	0.78	0.05	0.8
(2,954)	1:56:A:ILE:HG23	1:57:A:VAL:H	20	0.78	0.05	0.8
(2,954)	1:56:A:ILE:HG21	1:57:A:VAL:H	20	0.78	0.05	0.8
(2,3462)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	20	0.77	0.1	0.78
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	20	0.77	0.1	0.78
(2,3462)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	20	0.77	0.1	0.78
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	20	0.76	0.1	0.77
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	20	0.76	0.07	0.76
(2,1473)	1:110:A:LEU:HD13	1:110:A:LEU:H	20	0.76	0.07	0.76
(2,1473)	1:110:A:LEU:HD11	1:110:A:LEU:H	20	0.76	0.07	0.76
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	20	0.76	0.09	0.74
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	20	0.76	0.01	0.75
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	20	0.75	0.02	0.75
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	20	0.74	0.21	0.82
(4,244)	1:51:A:GLU:HG2	1:67:A:PHE:HD1	20	0.74	0.21	0.82
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	20	0.74	0.23	0.66
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	20	0.74	0.23	0.66
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	20	0.74	0.07	0.75
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	20	0.74	0.07	0.75
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	20	0.74	0.08	0.73
(2,1742)	1:110:A:LEU:HD11	1:173:A:ALA:HA	20	0.74	0.08	0.73
(2,1742)	1:110:A:LEU:HD13	1:173:A:ALA:HA	20	0.74	0.08	0.73
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	20	0.73	0.06	0.71
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	20	0.73	0.36	0.75
(4,7)	1:65:A:PHE:HZ	1:37:A:LEU:HD21	20	0.73	0.36	0.75
(4,7)	1:65:A:PHE:HZ	1:37:A:LEU:HD23	20	0.73	0.36	0.75
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	20	0.73	0.29	0.73

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG23	20	0.73	0.29	0.73
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG21	20	0.73	0.29	0.73
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	20	0.72	0.24	0.72
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD12	20	0.72	0.24	0.72
(2,1865)	1:109:A:ILE:HD11	1:144:A:LEU:HD13	20	0.72	0.24	0.72
(2,1865)	1:109:A:ILE:HD11	1:144:A:LEU:HD11	20	0.72	0.24	0.72
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	20	0.72	0.01	0.72
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD23	20	0.72	0.01	0.72
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD22	20	0.72	0.01	0.72
(4,431)	1:13:A:LEU:HG	1:13:A:LEU:HD12	20	0.72	0.01	0.72
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	20	0.72	0.16	0.78
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	20	0.71	0.57	0.5
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	20	0.7	0.2	0.72
(4,204)	1:173:A:ALA:HB1	1:111:A:LYS:HG3	20	0.7	0.2	0.72
(4,204)	1:173:A:ALA:HB1	1:111:A:LYS:HG2	20	0.7	0.2	0.72
(4,204)	1:173:A:ALA:HB2	1:111:A:LYS:HG2	20	0.7	0.2	0.72
(4,204)	1:173:A:ALA:HB3	1:111:A:LYS:HG3	20	0.7	0.2	0.72
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	20	0.7	0.03	0.69
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	20	0.7	0.17	0.77
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	20	0.7	0.31	0.58
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD3	20	0.7	0.31	0.58
(4,167)	1:34:A:VAL:H	1:11:A:LEU:HB3	20	0.7	0.31	0.58
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	20	0.7	0.02	0.7
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	20	0.69	0.07	0.69
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	20	0.68	0.16	0.7
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	20	0.68	0.16	0.7
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	20	0.67	0.07	0.66
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD21	20	0.67	0.07	0.66
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD23	20	0.67	0.07	0.66
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	20	0.67	0.04	0.67
(2,2784)	1:53:A:LEU:HD21	1:53:A:LEU:H	20	0.67	0.04	0.67
(2,2784)	1:53:A:LEU:HD22	1:53:A:LEU:H	20	0.67	0.04	0.67
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	20	0.67	0.02	0.66
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	20	0.66	0.29	0.66
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG23	20	0.66	0.29	0.66
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG21	20	0.66	0.29	0.66
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	20	0.66	0.02	0.65
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	20	0.65	0.03	0.65
(2,1297)	1:57:A:VAL:HG13	1:67:A:PHE:HB3	20	0.65	0.03	0.65
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	20	0.64	0.02	0.64
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	20	0.64	0.03	0.63
(2,3271)	1:57:A:VAL:HG13	1:67:A:PHE:HB3	20	0.64	0.03	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	20	0.64	0.05	0.64
(2,3813)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	20	0.64	0.19	0.67
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	20	0.64	0.19	0.67
(2,3813)	1:56:A:ILE:HD12	1:11:A:LEU:HD11	20	0.64	0.19	0.67
(2,3813)	1:56:A:ILE:HD12	1:11:A:LEU:HD13	20	0.64	0.19	0.67
(2,3813)	1:56:A:ILE:HD11	1:11:A:LEU:HD13	20	0.64	0.19	0.67
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD13	20	0.64	0.19	0.67
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	20	0.64	0.18	0.72
(2,1425)	1:56:A:ILE:HG23	1:65:A:PHE:HD1	20	0.64	0.18	0.72
(2,1425)	1:56:A:ILE:HG21	1:65:A:PHE:HD1	20	0.64	0.18	0.72
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	20	0.63	0.14	0.64
(2,3470)	1:110:A:LEU:HD13	1:107:A:ASP:HA	20	0.63	0.14	0.64
(2,3470)	1:110:A:LEU:HD12	1:107:A:ASP:HA	20	0.63	0.14	0.64
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	20	0.63	0.06	0.64
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB2	20	0.63	0.2	0.67
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	20	0.63	0.2	0.67
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB3	20	0.63	0.2	0.67
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	20	0.63	0.04	0.63
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	20	0.63	0.07	0.64
(4,437)	1:178:A:VAL:HG23	1:177:A:LYS:HG2	20	0.63	0.07	0.64
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	20	0.61	0.05	0.61
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	20	0.61	0.14	0.66
(4,15)	1:177:A:LYS:H	1:96:A:VAL:HG21	20	0.61	0.14	0.66
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD12	20	0.61	0.14	0.66
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD11	20	0.61	0.14	0.66
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	20	0.61	0.15	0.69
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	20	0.6	0.03	0.6
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	20	0.6	0.1	0.6
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	20	0.59	0.14	0.65
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	20	0.59	0.02	0.59
(2,1808)	1:13:A:LEU:HD22	1:13:A:LEU:HG	20	0.59	0.02	0.59
(2,1808)	1:13:A:LEU:HD23	1:13:A:LEU:HG	20	0.59	0.02	0.59
(4,436)	1:178:A:VAL:HG13	1:110:A:LEU:HB3	20	0.58	0.37	0.43
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	20	0.58	0.37	0.43
(4,436)	1:178:A:VAL:HG11	1:110:A:LEU:HB3	20	0.58	0.37	0.43
(4,436)	1:34:A:VAL:HG11	1:35:A:LYS:HG3	20	0.58	0.37	0.43
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	20	0.58	0.11	0.6
(4,278)	1:142:A:VAL:HG12	1:102:A:ALA:H	20	0.58	0.11	0.6
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	20	0.58	0.06	0.6
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	20	0.57	0.14	0.57
(4,303)	1:110:A:LEU:HD13	1:107:A:ASP:HA	20	0.57	0.14	0.57
(4,303)	1:110:A:LEU:HD12	1:107:A:ASP:HA	20	0.57	0.14	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	20	0.56	0.03	0.57
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	20	0.56	0.03	0.57
(2,1462)	1:14:A:VAL:HG23	1:14:A:VAL:H	20	0.56	0.03	0.57
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	20	0.55	0.2	0.57
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	20	0.54	0.02	0.55
(4,449)	1:74:A:ILE:HD11	1:57:A:VAL:HG23	20	0.54	0.04	0.54
(4,449)	1:74:A:ILE:HD12	1:11:A:LEU:HD23	20	0.54	0.04	0.54
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG23	20	0.54	0.04	0.54
(4,449)	1:57:A:VAL:HG21	1:74:A:ILE:HD11	20	0.54	0.04	0.54
(4,449)	1:74:A:ILE:HD11	1:11:A:LEU:HD21	20	0.54	0.04	0.54
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG21	20	0.54	0.04	0.54
(4,449)	1:74:A:ILE:HD12	1:11:A:LEU:HD21	20	0.54	0.04	0.54
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD12	20	0.54	0.04	0.55
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	20	0.54	0.04	0.55
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD13	20	0.54	0.04	0.55
(4,368)	1:20:A:ALA:HB3	1:22:A:ILE:HB	20	0.53	0.08	0.53
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	20	0.53	0.08	0.53
(4,368)	1:20:A:ALA:HB1	1:22:A:ILE:HB	20	0.53	0.08	0.53
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	20	0.53	0.02	0.54
(2,1813)	1:53:A:LEU:HD11	1:53:A:LEU:HG	20	0.53	0.02	0.54
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	20	0.51	0.09	0.52
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	20	0.51	0.09	0.52
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD11	20	0.51	0.06	0.5
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	20	0.51	0.06	0.5
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD12	20	0.51	0.06	0.5
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	20	0.51	0.11	0.5
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	20	0.5	0.06	0.49
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	20	0.5	0.06	0.49
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD12	20	0.5	0.06	0.49
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD13	20	0.49	0.04	0.48
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD12	20	0.49	0.04	0.48
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG23	20	0.49	0.04	0.48
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD11	20	0.49	0.04	0.48
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG22	20	0.49	0.04	0.48
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG21	20	0.49	0.04	0.48
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	20	0.49	0.15	0.5
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	20	0.48	0.01	0.49
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	20	0.48	0.02	0.48
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	20	0.48	0.05	0.48
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	20	0.48	0.1	0.46
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	20	0.48	0.1	0.46
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG22	20	0.48	0.08	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1859)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	20	0.48	0.08	0.47
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	20	0.48	0.08	0.47
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG23	20	0.48	0.08	0.47
(2,1827)	1:21:A:LEU:HD22	1:21:A:LEU:HG	20	0.47	0.06	0.46
(2,1827)	1:21:A:LEU:HD23	1:21:A:LEU:HG	20	0.47	0.06	0.46
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	20	0.47	0.06	0.46
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	20	0.47	0.05	0.46
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	20	0.47	0.05	0.46
(2,1834)	1:14:A:VAL:HG22	1:21:A:LEU:HG	20	0.47	0.05	0.46
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD21	20	0.47	0.03	0.48
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	20	0.47	0.03	0.48
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD23	20	0.47	0.03	0.48
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	20	0.47	0.03	0.46
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	20	0.47	0.03	0.47
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	20	0.46	0.08	0.44
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	20	0.46	0.08	0.44
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD22	20	0.46	0.08	0.44
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	20	0.46	0.04	0.47
(2,1872)	1:168:A:ILE:HD11	1:168:A:ILE:HG13	20	0.46	0.04	0.47
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	20	0.46	0.03	0.45
(2,3676)	1:86:A:LEU:HD23	1:86:A:LEU:HA	20	0.46	0.03	0.45
(2,3676)	1:86:A:LEU:HD21	1:86:A:LEU:HA	20	0.46	0.03	0.45
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	20	0.46	0.17	0.45
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	20	0.46	0.17	0.45
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	20	0.46	0.01	0.46
(2,1821)	1:143:A:VAL:HG21	1:143:A:VAL:HB	20	0.46	0.01	0.46
(2,1821)	1:143:A:VAL:HG22	1:143:A:VAL:HB	20	0.46	0.01	0.46
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	20	0.46	0.06	0.47
(2,1820)	1:142:A:VAL:HG11	1:142:A:VAL:HB	20	0.46	0.06	0.47
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD13	20	0.45	0.04	0.46
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	20	0.45	0.04	0.46
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD11	20	0.45	0.04	0.46
(2,1744)	1:109:A:ILE:HG23	1:109:A:ILE:HA	20	0.45	0.02	0.44
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	20	0.45	0.02	0.44
(2,1744)	1:109:A:ILE:HG21	1:109:A:ILE:HA	20	0.45	0.02	0.44
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	20	0.45	0.22	0.36
(2,1869)	1:97:A:LEU:HD23	1:96:A:VAL:HB	20	0.45	0.22	0.36
(2,1869)	1:97:A:LEU:HD22	1:96:A:VAL:HB	20	0.45	0.22	0.36
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	20	0.45	0.01	0.45
(2,3782)	1:143:A:VAL:HG21	1:143:A:VAL:HB	20	0.45	0.01	0.45
(2,3782)	1:143:A:VAL:HG22	1:143:A:VAL:HB	20	0.45	0.01	0.45
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	20	0.45	0.11	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	20	0.44	0.02	0.44
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	20	0.44	0.06	0.44
(2,175)	1:53:A:LEU:HD21	1:56:A:ILE:H	20	0.44	0.06	0.44
(2,175)	1:53:A:LEU:HD22	1:56:A:ILE:H	20	0.44	0.06	0.44
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	20	0.44	0.02	0.44
(2,3411)	1:56:A:ILE:HG23	1:56:A:ILE:H	20	0.44	0.02	0.44
(2,3411)	1:56:A:ILE:HG21	1:56:A:ILE:H	20	0.44	0.02	0.44
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	20	0.44	0.05	0.44
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	20	0.44	0.09	0.45
(2,1407)	1:95:A:ALA:HB3	1:95:A:ALA:H	20	0.44	0.09	0.45
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	20	0.44	0.07	0.45
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD21	20	0.43	0.06	0.44
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD22	20	0.43	0.06	0.44
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	20	0.43	0.06	0.44
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD21	20	0.43	0.06	0.44
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD12	20	0.43	0.05	0.45
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	20	0.43	0.05	0.45
(4,447)	1:53:A:LEU:HD12	1:11:A:LEU:HD23	20	0.43	0.05	0.45
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD11	20	0.43	0.05	0.45
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	20	0.43	0.02	0.43
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	20	0.43	0.02	0.43
(2,3798)	1:48:A:ILE:HD11	1:48:A:ILE:HG13	20	0.43	0.02	0.43
(2,3399)	1:21:A:LEU:HD13	1:21:A:LEU:H	20	0.43	0.09	0.46
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	20	0.43	0.09	0.46
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	20	0.43	0.06	0.44
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	20	0.43	0.06	0.44
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG22	20	0.43	0.06	0.44
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	20	0.43	0.05	0.44
(2,1819)	1:86:A:LEU:HD22	1:86:A:LEU:HG	20	0.43	0.05	0.44
(2,1819)	1:86:A:LEU:HD23	1:86:A:LEU:HG	20	0.43	0.05	0.44
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	20	0.42	0.07	0.44
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG23	20	0.42	0.07	0.44
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	20	0.42	0.09	0.43
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	20	0.42	0.09	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	20	0.42	0.01	0.42
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	20	0.42	0.04	0.42
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	20	0.41	0.08	0.44
(4,446)	1:110:A:LEU:HD12	1:110:A:LEU:HG	20	0.41	0.08	0.44
(4,446)	1:110:A:LEU:HD11	1:110:A:LEU:HG	20	0.41	0.08	0.44
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD11	20	0.41	0.08	0.44
(4,446)	1:110:A:LEU:HD13	1:110:A:LEU:HG	20	0.41	0.08	0.44
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	20	0.41	0.04	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	20	0.41	0.11	0.48
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	20	0.41	0.18	0.4
(4,259)	1:117:A:MET:HE2	2:201:A:NAD:H2A	20	0.41	0.18	0.4
(4,259)	1:117:A:MET:HE3	2:201:A:NAD:H2A	20	0.41	0.18	0.4
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	20	0.41	0.02	0.42
(2,3544)	1:66:A:ALA:HB3	1:66:A:ALA:HA	20	0.41	0.02	0.42
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	20	0.41	0.11	0.42
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	20	0.41	0.11	0.42
(2,1849)	1:15:A:LEU:HD13	1:74:A:ILE:HD11	20	0.41	0.11	0.42
(2,1849)	1:15:A:LEU:HD11	1:74:A:ILE:HD12	20	0.41	0.11	0.42
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD21	20	0.4	0.04	0.41
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	20	0.4	0.04	0.41
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD23	20	0.4	0.04	0.41
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	20	0.4	0.04	0.41
(2,3833)	1:168:A:ILE:HD11	1:168:A:ILE:HG13	20	0.4	0.04	0.41
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	20	0.4	0.04	0.4
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	20	0.4	0.02	0.4
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	20	0.4	0.02	0.4
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	20	0.4	0.05	0.42
(2,1699)	1:43:A:ALA:HB1	1:43:A:ALA:HA	20	0.39	0.01	0.4
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	20	0.39	0.01	0.4
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB2	20	0.39	0.01	0.4
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	20	0.39	0.08	0.4
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	20	0.39	0.05	0.38
(2,1793)	1:53:A:LEU:HD12	1:53:A:LEU:HB2	20	0.39	0.05	0.38
(2,3666)	1:43:A:ALA:HB1	1:43:A:ALA:HA	20	0.39	0.01	0.39
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	20	0.39	0.01	0.39
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB2	20	0.39	0.01	0.39
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	20	0.39	0.23	0.22
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	20	0.39	0.01	0.39
(2,1221)	1:176:A:ILE:HG22	1:176:A:ILE:HB	20	0.39	0.01	0.39
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	20	0.39	0.03	0.4
(2,3677)	1:15:A:LEU:HD22	1:15:A:LEU:HA	20	0.39	0.03	0.4
(2,3677)	1:15:A:LEU:HD23	1:15:A:LEU:HA	20	0.39	0.03	0.4
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	20	0.38	0.07	0.4
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD21	20	0.37	0.04	0.36
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	20	0.37	0.04	0.36
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD23	20	0.37	0.04	0.36
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	20	0.37	0.04	0.38
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG22	20	0.37	0.04	0.38
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	20	0.36	0.02	0.36
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	20	0.36	0.02	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD12	20	0.36	0.02	0.36
(2,1546)	1:48:A:ILE:HD11	1:53:A:LEU:HB2	20	0.36	0.01	0.36
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	20	0.36	0.01	0.36
(2,1546)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	20	0.36	0.01	0.36
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD22	20	0.36	0.02	0.36
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	20	0.36	0.02	0.36
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD21	20	0.36	0.02	0.36
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD11	20	0.35	0.04	0.35
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	20	0.35	0.04	0.35
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD12	20	0.35	0.04	0.35
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	20	0.35	0.04	0.36
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	20	0.35	0.06	0.36
(2,3781)	1:142:A:VAL:HG11	1:142:A:VAL:HB	20	0.35	0.06	0.36
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	20	0.35	0.02	0.35
(2,1692)	1:20:A:ALA:HB1	1:20:A:ALA:HA	20	0.35	0.02	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	20	0.35	0.01	0.35
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	20	0.34	0.03	0.36
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	20	0.34	0.03	0.36
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	20	0.34	0.01	0.34
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	20	0.34	0.01	0.34
(2,3783)	1:143:A:VAL:HG11	1:143:A:VAL:HB	20	0.34	0.01	0.34
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	20	0.34	0.04	0.32
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	20	0.34	0.04	0.32
(2,1838)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	20	0.34	0.03	0.34
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	20	0.34	0.03	0.34
(2,1838)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	20	0.34	0.03	0.34
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	20	0.34	0.07	0.32
(2,3439)	1:110:A:LEU:HD13	1:110:A:LEU:H	20	0.34	0.07	0.32
(2,3439)	1:110:A:LEU:HD11	1:110:A:LEU:H	20	0.34	0.07	0.32
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	20	0.34	0.09	0.35
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	20	0.33	0.11	0.35
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD12	20	0.33	0.11	0.35
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	20	0.33	0.05	0.34
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	20	0.33	0.02	0.33
(2,1532)	1:34:A:VAL:HG13	1:34:A:VAL:HA	20	0.33	0.02	0.34
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	20	0.33	0.02	0.34
(2,1201)	1:144:A:LEU:HD23	1:144:A:LEU:HG	20	0.33	0.02	0.33
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	20	0.33	0.02	0.33
(2,1201)	1:144:A:LEU:HD22	1:144:A:LEU:HG	20	0.33	0.02	0.33
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	20	0.33	0.04	0.32
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	20	0.33	0.04	0.32
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	20	0.33	0.03	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	20	0.33	0.04	0.31
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	20	0.33	0.02	0.32
(2,1832)	1:53:A:LEU:HD21	1:56:A:ILE:HB	20	0.33	0.02	0.32
(2,1832)	1:53:A:LEU:HD22	1:56:A:ILE:HB	20	0.33	0.02	0.32
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	20	0.33	0.05	0.32
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	20	0.33	0.05	0.32
(2,3387)	1:21:A:LEU:HD21	1:10:A:PHE:HE1	20	0.33	0.05	0.32
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	20	0.33	0.01	0.32
(2,1405)	1:20:A:ALA:HB3	1:20:A:ALA:H	20	0.33	0.01	0.32
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	20	0.32	0.04	0.33
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	20	0.32	0.09	0.36
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	20	0.32	0.01	0.32
(2,3196)	1:176:A:ILE:HG22	1:176:A:ILE:HB	20	0.32	0.01	0.32
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD22	20	0.32	0.02	0.32
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	20	0.32	0.02	0.32
(2,1850)	1:97:A:LEU:HD12	1:124:A:LEU:HD23	20	0.32	0.02	0.32
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	20	0.32	0.02	0.32
(2,1850)	1:97:A:LEU:HD12	1:124:A:LEU:HD22	20	0.32	0.02	0.32
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD21	20	0.32	0.02	0.32
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD23	20	0.32	0.02	0.32
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD21	20	0.32	0.02	0.32
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	20	0.32	0.02	0.32
(2,3659)	1:20:A:ALA:HB1	1:20:A:ALA:HA	20	0.32	0.02	0.32
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	20	0.32	0.02	0.32
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	20	0.32	0.01	0.32
(2,3556)	1:28:A:ALA:HB3	1:28:A:ALA:HA	20	0.32	0.01	0.32
(2,3556)	1:28:A:ALA:HB2	1:28:A:ALA:HA	20	0.32	0.01	0.32
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	20	0.32	0.02	0.32
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD22	20	0.32	0.02	0.32
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	20	0.32	0.02	0.32
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD21	20	0.32	0.02	0.32
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	20	0.31	0.06	0.3
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	20	0.31	0.06	0.3
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD12	20	0.31	0.06	0.3
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	20	0.31	0.01	0.31
(2,1395)	1:39:A:ALA:HB3	1:40:A:LYS:H	20	0.31	0.01	0.31
(2,3175)	1:144:A:LEU:HD23	1:144:A:LEU:HG	20	0.31	0.02	0.31
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	20	0.31	0.02	0.31
(2,3175)	1:144:A:LEU:HD22	1:144:A:LEU:HG	20	0.31	0.02	0.31
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	20	0.31	0.01	0.32
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD12	20	0.31	0.04	0.33
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	20	0.31	0.04	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD13	20	0.31	0.04	0.33
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	20	0.31	0.06	0.28
(2,3769)	1:5:A:VAL:HG23	1:5:A:VAL:HB	20	0.31	0.06	0.28
(2,3769)	1:5:A:VAL:HG22	1:5:A:VAL:HB	20	0.31	0.06	0.28
(2,1874)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	20	0.31	0.06	0.31
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	20	0.31	0.06	0.31
(2,1874)	1:168:A:ILE:HD12	1:171:A:VAL:HG13	20	0.31	0.06	0.31
(2,1874)	1:168:A:ILE:HD12	1:171:A:VAL:HG11	20	0.31	0.06	0.31
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	20	0.31	0.04	0.31
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	20	0.31	0.03	0.32
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	20	0.31	0.03	0.32
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	20	0.31	0.03	0.32
(2,1839)	1:56:A:ILE:HG21	1:56:A:ILE:HG12	20	0.31	0.03	0.32
(2,1839)	1:56:A:ILE:HG22	1:56:A:ILE:HG12	20	0.31	0.03	0.32
(2,1858)	1:109:A:ILE:HG21	1:109:A:ILE:HD11	20	0.3	0.03	0.3
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	20	0.3	0.03	0.3
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	20	0.3	0.03	0.3
(2,1858)	1:109:A:ILE:HG22	1:109:A:ILE:HD11	20	0.3	0.03	0.3
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	20	0.3	0.01	0.31
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	20	0.3	0.1	0.26
(2,1435)	1:15:A:LEU:HD22	1:15:A:LEU:H	20	0.3	0.1	0.26
(2,1435)	1:15:A:LEU:HD23	1:15:A:LEU:H	20	0.3	0.1	0.26
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	20	0.3	0.02	0.3
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG12	20	0.3	0.02	0.3
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	20	0.3	0.02	0.3
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	20	0.3	0.02	0.3
(2,1686)	1:14:A:VAL:HG23	1:19:A:PRO:HA	20	0.3	0.02	0.3
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	20	0.3	0.01	0.3
(2,1586)	1:28:A:ALA:HB3	1:28:A:ALA:HA	20	0.3	0.01	0.3
(2,1586)	1:28:A:ALA:HB2	1:28:A:ALA:HA	20	0.3	0.01	0.3
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	20	0.3	0.07	0.28
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG23	20	0.3	0.07	0.28
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG21	20	0.3	0.07	0.28
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	20	0.3	0.03	0.29
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	20	0.3	0.01	0.3
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	20	0.3	0.02	0.3
(2,1573)	1:66:A:ALA:HB3	1:66:A:ALA:HA	20	0.3	0.02	0.3
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	20	0.3	0.02	0.29
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	20	0.3	0.05	0.31
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	20	0.29	0.01	0.29
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	20	0.29	0.01	0.29
(2,1822)	1:143:A:VAL:HG11	1:143:A:VAL:HB	20	0.29	0.01	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	20	0.29	0.02	0.28
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	20	0.29	0.04	0.29
(4,451)	1:168:A:ILE:HD12	1:168:A:ILE:HG12	20	0.29	0.04	0.29
(4,451)	1:168:A:ILE:HD11	1:168:A:ILE:HG12	20	0.29	0.04	0.29
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	20	0.28	0.02	0.28
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	20	0.28	0.01	0.28
(4,426)	1:53:A:LEU:HD13	1:37:A:LEU:HG	20	0.28	0.01	0.28
(2,1301)	1:34:A:VAL:HG13	1:38:A:LEU:H	20	0.28	0.09	0.27
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	20	0.28	0.09	0.27
(2,1301)	1:34:A:VAL:HG12	1:38:A:LEU:H	20	0.28	0.09	0.27
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	20	0.28	0.06	0.3
(2,3826)	1:11:A:LEU:HD13	1:11:A:LEU:HB3	20	0.28	0.06	0.3
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG22	20	0.28	0.08	0.27
(2,3821)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	20	0.28	0.08	0.27
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	20	0.28	0.08	0.27
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG23	20	0.28	0.08	0.27
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	20	0.28	0.04	0.28
(4,395)	1:56:A:ILE:HG22	1:56:A:ILE:HA	20	0.28	0.04	0.28
(4,395)	1:56:A:ILE:HG23	1:56:A:ILE:HA	20	0.28	0.04	0.28
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	20	0.28	0.02	0.27
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	20	0.28	0.01	0.28
(2,1796)	1:76:A:ALA:HB2	1:15:A:LEU:HD11	20	0.27	0.04	0.28
(2,1796)	1:76:A:ALA:HB2	1:15:A:LEU:HD12	20	0.27	0.04	0.28
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	20	0.27	0.04	0.28
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	20	0.27	0.04	0.28
(2,1796)	1:76:A:ALA:HB1	1:15:A:LEU:HD11	20	0.27	0.04	0.28
(2,1796)	1:76:A:ALA:HB1	1:15:A:LEU:HD12	20	0.27	0.04	0.28
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	20	0.27	0.06	0.24
(2,1804)	1:5:A:VAL:HG23	1:5:A:VAL:HB	20	0.27	0.06	0.24
(2,1804)	1:5:A:VAL:HG22	1:5:A:VAL:HB	20	0.27	0.06	0.24
(2,1857)	1:151:A:MET:HE1	1:171:A:VAL:HG12	20	0.27	0.04	0.27
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	20	0.27	0.04	0.27
(2,1857)	1:151:A:MET:HE2	1:171:A:VAL:HG12	20	0.27	0.04	0.27
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	20	0.27	0.03	0.28
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	20	0.27	0.02	0.28
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	20	0.27	0.05	0.26
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	20	0.27	0.05	0.26
(2,3795)	1:14:A:VAL:HG22	1:21:A:LEU:HG	20	0.27	0.05	0.26
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	20	0.26	0.06	0.25
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	20	0.26	0.02	0.26
(2,1576)	1:22:A:ILE:HG21	1:22:A:ILE:HA	20	0.26	0.02	0.26
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	20	0.26	0.04	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE3	20	0.26	0.04	0.25
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE1	20	0.26	0.04	0.25
(2,2041)	1:152:A:ALA:HB2	1:152:A:ALA:H	20	0.26	0.03	0.26
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	20	0.26	0.03	0.26
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	20	0.26	0.03	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	20	0.26	0.01	0.26
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	20	0.26	0.03	0.25
(2,1709)	1:86:A:LEU:HD23	1:86:A:LEU:HA	20	0.26	0.03	0.25
(2,1709)	1:86:A:LEU:HD21	1:86:A:LEU:HA	20	0.26	0.03	0.25
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	20	0.26	0.03	0.26
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD22	20	0.26	0.03	0.26
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD21	20	0.26	0.03	0.26
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	20	0.26	0.03	0.25
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	20	0.26	0.03	0.25
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	20	0.26	0.07	0.24
(4,439)	1:176:A:ILE:HG22	1:109:A:ILE:HB	20	0.26	0.07	0.24
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	20	0.25	0.06	0.26
(2,1863)	1:11:A:LEU:HD13	1:11:A:LEU:HB3	20	0.25	0.06	0.26
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	20	0.25	0.05	0.25
(2,3809)	1:176:A:ILE:HB	1:110:A:LEU:HD11	20	0.25	0.05	0.25
(2,3809)	1:110:A:LEU:HD13	1:176:A:ILE:HB	20	0.25	0.05	0.25
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	20	0.25	0.06	0.23
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG23	20	0.25	0.06	0.23
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG21	20	0.25	0.06	0.23
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	20	0.25	0.02	0.24
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	20	0.25	0.01	0.24
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	20	0.24	0.02	0.25
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	20	0.24	0.02	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	20	0.24	0.02	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG22	20	0.24	0.02	0.24
(2,1854)	1:22:A:ILE:HG23	1:14:A:VAL:HG21	20	0.24	0.02	0.24
(2,3836)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	20	0.24	0.06	0.24
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	20	0.24	0.06	0.24
(2,3836)	1:168:A:ILE:HD12	1:171:A:VAL:HG13	20	0.24	0.06	0.24
(2,3836)	1:168:A:ILE:HD12	1:171:A:VAL:HG11	20	0.24	0.06	0.24
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	20	0.24	0.05	0.23
(2,3759)	1:53:A:LEU:HD12	1:53:A:LEU:HB2	20	0.24	0.05	0.23
(2,1844)	1:110:A:LEU:HD23	1:110:A:LEU:HB3	20	0.24	0.03	0.25
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	20	0.24	0.03	0.25
(2,1844)	1:110:A:LEU:HD22	1:110:A:LEU:HB3	20	0.24	0.03	0.25
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	20	0.24	0.03	0.24
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	20	0.24	0.03	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3710)	1:14:A:VAL:HG23	1:14:A:VAL:HA	20	0.24	0.03	0.24
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	20	0.24	0.05	0.24
(2,1810)	1:21:A:LEU:HD12	1:21:A:LEU:HB3	20	0.24	0.05	0.25
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	20	0.24	0.05	0.25
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	20	0.23	0.04	0.24
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	20	0.23	0.01	0.23
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	20	0.23	0.05	0.24
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	20	0.23	0.02	0.23
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	20	0.23	0.03	0.24
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	20	0.23	0.05	0.24
(2,3800)	1:56:A:ILE:HD11	1:56:A:ILE:HG12	20	0.23	0.02	0.22
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	20	0.23	0.02	0.22
(2,3800)	1:56:A:ILE:HD12	1:56:A:ILE:HG12	20	0.23	0.02	0.22
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	20	0.23	0.02	0.23
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	20	0.23	0.03	0.23
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	20	0.23	0.04	0.24
(2,3424)	1:165:A:VAL:HG23	2:201:A:NAD:H5N	20	0.23	0.04	0.24
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	20	0.22	0.03	0.22
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	20	0.22	0.04	0.21
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE3	20	0.22	0.04	0.21
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE1	20	0.22	0.04	0.21
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	20	0.22	0.02	0.22
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	20	0.22	0.02	0.22
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	20	0.22	0.06	0.2
(2,1861)	1:41:A:MET:HE1	1:11:A:LEU:HD12	20	0.22	0.06	0.2
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD11	20	0.22	0.06	0.2
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	20	0.22	0.01	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	20	0.22	0.02	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	20	0.22	0.02	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG22	20	0.22	0.02	0.22
(2,3816)	1:22:A:ILE:HG23	1:14:A:VAL:HG21	20	0.22	0.02	0.22
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	20	0.22	0.02	0.21
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	20	0.22	0.01	0.22
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	20	0.22	0.02	0.22
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	20	0.22	0.02	0.22
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	20	0.22	0.04	0.22
(2,1455)	1:165:A:VAL:HG23	2:201:A:NAD:H5N	20	0.22	0.04	0.22
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	20	0.22	0.01	0.22
(2,3372)	1:20:A:ALA:HB3	1:20:A:ALA:H	20	0.22	0.01	0.22
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	20	0.21	0.06	0.19
(2,3824)	1:41:A:MET:HE1	1:11:A:LEU:HD12	20	0.21	0.06	0.19
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD11	20	0.21	0.06	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	20	0.21	0.01	0.21
(2,3841)	1:76:A:ALA:HB1	1:76:A:ALA:H	20	0.21	0.03	0.2
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	20	0.21	0.03	0.2
(2,3841)	1:76:A:ALA:HB3	1:76:A:ALA:H	20	0.21	0.03	0.2
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	20	0.21	0.02	0.21
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	20	0.21	0.01	0.21
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	20	0.21	0.02	0.21
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	20	0.21	0.02	0.2
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	20	0.21	0.02	0.2
(2,3653)	1:14:A:VAL:HG23	1:19:A:PRO:HA	20	0.21	0.02	0.2
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	20	0.21	0.03	0.21
(2,1524)	1:82:A:VAL:HG11	1:82:A:VAL:HA	20	0.21	0.03	0.21
(2,1524)	1:82:A:VAL:HG12	1:82:A:VAL:HA	20	0.21	0.03	0.21
(2,1524)	1:82:A:VAL:HG13	1:82:A:VAL:HA	20	0.21	0.03	0.21
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	20	0.21	0.04	0.21
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	20	0.2	0.01	0.2
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	20	0.2	0.02	0.2
(2,1800)	1:53:A:LEU:HD13	1:37:A:LEU:HG	20	0.2	0.02	0.2
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	20	0.2	0.03	0.21
(4,452)	1:59:A:THR:HB	1:59:A:THR:HG22	20	0.2	0.03	0.21
(2,3819)	1:151:A:MET:HE1	1:171:A:VAL:HG12	20	0.2	0.04	0.2
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	20	0.2	0.04	0.2
(2,3819)	1:151:A:MET:HE2	1:171:A:VAL:HG12	20	0.2	0.04	0.2
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	20	0.2	0.03	0.21
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	20	0.2	0.03	0.21
(2,3495)	1:82:A:VAL:HG11	1:82:A:VAL:HA	20	0.2	0.03	0.21
(2,3495)	1:82:A:VAL:HG12	1:82:A:VAL:HA	20	0.2	0.03	0.21
(2,3495)	1:82:A:VAL:HG13	1:82:A:VAL:HA	20	0.2	0.03	0.21
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	20	0.2	0.03	0.2
(2,1194)	1:176:A:ILE:HD12	1:114:A:ILE:HD13	20	0.2	0.03	0.2
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	20	0.2	0.02	0.21
(2,3503)	1:34:A:VAL:HG13	1:34:A:VAL:HA	20	0.2	0.02	0.2
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	20	0.2	0.02	0.2
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	20	0.2	0.06	0.18
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	20	0.2	0.06	0.18
(2,3794)	1:14:A:VAL:HG22	1:14:A:VAL:HB	20	0.2	0.06	0.18
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	20	0.2	0.02	0.2
(2,3547)	1:22:A:ILE:HG21	1:22:A:ILE:HA	20	0.2	0.02	0.2
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	20	0.2	0.03	0.21
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	20	0.2	0.01	0.2
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	20	0.19	0.02	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	20	0.19	0.01	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	20	0.19	0.02	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	20	0.19	0.0	0.19
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	20	0.18	0.02	0.18
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	20	0.18	0.02	0.18
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD12	20	0.18	0.02	0.18
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	20	0.18	0.01	0.18
(2,3654)	1:96:A:VAL:HG22	1:96:A:VAL:HA	20	0.18	0.01	0.18
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	20	0.18	0.02	0.18
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	20	0.18	0.01	0.18
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	20	0.18	0.02	0.18
(2,3793)	1:53:A:LEU:HD21	1:56:A:ILE:HB	20	0.18	0.02	0.18
(2,3793)	1:53:A:LEU:HD22	1:56:A:ILE:HB	20	0.18	0.02	0.18
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	20	0.18	0.02	0.17
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD22	20	0.17	0.02	0.18
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	20	0.17	0.02	0.18
(2,3127)	1:97:A:LEU:HD12	1:124:A:LEU:HD23	20	0.17	0.02	0.18
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	20	0.17	0.02	0.18
(2,3127)	1:97:A:LEU:HD12	1:124:A:LEU:HD22	20	0.17	0.02	0.18
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD21	20	0.17	0.02	0.18
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD23	20	0.17	0.02	0.18
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD21	20	0.17	0.02	0.18
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	20	0.17	0.01	0.17
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	20	0.17	0.03	0.17
(2,3167)	1:176:A:ILE:HD12	1:114:A:ILE:HD13	20	0.17	0.03	0.17
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	20	0.16	0.02	0.16
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	20	0.16	0.03	0.15
(2,3773)	1:34:A:VAL:HG13	1:37:A:LEU:HB3	20	0.16	0.02	0.16
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	20	0.16	0.02	0.16
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	20	0.16	0.01	0.16
(2,1962)	1:110:A:LEU:HD13	1:106:A:PHE:HE1	20	0.16	0.01	0.16
(2,1962)	1:110:A:LEU:HD12	1:106:A:PHE:HE1	20	0.16	0.01	0.16
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	20	0.15	0.02	0.16
(2,3770)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	20	0.15	0.02	0.15
(2,3770)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	20	0.15	0.02	0.15
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	20	0.15	0.02	0.15
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	20	0.15	0.02	0.15
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	20	0.15	0.02	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	20	0.15	0.01	0.15
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	20	0.15	0.01	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	20	0.14	0.01	0.14
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	20	0.13	0.01	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	20	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,274)	1:124:A:LEU:HD22	1:159:A:TYR:HE1	19	1.6	0.43	1.5
(4,274)	1:124:A:LEU:HD23	1:159:A:TYR:HE1	19	1.6	0.43	1.5
(4,274)	1:124:A:LEU:HD21	1:156:A:PHE:HZ	19	1.6	0.43	1.5
(4,274)	1:124:A:LEU:HD22	1:156:A:PHE:HZ	19	1.6	0.43	1.5
(4,274)	1:124:A:LEU:HD23	1:156:A:PHE:HZ	19	1.6	0.43	1.5
(4,274)	1:124:A:LEU:HD21	1:159:A:TYR:HE1	19	1.6	0.43	1.5
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	19	1.39	0.77	1.54
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	19	0.95	0.28	0.94
(2,1468)	1:22:A:ILE:HG21	1:10:A:PHE:HZ	19	0.95	0.28	0.94
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD11	19	0.87	0.12	0.87
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	19	0.87	0.12	0.87
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	19	0.87	0.12	0.87
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	19	0.87	0.12	0.87
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD12	19	0.87	0.12	0.87
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	19	0.82	0.27	0.97
(2,1549)	1:37:A:LEU:HD12	1:41:A:MET:HG2	19	0.78	0.32	0.85
(2,1549)	1:37:A:LEU:HD13	1:41:A:MET:HG2	19	0.78	0.32	0.85
(2,1549)	1:37:A:LEU:HD11	1:41:A:MET:HG2	19	0.78	0.32	0.85
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD22	19	0.76	0.15	0.77
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD23	19	0.76	0.15	0.77
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD23	19	0.76	0.15	0.77
(4,450)	1:97:A:LEU:HD21	1:124:A:LEU:HD23	19	0.76	0.15	0.77
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD22	19	0.76	0.15	0.77
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD21	19	0.76	0.15	0.77
(4,450)	1:97:A:LEU:HD21	1:124:A:LEU:HD22	19	0.76	0.15	0.77
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD21	19	0.76	0.15	0.77
(2,3790)	1:34:A:VAL:HG12	1:50:A:MET:HE2	19	0.68	0.16	0.72
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	19	0.68	0.16	0.72
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE2	19	0.68	0.16	0.72
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE1	19	0.68	0.16	0.72
(2,3790)	1:34:A:VAL:HG12	1:50:A:MET:HE1	19	0.68	0.16	0.72
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	19	0.6	0.24	0.66
(2,1424)	1:56:A:ILE:HG23	1:65:A:PHE:HE1	19	0.6	0.24	0.66
(2,1424)	1:56:A:ILE:HG21	1:65:A:PHE:HE1	19	0.6	0.24	0.66
(2,1807)	1:151:A:MET:HE2	1:174:A:GLU:HG2	19	0.55	0.24	0.53
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	19	0.55	0.24	0.53
(2,1807)	1:151:A:MET:HE3	1:174:A:GLU:HG2	19	0.55	0.24	0.53
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	19	0.55	0.18	0.51
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	19	0.55	0.18	0.51
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	19	0.55	0.18	0.51
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	19	0.54	0.14	0.54
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB3	19	0.54	0.14	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3837)	1:5:A:VAL:HG23	1:5:A:VAL:HA	19	0.54	0.33	0.76
(2,3837)	1:5:A:VAL:HG21	1:5:A:VAL:HA	19	0.54	0.33	0.76
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	19	0.54	0.33	0.76
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	19	0.47	0.16	0.48
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	19	0.44	0.05	0.43
(2,1750)	1:158:A:PHE:HB2	1:168:A:ILE:HG12	19	0.44	0.05	0.43
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	19	0.4	0.07	0.41
(2,405)	1:95:A:ALA:HB2	1:149:A:LYS:H	19	0.4	0.07	0.41
(2,1531)	1:21:A:LEU:HD11	1:14:A:VAL:HA	19	0.39	0.04	0.37
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	19	0.39	0.04	0.37
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	19	0.38	0.05	0.39
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	19	0.38	0.11	0.45
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG12	19	0.38	0.11	0.45
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG13	19	0.38	0.11	0.45
(2,16)	1:21:A:LEU:HD13	1:10:A:PHE:HE1	19	0.36	0.11	0.38
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	19	0.36	0.11	0.38
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	19	0.35	0.09	0.35
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	19	0.35	0.09	0.35
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	19	0.35	0.04	0.34
(2,3718)	1:158:A:PHE:HB2	1:168:A:ILE:HG12	19	0.35	0.04	0.34
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	19	0.34	0.07	0.35
(2,2376)	1:95:A:ALA:HB2	1:149:A:LYS:H	19	0.34	0.07	0.35
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	19	0.34	0.08	0.35
(2,3474)	1:146:A:VAL:HG12	1:96:A:VAL:HA	19	0.34	0.08	0.35
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD11	19	0.34	0.12	0.34
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	19	0.34	0.12	0.34
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	19	0.34	0.12	0.34
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	19	0.34	0.12	0.34
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD12	19	0.34	0.12	0.34
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	19	0.32	0.09	0.31
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	19	0.32	0.09	0.31
(2,3811)	1:15:A:LEU:HD13	1:74:A:ILE:HD11	19	0.32	0.09	0.31
(2,3811)	1:15:A:LEU:HD11	1:74:A:ILE:HD12	19	0.32	0.09	0.31
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	19	0.29	0.11	0.25
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	19	0.28	0.05	0.28
(2,3490)	1:48:A:ILE:HD13	1:53:A:LEU:HA	19	0.28	0.06	0.27
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	19	0.28	0.06	0.27
(2,3490)	1:48:A:ILE:HD12	1:53:A:LEU:HA	19	0.28	0.06	0.27
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	19	0.25	0.06	0.24
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	19	0.23	0.04	0.23
(2,3502)	1:21:A:LEU:HD11	1:14:A:VAL:HA	19	0.23	0.04	0.22
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	19	0.23	0.04	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	19	0.22	0.02	0.22
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	19	0.22	0.05	0.23
(2,1410)	1:95:A:ALA:HB3	1:96:A:VAL:H	19	0.22	0.05	0.23
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	19	0.21	0.03	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	19	0.21	0.02	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD21	19	0.21	0.02	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD22	19	0.21	0.02	0.21
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	19	0.2	0.02	0.2
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	19	0.18	0.03	0.18
(2,3763)	1:76:A:ALA:HB2	1:15:A:LEU:HD11	19	0.18	0.04	0.18
(2,3763)	1:76:A:ALA:HB2	1:15:A:LEU:HD12	19	0.18	0.04	0.18
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	19	0.18	0.04	0.18
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	19	0.18	0.04	0.18
(2,3763)	1:76:A:ALA:HB1	1:15:A:LEU:HD11	19	0.18	0.04	0.18
(2,3763)	1:76:A:ALA:HB1	1:15:A:LEU:HD12	19	0.18	0.04	0.18
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	19	0.18	0.03	0.18
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG22	19	0.18	0.03	0.18
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	19	0.17	0.04	0.17
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	19	0.16	0.04	0.15
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	19	0.16	0.06	0.14
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	19	0.16	0.06	0.14
(2,1833)	1:14:A:VAL:HG22	1:14:A:VAL:HB	19	0.16	0.06	0.14
(2,1474)	1:110:A:LEU:HD23	1:110:A:LEU:H	19	0.16	0.03	0.16
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	19	0.16	0.03	0.16
(2,1474)	1:110:A:LEU:HD21	1:110:A:LEU:H	19	0.16	0.03	0.16
(2,1809)	1:34:A:VAL:HG13	1:37:A:LEU:HB3	19	0.15	0.02	0.15
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	19	0.15	0.02	0.15
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	19	0.14	0.02	0.15
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	19	0.14	0.02	0.14
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	19	0.14	0.03	0.13
(2,1805)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	19	0.13	0.02	0.13
(2,1805)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	19	0.13	0.02	0.13
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	19	0.13	0.02	0.13
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	19	0.13	0.02	0.13
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	19	0.13	0.02	0.14
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	19	0.12	0.01	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	19	0.12	0.01	0.12
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	19	0.12	0.01	0.11
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	18	1.81	0.83	2.13
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG12	18	1.81	0.83	2.13
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG11	18	1.81	0.83	2.13
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	18	0.85	0.31	1.02

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	18	0.78	0.2	0.79
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	18	0.73	0.16	0.76
(2,3524)	1:13:A:LEU:HD11	1:18:A:ASN:HB2	18	0.73	0.16	0.76
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	18	0.66	0.05	0.66
(4,6)	1:65:A:PHE:HE1	1:74:A:ILE:HG23	18	0.58	0.15	0.58
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD22	18	0.58	0.15	0.58
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD21	18	0.58	0.15	0.58
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD23	18	0.58	0.15	0.58
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	18	0.47	0.11	0.44
(2,1565)	1:22:A:ILE:HG22	1:41:A:MET:HB2	18	0.47	0.11	0.44
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	18	0.43	0.11	0.44
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	18	0.42	0.09	0.43
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	18	0.39	0.07	0.41
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	18	0.38	0.12	0.41
(2,1314)	1:142:A:VAL:HG11	1:103:A:GLU:HA	18	0.38	0.12	0.41
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	18	0.37	0.05	0.37
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	18	0.33	0.09	0.34
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	18	0.27	0.07	0.28
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	18	0.26	0.12	0.22
(4,208)	1:171:A:VAL:HG23	1:173:A:ALA:HA	18	0.26	0.12	0.22
(4,208)	1:14:A:VAL:HG22	1:11:A:LEU:HA	18	0.26	0.12	0.22
(4,208)	1:14:A:VAL:HG21	1:11:A:LEU:HA	18	0.26	0.12	0.22
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	18	0.26	0.03	0.26
(4,307)	1:38:A:LEU:HD11	1:50:A:MET:HA	18	0.24	0.06	0.27
(4,307)	1:38:A:LEU:HD13	1:50:A:MET:HA	18	0.24	0.06	0.27
(4,307)	1:26:A:LEU:HD22	1:15:A:LEU:HA	18	0.24	0.06	0.27
(4,307)	1:26:A:LEU:HD23	1:15:A:LEU:HA	18	0.24	0.06	0.27
(4,307)	1:38:A:LEU:HD12	1:50:A:MET:HA	18	0.24	0.06	0.27
(4,307)	1:26:A:LEU:HD21	1:15:A:LEU:HA	18	0.24	0.06	0.27
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	18	0.24	0.06	0.26
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	18	0.24	0.04	0.24
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	18	0.24	0.04	0.24
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG22	18	0.24	0.04	0.24
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	18	0.23	0.09	0.24
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	18	0.23	0.09	0.24
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG11	18	0.22	0.04	0.24
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	18	0.22	0.04	0.24
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	18	0.21	0.03	0.22
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	18	0.2	0.05	0.22
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	18	0.2	0.05	0.19
(2,3266)	1:53:A:LEU:HD11	1:67:A:PHE:HE1	18	0.2	0.05	0.19
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	18	0.19	0.03	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	18	0.18	0.03	0.2
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD21	18	0.17	0.03	0.17
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	18	0.17	0.03	0.17
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD23	18	0.17	0.03	0.17
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	18	0.17	0.03	0.16
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	18	0.17	0.02	0.16
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB1	18	0.17	0.02	0.16
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB3	18	0.17	0.02	0.16
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	18	0.16	0.02	0.16
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	18	0.16	0.02	0.17
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	18	0.15	0.02	0.15
(2,85)	1:152:A:ALA:HB2	1:152:A:ALA:H	18	0.14	0.02	0.14
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	18	0.14	0.02	0.14
(2,3802)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	18	0.14	0.02	0.14
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	18	0.14	0.02	0.14
(2,3802)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	18	0.14	0.02	0.14
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	18	0.13	0.01	0.13
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	18	0.13	0.02	0.13
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	18	0.12	0.01	0.13
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	18	0.12	0.01	0.12
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	17	0.77	0.35	0.81
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	17	0.77	0.35	0.81
(4,353)	1:84:A:VAL:HB	1:87:A:GLY:HA2	17	0.77	0.35	0.81
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	17	0.77	0.12	0.8
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	17	0.7	0.21	0.69
(4,95)	1:51:A:GLU:H	1:58:A:GLU:HG3	17	0.7	0.21	0.69
(4,332)	1:37:A:LEU:HD12	1:41:A:MET:HB2	17	0.65	0.1	0.63
(4,332)	1:37:A:LEU:HD13	1:41:A:MET:HB2	17	0.65	0.1	0.63
(4,332)	1:37:A:LEU:HD11	1:41:A:MET:HB2	17	0.65	0.1	0.63
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	17	0.55	0.23	0.59
(2,1601)	1:41:A:MET:HE2	1:10:A:PHE:HB3	17	0.55	0.23	0.59
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	17	0.47	0.17	0.44
(2,3772)	1:151:A:MET:HE2	1:174:A:GLU:HG2	17	0.44	0.21	0.44
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	17	0.44	0.21	0.44
(2,3772)	1:151:A:MET:HE3	1:174:A:GLU:HG2	17	0.44	0.21	0.44
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	17	0.44	0.38	0.3
(2,815)	1:102:A:ALA:H	1:101:A:THR:HG23	17	0.44	0.38	0.3
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	17	0.43	0.1	0.47
(2,3391)	1:56:A:ILE:HG23	1:65:A:PHE:HD1	17	0.43	0.1	0.47
(2,3391)	1:56:A:ILE:HG21	1:65:A:PHE:HD1	17	0.43	0.1	0.47
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	17	0.41	0.2	0.35
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	17	0.38	0.05	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG21	17	0.38	0.05	0.37
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	17	0.37	0.02	0.37
(2,521)	1:129:A:THR:HG23	1:129:A:THR:H	17	0.37	0.02	0.37
(2,521)	1:129:A:THR:HG22	1:129:A:THR:H	17	0.37	0.02	0.37
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	17	0.31	0.17	0.28
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	17	0.31	0.17	0.28
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	17	0.31	0.17	0.28
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	17	0.28	0.14	0.27
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	17	0.28	0.14	0.27
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	17	0.25	0.08	0.22
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD13	17	0.24	0.06	0.23
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD11	17	0.24	0.06	0.23
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD12	17	0.24	0.06	0.23
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	17	0.22	0.05	0.22
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	17	0.2	0.05	0.2
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG23	17	0.2	0.05	0.2
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	17	0.2	0.04	0.21
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	17	0.19	0.03	0.19
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	17	0.18	0.05	0.17
(4,290)	1:53:A:LEU:HD22	1:56:A:ILE:H	17	0.18	0.05	0.17
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	17	0.18	0.05	0.18
(4,442)	1:178:A:VAL:HG21	1:144:A:LEU:HG	17	0.18	0.05	0.18
(4,442)	1:178:A:VAL:HG22	1:176:A:ILE:HB	17	0.18	0.05	0.18
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	17	0.17	0.03	0.18
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	17	0.17	0.02	0.17
(2,3382)	1:53:A:LEU:HD11	1:67:A:PHE:HZ	17	0.17	0.02	0.17
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	17	0.16	0.03	0.15
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	17	0.16	0.03	0.15
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG11	17	0.16	0.02	0.16
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	17	0.16	0.02	0.16
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	17	0.15	0.03	0.15
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	17	0.15	0.03	0.15
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG22	17	0.15	0.03	0.15
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	17	0.13	0.02	0.14
(2,3405)	1:56:A:ILE:HG23	1:57:A:VAL:H	17	0.13	0.02	0.14
(2,3405)	1:56:A:ILE:HG21	1:57:A:VAL:H	17	0.13	0.02	0.14
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	17	0.13	0.02	0.13
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB1	17	0.13	0.02	0.13
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB3	17	0.13	0.02	0.13
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	17	0.12	0.01	0.12
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	17	0.12	0.01	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	17	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1291)	1:84:A:VAL:HG13	1:84:A:VAL:H	16	0.98	0.29	0.94
(2,1291)	1:84:A:VAL:HG12	1:84:A:VAL:H	16	0.98	0.29	0.94
(2,1291)	1:84:A:VAL:HG11	1:84:A:VAL:H	16	0.98	0.29	0.94
(2,3416)	1:143:A:VAL:HG13	1:143:A:VAL:H	16	0.71	0.05	0.71
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	16	0.71	0.05	0.71
(2,3416)	1:143:A:VAL:HG11	1:143:A:VAL:H	16	0.71	0.05	0.71
(2,3265)	1:84:A:VAL:HG13	1:84:A:VAL:H	16	0.71	0.29	0.66
(2,3265)	1:84:A:VAL:HG12	1:84:A:VAL:H	16	0.71	0.29	0.66
(2,3265)	1:84:A:VAL:HG11	1:84:A:VAL:H	16	0.71	0.29	0.66
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE1	16	0.67	0.1	0.66
(2,3784)	1:37:A:LEU:HD11	1:41:A:MET:HE1	16	0.67	0.1	0.66
(2,3784)	1:37:A:LEU:HD13	1:41:A:MET:HE3	16	0.67	0.1	0.66
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE3	16	0.67	0.1	0.66
(2,3784)	1:37:A:LEU:HD13	1:41:A:MET:HE1	16	0.67	0.1	0.66
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE1	16	0.61	0.1	0.6
(2,1823)	1:37:A:LEU:HD11	1:41:A:MET:HE1	16	0.61	0.1	0.6
(2,1823)	1:37:A:LEU:HD13	1:41:A:MET:HE3	16	0.61	0.1	0.6
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE3	16	0.61	0.1	0.6
(2,1823)	1:37:A:LEU:HD13	1:41:A:MET:HE1	16	0.61	0.1	0.6
(2,3570)	1:4:A:MET:HE3	1:52:A:GLU:HA	16	0.5	0.21	0.48
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	16	0.5	0.21	0.48
(2,3570)	1:4:A:MET:HE2	1:52:A:GLU:HA	16	0.5	0.21	0.48
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	16	0.4	0.13	0.4
(2,187)	1:26:A:LEU:HD22	1:26:A:LEU:H	16	0.4	0.13	0.4
(2,187)	1:26:A:LEU:HD23	1:26:A:LEU:H	16	0.4	0.13	0.4
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	16	0.34	0.08	0.34
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	16	0.32	0.16	0.24
(2,1388)	1:41:A:MET:HE2	1:41:A:MET:H	16	0.32	0.16	0.24
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	16	0.23	0.07	0.22
(2,1509)	1:151:A:MET:HE2	1:171:A:VAL:HA	16	0.23	0.07	0.22
(2,1509)	1:151:A:MET:HE3	1:171:A:VAL:HA	16	0.23	0.07	0.22
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	16	0.21	0.11	0.16
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	16	0.2	0.02	0.2
(2,594)	1:43:A:ALA:HB1	1:44:A:LYS:H	16	0.2	0.02	0.2
(2,594)	1:43:A:ALA:HB3	1:44:A:LYS:H	16	0.2	0.02	0.2
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	16	0.17	0.04	0.17
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	16	0.16	0.02	0.16
(2,2367)	1:48:A:ILE:HG23	1:48:A:ILE:H	16	0.16	0.02	0.16
(2,2367)	1:48:A:ILE:HG22	1:48:A:ILE:H	16	0.16	0.02	0.16
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	16	0.16	0.05	0.15
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG21	16	0.16	0.05	0.15
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	16	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	16	0.14	0.04	0.11
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	16	0.13	0.03	0.11
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	16	0.12	0.01	0.12
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	16	0.12	0.01	0.12
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG23	16	0.12	0.01	0.12
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	16	0.12	0.01	0.12
(4,41)	1:5:A:VAL:HG22	1:5:A:VAL:H	16	0.12	0.01	0.12
(4,41)	1:5:A:VAL:HG23	1:5:A:VAL:H	16	0.12	0.01	0.12
(4,41)	1:5:A:VAL:HG21	1:5:A:VAL:H	16	0.12	0.01	0.12
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	16	0.12	0.01	0.12
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG23	16	0.12	0.01	0.12
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	15	0.76	0.43	1.01
(4,440)	1:15:A:LEU:HD23	1:74:A:ILE:HB	15	0.76	0.43	1.01
(4,440)	1:15:A:LEU:HD23	1:13:A:LEU:HB2	15	0.76	0.43	1.01
(4,440)	1:15:A:LEU:HD22	1:13:A:LEU:HB2	15	0.76	0.43	1.01
(4,320)	1:151:A:MET:HE2	1:147:A:ASP:HB2	15	0.75	0.4	0.71
(4,320)	1:151:A:MET:HE3	1:158:A:PHE:HB3	15	0.75	0.4	0.71
(4,320)	1:151:A:MET:HE1	1:147:A:ASP:HB2	15	0.75	0.4	0.71
(4,320)	1:151:A:MET:HE3	1:147:A:ASP:HB2	15	0.75	0.4	0.71
(4,320)	1:151:A:MET:HE2	1:158:A:PHE:HB2	15	0.75	0.4	0.71
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	15	0.57	0.16	0.59
(2,1482)	1:11:A:LEU:HD11	1:11:A:LEU:H	15	0.57	0.16	0.59
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	15	0.45	0.13	0.48
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HG3	15	0.45	0.13	0.48
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	15	0.43	0.21	0.38
(2,1871)	1:97:A:LEU:HD22	1:151:A:MET:HG3	15	0.43	0.21	0.38
(2,1871)	1:97:A:LEU:HD21	1:151:A:MET:HG3	15	0.43	0.21	0.38
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	15	0.41	0.21	0.3
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	15	0.35	0.18	0.28
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	15	0.31	0.06	0.31
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	15	0.31	0.09	0.31
(2,3467)	1:11:A:LEU:HD12	1:38:A:LEU:HA	15	0.31	0.09	0.31
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	15	0.26	0.1	0.26
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	15	0.23	0.08	0.21
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	15	0.23	0.05	0.21
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	15	0.23	0.05	0.22
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	15	0.22	0.04	0.22
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	15	0.2	0.03	0.2
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	15	0.2	0.04	0.21
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	15	0.19	0.04	0.2
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	15	0.16	0.03	0.16
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	15	0.15	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	15	0.14	0.02	0.13
(4,69)	1:37:A:LEU:H	1:53:A:LEU:HD11	15	0.14	0.02	0.13
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	15	0.13	0.02	0.13
(2,2566)	1:43:A:ALA:HB1	1:44:A:LYS:H	15	0.13	0.02	0.13
(2,2566)	1:43:A:ALA:HB3	1:44:A:LYS:H	15	0.13	0.02	0.13
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	15	0.13	0.01	0.13
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD12	15	0.13	0.01	0.13
(2,1492)	1:167:A:LEU:HD22	1:123:A:HIS:HA	14	0.84	0.34	0.82
(2,1492)	1:167:A:LEU:HD23	1:123:A:HIS:HA	14	0.84	0.34	0.82
(2,1492)	1:167:A:LEU:HD21	1:123:A:HIS:HA	14	0.84	0.34	0.82
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	14	0.84	0.25	0.92
(2,21)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	14	0.84	0.25	0.92
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD12	14	0.84	0.25	0.92
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	14	0.49	0.14	0.52
(4,283)	1:143:A:VAL:HG12	1:143:A:VAL:H	14	0.49	0.14	0.52
(4,311)	1:143:A:VAL:HG13	1:178:A:VAL:HA	14	0.38	0.22	0.36
(4,311)	1:96:A:VAL:HG11	1:94:A:PRO:HA	14	0.38	0.22	0.36
(4,311)	1:143:A:VAL:HG11	1:178:A:VAL:HA	14	0.38	0.22	0.36
(4,311)	1:143:A:VAL:HG12	1:178:A:VAL:HA	14	0.38	0.22	0.36
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	14	0.38	0.15	0.4
(2,3390)	1:56:A:ILE:HG23	1:65:A:PHE:HE1	14	0.38	0.15	0.4
(2,3390)	1:56:A:ILE:HG21	1:65:A:PHE:HE1	14	0.38	0.15	0.4
(4,328)	1:122:A:VAL:HG13	1:113:A:GLY:HA2	14	0.37	0.18	0.32
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	14	0.37	0.18	0.32
(4,328)	1:122:A:VAL:HG12	1:113:A:GLY:HA2	14	0.37	0.18	0.32
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	14	0.22	0.05	0.21
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	14	0.21	0.08	0.18
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD23	14	0.21	0.08	0.18
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD22	14	0.21	0.08	0.18
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	14	0.18	0.04	0.17
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	14	0.15	0.02	0.14
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	14	0.15	0.02	0.14
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	14	0.14	0.03	0.13
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	14	0.14	0.03	0.13
(2,3473)	1:146:A:VAL:HG23	1:96:A:VAL:HA	14	0.14	0.03	0.13
(2,3473)	1:146:A:VAL:HG22	1:96:A:VAL:HA	14	0.14	0.03	0.13
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	14	0.14	0.03	0.14
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	14	0.13	0.02	0.13
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	14	0.12	0.02	0.12
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	14	0.12	0.02	0.12
(2,3519)	1:48:A:ILE:HD11	1:53:A:LEU:HB2	14	0.12	0.01	0.12
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	14	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3519)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	14	0.12	0.01	0.12
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	13	1.43	0.67	1.4
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	13	1.11	0.18	1.12
(4,292)	1:122:A:VAL:HG23	1:118:A:SER:H	13	0.91	0.45	0.87
(4,292)	1:122:A:VAL:HG22	1:118:A:SER:H	13	0.91	0.45	0.87
(4,292)	1:122:A:VAL:HG21	1:118:A:SER:H	13	0.91	0.45	0.87
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	13	0.7	0.04	0.72
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	13	0.6	0.34	0.58
(4,350)	1:42:A:LYS:HE3	1:44:A:LYS:HG2	13	0.6	0.34	0.58
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG2	13	0.6	0.34	0.58
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	13	0.47	0.17	0.49
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE2	13	0.38	0.11	0.42
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	13	0.38	0.11	0.42
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	13	0.35	0.04	0.34
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	13	0.34	0.11	0.35
(2,2521)	1:105:A:ASN:H	1:102:A:ALA:HB3	13	0.34	0.11	0.35
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB3	13	0.33	0.14	0.29
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB2	13	0.33	0.14	0.29
(2,3484)	1:124:A:LEU:HD12	1:167:A:LEU:HA	13	0.29	0.07	0.29
(2,3484)	1:124:A:LEU:HD11	1:167:A:LEU:HA	13	0.29	0.07	0.29
(2,3484)	1:124:A:LEU:HD13	1:167:A:LEU:HA	13	0.29	0.07	0.29
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	13	0.28	0.11	0.3
(2,1710)	1:26:A:LEU:HD21	1:15:A:LEU:HA	13	0.28	0.11	0.3
(2,1710)	1:26:A:LEU:HD22	1:15:A:LEU:HA	13	0.28	0.11	0.3
(2,1514)	1:124:A:LEU:HD12	1:167:A:LEU:HA	13	0.27	0.07	0.27
(2,1514)	1:124:A:LEU:HD11	1:167:A:LEU:HA	13	0.27	0.07	0.27
(2,1514)	1:124:A:LEU:HD13	1:167:A:LEU:HA	13	0.27	0.07	0.27
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	13	0.2	0.04	0.21
(2,3479)	1:151:A:MET:HE1	1:171:A:VAL:HA	13	0.19	0.07	0.19
(2,3479)	1:151:A:MET:HE2	1:171:A:VAL:HA	13	0.19	0.07	0.19
(2,3479)	1:151:A:MET:HE3	1:171:A:VAL:HA	13	0.19	0.07	0.19
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	13	0.15	0.02	0.15
(2,3575)	1:50:A:MET:HE1	1:50:A:MET:HG3	13	0.15	0.03	0.14
(2,3575)	1:50:A:MET:HE2	1:50:A:MET:HG3	13	0.15	0.03	0.14
(2,3575)	1:50:A:MET:HE3	1:50:A:MET:HG3	13	0.15	0.03	0.14
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	13	0.15	0.02	0.14
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	13	0.13	0.04	0.12
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	13	0.13	0.02	0.13
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	13	0.13	0.06	0.11
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	12	0.85	0.23	0.77
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	12	0.66	0.23	0.65
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	12	0.54	0.11	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1974)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	12	0.54	0.11	0.58
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD12	12	0.54	0.11	0.58
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	12	0.51	0.26	0.5
(2,1534)	1:151:A:MET:HE2	1:151:A:MET:HA	12	0.44	0.1	0.45
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	12	0.44	0.1	0.45
(2,1534)	1:151:A:MET:HE3	1:151:A:MET:HA	12	0.44	0.1	0.45
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	12	0.43	0.26	0.34
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	12	0.37	0.14	0.42
(2,1599)	1:4:A:MET:HE3	1:52:A:GLU:HA	12	0.26	0.17	0.2
(2,1599)	1:4:A:MET:HE1	1:52:A:GLU:HA	12	0.26	0.17	0.2
(2,1599)	1:4:A:MET:HE2	1:52:A:GLU:HA	12	0.26	0.17	0.2
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	12	0.23	0.08	0.22
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB3	12	0.23	0.08	0.22
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	12	0.22	0.09	0.25
(2,3371)	1:20:A:ALA:HB2	1:18:A:ASN:HD21	12	0.22	0.09	0.25
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	12	0.22	0.11	0.16
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	12	0.22	0.05	0.23
(2,3434)	1:15:A:LEU:HD11	1:65:A:PHE:HE1	12	0.22	0.09	0.22
(2,3434)	1:15:A:LEU:HD12	1:65:A:PHE:HE1	12	0.22	0.09	0.22
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	12	0.22	0.04	0.22
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	12	0.19	0.03	0.21
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	12	0.17	0.04	0.16
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	12	0.17	0.04	0.16
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	12	0.15	0.02	0.15
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	12	0.13	0.02	0.13
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG23	12	0.13	0.02	0.13
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	12	0.12	0.02	0.12
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	11	0.87	0.48	0.85
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	11	0.68	0.05	0.66
(2,1875)	1:5:A:VAL:HG23	1:5:A:VAL:HA	11	0.68	0.05	0.66
(2,3527)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	11	0.62	0.29	0.52
(2,3527)	1:84:A:VAL:HG21	1:85:A:ASP:HB2	11	0.62	0.29	0.52
(2,3527)	1:84:A:VAL:HG23	1:85:A:ASP:HB2	11	0.62	0.29	0.52
(2,1490)	1:167:A:LEU:HD12	1:166:A:TRP:HA	11	0.57	0.19	0.53
(2,1490)	1:167:A:LEU:HD13	1:166:A:TRP:HA	11	0.57	0.19	0.53
(2,1490)	1:167:A:LEU:HD11	1:166:A:TRP:HA	11	0.57	0.19	0.53
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	11	0.49	0.28	0.43
(2,3514)	1:143:A:VAL:HG12	1:132:A:ARG:HA	11	0.43	0.15	0.46
(2,3514)	1:143:A:VAL:HG11	1:132:A:ARG:HA	11	0.43	0.15	0.46
(2,3514)	1:143:A:VAL:HG13	1:132:A:ARG:HA	11	0.43	0.15	0.46
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	11	0.42	0.4	0.24
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB2	11	0.42	0.4	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	11	0.25	0.07	0.25
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	11	0.25	0.07	0.24
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	11	0.23	0.08	0.22
(2,2148)	1:26:A:LEU:HD23	1:26:A:LEU:H	11	0.23	0.08	0.22
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	11	0.21	0.09	0.17
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	11	0.17	0.04	0.17
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	11	0.16	0.06	0.16
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	11	0.15	0.03	0.14
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	11	0.14	0.02	0.14
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	11	0.13	0.02	0.14
(2,1540)	1:56:A:ILE:HG23	1:56:A:ILE:HA	11	0.13	0.02	0.14
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	11	0.12	0.01	0.12
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	10	0.64	0.24	0.64
(4,458)	1:50:A:MET:HE2	1:50:A:MET:HA	10	0.64	0.24	0.64
(4,458)	1:50:A:MET:HE2	1:51:A:GLU:HA	10	0.64	0.24	0.64
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	10	0.48	0.29	0.45
(2,1377)	1:4:A:MET:HE3	1:55:A:HIS:HD2	10	0.45	0.13	0.42
(2,1377)	1:4:A:MET:HE1	1:55:A:HIS:HD2	10	0.45	0.13	0.42
(2,1377)	1:4:A:MET:HE2	1:55:A:HIS:HD2	10	0.45	0.13	0.42
(2,3346)	1:4:A:MET:HE3	1:55:A:HIS:HD2	10	0.43	0.14	0.41
(2,3346)	1:4:A:MET:HE1	1:55:A:HIS:HD2	10	0.43	0.14	0.41
(2,3346)	1:4:A:MET:HE2	1:55:A:HIS:HD2	10	0.43	0.14	0.41
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	10	0.41	0.18	0.36
(2,1378)	1:50:A:MET:HE2	1:67:A:PHE:HZ	10	0.41	0.18	0.36
(2,1378)	1:50:A:MET:HE1	1:67:A:PHE:HZ	10	0.41	0.18	0.36
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	10	0.36	0.12	0.38
(2,1541)	1:143:A:VAL:HG11	1:132:A:ARG:HA	10	0.36	0.11	0.36
(2,1541)	1:143:A:VAL:HG13	1:132:A:ARG:HA	10	0.36	0.11	0.36
(2,1541)	1:143:A:VAL:HG12	1:132:A:ARG:HA	10	0.36	0.11	0.36
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	10	0.33	0.1	0.34
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	10	0.32	0.09	0.34
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	10	0.32	0.07	0.33
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	10	0.3	0.11	0.28
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	10	0.25	0.13	0.18
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	10	0.25	0.13	0.18
(2,3288)	1:142:A:VAL:HG13	1:103:A:GLU:HA	10	0.18	0.07	0.16
(2,3288)	1:142:A:VAL:HG11	1:103:A:GLU:HA	10	0.18	0.07	0.16
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	10	0.18	0.02	0.18
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	10	0.17	0.04	0.16
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	10	0.14	0.04	0.14
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	10	0.14	0.02	0.14
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD13	10	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3812)	1:56:A:ILE:HG21	1:11:A:LEU:HD11	10	0.14	0.02	0.14
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	10	0.14	0.03	0.13
(2,3820)	1:109:A:ILE:HG21	1:109:A:ILE:HD11	10	0.14	0.03	0.12
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	10	0.14	0.03	0.12
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	10	0.14	0.03	0.12
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	10	0.13	0.03	0.12
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	10	0.13	0.03	0.12
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	10	0.12	0.02	0.12
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	10	0.12	0.04	0.12
(2,3376)	1:95:A:ALA:HB3	1:96:A:VAL:H	10	0.12	0.04	0.12
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	10	0.12	0.02	0.12
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	10	0.12	0.01	0.12
(2,1440)	1:37:A:LEU:HD12	1:37:A:LEU:H	10	0.11	0.01	0.11
(2,1440)	1:37:A:LEU:HD11	1:37:A:LEU:H	10	0.11	0.01	0.11
(2,1440)	1:37:A:LEU:HD13	1:37:A:LEU:H	10	0.11	0.01	0.11
(4,415)	1:19:A:PRO:HB3	1:36:A:GLU:HG2	9	1.08	0.46	1.16
(4,415)	1:19:A:PRO:HB2	1:33:A:PRO:HG2	9	1.08	0.46	1.16
(4,415)	1:19:A:PRO:HB2	1:36:A:GLU:HG2	9	1.08	0.46	1.16
(4,415)	1:19:A:PRO:HB3	1:33:A:PRO:HG2	9	1.08	0.46	1.16
(2,3847)	1:41:A:MET:HE2	1:46:A:HIS:HA	9	0.83	0.22	0.92
(2,3847)	1:41:A:MET:HE1	1:46:A:HIS:HA	9	0.83	0.22	0.92
(2,3847)	1:41:A:MET:HE3	1:46:A:HIS:HA	9	0.83	0.22	0.92
(4,166)	1:171:A:VAL:H	1:168:A:ILE:HG13	9	0.52	0.28	0.65
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD12	9	0.52	0.28	0.65
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD13	9	0.52	0.28	0.65
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD11	9	0.52	0.28	0.65
(2,3600)	1:42:A:LYS:HE2	1:39:A:ALA:HA	9	0.41	0.09	0.36
(2,3600)	1:42:A:LYS:HE3	1:39:A:ALA:HA	9	0.41	0.09	0.36
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	9	0.37	0.21	0.27
(2,3428)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	9	0.35	0.13	0.34
(2,3428)	1:108:A:LEU:HD12	2:201:A:NAD:H2A	9	0.35	0.13	0.34
(2,3428)	1:108:A:LEU:HD13	2:201:A:NAD:H2A	9	0.35	0.13	0.34
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	9	0.34	0.16	0.35
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE3	9	0.31	0.07	0.31
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE1	9	0.31	0.07	0.31
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE2	9	0.31	0.07	0.31
(4,325)	1:7:A:VAL:HG13	1:10:A:PHE:HB3	9	0.28	0.15	0.2
(4,325)	1:7:A:VAL:HG11	1:10:A:PHE:HB3	9	0.28	0.15	0.2
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	9	0.27	0.06	0.27
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	9	0.27	0.08	0.29
(4,379)	1:50:A:MET:HA	1:39:A:ALA:HB3	9	0.26	0.13	0.21
(4,379)	1:50:A:MET:HA	1:35:A:LYS:HG2	9	0.26	0.13	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3409)	1:84:A:VAL:HG13	1:85:A:ASP:H	9	0.26	0.12	0.24
(2,3409)	1:84:A:VAL:HG11	1:85:A:ASP:H	9	0.26	0.12	0.24
(2,3409)	1:84:A:VAL:HG12	1:85:A:ASP:H	9	0.26	0.12	0.24
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD13	9	0.25	0.05	0.24
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD11	9	0.25	0.05	0.24
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE3	9	0.23	0.07	0.23
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE1	9	0.23	0.07	0.23
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE2	9	0.23	0.07	0.23
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	9	0.22	0.07	0.22
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB3	9	0.22	0.07	0.22
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD13	9	0.22	0.05	0.22
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD11	9	0.22	0.05	0.22
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	9	0.2	0.06	0.2
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	9	0.18	0.03	0.18
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	9	0.17	0.06	0.22
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB3	9	0.17	0.06	0.22
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	9	0.15	0.07	0.14
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	9	0.15	0.02	0.15
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	9	0.15	0.04	0.14
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	9	0.14	0.03	0.14
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	9	0.13	0.03	0.12
(4,198)	1:176:A:ILE:HD13	1:106:A:PHE:HE1	9	0.13	0.03	0.12
(4,198)	1:176:A:ILE:HD11	1:106:A:PHE:HE1	9	0.13	0.03	0.12
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	9	0.12	0.02	0.11
(2,3362)	1:39:A:ALA:HB2	1:40:A:LYS:H	9	0.12	0.01	0.12
(2,3362)	1:39:A:ALA:HB3	1:40:A:LYS:H	9	0.12	0.01	0.12
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	9	0.12	0.01	0.11
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	9	0.11	0.01	0.11
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	8	1.16	0.54	1.26
(2,3466)	1:97:A:LEU:HD21	1:166:A:TRP:HB2	8	0.59	0.11	0.64
(2,3466)	1:97:A:LEU:HD22	1:166:A:TRP:HB2	8	0.59	0.11	0.64
(2,1884)	1:41:A:MET:HE2	1:46:A:HIS:HA	8	0.59	0.17	0.63
(2,1884)	1:41:A:MET:HE1	1:46:A:HIS:HA	8	0.59	0.17	0.63
(2,1884)	1:41:A:MET:HE3	1:46:A:HIS:HA	8	0.59	0.17	0.63
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	8	0.44	0.1	0.46
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	8	0.42	0.01	0.42
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	8	0.41	0.01	0.4
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	8	0.39	0.22	0.33
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	8	0.37	0.03	0.38
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD21	8	0.36	0.12	0.37
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD23	8	0.36	0.12	0.37
(2,3832)	1:97:A:LEU:HD23	1:151:A:MET:HG3	8	0.36	0.13	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3832)	1:97:A:LEU:HD22	1:151:A:MET:HG3	8	0.36	0.13	0.38
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	8	0.32	0.2	0.29
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	8	0.28	0.07	0.3
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	8	0.21	0.03	0.22
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	8	0.21	0.09	0.2
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD11	8	0.21	0.09	0.2
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD13	8	0.21	0.09	0.2
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	8	0.17	0.09	0.12
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	8	0.17	0.02	0.18
(2,3518)	1:128:A:ILE:HD12	1:128:A:ILE:HA	8	0.15	0.03	0.15
(2,3518)	1:128:A:ILE:HD13	1:128:A:ILE:HA	8	0.15	0.03	0.15
(2,3518)	1:128:A:ILE:HD11	1:128:A:ILE:HA	8	0.15	0.03	0.15
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	8	0.15	0.03	0.15
(2,2210)	1:48:A:ILE:HD13	1:53:A:LEU:H	8	0.14	0.04	0.13
(2,2210)	1:48:A:ILE:HD12	1:53:A:LEU:H	8	0.14	0.04	0.13
(2,2210)	1:48:A:ILE:HD11	1:53:A:LEU:H	8	0.14	0.04	0.13
(4,61)	1:37:A:LEU:H	1:24:A:LEU:HD12	8	0.14	0.02	0.13
(4,61)	1:37:A:LEU:H	1:38:A:LEU:HD23	8	0.14	0.02	0.13
(2,1723)	1:38:A:LEU:HD13	1:50:A:MET:HA	8	0.12	0.02	0.12
(2,1723)	1:38:A:LEU:HD11	1:50:A:MET:HA	8	0.12	0.02	0.12
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	8	0.12	0.01	0.12
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HZ	8	0.12	0.01	0.12
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HE1	8	0.12	0.01	0.12
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	8	0.12	0.01	0.12
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	8	0.11	0.01	0.11
(2,339)	1:108:A:LEU:HD22	1:108:A:LEU:H	7	0.67	0.18	0.61
(2,339)	1:108:A:LEU:HD23	1:108:A:LEU:H	7	0.67	0.18	0.61
(2,339)	1:108:A:LEU:HD21	1:108:A:LEU:H	7	0.67	0.18	0.61
(4,338)	1:111:A:LYS:HD3	1:104:A:LYS:HA	7	0.54	0.11	0.51
(2,3964)	1:123:A:HIS:HB3	2:201:A:NAD:H6N	7	0.51	0.19	0.48
(2,3415)	1:122:A:VAL:HG21	1:122:A:VAL:H	7	0.5	0.06	0.48
(2,3415)	1:122:A:VAL:HG22	1:122:A:VAL:H	7	0.5	0.06	0.48
(2,3415)	1:122:A:VAL:HG23	1:122:A:VAL:H	7	0.5	0.06	0.48
(4,300)	1:97:A:LEU:HD23	1:156:A:PHE:HB3	7	0.46	0.24	0.43
(4,300)	1:97:A:LEU:HD21	1:175:A:PHE:HB3	7	0.46	0.24	0.43
(4,300)	1:97:A:LEU:HD23	1:175:A:PHE:HB3	7	0.46	0.24	0.43
(2,1276)	1:160:A:LEU:HD21	1:166:A:TRP:HE1	7	0.43	0.16	0.53
(2,3459)	1:167:A:LEU:HD23	1:123:A:HIS:HA	7	0.41	0.17	0.37
(2,3459)	1:167:A:LEU:HD22	1:123:A:HIS:HA	7	0.41	0.17	0.37
(2,2308)	1:108:A:LEU:HD22	1:108:A:LEU:H	7	0.33	0.18	0.27
(2,2308)	1:108:A:LEU:HD23	1:108:A:LEU:H	7	0.33	0.18	0.27
(2,2308)	1:108:A:LEU:HD21	1:108:A:LEU:H	7	0.33	0.18	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1288)	1:167:A:LEU:HD22	1:167:A:LEU:HA	7	0.3	0.09	0.25
(2,1288)	1:167:A:LEU:HD23	1:167:A:LEU:HA	7	0.3	0.09	0.25
(2,1459)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	7	0.3	0.1	0.29
(2,1459)	1:108:A:LEU:HD12	2:201:A:NAD:H2A	7	0.3	0.1	0.29
(2,1459)	1:108:A:LEU:HD13	2:201:A:NAD:H2A	7	0.3	0.1	0.29
(2,3182)	1:114:A:ILE:HD13	1:171:A:VAL:HB	7	0.29	0.14	0.26
(2,708)	1:113:A:GLY:H	1:109:A:ILE:HG21	7	0.26	0.07	0.26
(4,319)	1:26:A:LEU:HD23	1:14:A:VAL:HA	7	0.24	0.08	0.24
(4,319)	1:26:A:LEU:HD21	1:14:A:VAL:HA	7	0.24	0.08	0.24
(4,319)	1:26:A:LEU:HD22	1:14:A:VAL:HA	7	0.24	0.08	0.24
(2,1563)	1:48:A:ILE:HG23	1:53:A:LEU:HB2	7	0.23	0.07	0.23
(2,1563)	1:48:A:ILE:HG22	1:53:A:LEU:HB2	7	0.23	0.07	0.23
(2,3829)	1:109:A:ILE:HD11	1:101:A:THR:HG23	7	0.22	0.06	0.21
(2,1131)	1:136:A:MET:H	1:105:A:ASN:HD22	7	0.22	0.02	0.22
(2,726)	1:20:A:ALA:HB2	1:23:A:GLY:H	7	0.2	0.03	0.19
(2,550)	1:102:A:ALA:HB1	1:105:A:ASN:H	7	0.2	0.05	0.21
(2,550)	1:105:A:ASN:H	1:102:A:ALA:HB3	7	0.2	0.05	0.21
(2,1172)	1:144:A:LEU:HD11	1:106:A:PHE:HE1	7	0.19	0.04	0.2
(1,92)	1:133:A:LYS:N	1:129:A:THR:O	7	0.18	0.04	0.19
(1,4)	1:8:A:SER:N	1:4:A:MET:O	7	0.16	0.03	0.16
(2,1973)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	7	0.14	0.01	0.15
(2,431)	1:73:A:LYS:H	1:34:A:VAL:HG21	7	0.13	0.02	0.13
(2,1860)	1:57:A:VAL:HG21	1:57:A:VAL:HB	7	0.13	0.02	0.11
(2,3180)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	7	0.11	0.01	0.11
(2,1361)	1:177:A:LYS:HE2	1:147:A:ASP:H	6	1.5	0.46	1.52
(2,1554)	1:38:A:LEU:HD21	1:50:A:MET:HG2	6	0.75	0.17	0.78
(2,3657)	1:63:A:LYS:HG2	1:62:A:LYS:HA	6	0.69	0.06	0.7
(2,3657)	1:63:A:LYS:HG3	1:62:A:LYS:HA	6	0.69	0.06	0.7
(2,1690)	1:63:A:LYS:HG2	1:62:A:LYS:HA	6	0.62	0.06	0.63
(2,1690)	1:63:A:LYS:HG3	1:62:A:LYS:HA	6	0.62	0.06	0.63
(2,3508)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	6	0.52	0.28	0.41
(2,1831)	1:142:A:VAL:HG23	1:143:A:VAL:HB	6	0.52	0.15	0.59
(2,1211)	1:177:A:LYS:HD2	1:177:A:LYS:HA	6	0.32	0.11	0.36
(1,112)	1:159:A:TYR:N	1:167:A:LEU:O	6	0.22	0.0	0.22
(1,77)	1:112:A:ASP:H	1:108:A:LEU:O	6	0.19	0.03	0.2
(1,111)	1:159:A:TYR:H	1:167:A:LEU:O	6	0.18	0.01	0.18
(1,118)	1:168:A:ILE:N	1:122:A:VAL:O	6	0.18	0.05	0.18
(2,3345)	1:41:A:MET:HE1	1:10:A:PHE:HE1	6	0.18	0.04	0.18
(2,3345)	1:41:A:MET:HE2	1:10:A:PHE:HE1	6	0.18	0.04	0.18
(2,2657)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	6	0.16	0.04	0.16
(2,3509)	1:13:A:LEU:HD23	1:17:A:HIS:HB2	6	0.16	0.03	0.16
(2,3509)	1:13:A:LEU:HD21	1:17:A:HIS:HB2	6	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3509)	1:13:A:LEU:HD22	1:17:A:HIS:HB2	6	0.16	0.03	0.16
(1,24)	1:37:A:LEU:N	1:33:A:PRO:O	6	0.15	0.03	0.15
(2,268)	1:14:A:VAL:HG21	1:21:A:LEU:H	6	0.14	0.03	0.14
(2,268)	1:14:A:VAL:HG22	1:21:A:LEU:H	6	0.14	0.03	0.14
(2,268)	1:14:A:VAL:HG23	1:21:A:LEU:H	6	0.14	0.03	0.14
(2,1432)	1:38:A:LEU:HD12	1:39:A:ALA:H	6	0.13	0.03	0.12
(2,1432)	1:38:A:LEU:HD13	1:39:A:ALA:H	6	0.13	0.03	0.12
(2,1432)	1:38:A:LEU:HD11	1:39:A:ALA:H	6	0.13	0.03	0.12
(2,2651)	1:78:A:GLN:HG3	1:78:A:GLN:HE22	6	0.13	0.0	0.13
(2,1110)	1:76:A:ALA:H	1:75:A:ARG:H	6	0.13	0.03	0.12
(2,3468)	1:110:A:LEU:HD12	1:110:A:LEU:HA	6	0.12	0.01	0.12
(2,3468)	1:110:A:LEU:HD11	1:110:A:LEU:HA	6	0.12	0.01	0.12
(2,62)	1:178:A:VAL:H	1:177:A:LYS:H	6	0.11	0.01	0.11
(2,2010)	1:34:A:VAL:H	1:73:A:LYS:HA	6	0.11	0.01	0.11
(2,3173)	1:176:A:ILE:HD11	1:176:A:ILE:HA	6	0.1	0.0	0.11
(2,1840)	1:128:A:ILE:HG21	1:129:A:THR:HG22	5	0.6	0.06	0.62
(2,1840)	1:128:A:ILE:HG21	1:129:A:THR:HG21	5	0.6	0.06	0.62
(2,1840)	1:128:A:ILE:HG23	1:129:A:THR:HG21	5	0.6	0.06	0.62
(4,409)	1:4:A:MET:HE1	1:59:A:THR:HG23	5	0.47	0.21	0.52
(4,409)	1:4:A:MET:HE3	1:59:A:THR:HG23	5	0.47	0.21	0.52
(4,299)	1:168:A:ILE:HD12	1:152:A:ALA:HA	5	0.37	0.16	0.36
(4,299)	1:168:A:ILE:HD12	1:96:A:VAL:HA	5	0.37	0.16	0.36
(4,299)	1:168:A:ILE:HD11	1:96:A:VAL:HA	5	0.37	0.16	0.36
(2,19)	1:13:A:LEU:HA	1:17:A:HIS:HD2	5	0.36	0.12	0.43
(2,3791)	1:142:A:VAL:HG23	1:143:A:VAL:HB	5	0.35	0.09	0.38
(2,1555)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	5	0.35	0.12	0.36
(2,1555)	1:84:A:VAL:HG21	1:85:A:ASP:HB2	5	0.35	0.12	0.36
(2,3804)	1:128:A:ILE:HG21	1:129:A:THR:HG22	5	0.28	0.06	0.3
(2,3804)	1:128:A:ILE:HG21	1:129:A:THR:HG21	5	0.28	0.06	0.3
(2,3804)	1:128:A:ILE:HG23	1:129:A:THR:HG21	5	0.28	0.06	0.3
(2,120)	1:177:A:LYS:HB3	1:178:A:VAL:H	5	0.26	0.02	0.25
(2,3789)	1:22:A:ILE:HG22	1:44:A:LYS:HB3	5	0.24	0.08	0.23
(2,3785)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	5	0.22	0.09	0.2
(2,3785)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	5	0.22	0.09	0.2
(2,1420)	1:22:A:ILE:HG23	1:10:A:PHE:HE1	5	0.22	0.05	0.21
(2,1420)	1:22:A:ILE:HG21	1:10:A:PHE:HE1	5	0.22	0.05	0.21
(4,443)	1:48:A:ILE:HD12	1:38:A:LEU:HB2	5	0.22	0.06	0.21
(4,443)	1:48:A:ILE:HD13	1:38:A:LEU:HB2	5	0.22	0.06	0.21
(2,1218)	1:177:A:LYS:HG2	1:177:A:LYS:HA	5	0.2	0.03	0.19
(2,3940)	1:134:A:VAL:HG11	2:201:A:NAD:H2N	5	0.17	0.03	0.17
(1,88)	1:131:A:ALA:N	1:127:A:ASP:O	5	0.16	0.04	0.13
(4,8)	1:22:A:ILE:HG23	1:10:A:PHE:HD1	5	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2175)	1:57:A:VAL:HG21	1:66:A:ALA:H	5	0.15	0.04	0.13
(2,2175)	1:57:A:VAL:HG22	1:66:A:ALA:H	5	0.15	0.04	0.13
(1,89)	1:132:A:ARG:H	1:128:A:ILE:O	5	0.14	0.02	0.13
(1,119)	1:171:A:VAL:H	1:114:A:ILE:O	5	0.13	0.03	0.12
(1,55)	1:74:A:ILE:H	1:32:A:ALA:O	5	0.13	0.01	0.12
(2,2192)	1:82:A:VAL:HB	1:82:A:VAL:H	5	0.13	0.02	0.12
(2,3478)	1:38:A:LEU:HD13	1:50:A:MET:HA	5	0.12	0.01	0.12
(2,3478)	1:38:A:LEU:HD11	1:50:A:MET:HA	5	0.12	0.01	0.12
(2,3825)	1:11:A:LEU:HD11	1:11:A:LEU:HB2	5	0.12	0.02	0.12
(2,3825)	1:11:A:LEU:HD13	1:11:A:LEU:HB2	5	0.12	0.02	0.12
(4,65)	1:7:A:VAL:H	1:7:A:VAL:HB	5	0.12	0.01	0.12
(4,65)	1:6:A:LYS:HB3	1:7:A:VAL:H	5	0.12	0.01	0.12
(2,2520)	1:8:A:SER:H	1:6:A:LYS:HA	5	0.12	0.02	0.1
(2,2887)	1:176:A:ILE:H	1:146:A:VAL:HG11	5	0.12	0.01	0.11
(1,39)	1:54:A:LYS:H	1:50:A:MET:O	5	0.11	0.01	0.12
(2,3775)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	5	0.11	0.0	0.11
(2,42)	1:148:A:ALA:H	1:148:A:ALA:HB1	5	0.11	0.0	0.11
(2,950)	1:76:A:ALA:H	1:76:A:ALA:HA	5	0.11	0.0	0.11
(2,2980)	1:40:A:LYS:H	1:39:A:ALA:H	5	0.11	0.0	0.11
(2,1217)	1:177:A:LYS:HE2	1:177:A:LYS:HB2	4	1.18	0.31	1.09
(4,313)	1:143:A:VAL:HG12	1:145:A:SER:HA	4	0.97	0.11	0.98
(4,313)	1:96:A:VAL:HG13	1:145:A:SER:HA	4	0.97	0.11	0.98
(2,1794)	1:117:A:MET:HE1	1:117:A:MET:HB2	4	0.55	0.19	0.55
(2,1794)	1:117:A:MET:HE3	1:117:A:MET:HB2	4	0.55	0.19	0.55
(2,3500)	1:144:A:LEU:HD22	1:145:A:SER:HB2	4	0.52	0.4	0.47
(2,3500)	1:144:A:LEU:HD21	1:145:A:SER:HB2	4	0.52	0.4	0.47
(2,3500)	1:144:A:LEU:HD23	1:145:A:SER:HB2	4	0.52	0.4	0.47
(2,948)	1:76:A:ALA:HB1	1:78:A:GLN:HE22	4	0.48	0.21	0.57
(2,948)	1:76:A:ALA:HB3	1:78:A:GLN:HE22	4	0.48	0.21	0.57
(2,3722)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	4	0.48	0.22	0.6
(2,3177)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	4	0.47	0.06	0.44
(2,305)	1:42:A:LYS:HA	1:46:A:HIS:H	4	0.46	0.21	0.57
(2,3761)	1:117:A:MET:HE1	1:117:A:MET:HB2	4	0.44	0.19	0.44
(2,3761)	1:117:A:MET:HE3	1:117:A:MET:HB2	4	0.44	0.19	0.44
(2,29)	1:88:A:TYR:HD1	1:159:A:TYR:HD1	4	0.43	0.04	0.42
(4,227)	1:8:A:SER:HB3	1:65:A:PHE:HE1	4	0.41	0.24	0.41
(4,227)	1:8:A:SER:HB3	1:55:A:HIS:HD2	4	0.41	0.24	0.41
(2,342)	1:41:A:MET:H	1:41:A:MET:HG2	4	0.41	0.25	0.42
(2,1511)	1:82:A:VAL:HG21	1:80:A:HIS:HA	4	0.4	0.28	0.38
(2,3481)	1:82:A:VAL:HG21	1:80:A:HIS:HA	4	0.4	0.28	0.37
(4,70)	1:130:A:THR:H	2:201:A:NAD:H4D	4	0.36	0.2	0.34
(2,1588)	1:152:A:ALA:HB2	1:149:A:LYS:HA	4	0.29	0.15	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2738)	1:30:A:GLY:H	1:26:A:LEU:HD23	4	0.28	0.11	0.3
(2,2738)	1:30:A:GLY:H	1:26:A:LEU:HD21	4	0.28	0.11	0.3
(2,2738)	1:30:A:GLY:H	1:26:A:LEU:HD22	4	0.28	0.11	0.3
(2,2748)	1:86:A:LEU:HD11	1:87:A:GLY:H	4	0.27	0.13	0.28
(2,3355)	1:41:A:MET:HE2	1:41:A:MET:H	4	0.27	0.13	0.23
(2,3430)	1:128:A:ILE:HD11	1:127:A:ASP:H	4	0.26	0.1	0.2
(2,3430)	1:128:A:ILE:HD12	1:127:A:ASP:H	4	0.26	0.1	0.2
(2,3430)	1:128:A:ILE:HD13	1:127:A:ASP:H	4	0.26	0.1	0.2
(2,985)	1:46:A:HIS:H	1:45:A:GLY:H	4	0.24	0.01	0.24
(2,3531)	1:151:A:MET:HE1	1:175:A:PHE:HB3	4	0.23	0.05	0.21
(2,3531)	1:151:A:MET:HE2	1:175:A:PHE:HB3	4	0.23	0.05	0.21
(2,1075)	1:56:A:ILE:H	1:58:A:GLU:H	4	0.22	0.06	0.21
(2,1889)	1:4:A:MET:HE1	1:4:A:MET:HA	4	0.2	0.03	0.18
(2,718)	1:91:A:GLN:HE21	1:89:A:GLU:HB2	4	0.19	0.01	0.19
(2,2417)	1:36:A:GLU:H	1:36:A:GLU:HB3	4	0.19	0.03	0.18
(2,1590)	1:32:A:ALA:HB2	1:33:A:PRO:HD3	4	0.17	0.07	0.14
(2,224)	1:81:A:SER:HA	1:82:A:VAL:H	4	0.16	0.04	0.16
(2,2189)	1:81:A:SER:HA	1:82:A:VAL:H	4	0.15	0.04	0.15
(2,3920)	1:115:A:LYS:H	2:201:A:NAD:H8A	4	0.14	0.03	0.14
(2,453)	1:34:A:VAL:HB	1:35:A:LYS:H	4	0.13	0.02	0.14
(2,2649)	1:70:A:ASN:HD22	1:50:A:MET:HB2	4	0.12	0.01	0.12
(2,3102)	1:136:A:MET:H	1:105:A:ASN:HD22	4	0.12	0.01	0.12
(1,97)	1:136:A:MET:H	1:132:A:ARG:O	4	0.12	0.01	0.12
(2,3036)	1:161:A:SER:H	2:201:A:NAD:H6N	4	0.12	0.01	0.12
(2,3924)	1:109:A:ILE:HD11	2:201:A:NAD:H2A	4	0.12	0.01	0.12
(2,1964)	1:15:A:LEU:HD11	1:65:A:PHE:HD1	4	0.11	0.01	0.11
(2,3712)	1:109:A:ILE:HG22	1:109:A:ILE:HA	4	0.11	0.0	0.11
(2,3712)	1:109:A:ILE:HG21	1:109:A:ILE:HA	4	0.11	0.0	0.11
(2,3184)	1:92:A:VAL:HG21	1:92:A:VAL:H	4	0.1	0.0	0.1
(2,3197)	1:176:A:ILE:HD11	1:176:A:ILE:HB	4	0.1	0.0	0.1
(2,1984)	1:106:A:PHE:HD1	1:106:A:PHE:HE1	4	0.1	0.0	0.1
(2,1236)	1:151:A:MET:HE2	1:156:A:PHE:HZ	3	1.02	0.23	0.93
(2,1236)	1:151:A:MET:HE3	1:156:A:PHE:HZ	3	1.02	0.23	0.93
(2,1236)	1:151:A:MET:HE1	1:156:A:PHE:HZ	3	1.02	0.23	0.93
(2,32)	1:88:A:TYR:HE1	1:159:A:TYR:HD1	3	0.9	0.74	0.46
(4,160)	1:22:A:ILE:HD12	1:22:A:ILE:H	3	0.75	0.02	0.75
(4,160)	1:22:A:ILE:HD11	1:22:A:ILE:H	3	0.75	0.02	0.75
(4,160)	1:22:A:ILE:HD13	1:22:A:ILE:H	3	0.75	0.02	0.75
(4,301)	1:97:A:LEU:HD23	1:156:A:PHE:HB2	3	0.65	0.22	0.52
(4,301)	1:97:A:LEU:HD22	1:156:A:PHE:HB2	3	0.65	0.22	0.52
(4,301)	1:97:A:LEU:HD23	1:175:A:PHE:HB2	3	0.65	0.22	0.52
(2,1535)	1:22:A:ILE:HG21	1:44:A:LYS:HE3	3	0.61	0.26	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1535)	1:22:A:ILE:HG22	1:44:A:LYS:HE3	3	0.61	0.26	0.67
(2,2266)	1:153:A:ASP:H	1:95:A:ALA:HB1	3	0.57	0.27	0.56
(2,3839)	1:129:A:THR:HG22	1:129:A:THR:HA	3	0.56	0.03	0.55
(2,3839)	1:129:A:THR:HG21	1:129:A:THR:HA	3	0.56	0.03	0.55
(2,1426)	1:86:A:LEU:HD11	1:88:A:TYR:HD1	3	0.48	0.19	0.44
(2,1426)	1:86:A:LEU:HD12	1:88:A:TYR:HD1	3	0.48	0.19	0.44
(2,1877)	1:129:A:THR:HG22	1:129:A:THR:HA	3	0.47	0.03	0.46
(2,1877)	1:129:A:THR:HG21	1:129:A:THR:HA	3	0.47	0.03	0.46
(2,300)	1:153:A:ASP:H	1:95:A:ALA:HB1	3	0.45	0.27	0.44
(2,1412)	1:66:A:ALA:HB2	1:31:A:TRP:HZ3	3	0.41	0.19	0.35
(2,3211)	1:151:A:MET:HE2	1:156:A:PHE:HZ	3	0.37	0.24	0.28
(2,3211)	1:151:A:MET:HE3	1:156:A:PHE:HZ	3	0.37	0.24	0.28
(2,3211)	1:151:A:MET:HE1	1:156:A:PHE:HZ	3	0.37	0.24	0.28
(2,3378)	1:66:A:ALA:HB2	1:31:A:TRP:HZ3	3	0.36	0.19	0.31
(2,629)	1:44:A:LYS:H	1:42:A:LYS:HG3	3	0.31	0.01	0.31
(4,364)	1:4:A:MET:HE2	1:58:A:GLU:HG3	3	0.29	0.07	0.25
(4,364)	1:4:A:MET:HE3	1:58:A:GLU:HG3	3	0.29	0.07	0.25
(4,364)	1:4:A:MET:HE2	1:53:A:LEU:HB2	3	0.29	0.07	0.25
(4,195)	1:114:A:ILE:HD11	1:117:A:MET:HE1	3	0.29	0.11	0.3
(2,2625)	1:29:A:ASN:H	1:29:A:ASN:HB3	3	0.25	0.0	0.25
(2,653)	1:29:A:ASN:H	1:29:A:ASN:HB3	3	0.24	0.0	0.24
(2,1754)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	3	0.23	0.0	0.23
(2,2918)	1:76:A:ALA:HB1	1:78:A:GLN:HE22	3	0.23	0.04	0.22
(2,2918)	1:76:A:ALA:HB3	1:78:A:GLN:HE22	3	0.23	0.04	0.22
(2,1014)	1:160:A:LEU:H	1:89:A:GLU:H	3	0.22	0.07	0.19
(2,1155)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	3	0.21	0.03	0.22
(4,453)	1:48:A:ILE:HG13	1:38:A:LEU:HA	3	0.21	0.03	0.22
(2,3559)	1:102:A:ALA:HB1	2:201:A:NAD:H4B	3	0.19	0.07	0.17
(2,3679)	1:97:A:LEU:HD21	1:97:A:LEU:HA	3	0.19	0.09	0.15
(2,3679)	1:97:A:LEU:HD23	1:97:A:LEU:HA	3	0.19	0.09	0.15
(1,117)	1:168:A:ILE:H	1:122:A:VAL:O	3	0.18	0.02	0.19
(2,2949)	1:165:A:VAL:H	1:91:A:GLN:HE22	3	0.18	0.09	0.14
(2,3959)	1:123:A:HIS:HB3	2:201:A:NAD:H5N	3	0.18	0.06	0.16
(1,2)	1:7:A:VAL:N	1:3:A:HIS:O	3	0.16	0.02	0.16
(2,2232)	1:21:A:LEU:H	1:24:A:LEU:HD23	3	0.16	0.02	0.17
(2,2232)	1:21:A:LEU:H	1:24:A:LEU:HD21	3	0.16	0.02	0.17
(4,213)	1:165:A:VAL:HB	1:123:A:HIS:HA	3	0.15	0.04	0.13
(4,213)	1:143:A:VAL:HB	1:144:A:LEU:HA	3	0.15	0.04	0.13
(2,2234)	1:14:A:VAL:HG23	1:21:A:LEU:H	3	0.14	0.02	0.14
(2,2234)	1:14:A:VAL:HG22	1:21:A:LEU:H	3	0.14	0.02	0.14
(2,2680)	1:113:A:GLY:H	1:109:A:ILE:HG21	3	0.14	0.05	0.11
(2,1158)	1:165:A:VAL:HG21	1:165:A:VAL:H	3	0.14	0.0	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,9)	1:11:A:LEU:H	1:7:A:VAL:O	3	0.13	0.0	0.13
(1,110)	1:153:A:ASP:N	1:149:A:LYS:O	3	0.13	0.01	0.12
(2,1399)	1:86:A:LEU:HG	1:86:A:LEU:H	3	0.13	0.02	0.14
(2,96)	1:25:A:ASP:HB3	1:25:A:ASP:H	3	0.13	0.02	0.12
(2,673)	1:70:A:ASN:HD22	1:50:A:MET:HG3	3	0.13	0.04	0.1
(2,1745)	1:34:A:VAL:HA	1:37:A:LEU:HD21	3	0.13	0.02	0.13
(2,3884)	2:201:A:NAD:H1B	1:109:A:ILE:HD12	3	0.13	0.02	0.12
(1,59)	1:77:A:ASN:H	1:64:A:ARG:O	3	0.12	0.03	0.11
(1,91)	1:133:A:LYS:H	1:129:A:THR:O	3	0.12	0.0	0.12
(2,54)	1:34:A:VAL:H	1:74:A:ILE:HG21	3	0.12	0.01	0.13
(2,54)	1:34:A:VAL:H	1:74:A:ILE:HG22	3	0.12	0.01	0.13
(2,904)	1:92:A:VAL:H	1:92:A:VAL:HA	3	0.12	0.0	0.12
(2,445)	1:36:A:GLU:H	1:36:A:GLU:HB3	3	0.12	0.02	0.11
(2,1842)	1:11:A:LEU:HD21	1:11:A:LEU:HB2	3	0.12	0.01	0.13
(2,1842)	1:11:A:LEU:HD22	1:11:A:LEU:HB2	3	0.12	0.01	0.13
(2,2722)	1:139:A:GLY:H	1:103:A:GLU:HA	3	0.12	0.01	0.12
(2,3295)	1:50:A:MET:HA	1:70:A:ASN:HD22	3	0.12	0.0	0.12
(4,425)	1:34:A:VAL:HG21	1:35:A:LYS:HB2	3	0.12	0.02	0.11
(2,1308)	1:13:A:LEU:HD11	1:13:A:LEU:HA	3	0.11	0.0	0.11
(2,2492)	1:129:A:THR:HG21	1:129:A:THR:H	3	0.11	0.01	0.11
(2,2492)	1:129:A:THR:HG22	1:129:A:THR:H	3	0.11	0.01	0.11
(2,1207)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	3	0.11	0.01	0.1
(2,3764)	1:160:A:LEU:HG	1:160:A:LEU:HD13	3	0.11	0.0	0.11
(2,1733)	1:7:A:VAL:HA	1:7:A:VAL:HB	3	0.1	0.0	0.1
(2,1610)	1:13:A:LEU:HG	1:17:A:HIS:HB2	2	0.78	0.04	0.78
(2,1529)	1:144:A:LEU:HD22	1:145:A:SER:HB2	2	0.75	0.12	0.75
(2,1529)	1:144:A:LEU:HD23	1:145:A:SER:HB2	2	0.75	0.12	0.75
(4,402)	1:6:A:LYS:HE2	1:6:A:LYS:HG3	2	0.73	0.01	0.73
(4,402)	1:42:A:LYS:HG3	1:42:A:LYS:HE3	2	0.73	0.01	0.73
(4,9)	1:22:A:ILE:HD13	1:10:A:PHE:HD1	2	0.58	0.35	0.58
(4,9)	1:10:A:PHE:HD1	1:7:A:VAL:HG11	2	0.58	0.35	0.58
(2,1846)	1:160:A:LEU:HD13	1:91:A:GLN:HB2	2	0.56	0.06	0.56
(2,1846)	1:160:A:LEU:HD11	1:91:A:GLN:HB2	2	0.56	0.06	0.56
(2,3788)	1:151:A:MET:HE1	1:151:A:MET:HG3	2	0.52	0.02	0.52
(2,3788)	1:151:A:MET:HE2	1:151:A:MET:HG3	2	0.52	0.02	0.52
(2,2348)	1:156:A:PHE:H	1:168:A:ILE:HD12	2	0.52	0.29	0.52
(2,2348)	1:156:A:PHE:H	1:168:A:ILE:HD11	2	0.52	0.29	0.52
(2,3843)	1:76:A:ALA:HB1	1:16:A:ARG:HA	2	0.51	0.05	0.51
(2,3843)	1:76:A:ALA:HB3	1:16:A:ARG:HA	2	0.51	0.05	0.51
(4,129)	1:13:A:LEU:HD23	1:18:A:ASN:H	2	0.48	0.04	0.48
(4,129)	1:13:A:LEU:HD21	1:18:A:ASN:H	2	0.48	0.04	0.48
(2,2221)	1:168:A:ILE:HD12	1:157:A:ASP:H	2	0.45	0.35	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3461)	1:168:A:ILE:HD12	1:156:A:PHE:HB2	2	0.41	0.12	0.41
(2,3461)	1:168:A:ILE:HD11	1:156:A:PHE:HB2	2	0.41	0.12	0.41
(4,410)	1:50:A:MET:HE3	1:54:A:LYS:HD3	2	0.4	0.18	0.4
(4,410)	1:50:A:MET:HE3	1:54:A:LYS:HD2	2	0.4	0.18	0.4
(4,223)	1:13:A:LEU:HD12	1:10:A:PHE:HE1	2	0.36	0.21	0.36
(2,3446)	1:74:A:ILE:HD12	1:67:A:PHE:HE1	2	0.33	0.22	0.33
(2,3384)	1:21:A:LEU:HD11	1:18:A:ASN:HD22	2	0.32	0.02	0.32
(4,322)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	2	0.32	0.02	0.32
(2,2123)	1:86:A:LEU:H	1:86:A:LEU:HB3	2	0.27	0.02	0.27
(4,411)	1:84:A:VAL:HB	1:86:A:LEU:HB3	2	0.27	0.06	0.27
(4,411)	1:172:A:PRO:HB2	1:114:A:ILE:HG12	2	0.27	0.06	0.27
(4,387)	1:83:A:GLU:HA	1:82:A:VAL:HG12	2	0.26	0.08	0.26
(4,40)	1:5:A:VAL:H	1:5:A:VAL:HB	2	0.26	0.0	0.26
(2,164)	1:86:A:LEU:H	1:86:A:LEU:HB3	2	0.26	0.03	0.26
(2,1274)	1:160:A:LEU:HD22	1:91:A:GLN:HE22	2	0.25	0.1	0.25
(2,1274)	1:160:A:LEU:HD21	1:91:A:GLN:HE22	2	0.25	0.1	0.25
(2,486)	1:58:A:GLU:H	1:58:A:GLU:HB3	2	0.24	0.01	0.24
(2,3248)	1:160:A:LEU:HD22	1:91:A:GLN:HE22	2	0.24	0.1	0.24
(2,3248)	1:160:A:LEU:HD21	1:91:A:GLN:HE22	2	0.24	0.1	0.24
(2,768)	1:30:A:GLY:H	1:26:A:LEU:HD21	2	0.22	0.04	0.22
(2,768)	1:30:A:GLY:H	1:26:A:LEU:HD22	2	0.22	0.04	0.22
(2,1208)	1:114:A:ILE:HD13	1:171:A:VAL:HB	2	0.22	0.1	0.22
(2,3558)	1:152:A:ALA:HB2	1:149:A:LYS:HA	2	0.21	0.01	0.21
(2,1633)	1:42:A:LYS:HE2	1:39:A:ALA:HA	2	0.2	0.06	0.2
(1,18)	1:15:A:LEU:N	1:11:A:LEU:O	2	0.2	0.0	0.2
(2,190)	1:13:A:LEU:H	1:13:A:LEU:HB3	2	0.19	0.01	0.19
(2,1828)	1:151:A:MET:HE1	1:151:A:MET:HG3	2	0.18	0.02	0.18
(2,1828)	1:151:A:MET:HE2	1:151:A:MET:HG3	2	0.18	0.02	0.18
(2,2852)	1:85:A:ASP:H	1:86:A:LEU:H	2	0.18	0.02	0.18
(2,1880)	1:76:A:ALA:HB1	1:16:A:ARG:HA	2	0.18	0.04	0.18
(2,1880)	1:76:A:ALA:HB3	1:16:A:ARG:HA	2	0.18	0.04	0.18
(4,392)	1:8:A:SER:HB2	1:7:A:VAL:HB	2	0.17	0.03	0.17
(2,811)	1:14:A:VAL:HG23	1:22:A:ILE:H	2	0.17	0.07	0.17
(2,811)	1:14:A:VAL:HG21	1:22:A:ILE:H	2	0.17	0.07	0.17
(1,17)	1:15:A:LEU:H	1:11:A:LEU:O	2	0.16	0.02	0.16
(2,2506)	1:64:A:ARG:H	1:76:A:ALA:HB1	2	0.16	0.03	0.16
(2,2506)	1:64:A:ARG:H	1:76:A:ALA:HB3	2	0.16	0.03	0.16
(4,448)	1:110:A:LEU:HD21	1:144:A:LEU:HG	2	0.16	0.01	0.16
(4,448)	1:110:A:LEU:HD22	1:144:A:LEU:HG	2	0.16	0.01	0.16
(2,3445)	1:97:A:LEU:HD23	1:166:A:TRP:HE3	2	0.16	0.01	0.16
(2,3445)	1:97:A:LEU:HD21	1:166:A:TRP:HE3	2	0.16	0.01	0.16
(1,94)	1:134:A:VAL:N	1:130:A:THR:O	2	0.15	0.03	0.15

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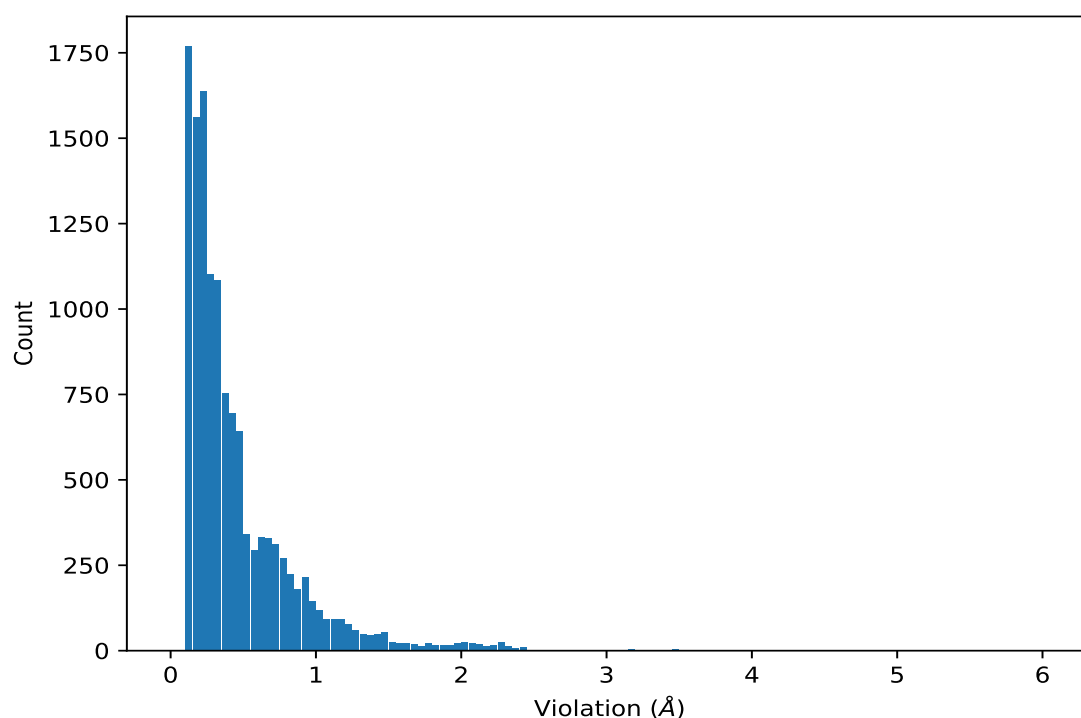
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,61)	1:166:A:TRP:HE1	1:126:A:GLN:HB2	2	0.15	0.04	0.15
(2,184)	1:26:A:LEU:H	1:19:A:PRO:HA	2	0.15	0.03	0.15
(2,1932)	2:201:A:NAD:H3D	2:201:A:NAD:H2N	2	0.15	0.02	0.15
(2,3896)	2:201:A:NAD:H3D	2:201:A:NAD:H2N	2	0.15	0.02	0.15
(2,198)	1:20:A:ALA:HA	1:24:A:LEU:H	2	0.14	0.01	0.14
(4,209)	1:76:A:ALA:HB3	1:16:A:ARG:H	2	0.14	0.02	0.14
(4,209)	1:76:A:ALA:HB1	1:16:A:ARG:H	2	0.14	0.02	0.14
(2,723)	1:20:A:ALA:HA	1:23:A:GLY:H	2	0.14	0.01	0.14
(2,1591)	1:95:A:ALA:HB1	1:149:A:LYS:HA	2	0.14	0.02	0.14
(2,3918)	1:114:A:ILE:HD11	2:201:A:NAD:H8A	2	0.14	0.01	0.14
(2,43)	1:96:A:VAL:HG21	1:148:A:ALA:H	2	0.12	0.01	0.12
(2,1099)	1:100:A:GLY:H	1:166:A:TRP:H	2	0.12	0.01	0.12
(2,2151)	1:13:A:LEU:H	1:13:A:LEU:HB3	2	0.12	0.01	0.12
(2,2216)	1:26:A:LEU:HD11	1:27:A:ASP:H	2	0.12	0.02	0.12
(2,2216)	1:26:A:LEU:HD13	1:27:A:ASP:H	2	0.12	0.02	0.12
(2,3947)	1:165:A:VAL:HG21	2:201:A:NAD:H4N	2	0.12	0.01	0.12
(1,121)	1:175:A:PHE:H	1:172:A:PRO:O	2	0.12	0.0	0.12
(2,2550)	1:86:A:LEU:H	1:88:A:TYR:H	2	0.12	0.01	0.12
(2,3335)	1:16:A:ARG:HD2	1:12:A:SER:H	2	0.12	0.01	0.12
(3,20)	1:163:A:ASN:OD1	2:201:A:NAD:H71N	2	0.12	0.02	0.12
(2,99)	1:140:A:LYS:H	1:103:A:GLU:HA	2	0.12	0.0	0.12
(2,1687)	1:96:A:VAL:HG21	1:96:A:VAL:HA	2	0.11	0.01	0.11
(2,1989)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	2	0.11	0.0	0.11
(2,2132)	1:56:A:ILE:HD11	1:56:A:ILE:H	2	0.11	0.01	0.11
(2,2212)	1:53:A:LEU:H	1:48:A:ILE:HG12	2	0.11	0.01	0.11
(2,2269)	1:84:A:VAL:HA	1:84:A:VAL:H	2	0.11	0.0	0.11
(2,2305)	1:173:A:ALA:HB1	1:176:A:ILE:H	2	0.11	0.0	0.11
(2,2597)	1:44:A:LYS:H	1:21:A:LEU:HA	2	0.11	0.0	0.11
(2,439)	1:55:A:HIS:H	1:54:A:LYS:HB2	2	0.11	0.0	0.11
(2,3302)	1:82:A:VAL:HA	1:83:A:GLU:H	2	0.11	0.0	0.11
(2,2822)	1:74:A:ILE:H	1:73:A:LYS:HB2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	2	6.05
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	14	5.97
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	9	5.03
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	16	4.57
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	20	4.4
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	14	4.38
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	6	4.35
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	10	4.05
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	12	4.02
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	18	3.83
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	11	3.78
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	5	3.73
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	18	3.72
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	1	3.67
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	17	3.66
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	7	3.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	17	3.6
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	7	3.58
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	4	3.55
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	19	3.54
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	8	3.49
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	2	3.46
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	2	3.46
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	9	3.44
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	3	3.38
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	4	3.36
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	15	3.24
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	9	3.21
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	15	3.18
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	3	3.15
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	9	3.15
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG11	9	2.99
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	18	2.86
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	8	2.85
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	6	2.81
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	20	2.79
(2,1635)	1:73:A:LYS:HE3	1:33:A:PRO:HB2	13	2.77
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	1	2.71
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG11	8	2.7
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	3	2.66
(4,186)	1:175:A:PHE:H	2:201:A:NAD:H2A	3	2.65
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	7	2.64
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	7	2.59
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG11	14	2.56
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	10	2.53
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	1	2.49
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	6	2.49
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	17	2.44
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	7	2.43
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	18	2.42
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD13	18	2.42
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	10	2.42
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	15	2.41
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG11	12	2.41
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD13	6	2.4
(2,1527)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	10	2.4
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	5	2.39
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	13	2.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	8	2.37
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD13	10	2.37
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	11	2.37
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	6	2.37
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	20	2.36
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	3	2.36
(4,274)	1:124:A:LEU:HD22	1:159:A:TYR:HE1	1	2.34
(2,1527)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	1	2.34
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	15	2.34
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	19	2.34
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	9	2.33
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	18	2.33
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	15	2.32
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	14	2.32
(2,1527)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	4	2.32
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	16	2.31
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	1	2.3
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	10	2.3
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	19	2.3
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	7	2.29
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	19	2.29
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	13	2.29
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	12	2.28
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	19	2.28
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	2	2.28
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	4	2.28
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	5	2.28
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	11	2.27
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG12	18	2.27
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	11	2.27
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	5	2.27
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	7	2.27
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	11	2.27
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	6	2.27
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	13	2.26
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	15	2.26
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	3	2.26
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	15	2.26
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	11	2.25
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	9	2.25
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	9	2.25
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	11	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	20	2.25
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	8	2.25
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	16	2.24
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	17	2.24
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	5	2.23
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	17	2.23
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	7	2.22
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	4	2.21
(2,1527)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	3	2.21
(2,1471)	1:57:A:VAL:HG23	1:57:A:VAL:H	12	2.21
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	16	2.21
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	13	2.2
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	15	2.2
(2,1527)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	9	2.2
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	8	2.2
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	14	2.2
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	6	2.2
(4,315)	1:56:A:ILE:HG21	1:6:A:LYS:HA	6	2.19
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	8	2.19
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	3	2.19
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	19	2.18
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	20	2.18
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	16	2.18
(2,1471)	1:57:A:VAL:HG21	1:57:A:VAL:H	6	2.18
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	2	2.18
(2,1527)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	7	2.17
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	16	2.17
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	19	2.17
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	12	2.16
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	20	2.16
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	17	2.15
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	15	2.14
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	18	2.14
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	1	2.14
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	15	2.14
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	2	2.14
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	3	2.14
(4,315)	1:56:A:ILE:HG21	1:6:A:LYS:HA	18	2.13
(4,274)	1:124:A:LEU:HD21	1:156:A:PHE:HZ	13	2.13
(4,186)	1:175:A:PHE:H	2:201:A:NAD:H2A	6	2.13
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	1	2.13
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	8	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	19	2.12
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	16	2.12
(4,326)	1:124:A:LEU:HD22	1:177:A:LYS:HE2	3	2.11
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	3	2.11
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	15	2.11
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	8	2.1
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	16	2.1
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	10	2.09
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	8	2.09
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	1	2.09
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	18	2.08
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	20	2.08
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	18	2.08
(4,315)	1:56:A:ILE:HG22	1:6:A:LYS:HA	9	2.07
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	15	2.07
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG12	2	2.07
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	20	2.07
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	7	2.07
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	13	2.07
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	20	2.07
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	11	2.07
(4,326)	1:124:A:LEU:HD23	1:177:A:LYS:HE2	10	2.06
(4,326)	1:124:A:LEU:HD21	1:177:A:LYS:HE2	13	2.06
(4,274)	1:124:A:LEU:HD21	1:156:A:PHE:HZ	4	2.06
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	19	2.06
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	6	2.05
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	14	2.05
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG22	12	2.05
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	13	2.05
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	14	2.04
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	3	2.04
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	17	2.04
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	4	2.04
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	2	2.03
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	17	2.03
(4,326)	1:124:A:LEU:HD22	1:177:A:LYS:HE2	4	2.02
(4,326)	1:124:A:LEU:HD23	1:177:A:LYS:HE2	8	2.02
(4,326)	1:124:A:LEU:HD21	1:177:A:LYS:HE2	18	2.02
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	1	2.02
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	4	2.02
(4,274)	1:124:A:LEU:HD22	1:159:A:TYR:HE1	10	2.02
(4,274)	1:124:A:LEU:HD21	1:156:A:PHE:HZ	12	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	13	2.02
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	5	2.01
(4,274)	1:124:A:LEU:HD23	1:156:A:PHE:HZ	8	2.01
(2,1803)	1:56:A:ILE:HG12	1:53:A:LEU:HD12	2	2.01
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	9	2.01
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	20	2.01
(4,326)	1:124:A:LEU:HD21	1:177:A:LYS:HE2	1	2.0
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	16	2.0
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	17	2.0
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	12	2.0
(2,1361)	1:177:A:LYS:HE2	1:147:A:ASP:H	16	2.0
(4,326)	1:124:A:LEU:HD21	1:177:A:LYS:HE2	12	1.99
(4,186)	1:175:A:PHE:H	2:201:A:NAD:H2A	19	1.99
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG22	2	1.99
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	2	1.99
(2,1361)	1:177:A:LYS:HE2	1:147:A:ASP:H	7	1.99
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	7	1.98
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	14	1.98
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	19	1.97
(4,186)	1:175:A:PHE:H	2:201:A:NAD:H2A	16	1.97
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	7	1.97
(4,326)	1:124:A:LEU:HD23	1:177:A:LYS:HE2	5	1.96
(4,326)	1:124:A:LEU:HD23	1:177:A:LYS:HE2	15	1.96
(4,326)	1:124:A:LEU:HD21	1:177:A:LYS:HE2	17	1.96
(4,316)	1:37:A:LEU:HD21	1:8:A:SER:HB2	6	1.96
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	4	1.96
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	10	1.96
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	4	1.96
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	10	1.95
(2,1802)	1:53:A:LEU:HD13	1:74:A:ILE:HG23	10	1.95
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	8	1.95
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	20	1.95
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	11	1.94
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	4	1.94
(2,32)	1:88:A:TYR:HE1	1:159:A:TYR:HD1	20	1.94
(4,326)	1:124:A:LEU:HD21	1:177:A:LYS:HE2	19	1.93
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	2	1.93
(4,316)	1:37:A:LEU:HD21	1:8:A:SER:HB2	13	1.92
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG21	7	1.92
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	5	1.91
(4,326)	1:124:A:LEU:HD23	1:177:A:LYS:HE2	20	1.91
(4,186)	1:175:A:PHE:H	2:201:A:NAD:H2A	2	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	3	1.91
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	14	1.91
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	1	1.91
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	17	1.91
(4,186)	1:175:A:PHE:H	2:201:A:NAD:H2A	5	1.9
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	19	1.9
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	19	1.88
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	8	1.88
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	12	1.88
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD13	18	1.87
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	8	1.87
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	11	1.87
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	3	1.87
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	16	1.87
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	1	1.86
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	15	1.85
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	1	1.85
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	17	1.85
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	12	1.85
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	5	1.85
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	18	1.85
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	14	1.84
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	12	1.84
(2,1802)	1:53:A:LEU:HD13	1:74:A:ILE:HG23	18	1.84
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	11	1.84
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	3	1.83
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	16	1.83
(4,441)	1:56:A:ILE:HD11	1:38:A:LEU:HB2	7	1.82
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	12	1.82
(4,316)	1:37:A:LEU:HD23	1:23:A:GLY:HA3	5	1.82
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	5	1.82
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	5	1.82
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	7	1.81
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	11	1.81
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	17	1.81
(4,315)	1:56:A:ILE:HG23	1:38:A:LEU:HA	20	1.81
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	11	1.81
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD13	10	1.8
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	13	1.79
(4,326)	1:124:A:LEU:HD22	1:163:A:ASN:HB2	9	1.79
(4,316)	1:37:A:LEU:HD21	1:8:A:SER:HB2	9	1.79
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	7	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1361)	1:177:A:LYS:HE2	1:147:A:ASP:H	9	1.79
(2,1174)	1:101:A:THR:HG21	1:144:A:LEU:HD11	12	1.79
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	4	1.78
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD13	6	1.78
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	20	1.78
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	2	1.77
(4,292)	1:122:A:VAL:HG23	1:118:A:SER:H	3	1.77
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	9	1.77
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	1	1.76
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	20	1.76
(4,441)	1:56:A:ILE:HD12	1:6:A:LYS:HB3	13	1.75
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	18	1.75
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	16	1.75
(4,326)	1:124:A:LEU:HD21	1:177:A:LYS:HE2	6	1.75
(4,315)	1:56:A:ILE:HG22	1:38:A:LEU:HA	14	1.75
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG21	19	1.75
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	13	1.75
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	16	1.75
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	8	1.75
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	8	1.74
(4,274)	1:124:A:LEU:HD23	1:156:A:PHE:HZ	6	1.74
(4,186)	1:175:A:PHE:H	2:201:A:NAD:H2A	18	1.74
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	9	1.73
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	18	1.73
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	17	1.73
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	2	1.73
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	17	1.72
(2,1802)	1:53:A:LEU:HD13	1:74:A:ILE:HG23	6	1.72
(4,441)	1:56:A:ILE:HD11	1:38:A:LEU:HB2	6	1.71
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	13	1.71
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	3	1.7
(4,441)	1:56:A:ILE:HD12	1:6:A:LYS:HB3	16	1.69
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	15	1.69
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG12	15	1.69
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	13	1.69
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	13	1.69
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	14	1.68
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	5	1.68
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	4	1.68
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	10	1.67
(4,435)	1:24:A:LEU:HB3	1:53:A:LEU:HD12	19	1.67
(4,414)	1:133:A:LYS:HB2	1:128:A:ILE:HG21	5	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	3	1.67
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	8	1.67
(2,1217)	1:177:A:LYS:HE2	1:177:A:LYS:HB2	14	1.67
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	9	1.67
(4,274)	1:124:A:LEU:HD22	1:159:A:TYR:HE1	15	1.66
(4,274)	1:124:A:LEU:HD23	1:159:A:TYR:HE1	19	1.66
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	17	1.66
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	15	1.65
(2,3498)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	10	1.65
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	19	1.64
(4,441)	1:56:A:ILE:HD13	1:6:A:LYS:HB3	17	1.63
(4,415)	1:19:A:PRO:HB2	1:36:A:GLU:HG2	3	1.63
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	18	1.63
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	15	1.63
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	4	1.63
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	5	1.63
(4,441)	1:56:A:ILE:HD11	1:38:A:LEU:HB2	9	1.62
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	16	1.62
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	20	1.62
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	6	1.62
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	6	1.62
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	10	1.61
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	5	1.61
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	5	1.61
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	2	1.61
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	3	1.61
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	9	1.6
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	11	1.6
(2,3498)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	1	1.6
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	17	1.6
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	14	1.6
(4,326)	1:124:A:LEU:HD23	1:163:A:ASN:HB2	14	1.59
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	11	1.59
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	15	1.59
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	19	1.59
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	17	1.59
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	12	1.59
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	20	1.59
(4,292)	1:122:A:VAL:HG22	1:118:A:SER:H	2	1.58
(2,3498)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	4	1.58
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	7	1.58
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	11	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,415)	1:19:A:PRO:HB2	1:33:A:PRO:HG2	13	1.57
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	1	1.57
(4,441)	1:56:A:ILE:HD11	1:38:A:LEU:HB2	1	1.56
(4,326)	1:124:A:LEU:HD22	1:163:A:ASN:HB2	16	1.56
(4,320)	1:151:A:MET:HE2	1:147:A:ASP:HB2	5	1.56
(4,316)	1:37:A:LEU:HD22	1:8:A:SER:HB2	3	1.56
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	19	1.56
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	20	1.56
(4,326)	1:124:A:LEU:HD23	1:163:A:ASN:HB2	11	1.55
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD11	16	1.55
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	2	1.54
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD11	17	1.54
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	12	1.54
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	7	1.54
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	2	1.54
(2,3454)	1:168:A:ILE:HD13	1:149:A:LYS:H	12	1.53
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	20	1.53
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	3	1.53
(2,1291)	1:84:A:VAL:HG12	1:84:A:VAL:H	2	1.53
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	13	1.53
(4,415)	1:19:A:PRO:HB3	1:33:A:PRO:HG2	4	1.52
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	10	1.52
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	11	1.52
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	14	1.52
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	19	1.52
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	15	1.51
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB2	17	1.51
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	12	1.51
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	2	1.51
(4,274)	1:124:A:LEU:HD23	1:159:A:TYR:HE1	16	1.5
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	17	1.5
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	3	1.5
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	4	1.5
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	11	1.5
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	5	1.5
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	18	1.49
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	8	1.49
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	10	1.49
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	14	1.49
(4,326)	1:124:A:LEU:HD21	1:163:A:ASN:HB2	7	1.48
(4,320)	1:151:A:MET:HE2	1:147:A:ASP:HB2	1	1.48
(4,274)	1:124:A:LEU:HD22	1:156:A:PHE:HZ	5	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	5	1.48
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	13	1.48
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	15	1.48
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	1	1.48
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	16	1.48
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	12	1.48
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	3	1.48
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	9	1.48
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	12	1.48
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	2	1.47
(4,326)	1:124:A:LEU:HD22	1:163:A:ASN:HB2	2	1.47
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	3	1.47
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	13	1.47
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	12	1.47
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	2	1.47
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD11	6	1.47
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD11	7	1.47
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD11	18	1.47
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	14	1.47
(4,441)	1:56:A:ILE:HD12	1:38:A:LEU:HB2	5	1.46
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	10	1.46
(2,3498)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	3	1.46
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	16	1.46
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	14	1.46
(2,1421)	1:21:A:LEU:HD21	1:10:A:PHE:HE1	11	1.46
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	13	1.46
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	14	1.46
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	20	1.46
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD12	11	1.46
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	15	1.46
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD13	20	1.46
(4,441)	1:56:A:ILE:HD11	1:38:A:LEU:HB2	8	1.45
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	20	1.45
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	20	1.45
(4,274)	1:124:A:LEU:HD21	1:156:A:PHE:HZ	3	1.45
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	5	1.45
(2,3498)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	9	1.45
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	4	1.45
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	7	1.45
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	4	1.45
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	8	1.45
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	19	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	8	1.45
(2,1421)	1:21:A:LEU:HD21	1:10:A:PHE:HE1	4	1.45
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	9	1.45
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD11	4	1.45
(4,350)	1:42:A:LYS:HE3	1:44:A:LYS:HG2	12	1.44
(2,1802)	1:53:A:LEU:HD12	1:74:A:ILE:HG23	5	1.44
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	20	1.44
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	2	1.44
(2,1421)	1:21:A:LEU:HD21	1:10:A:PHE:HE1	6	1.44
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	7	1.44
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	15	1.44
(4,441)	1:56:A:ILE:HD11	1:6:A:LYS:HB3	11	1.43
(4,441)	1:56:A:ILE:HD12	1:38:A:LEU:HB2	12	1.43
(4,274)	1:124:A:LEU:HD21	1:159:A:TYR:HE1	14	1.43
(4,274)	1:124:A:LEU:HD21	1:156:A:PHE:HZ	18	1.43
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	16	1.43
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	2	1.43
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	12	1.43
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	6	1.43
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	18	1.43
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	17	1.43
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	19	1.43
(2,1291)	1:84:A:VAL:HG12	1:84:A:VAL:H	15	1.43
(4,316)	1:37:A:LEU:HD21	1:8:A:SER:HB2	20	1.42
(2,3498)	1:38:A:LEU:HD22	1:47:A:GLY:HA2	7	1.42
(2,3454)	1:168:A:ILE:HD12	1:149:A:LYS:H	9	1.42
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	16	1.42
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	7	1.42
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	18	1.42
(4,292)	1:122:A:VAL:HG22	1:118:A:SER:H	13	1.41
(4,202)	1:173:A:ALA:HA	1:145:A:SER:HB2	4	1.41
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	1	1.41
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	6	1.41
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	8	1.41
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	1	1.41
(2,1530)	1:178:A:VAL:HG21	1:109:A:ILE:HA	3	1.41
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	18	1.41
(2,1421)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	10	1.41
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	3	1.41
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB1	9	1.4
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	12	1.4
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	1	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	8	1.4
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	18	1.4
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	3	1.4
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	20	1.4
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	16	1.4
(2,1492)	1:167:A:LEU:HD23	1:123:A:HIS:HA	11	1.4
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	6	1.4
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	11	1.4
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	18	1.4
(4,274)	1:124:A:LEU:HD22	1:159:A:TYR:HE1	20	1.39
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD3	2	1.39
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	7	1.39
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	2	1.39
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	14	1.39
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	7	1.39
(2,1530)	1:178:A:VAL:HG21	1:109:A:ILE:HA	2	1.39
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	11	1.39
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	12	1.39
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	10	1.39
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	14	1.38
(2,3454)	1:168:A:ILE:HD11	1:149:A:LYS:H	19	1.38
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	9	1.38
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	10	1.38
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	19	1.38
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	1	1.38
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	3	1.38
(4,415)	1:19:A:PRO:HB2	1:33:A:PRO:HG2	2	1.37
(4,184)	1:105:A:ASN:H	1:136:A:MET:H	17	1.37
(2,3830)	1:97:A:LEU:HD22	1:95:A:ALA:HB2	4	1.37
(2,3830)	1:97:A:LEU:HD23	1:95:A:ALA:HB2	5	1.37
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	15	1.37
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG22	16	1.37
(2,1738)	1:7:A:VAL:HA	1:22:A:ILE:HG23	17	1.37
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	14	1.37
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	14	1.37
(2,1530)	1:178:A:VAL:HG21	1:109:A:ILE:HA	19	1.37
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	20	1.37
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	17	1.37
(2,817)	1:53:A:LEU:H	1:38:A:LEU:HD11	1	1.37
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	18	1.36
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	8	1.36
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	9	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	13	1.36
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	17	1.36
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	5	1.36
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	7	1.36
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	11	1.36
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	1	1.35
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	8	1.35
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	7	1.35
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	14	1.35
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	19	1.35
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	15	1.35
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	1	1.35
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	13	1.34
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	8	1.34
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	13	1.34
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	2	1.34
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	11	1.34
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	20	1.34
(2,1421)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	8	1.34
(2,1236)	1:151:A:MET:HE2	1:156:A:PHE:HZ	9	1.34
(4,184)	1:105:A:ASN:H	1:136:A:MET:H	11	1.33
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD3	18	1.33
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	5	1.33
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	12	1.33
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	18	1.33
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD21	6	1.33
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	9	1.33
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	17	1.33
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	4	1.33
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	12	1.33
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	14	1.32
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	8	1.32
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	10	1.32
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	4	1.32
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	6	1.32
(2,1530)	1:178:A:VAL:HG22	1:109:A:ILE:HA	10	1.32
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	20	1.32
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	8	1.32
(4,274)	1:124:A:LEU:HD23	1:159:A:TYR:HE1	2	1.31
(4,202)	1:173:A:ALA:HA	1:145:A:SER:HB2	19	1.31
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	20	1.31
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	4	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	19	1.31
(2,1530)	1:178:A:VAL:HG21	1:109:A:ILE:HA	5	1.31
(2,1487)	1:168:A:ILE:HD13	1:149:A:LYS:H	12	1.31
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	20	1.31
(4,441)	1:56:A:ILE:HD11	1:6:A:LYS:HB3	4	1.3
(4,441)	1:56:A:ILE:HD13	1:38:A:LEU:HB2	14	1.3
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	6	1.3
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD3	13	1.3
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	15	1.3
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	17	1.3
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	11	1.3
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	18	1.3
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	8	1.3
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	13	1.3
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	16	1.3
(2,1492)	1:167:A:LEU:HD23	1:123:A:HIS:HA	5	1.3
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	14	1.3
(4,292)	1:122:A:VAL:HG22	1:118:A:SER:H	4	1.29
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	8	1.29
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	6	1.29
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	17	1.29
(2,1856)	1:22:A:ILE:HD12	1:14:A:VAL:HG23	1	1.29
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	8	1.29
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	9	1.29
(2,1260)	1:142:A:VAL:HG23	1:178:A:VAL:HG11	8	1.29
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	9	1.28
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	18	1.28
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	19	1.28
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	14	1.28
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	3	1.28
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB3	19	1.28
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	14	1.28
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	18	1.28
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	15	1.28
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	3	1.28
(2,1291)	1:84:A:VAL:HG12	1:84:A:VAL:H	6	1.28
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	17	1.28
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	4	1.28
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	15	1.28
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	16	1.28
(4,440)	1:15:A:LEU:HD22	1:13:A:LEU:HB2	20	1.27
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	11	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	12	1.27
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	11	1.27
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	1	1.27
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	20	1.27
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	13	1.27
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD12	2	1.27
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	6	1.27
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	10	1.27
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	18	1.27
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	4	1.27
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	13	1.26
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	12	1.26
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	3	1.26
(2,3265)	1:84:A:VAL:HG12	1:84:A:VAL:H	2	1.26
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD21	11	1.26
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	14	1.26
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	13	1.26
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	15	1.26
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	12	1.26
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	7	1.26
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	3	1.26
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	5	1.26
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	6	1.26
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	20	1.26
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	15	1.25
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB1	9	1.25
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	12	1.25
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	10	1.25
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	10	1.25
(2,1291)	1:84:A:VAL:HG12	1:84:A:VAL:H	20	1.25
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	7	1.25
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	8	1.25
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	10	1.25
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	17	1.25
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	19	1.25
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	13	1.24
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	13	1.24
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	2	1.24
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	10	1.24
(2,1843)	1:110:A:LEU:HD13	1:110:A:LEU:HB3	14	1.24
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	13	1.24
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	19	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	4	1.24
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	16	1.24
(2,1361)	1:177:A:LYS:HE2	1:147:A:ASP:H	11	1.24
(2,1361)	1:177:A:LYS:HE2	1:147:A:ASP:H	14	1.24
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	5	1.23
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	3	1.23
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	14	1.23
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG23	3	1.23
(2,1843)	1:110:A:LEU:HD12	1:110:A:LEU:HB3	15	1.23
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	2	1.23
(2,1452)	1:38:A:LEU:HD12	1:38:A:LEU:H	6	1.23
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	4	1.23
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	1	1.23
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	4	1.22
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	19	1.22
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	10	1.22
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	1	1.22
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	3	1.22
(2,3830)	1:97:A:LEU:HD22	1:95:A:ALA:HB1	10	1.22
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	13	1.22
(2,1868)	1:97:A:LEU:HD22	1:95:A:ALA:HB2	4	1.22
(2,1868)	1:97:A:LEU:HD23	1:95:A:ALA:HB2	5	1.22
(2,1843)	1:110:A:LEU:HD13	1:110:A:LEU:HB3	5	1.22
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	6	1.22
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	5	1.22
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	12	1.22
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	3	1.22
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	15	1.22
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	9	1.22
(2,1452)	1:38:A:LEU:HD11	1:38:A:LEU:H	19	1.22
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	20	1.22
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	13	1.22
(4,274)	1:124:A:LEU:HD21	1:159:A:TYR:HE1	7	1.21
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB3	7	1.21
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	4	1.21
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	7	1.21
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	20	1.21
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	2	1.21
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	8	1.21
(2,1843)	1:110:A:LEU:HD13	1:110:A:LEU:HB3	9	1.21
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	12	1.21
(2,1806)	1:13:A:LEU:HD21	1:13:A:LEU:HB2	12	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	1	1.21
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	12	1.21
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	17	1.21
(2,1452)	1:38:A:LEU:HD12	1:38:A:LEU:H	1	1.21
(2,1452)	1:38:A:LEU:HD12	1:38:A:LEU:H	4	1.21
(2,1452)	1:38:A:LEU:HD12	1:38:A:LEU:H	14	1.21
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	15	1.21
(2,1291)	1:84:A:VAL:HG13	1:84:A:VAL:H	1	1.21
(4,436)	1:178:A:VAL:HG13	1:110:A:LEU:HB3	3	1.2
(4,103)	1:114:A:ILE:H	1:123:A:HIS:HA	6	1.2
(4,103)	1:114:A:ILE:H	1:123:A:HIS:HA	16	1.2
(4,7)	1:65:A:PHE:HZ	1:37:A:LEU:HD21	5	1.2
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	16	1.2
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	2	1.2
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	12	1.2
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	13	1.2
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	13	1.2
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	16	1.2
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	19	1.2
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	19	1.2
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD21	4	1.2
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	9	1.2
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	14	1.2
(2,1487)	1:168:A:ILE:HD12	1:149:A:LYS:H	9	1.2
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	1	1.2
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	3	1.2
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	10	1.2
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	4	1.2
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	11	1.2
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	18	1.2
(4,184)	1:105:A:ASN:H	1:136:A:MET:H	16	1.19
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	17	1.19
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	18	1.19
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	17	1.19
(2,1492)	1:167:A:LEU:HD23	1:123:A:HIS:HA	2	1.19
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	2	1.19
(2,1452)	1:38:A:LEU:HD11	1:38:A:LEU:H	7	1.19
(2,1452)	1:38:A:LEU:HD12	1:38:A:LEU:H	11	1.19
(2,1452)	1:38:A:LEU:HD12	1:38:A:LEU:H	17	1.19
(2,1452)	1:38:A:LEU:HD11	1:38:A:LEU:H	18	1.19
(2,1260)	1:142:A:VAL:HG23	1:178:A:VAL:HG11	15	1.19
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	13	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	2	1.19
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	7	1.18
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	8	1.18
(4,320)	1:151:A:MET:HE1	1:147:A:ASP:HB2	19	1.18
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	9	1.18
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	18	1.18
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD13	14	1.18
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	15	1.18
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	8	1.18
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	5	1.18
(2,1260)	1:142:A:VAL:HG23	1:178:A:VAL:HG11	10	1.18
(2,1217)	1:177:A:LYS:HE2	1:177:A:LYS:HB2	7	1.18
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	5	1.18
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	1	1.18
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	13	1.17
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	3	1.17
(2,3830)	1:97:A:LEU:HD23	1:95:A:ALA:HB2	6	1.17
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	1	1.17
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	6	1.17
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	18	1.17
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	11	1.17
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	18	1.17
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	18	1.17
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	14	1.17
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	20	1.17
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	7	1.17
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	8	1.17
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	13	1.17
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	1	1.17
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	16	1.17
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	9	1.17
(2,336)	1:176:A:ILE:H	1:176:A:ILE:HG12	14	1.17
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	12	1.17
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	19	1.16
(4,415)	1:19:A:PRO:HB2	1:36:A:GLU:HG2	7	1.16
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	1	1.16
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	7	1.16
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	15	1.16
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	16	1.16
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	8	1.16
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	7	1.16
(2,3265)	1:84:A:VAL:HG12	1:84:A:VAL:H	15	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	3	1.16
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	5	1.16
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	6	1.16
(2,1806)	1:13:A:LEU:HD23	1:13:A:LEU:HB2	8	1.16
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	16	1.16
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	19	1.16
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	3	1.16
(2,1452)	1:38:A:LEU:HD13	1:38:A:LEU:H	12	1.16
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG12	7	1.16
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	18	1.16
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG12	19	1.16
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	10	1.16
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	2	1.15
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	3	1.15
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	4	1.15
(4,378)	1:24:A:LEU:HA	1:15:A:LEU:HB2	11	1.15
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	13	1.15
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	8	1.15
(4,202)	1:173:A:ALA:HA	1:145:A:SER:HB2	5	1.15
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	10	1.15
(2,3807)	1:110:A:LEU:HD13	1:110:A:LEU:HB3	14	1.15
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	9	1.15
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	10	1.15
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	19	1.15
(2,3501)	1:178:A:VAL:HG21	1:109:A:ILE:HA	3	1.15
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	11	1.15
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	1	1.15
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	3	1.15
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	7	1.15
(2,1806)	1:13:A:LEU:HD21	1:13:A:LEU:HB2	11	1.15
(2,1806)	1:13:A:LEU:HD23	1:13:A:LEU:HB2	13	1.15
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	14	1.15
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG23	10	1.15
(2,1561)	1:21:A:LEU:HD13	1:41:A:MET:HB2	20	1.15
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	18	1.15
(2,1487)	1:168:A:ILE:HD11	1:149:A:LYS:H	19	1.15
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	4	1.15
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	20	1.15
(4,436)	1:178:A:VAL:HG13	1:110:A:LEU:HB3	17	1.14
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	15	1.14
(4,274)	1:124:A:LEU:HD21	1:159:A:TYR:HE1	11	1.14
(2,3807)	1:110:A:LEU:HD13	1:110:A:LEU:HB3	5	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3807)	1:110:A:LEU:HD12	1:110:A:LEU:HB3	15	1.14
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	15	1.14
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG23	17	1.14
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	11	1.14
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	16	1.14
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	8	1.14
(2,1856)	1:22:A:ILE:HD13	1:14:A:VAL:HG21	20	1.14
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE2	5	1.14
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	4	1.14
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG21	5	1.14
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	15	1.14
(2,1561)	1:21:A:LEU:HD12	1:41:A:MET:HB2	5	1.14
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	13	1.14
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	16	1.14
(2,1549)	1:37:A:LEU:HD12	1:41:A:MET:HG2	1	1.14
(2,1452)	1:38:A:LEU:HD12	1:38:A:LEU:H	16	1.14
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	18	1.14
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	6	1.14
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	19	1.14
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	6	1.14
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD23	2	1.13
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	3	1.13
(4,440)	1:15:A:LEU:HD23	1:74:A:ILE:HB	4	1.13
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	18	1.13
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	12	1.13
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	6	1.13
(2,3704)	1:7:A:VAL:HA	1:22:A:ILE:HG22	16	1.13
(2,3501)	1:178:A:VAL:HG21	1:109:A:ILE:HA	2	1.13
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	12	1.13
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB3	19	1.13
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	18	1.13
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	13	1.13
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	4	1.13
(4,313)	1:96:A:VAL:HG13	1:145:A:SER:HA	5	1.12
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	2	1.12
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	8	1.12
(2,3807)	1:110:A:LEU:HD13	1:110:A:LEU:HB3	9	1.12
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	12	1.12
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	13	1.12
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	1	1.12
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG22	20	1.12
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD13	10	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1559)	1:21:A:LEU:HD21	1:41:A:MET:HB2	6	1.12
(2,1549)	1:37:A:LEU:HD12	1:41:A:MET:HG2	3	1.12
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	7	1.12
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	5	1.12
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	8	1.12
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	17	1.12
(4,103)	1:114:A:ILE:H	1:123:A:HIS:HA	8	1.11
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD23	6	1.11
(4,7)	1:65:A:PHE:HZ	1:37:A:LEU:HD23	12	1.11
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	16	1.11
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	19	1.11
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	10	1.11
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	8	1.11
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	13	1.11
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	14	1.11
(2,3501)	1:178:A:VAL:HG21	1:109:A:ILE:HA	19	1.11
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	20	1.11
(2,1806)	1:13:A:LEU:HD21	1:13:A:LEU:HB2	2	1.11
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	15	1.11
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	20	1.11
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	3	1.11
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	5	1.11
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	10	1.11
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	11	1.11
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	13	1.11
(4,436)	1:178:A:VAL:HG13	1:110:A:LEU:HB3	20	1.1
(4,353)	1:84:A:VAL:HB	1:87:A:GLY:HA2	20	1.1
(4,186)	1:133:A:LYS:H	2:201:A:NAD:H5N	4	1.1
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	20	1.1
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	18	1.1
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	9	1.1
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	17	1.1
(2,1851)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	17	1.1
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD11	13	1.1
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	9	1.1
(2,1806)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	10	1.1
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	12	1.1
(2,1559)	1:21:A:LEU:HD21	1:41:A:MET:HB2	11	1.1
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	2	1.1
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	9	1.1
(2,1500)	1:11:A:LEU:HD12	1:38:A:LEU:HA	6	1.1
(2,1492)	1:167:A:LEU:HD22	1:123:A:HIS:HA	18	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	19	1.1
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	8	1.1
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	16	1.1
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	17	1.09
(4,36)	1:76:A:ALA:H	1:57:A:VAL:HG23	15	1.09
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	9	1.09
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	7	1.09
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	14	1.09
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	15	1.09
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD11	7	1.09
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	2	1.09
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	11	1.09
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	1	1.09
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	3	1.09
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	9	1.09
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	18	1.09
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	12	1.08
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	20	1.08
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	3	1.08
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	4	1.08
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	12	1.08
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	19	1.08
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG21	5	1.08
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG23	10	1.08
(2,3527)	1:84:A:VAL:HG21	1:85:A:ASP:HB2	2	1.08
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	14	1.08
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	18	1.08
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	4	1.08
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	12	1.08
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	13	1.08
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG12	14	1.08
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	8	1.08
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	11	1.07
(4,436)	1:178:A:VAL:HG13	1:110:A:LEU:HB3	1	1.07
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	5	1.07
(4,378)	1:24:A:LEU:HA	1:15:A:LEU:HB2	7	1.07
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG2	20	1.07
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	6	1.07
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	4	1.07
(2,1868)	1:97:A:LEU:HD22	1:95:A:ALA:HB1	10	1.07
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	13	1.07
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	2	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	15	1.07
(2,1549)	1:37:A:LEU:HD11	1:41:A:MET:HG2	16	1.07
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	2	1.07
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	6	1.07
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	14	1.07
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	17	1.07
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	16	1.07
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD12	20	1.07
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD22	2	1.06
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	9	1.06
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	10	1.06
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	8	1.06
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	18	1.06
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	11	1.06
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD21	6	1.06
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	10	1.06
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	9	1.06
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	6	1.06
(2,3501)	1:178:A:VAL:HG22	1:109:A:ILE:HA	10	1.06
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB3	7	1.06
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	15	1.06
(2,1492)	1:167:A:LEU:HD22	1:123:A:HIS:HA	10	1.06
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	11	1.06
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	14	1.06
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	15	1.06
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	19	1.06
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	10	1.06
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	7	1.05
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	2	1.05
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	15	1.05
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	12	1.05
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	14	1.05
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	11	1.05
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	2	1.05
(2,3847)	1:41:A:MET:HE1	1:46:A:HIS:HA	7	1.05
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	2	1.05
(2,3501)	1:178:A:VAL:HG21	1:109:A:ILE:HA	5	1.05
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	16	1.05
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	20	1.05
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	18	1.05
(2,1559)	1:21:A:LEU:HD21	1:41:A:MET:HB2	4	1.05
(2,1559)	1:21:A:LEU:HD22	1:41:A:MET:HB2	9	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1549)	1:37:A:LEU:HD11	1:41:A:MET:HG2	11	1.05
(2,1549)	1:37:A:LEU:HD11	1:41:A:MET:HG2	15	1.05
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	7	1.05
(2,1492)	1:167:A:LEU:HD22	1:123:A:HIS:HA	15	1.05
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	10	1.05
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	16	1.05
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	17	1.05
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	6	1.05
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	9	1.05
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	2	1.05
(4,436)	1:178:A:VAL:HG13	1:110:A:LEU:HB3	4	1.04
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	10	1.04
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD13	16	1.04
(4,329)	1:142:A:VAL:HG21	1:106:A:PHE:HA	19	1.04
(4,184)	1:105:A:ASN:H	1:136:A:MET:H	6	1.04
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	10	1.04
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	11	1.04
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	15	1.04
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	17	1.04
(2,3500)	1:144:A:LEU:HD23	1:145:A:SER:HB2	6	1.04
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	17	1.04
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	17	1.04
(2,1851)	1:56:A:ILE:HD12	1:11:A:LEU:HD11	12	1.04
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD11	1	1.04
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	1	1.04
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	4	1.04
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	5	1.04
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	20	1.04
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	4	1.04
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	10	1.04
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	1	1.04
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	7	1.04
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	6	1.04
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	5	1.04
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD13	6	1.03
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD12	14	1.03
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	15	1.03
(2,3847)	1:41:A:MET:HE2	1:46:A:HIS:HA	8	1.03
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	8	1.03
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	17	1.03
(2,1807)	1:151:A:MET:HE3	1:174:A:GLU:HG2	14	1.03
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	6	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1500)	1:11:A:LEU:HD12	1:38:A:LEU:HA	10	1.03
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	18	1.03
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	11	1.03
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	4	1.03
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	14	1.03
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	18	1.03
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	6	1.03
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	16	1.03
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	1	1.03
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	2	1.03
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	12	1.03
(4,415)	1:19:A:PRO:HB2	1:36:A:GLU:HG2	8	1.02
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD13	11	1.02
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	2	1.02
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	13	1.02
(2,3847)	1:41:A:MET:HE2	1:46:A:HIS:HA	6	1.02
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	9	1.02
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	18	1.02
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	3	1.02
(2,1868)	1:97:A:LEU:HD23	1:95:A:ALA:HB2	6	1.02
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	17	1.02
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	9	1.02
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	13	1.02
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	10	1.02
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	13	1.02
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	17	1.02
(2,1441)	1:7:A:VAL:HG11	1:7:A:VAL:H	5	1.02
(2,1441)	1:7:A:VAL:HG13	1:7:A:VAL:H	20	1.02
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	1	1.02
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	2	1.02
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	11	1.02
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	19	1.02
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	20	1.02
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	7	1.02
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	8	1.02
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	11	1.02
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	12	1.02
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	14	1.02
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	18	1.02
(4,440)	1:15:A:LEU:HD23	1:13:A:LEU:HB2	5	1.01
(4,436)	1:178:A:VAL:HG11	1:110:A:LEU:HB3	7	1.01
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	2	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD21	5	1.01
(2,3830)	1:97:A:LEU:HD21	1:95:A:ALA:HB1	1	1.01
(2,3265)	1:84:A:VAL:HG12	1:84:A:VAL:H	6	1.01
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	15	1.01
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG23	17	1.01
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	3	1.01
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE2	8	1.01
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	8	1.01
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	3	1.01
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	9	1.01
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	12	1.01
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG23	14	1.01
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	2	1.01
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	10	1.01
(2,1549)	1:37:A:LEU:HD11	1:41:A:MET:HG2	12	1.01
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	5	1.01
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	3	1.01
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	8	1.01
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	17	1.01
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	4	1.01
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	13	1.01
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	17	1.01
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	8	1.01
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	3	1.0
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD21	11	1.0
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	15	1.0
(2,1851)	1:56:A:ILE:HD12	1:11:A:LEU:HD11	4	1.0
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	18	1.0
(2,1843)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	7	1.0
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	10	1.0
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	14	1.0
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	7	1.0
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	2	1.0
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	3	1.0
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	5	1.0
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	7	1.0
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	10	1.0
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	11	1.0
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	12	1.0
(2,1217)	1:177:A:LYS:HE2	1:177:A:LYS:HB2	16	1.0
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	17	1.0
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	15	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	2	1.0
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	10	1.0
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	15	1.0
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD21	9	0.99
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	8	0.99
(4,313)	1:96:A:VAL:HG13	1:145:A:SER:HA	7	0.99
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	12	0.99
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD13	19	0.99
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	20	0.99
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	9	0.99
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD12	18	0.99
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	18	0.99
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	8	0.99
(2,1495)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	12	0.99
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	2	0.99
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	4	0.99
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	16	0.99
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	19	0.99
(2,1291)	1:84:A:VAL:HG11	1:84:A:VAL:H	11	0.99
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	1	0.99
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	2	0.99
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	4	0.99
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	9	0.99
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	9	0.99
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	19	0.99
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	1	0.99
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	2	0.99
(2,21)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	7	0.99
(4,458)	1:50:A:MET:HE2	1:50:A:MET:HA	13	0.98
(4,320)	1:151:A:MET:HE3	1:147:A:ASP:HB2	7	0.98
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	8	0.98
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	19	0.98
(2,3265)	1:84:A:VAL:HG12	1:84:A:VAL:H	20	0.98
(2,1830)	1:34:A:VAL:HG12	1:50:A:MET:HE1	18	0.98
(2,1495)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	11	0.98
(2,1467)	1:14:A:VAL:HG13	1:10:A:PHE:HD1	5	0.98
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	1	0.98
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	6	0.98
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	8	0.98
(2,1444)	1:56:A:ILE:HG23	1:56:A:ILE:H	9	0.98
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	20	0.98
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	12	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	12	0.98
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	19	0.98
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	14	0.98
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	10	0.97
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	12	0.97
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	15	0.97
(4,301)	1:97:A:LEU:HD23	1:175:A:PHE:HB2	17	0.97
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	4	0.97
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	20	0.97
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	15	0.97
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	19	0.97
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	13	0.97
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	12	0.97
(2,3527)	1:84:A:VAL:HG21	1:85:A:ASP:HB2	15	0.97
(2,1830)	1:34:A:VAL:HG12	1:50:A:MET:HE2	1	0.97
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	17	0.97
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	18	0.97
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	16	0.97
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	5	0.97
(2,1559)	1:21:A:LEU:HD23	1:41:A:MET:HB2	19	0.97
(2,1554)	1:38:A:LEU:HD21	1:50:A:MET:HG2	12	0.97
(2,1549)	1:37:A:LEU:HD13	1:41:A:MET:HG2	2	0.97
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	4	0.97
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	8	0.97
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	15	0.97
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	16	0.97
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	6	0.97
(2,1444)	1:56:A:ILE:HG21	1:56:A:ILE:H	14	0.97
(2,1444)	1:56:A:ILE:HG22	1:56:A:ILE:H	15	0.97
(2,1291)	1:84:A:VAL:HG13	1:84:A:VAL:H	18	0.97
(2,1260)	1:142:A:VAL:HG21	1:178:A:VAL:HG11	9	0.97
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	7	0.97
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	13	0.97
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	16	0.97
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	7	0.97
(2,21)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	13	0.97
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD22	5	0.96
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	6	0.96
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD12	15	0.96
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	6	0.96
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	10	0.96
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	14	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,378)	1:24:A:LEU:HA	1:15:A:LEU:HB2	20	0.96
(4,313)	1:143:A:VAL:HG12	1:145:A:SER:HA	13	0.96
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	14	0.96
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	12	0.96
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	2	0.96
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	4	0.96
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	4	0.96
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	8	0.96
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	4	0.96
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	20	0.96
(2,3771)	1:13:A:LEU:HD21	1:13:A:LEU:HB2	12	0.96
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	2	0.96
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	5	0.96
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD23	5	0.96
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE2	6	0.96
(2,1742)	1:110:A:LEU:HD11	1:173:A:ALA:HA	5	0.96
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	7	0.96
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	12	0.96
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	3	0.96
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	17	0.96
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	13	0.96
(2,1495)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	1	0.96
(2,1291)	1:84:A:VAL:HG11	1:84:A:VAL:H	14	0.96
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	18	0.96
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	5	0.96
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	3	0.96
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	6	0.96
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	11	0.96
(2,339)	1:108:A:LEU:HD21	1:108:A:LEU:H	18	0.96
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD23	8	0.95
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD21	13	0.95
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	5	0.95
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	8	0.95
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	19	0.95
(4,349)	1:39:A:ALA:HB1	1:42:A:LYS:HE2	20	0.95
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	1	0.95
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	20	0.95
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	1	0.95
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	11	0.95
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	12	0.95
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	1	0.95
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	12	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG23	14	0.95
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	18	0.95
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	10	0.95
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	11	0.95
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD21	2	0.95
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	6	0.95
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD21	15	0.95
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	20	0.95
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE2	4	0.95
(2,1527)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	12	0.95
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	5	0.95
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	10	0.95
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	9	0.95
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	19	0.95
(2,1495)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	5	0.95
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	11	0.95
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	2	0.95
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	4	0.95
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	9	0.95
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	18	0.95
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	20	0.95
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	18	0.95
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG13	12	0.95
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	14	0.94
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD13	19	0.94
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	11	0.94
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	16	0.94
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD13	14	0.94
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	6	0.94
(4,292)	1:122:A:VAL:HG21	1:118:A:SER:H	19	0.94
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	11	0.94
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	3	0.94
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD13	8	0.94
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	17	0.94
(2,3847)	1:41:A:MET:HE2	1:46:A:HIS:HA	18	0.94
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	17	0.94
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD21	4	0.94
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	3	0.94
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	9	0.94
(2,3265)	1:84:A:VAL:HG13	1:84:A:VAL:H	1	0.94
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	8	0.94
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD23	13	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	16	0.94
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	19	0.94
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	11	0.94
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	19	0.94
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	17	0.94
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	9	0.94
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	1	0.94
(2,816)	1:53:A:LEU:HD22	1:53:A:LEU:H	6	0.94
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	10	0.94
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	19	0.94
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	10	0.94
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	7	0.94
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD12	5	0.93
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD22	18	0.93
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	7	0.93
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	16	0.93
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	16	0.93
(4,329)	1:142:A:VAL:HG21	1:106:A:PHE:HA	11	0.93
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	1	0.93
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD23	13	0.93
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	19	0.93
(4,9)	1:10:A:PHE:HD1	1:7:A:VAL:HG11	5	0.93
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD22	3	0.93
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD21	13	0.93
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	17	0.93
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	7	0.93
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD21	18	0.93
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG23	16	0.93
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	3	0.93
(2,1851)	1:56:A:ILE:HD12	1:11:A:LEU:HD11	11	0.93
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	13	0.93
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	15	0.93
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	16	0.93
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE2	10	0.93
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	14	0.93
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	19	0.93
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG23	18	0.93
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	5	0.93
(2,1549)	1:37:A:LEU:HD12	1:41:A:MET:HG2	9	0.93
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	4	0.93
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	13	0.93
(2,1236)	1:151:A:MET:HE1	1:156:A:PHE:HZ	17	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	5	0.93
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	10	0.93
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	14	0.93
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	7	0.93
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	11	0.93
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	5	0.93
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	10	0.93
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	7	0.92
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD13	20	0.92
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	1	0.92
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	3	0.92
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	8	0.92
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	13	0.92
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	18	0.92
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	15	0.92
(4,300)	1:97:A:LEU:HD21	1:175:A:PHE:HB3	9	0.92
(4,244)	1:51:A:GLU:HG2	1:67:A:PHE:HD1	5	0.92
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	19	0.92
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	12	0.92
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	15	0.92
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	14	0.92
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	8	0.92
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	1	0.92
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	5	0.92
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD22	10	0.92
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	18	0.92
(2,3847)	1:41:A:MET:HE3	1:46:A:HIS:HA	20	0.92
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD13	14	0.92
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	3	0.92
(2,3807)	1:110:A:LEU:HD11	1:110:A:LEU:HB3	7	0.92
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	20	0.92
(2,3527)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	20	0.92
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	4	0.92
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD23	7	0.92
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	9	0.92
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	12	0.92
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	17	0.92
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	19	0.92
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	11	0.92
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD12	12	0.92
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	17	0.92
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	18	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	20	0.92
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	4	0.92
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	17	0.92
(2,1549)	1:37:A:LEU:HD11	1:41:A:MET:HG2	4	0.92
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	1	0.92
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	5	0.92
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	17	0.92
(2,1468)	1:22:A:ILE:HG21	1:10:A:PHE:HZ	16	0.92
(2,1107)	1:118:A:SER:H	2:201:A:NAD:H51A	1	0.92
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	13	0.92
(2,816)	1:53:A:LEU:HD22	1:53:A:LEU:H	16	0.92
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	3	0.92
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	18	0.92
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	19	0.92
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD23	10	0.91
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	4	0.91
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	10	0.91
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	17	0.91
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	19	0.91
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	18	0.91
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	20	0.91
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	13	0.91
(4,202)	1:173:A:ALA:HA	1:145:A:SER:HB2	12	0.91
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	15	0.91
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	18	0.91
(2,3837)	1:5:A:VAL:HG23	1:5:A:VAL:HA	11	0.91
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE2	5	0.91
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	5	0.91
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	6	0.91
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	16	0.91
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	19	0.91
(2,3508)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	1	0.91
(2,3462)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	12	0.91
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	1	0.91
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	9	0.91
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	18	0.91
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	7	0.91
(2,1865)	1:109:A:ILE:HD11	1:144:A:LEU:HD11	12	0.91
(2,1851)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	1	0.91
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	6	0.91
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	19	0.91
(2,1807)	1:151:A:MET:HE2	1:174:A:GLU:HG2	20	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	10	0.91
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD21	13	0.91
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	14	0.91
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	16	0.91
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	6	0.91
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	19	0.91
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	20	0.91
(2,1495)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	7	0.91
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	18	0.91
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	18	0.91
(2,1291)	1:84:A:VAL:HG12	1:84:A:VAL:H	8	0.91
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	11	0.91
(2,339)	1:108:A:LEU:HD21	1:108:A:LEU:H	19	0.91
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	13	0.91
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	15	0.91
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	18	0.91
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	4	0.91
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	7	0.91
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	11	0.91
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	12	0.91
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	13	0.91
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	19	0.91
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	15	0.91
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	4	0.91
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	9	0.91
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD22	3	0.9
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	14	0.9
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	15	0.9
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	20	0.9
(4,292)	1:122:A:VAL:HG23	1:118:A:SER:H	1	0.9
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	3	0.9
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	4	0.9
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	16	0.9
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	19	0.9
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	7	0.9
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	13	0.9
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	3	0.9
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	12	0.9
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD22	2	0.9
(2,3837)	1:5:A:VAL:HG23	1:5:A:VAL:HA	10	0.9
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	3	0.9
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	7	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3771)	1:13:A:LEU:HD23	1:13:A:LEU:HB2	8	0.9
(2,3771)	1:13:A:LEU:HD23	1:13:A:LEU:HB2	13	0.9
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	14	0.9
(2,3462)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	11	0.9
(2,2266)	1:153:A:ASP:H	1:95:A:ALA:HB1	5	0.9
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	13	0.9
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	10	0.9
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD21	14	0.9
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	4	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD22	2	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD22	3	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	7	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD21	9	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	16	0.9
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	18	0.9
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	11	0.9
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	17	0.9
(2,1535)	1:22:A:ILE:HG22	1:44:A:LYS:HE3	12	0.9
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	9	0.9
(2,1495)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	14	0.9
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	20	0.9
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	16	0.9
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	12	0.9
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	6	0.9
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	8	0.9
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	9	0.9
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	17	0.9
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	8	0.9
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	5	0.9
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	9	0.89
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	18	0.89
(4,378)	1:24:A:LEU:HA	1:21:A:LEU:HG	17	0.89
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	9	0.89
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	7	0.89
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	20	0.89
(4,204)	1:173:A:ALA:HB1	1:111:A:LYS:HG3	2	0.89
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	2	0.89
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	11	0.89
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	10	0.89
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	7	0.89
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	1	0.89
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE1	14	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	1	0.89
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	4	0.89
(2,3771)	1:13:A:LEU:HD21	1:13:A:LEU:HB2	11	0.89
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	7	0.89
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	6	0.89
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	3	0.89
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB2	11	0.89
(2,1865)	1:109:A:ILE:HD11	1:144:A:LEU:HD13	19	0.89
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	20	0.89
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	10	0.89
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	8	0.89
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	8	0.89
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	17	0.89
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	19	0.89
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE2	11	0.89
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	1	0.89
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	12	0.89
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	15	0.89
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	8	0.89
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	18	0.89
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	2	0.89
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	7	0.89
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	18	0.89
(2,1490)	1:167:A:LEU:HD11	1:166:A:TRP:HA	17	0.89
(2,1291)	1:84:A:VAL:HG11	1:84:A:VAL:H	10	0.89
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	15	0.89
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	8	0.89
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	1	0.89
(2,816)	1:53:A:LEU:HD21	1:53:A:LEU:H	2	0.89
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	2	0.89
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	10	0.89
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	14	0.89
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	15	0.89
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	16	0.89
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	18	0.89
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	12	0.89
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD22	12	0.88
(4,397)	1:56:A:ILE:HA	1:54:A:LYS:HB2	12	0.88
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD13	3	0.88
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	13	0.88
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	7	0.88
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	14	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3837)	1:5:A:VAL:HG23	1:5:A:VAL:HA	5	0.88
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	18	0.88
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	19	0.88
(2,3508)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	3	0.88
(2,3421)	1:38:A:LEU:HD12	1:38:A:LEU:H	6	0.88
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	4	0.88
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD21	11	0.88
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD23	20	0.88
(2,1851)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	9	0.88
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	1	0.88
(2,1845)	1:176:A:ILE:HB	1:110:A:LEU:HD11	9	0.88
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	18	0.88
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD21	6	0.88
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	11	0.88
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD21	20	0.88
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	3	0.88
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	14	0.88
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	16	0.88
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	13	0.88
(2,1291)	1:84:A:VAL:HG11	1:84:A:VAL:H	9	0.88
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	16	0.88
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	3	0.88
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	4	0.88
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	10	0.88
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	13	0.88
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	9	0.88
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	19	0.88
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	11	0.88
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD13	9	0.87
(4,292)	1:122:A:VAL:HG22	1:118:A:SER:H	10	0.87
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	13	0.87
(4,103)	1:114:A:ILE:H	1:123:A:HIS:HA	20	0.87
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	1	0.87
(2,3772)	1:151:A:MET:HE3	1:174:A:GLU:HG2	14	0.87
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG23	18	0.87
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	17	0.87
(2,3462)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	1	0.87
(2,3462)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	5	0.87
(2,3421)	1:38:A:LEU:HD12	1:38:A:LEU:H	1	0.87
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	9	0.87
(2,3421)	1:38:A:LEU:HD11	1:38:A:LEU:H	19	0.87
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	20	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	8	0.87
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	15	0.87
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD22	3	0.87
(2,1851)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	7	0.87
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	15	0.87
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	13	0.87
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	12	0.87
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD23	8	0.87
(2,1554)	1:38:A:LEU:HD21	1:50:A:MET:HG2	3	0.87
(2,1529)	1:144:A:LEU:HD23	1:145:A:SER:HB2	6	0.87
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	12	0.87
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	2	0.87
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	17	0.87
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD23	12	0.86
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	13	0.86
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	14	0.86
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	10	0.86
(4,320)	1:151:A:MET:HE1	1:147:A:ASP:HB2	20	0.86
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	1	0.86
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	5	0.86
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	5	0.86
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	1	0.86
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	6	0.86
(4,166)	1:171:A:VAL:H	1:168:A:ILE:HG13	14	0.86
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	10	0.86
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	15	0.86
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD13	10	0.86
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	2	0.86
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	4	0.86
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	16	0.86
(2,3421)	1:38:A:LEU:HD12	1:38:A:LEU:H	4	0.86
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	10	0.86
(2,3421)	1:38:A:LEU:HD12	1:38:A:LEU:H	14	0.86
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	15	0.86
(2,1868)	1:97:A:LEU:HD21	1:95:A:ALA:HB1	1	0.86
(2,1865)	1:109:A:ILE:HD11	1:144:A:LEU:HD13	3	0.86
(2,1851)	1:56:A:ILE:HD11	1:11:A:LEU:HD13	6	0.86
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	3	0.86
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	12	0.86
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	17	0.86
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	11	0.86
(2,1500)	1:11:A:LEU:HD12	1:38:A:LEU:HA	14	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	15	0.86
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	2	0.86
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	3	0.86
(2,1492)	1:167:A:LEU:HD23	1:123:A:HIS:HA	9	0.86
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	7	0.86
(2,1473)	1:110:A:LEU:HD11	1:110:A:LEU:H	13	0.86
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	1	0.86
(2,1291)	1:84:A:VAL:HG11	1:84:A:VAL:H	12	0.86
(2,1217)	1:177:A:LYS:HE2	1:177:A:LYS:HB2	12	0.86
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	11	0.86
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	18	0.86
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD13	5	0.85
(4,332)	1:37:A:LEU:HD13	1:41:A:MET:HB2	18	0.85
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	2	0.85
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	18	0.85
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	5	0.85
(4,6)	1:65:A:PHE:HE1	1:74:A:ILE:HG23	1	0.85
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD21	6	0.85
(2,3771)	1:13:A:LEU:HD21	1:13:A:LEU:HB2	2	0.85
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	9	0.85
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	10	0.85
(2,3771)	1:13:A:LEU:HD22	1:13:A:LEU:HB2	15	0.85
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	12	0.85
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	7	0.85
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	11	0.85
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	2	0.85
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	3	0.85
(2,3421)	1:38:A:LEU:HD12	1:38:A:LEU:H	17	0.85
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	2	0.85
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	10	0.85
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE1	14	0.85
(2,1807)	1:151:A:MET:HE2	1:174:A:GLU:HG2	2	0.85
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	4	0.85
(2,1549)	1:37:A:LEU:HD12	1:41:A:MET:HG2	19	0.85
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	1	0.85
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	4	0.85
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	4	0.85
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	15	0.85
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	11	0.85
(2,816)	1:53:A:LEU:HD23	1:53:A:LEU:H	15	0.85
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	5	0.85
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD22	6	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,450)	1:97:A:LEU:HD21	1:124:A:LEU:HD22	10	0.84
(4,378)	1:24:A:LEU:HA	1:15:A:LEU:HB2	3	0.84
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	12	0.84
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	9	0.84
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	16	0.84
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	2	0.84
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	16	0.84
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	4	0.84
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	10	0.84
(2,3813)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	17	0.84
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	11	0.84
(2,3527)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	6	0.84
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	17	0.84
(2,3421)	1:38:A:LEU:HD11	1:38:A:LEU:H	7	0.84
(2,3421)	1:38:A:LEU:HD12	1:38:A:LEU:H	11	0.84
(2,3421)	1:38:A:LEU:HD11	1:38:A:LEU:H	18	0.84
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	14	0.84
(2,1899)	1:24:A:LEU:HA	1:24:A:LEU:HD21	1	0.84
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	2	0.84
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE1	14	0.84
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	18	0.84
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	20	0.84
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	16	0.84
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	11	0.84
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	15	0.84
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	16	0.84
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	17	0.84
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	14	0.84
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	17	0.84
(2,1291)	1:84:A:VAL:HG13	1:84:A:VAL:H	3	0.84
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	12	0.84
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	2	0.84
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	14	0.84
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	6	0.84
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	20	0.83
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	5	0.83
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	17	0.83
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	11	0.83
(4,222)	1:57:A:VAL:HG22	1:74:A:ILE:HB	17	0.83
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	20	0.83
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	9	0.83
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	16	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	14	0.83
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	17	0.83
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD21	9	0.83
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	17	0.83
(2,3964)	1:123:A:HIS:HB3	2:201:A:NAD:H6N	13	0.83
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	15	0.83
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	15	0.83
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	17	0.83
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	5	0.83
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	8	0.83
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	13	0.83
(2,1869)	1:97:A:LEU:HD23	1:96:A:VAL:HB	2	0.83
(2,1865)	1:109:A:ILE:HD11	1:144:A:LEU:HD13	16	0.83
(2,1856)	1:22:A:ILE:HD12	1:14:A:VAL:HG23	5	0.83
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	19	0.83
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	20	0.83
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	2	0.83
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	6	0.83
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	9	0.83
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	2	0.83
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG11	17	0.83
(2,1610)	1:13:A:LEU:HG	1:17:A:HIS:HB2	5	0.83
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	6	0.83
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	2	0.83
(2,1549)	1:37:A:LEU:HD13	1:41:A:MET:HG2	17	0.83
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	17	0.83
(2,1490)	1:167:A:LEU:HD13	1:166:A:TRP:HA	4	0.83
(2,1473)	1:110:A:LEU:HD11	1:110:A:LEU:H	11	0.83
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	2	0.83
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	6	0.83
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	15	0.83
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	3	0.83
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	11	0.83
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	16	0.83
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	13	0.83
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	17	0.83
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	6	0.83
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	17	0.83
(4,458)	1:50:A:MET:HE2	1:51:A:GLU:HA	14	0.82
(4,450)	1:97:A:LEU:HD21	1:124:A:LEU:HD23	4	0.82
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	6	0.82
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	11	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB2	9	0.82
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	20	0.82
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	10	0.82
(4,204)	1:173:A:ALA:HB1	1:111:A:LYS:HG2	6	0.82
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	19	0.82
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	9	0.82
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	14	0.82
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	12	0.82
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD11	11	0.82
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	4	0.82
(4,6)	1:65:A:PHE:HE1	1:74:A:ILE:HG23	3	0.82
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	19	0.82
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	16	0.82
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	8	0.82
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	8	0.82
(2,3462)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	7	0.82
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	20	0.82
(2,3421)	1:38:A:LEU:HD13	1:38:A:LEU:H	12	0.82
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	19	0.82
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	16	0.82
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	8	0.82
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	14	0.82
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	7	0.82
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	11	0.82
(2,1845)	1:176:A:ILE:HB	1:110:A:LEU:HD11	14	0.82
(2,1845)	1:110:A:LEU:HD13	1:176:A:ILE:HB	15	0.82
(2,1794)	1:117:A:MET:HE3	1:117:A:MET:HB2	12	0.82
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	5	0.82
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	11	0.82
(2,1549)	1:37:A:LEU:HD12	1:41:A:MET:HG2	13	0.82
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	16	0.82
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	17	0.82
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	10	0.82
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	12	0.82
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	18	0.82
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	19	0.82
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	7	0.82
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	5	0.82
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	8	0.82
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	12	0.82
(2,954)	1:56:A:ILE:HG21	1:57:A:VAL:H	14	0.82
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	20	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	1	0.82
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	6	0.82
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	8	0.82
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	14	0.82
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	9	0.82
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	1	0.82
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD22	8	0.81
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD22	17	0.81
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	2	0.81
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	17	0.81
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	19	0.81
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	3	0.81
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	14	0.81
(4,320)	1:151:A:MET:HE1	1:147:A:ASP:HB2	14	0.81
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	6	0.81
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	11	0.81
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	17	0.81
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	6	0.81
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	5	0.81
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	2	0.81
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	11	0.81
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	15	0.81
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	20	0.81
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	16	0.81
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	20	0.81
(2,3847)	1:41:A:MET:HE3	1:46:A:HIS:HA	17	0.81
(2,3784)	1:37:A:LEU:HD11	1:41:A:MET:HE1	12	0.81
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	14	0.81
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	4	0.81
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	2	0.81
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	19	0.81
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	2	0.81
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	15	0.81
(2,3462)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	14	0.81
(2,2348)	1:156:A:PHE:H	1:168:A:ILE:HD11	5	0.81
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	5	0.81
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	14	0.81
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	4	0.81
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	4	0.81
(2,1807)	1:151:A:MET:HE3	1:174:A:GLU:HG2	7	0.81
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	4	0.81
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	8	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	10	0.81
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	15	0.81
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	17	0.81
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG12	19	0.81
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	10	0.81
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	15	0.81
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	3	0.81
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	5	0.81
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	9	0.81
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	11	0.81
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	15	0.81
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	20	0.81
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	7	0.81
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	7	0.81
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	7	0.81
(2,954)	1:56:A:ILE:HG23	1:57:A:VAL:H	9	0.81
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	16	0.81
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	17	0.81
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	14	0.81
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	16	0.8
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	9	0.8
(4,313)	1:96:A:VAL:HG13	1:145:A:SER:HA	6	0.8
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	15	0.8
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD11	15	0.8
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD23	4	0.8
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	1	0.8
(2,3847)	1:41:A:MET:HE3	1:46:A:HIS:HA	16	0.8
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	13	0.8
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	17	0.8
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	19	0.8
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	17	0.8
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	11	0.8
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	7	0.8
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	7	0.8
(2,2221)	1:168:A:ILE:HD12	1:157:A:ASP:H	17	0.8
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	17	0.8
(2,1865)	1:109:A:ILE:HD11	1:144:A:LEU:HD13	10	0.8
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	10	0.8
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	1	0.8
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	13	0.8
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	16	0.8
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	11	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	18	0.8
(2,1554)	1:38:A:LEU:HD21	1:50:A:MET:HG2	14	0.8
(2,1473)	1:110:A:LEU:HD13	1:110:A:LEU:H	9	0.8
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	14	0.8
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	7	0.8
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	8	0.8
(2,1434)	1:38:A:LEU:HD23	1:39:A:ALA:H	13	0.8
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	13	0.8
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	17	0.8
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	19	0.8
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	4	0.8
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	6	0.8
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	7	0.8
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD23	7	0.79
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD21	15	0.79
(4,332)	1:37:A:LEU:HD13	1:41:A:MET:HB2	6	0.79
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	18	0.79
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	15	0.79
(4,204)	1:173:A:ALA:HB1	1:111:A:LYS:HG3	16	0.79
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	19	0.79
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	20	0.79
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	16	0.79
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	2	0.79
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	16	0.79
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	4	0.79
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	6	0.79
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	19	0.79
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	20	0.79
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	9	0.79
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	17	0.79
(2,3500)	1:144:A:LEU:HD22	1:145:A:SER:HB2	9	0.79
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	3	0.79
(2,3421)	1:38:A:LEU:HD12	1:38:A:LEU:H	16	0.79
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	4	0.79
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	7	0.79
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	8	0.79
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	9	0.79
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	11	0.79
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	12	0.79
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	13	0.79
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	19	0.79
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	3	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	9	0.79
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	16	0.79
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG23	8	0.79
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	10	0.79
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	16	0.79
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	3	0.79
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	9	0.79
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	1	0.79
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	3	0.79
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG12	14	0.79
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	9	0.79
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	6	0.79
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	17	0.79
(2,1236)	1:151:A:MET:HE3	1:156:A:PHE:HZ	5	0.79
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	12	0.79
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	6	0.79
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	11	0.79
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	9	0.79
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	15	0.79
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	17	0.79
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	8	0.79
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD23	3	0.78
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD22	15	0.78
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	16	0.78
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	12	0.78
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	16	0.78
(4,204)	1:173:A:ALA:HB3	1:111:A:LYS:HG3	14	0.78
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	3	0.78
(4,184)	1:105:A:ASN:H	1:136:A:MET:H	19	0.78
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	6	0.78
(4,160)	1:22:A:ILE:HD13	1:22:A:ILE:H	20	0.78
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	16	0.78
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE2	8	0.78
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	3	0.78
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	16	0.78
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	4	0.78
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	2	0.78
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	3	0.78
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD23	13	0.78
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	6	0.78
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	2	0.78
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	6	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	10	0.78
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	14	0.78
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	16	0.78
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	17	0.78
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	18	0.78
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	11	0.78
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	14	0.78
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	9	0.78
(2,1847)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	20	0.78
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	2	0.78
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	6	0.78
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	2	0.78
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	6	0.78
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	7	0.78
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG11	11	0.78
(2,1495)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	18	0.78
(2,1492)	1:167:A:LEU:HD22	1:123:A:HIS:HA	1	0.78
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	12	0.78
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	13	0.78
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	4	0.78
(2,1157)	1:144:A:LEU:HD21	1:106:A:PHE:HD1	13	0.78
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	1	0.78
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	2	0.78
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	3	0.78
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	15	0.78
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	19	0.78
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	3	0.78
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	16	0.78
(2,300)	1:153:A:ASP:H	1:95:A:ALA:HB1	5	0.78
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG11	8	0.78
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	15	0.78
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	8	0.78
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	15	0.78
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD22	1	0.77
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	12	0.77
(4,378)	1:24:A:LEU:HA	1:15:A:LEU:HB2	1	0.77
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	3	0.77
(4,311)	1:96:A:VAL:HG11	1:94:A:PRO:HA	13	0.77
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	17	0.77
(4,283)	1:143:A:VAL:HG12	1:143:A:VAL:H	3	0.77
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	20	0.77
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	11	0.77
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	15	0.77
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	9	0.77
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	11	0.77
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	14	0.77
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	4	0.77
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	5	0.77
(2,3813)	1:56:A:ILE:HD12	1:11:A:LEU:HD11	12	0.77
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE1	5	0.77
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	14	0.77
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	20	0.77
(2,3416)	1:143:A:VAL:HG13	1:143:A:VAL:H	15	0.77
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	18	0.77
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	15	0.77
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	8	0.77
(2,1875)	1:5:A:VAL:HG23	1:5:A:VAL:HA	11	0.77
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	7	0.77
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	15	0.77
(2,1740)	1:11:A:LEU:HA	1:37:A:LEU:HD21	5	0.77
(2,1554)	1:38:A:LEU:HD21	1:50:A:MET:HG2	20	0.77
(2,1549)	1:37:A:LEU:HD12	1:41:A:MET:HG2	20	0.77
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	20	0.77
(2,1473)	1:110:A:LEU:HD13	1:110:A:LEU:H	5	0.77
(2,1473)	1:110:A:LEU:HD11	1:110:A:LEU:H	10	0.77
(2,1388)	1:41:A:MET:HE2	1:41:A:MET:H	5	0.77
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	20	0.77
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	8	0.77
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	20	0.77
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	7	0.77
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	3	0.77
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	13	0.77
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	19	0.77
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	11	0.77
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	5	0.77
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD21	9	0.76
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD23	13	0.76
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD22	20	0.76
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	16	0.76
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD21	1	0.76
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	14	0.76
(4,332)	1:37:A:LEU:HD12	1:41:A:MET:HB2	7	0.76
(4,204)	1:173:A:ALA:HB1	1:111:A:LYS:HG3	17	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	2	0.76
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	3	0.76
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	7	0.76
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	8	0.76
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	17	0.76
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	17	0.76
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	19	0.76
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	7	0.76
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	13	0.76
(4,6)	1:65:A:PHE:HE1	1:74:A:ILE:HG23	20	0.76
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	3	0.76
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE1	16	0.76
(2,3784)	1:37:A:LEU:HD11	1:41:A:MET:HE1	17	0.76
(2,3772)	1:151:A:MET:HE2	1:174:A:GLU:HG2	20	0.76
(2,3657)	1:63:A:LYS:HG2	1:62:A:LYS:HA	6	0.76
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	17	0.76
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	8	0.76
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	13	0.76
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	16	0.76
(2,3524)	1:13:A:LEU:HD11	1:18:A:ASN:HB2	12	0.76
(2,3466)	1:97:A:LEU:HD22	1:166:A:TRP:HB2	9	0.76
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	10	0.76
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	7	0.76
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	14	0.76
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	6	0.76
(2,1875)	1:5:A:VAL:HG23	1:5:A:VAL:HA	10	0.76
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	1	0.76
(2,1845)	1:176:A:ILE:HB	1:110:A:LEU:HD11	5	0.76
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	11	0.76
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	10	0.76
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	13	0.76
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	12	0.76
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	19	0.76
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	4	0.76
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	6	0.76
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	10	0.76
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	11	0.76
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	13	0.76
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	1	0.76
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	3	0.76
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	5	0.76
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	10	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	15	0.76
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	16	0.76
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	15	0.76
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	2	0.76
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	18	0.76
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	7	0.76
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	16	0.76
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	9	0.76
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	6	0.76
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	9	0.76
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	16	0.76
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	17	0.76
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	20	0.76
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD23	19	0.75
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	12	0.75
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	4	0.75
(4,332)	1:37:A:LEU:HD13	1:41:A:MET:HB2	8	0.75
(4,320)	1:151:A:MET:HE1	1:147:A:ASP:HB2	13	0.75
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	13	0.75
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	12	0.75
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	18	0.75
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD13	12	0.75
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	14	0.75
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD11	16	0.75
(4,160)	1:22:A:ILE:HD11	1:22:A:ILE:H	3	0.75
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	8	0.75
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	18	0.75
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	6	0.75
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	17	0.75
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	20	0.75
(2,3790)	1:34:A:VAL:HG12	1:50:A:MET:HE1	18	0.75
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	13	0.75
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	15	0.75
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	10	0.75
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	8	0.75
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	9	0.75
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	20	0.75
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	17	0.75
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	12	0.75
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	10	0.75
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	12	0.75
(2,1884)	1:41:A:MET:HE1	1:46:A:HIS:HA	7	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1875)	1:5:A:VAL:HG23	1:5:A:VAL:HA	5	0.75
(2,1871)	1:97:A:LEU:HD22	1:151:A:MET:HG3	2	0.75
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	9	0.75
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	15	0.75
(2,1823)	1:37:A:LEU:HD11	1:41:A:MET:HE1	12	0.75
(2,1790)	1:144:A:LEU:HG	1:178:A:VAL:HG12	7	0.75
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	6	0.75
(2,1742)	1:110:A:LEU:HD11	1:173:A:ALA:HA	14	0.75
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	5	0.75
(2,1522)	1:142:A:VAL:HG23	1:178:A:VAL:HA	1	0.75
(2,1495)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	4	0.75
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	13	0.75
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	15	0.75
(2,1361)	1:177:A:LYS:HE2	1:147:A:ASP:H	2	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	2	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	6	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	7	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	8	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	11	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	13	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	17	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	18	0.75
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	19	0.75
(2,288)	1:6:A:LYS:H	1:5:A:VAL:HG12	9	0.75
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	19	0.75
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	7	0.75
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	4	0.75
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	7	0.75
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	10	0.75
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	12	0.75
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	13	0.75
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	14	0.75
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	19	0.75
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD23	18	0.74
(4,431)	1:13:A:LEU:HG	1:13:A:LEU:HD12	10	0.74
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	15	0.74
(4,402)	1:42:A:LYS:HG3	1:42:A:LYS:HE3	14	0.74
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	1	0.74
(4,259)	1:117:A:MET:HE2	2:201:A:NAD:H2A	4	0.74
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	19	0.74
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	10	0.74
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	9	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	4	0.74
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	4	0.74
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	4	0.74
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	20	0.74
(2,3813)	1:56:A:ILE:HD12	1:11:A:LEU:HD11	4	0.74
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	18	0.74
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	4	0.74
(2,3790)	1:34:A:VAL:HG12	1:50:A:MET:HE2	1	0.74
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	15	0.74
(2,3527)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	1	0.74
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	16	0.74
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	16	0.74
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	6	0.74
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	8	0.74
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	17	0.74
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	4	0.74
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	5	0.74
(2,1884)	1:41:A:MET:HE2	1:46:A:HIS:HA	8	0.74
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	2	0.74
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	16	0.74
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	3	0.74
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	4	0.74
(2,1742)	1:110:A:LEU:HD13	1:173:A:ALA:HA	15	0.74
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	18	0.74
(2,1610)	1:13:A:LEU:HG	1:17:A:HIS:HB2	12	0.74
(2,1601)	1:41:A:MET:HE2	1:10:A:PHE:HB3	15	0.74
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	5	0.74
(2,1549)	1:37:A:LEU:HD11	1:41:A:MET:HG2	10	0.74
(2,1549)	1:37:A:LEU:HD11	1:41:A:MET:HG2	14	0.74
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	16	0.74
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	12	0.74
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	2	0.74
(2,1426)	1:86:A:LEU:HD12	1:88:A:TYR:HD1	20	0.74
(2,1425)	1:56:A:ILE:HG23	1:65:A:PHE:HD1	9	0.74
(2,1424)	1:56:A:ILE:HG23	1:65:A:PHE:HE1	9	0.74
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	11	0.74
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	2	0.74
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	5	0.74
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	7	0.74
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	8	0.74
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	13	0.74
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	17	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	3	0.74
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	2	0.74
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	5	0.74
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	18	0.74
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	4	0.73
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD22	6	0.73
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	11	0.73
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD23	12	0.73
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD22	13	0.73
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	14	0.73
(4,431)	1:13:A:LEU:HG	1:13:A:LEU:HD12	18	0.73
(4,431)	1:13:A:LEU:HG	1:13:A:LEU:HD12	19	0.73
(4,414)	1:44:A:LYS:HB3	1:14:A:VAL:HG13	17	0.73
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	4	0.73
(4,338)	1:111:A:LYS:HD3	1:104:A:LYS:HA	1	0.73
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	3	0.73
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	7	0.73
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	14	0.73
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	18	0.73
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	4	0.73
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	6	0.73
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	8	0.73
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD12	10	0.73
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	9	0.73
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	19	0.73
(4,160)	1:22:A:ILE:HD12	1:22:A:ILE:H	1	0.73
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	7	0.73
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	14	0.73
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE2	6	0.73
(2,3657)	1:63:A:LYS:HG2	1:62:A:LYS:HA	17	0.73
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	7	0.73
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	11	0.73
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	6	0.73
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	10	0.73
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	14	0.73
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	18	0.73
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	16	0.73
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	1	0.73
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	15	0.73
(2,3416)	1:143:A:VAL:HG11	1:143:A:VAL:H	8	0.73
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	19	0.73
(2,3416)	1:143:A:VAL:HG11	1:143:A:VAL:H	20	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	14	0.73
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	17	0.73
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	7	0.73
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	13	0.73
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	10	0.73
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	1	0.73
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB3	7	0.73
(2,1783)	1:44:A:LYS:HG3	1:21:A:LEU:HD22	20	0.73
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG11	4	0.73
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	19	0.73
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	4	0.73
(2,1511)	1:82:A:VAL:HG21	1:80:A:HIS:HA	9	0.73
(2,1490)	1:167:A:LEU:HD12	1:166:A:TRP:HA	11	0.73
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	7	0.73
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	18	0.73
(2,1375)	1:41:A:MET:HE2	1:10:A:PHE:HD1	5	0.73
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	3	0.73
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	9	0.73
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	14	0.73
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	3	0.73
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	9	0.73
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	4	0.73
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	9	0.73
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	13	0.73
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	16	0.73
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	17	0.73
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	16	0.73
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	2	0.73
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	1	0.73
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	5	0.72
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	7	0.72
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	8	0.72
(4,402)	1:6:A:LYS:HE2	1:6:A:LYS:HG3	9	0.72
(4,311)	1:96:A:VAL:HG11	1:94:A:PRO:HA	6	0.72
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	19	0.72
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	14	0.72
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	7	0.72
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	7	0.72
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	9	0.72
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD23	15	0.72
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	8	0.72
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	17	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	19	0.72
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE2	4	0.72
(2,3481)	1:82:A:VAL:HG21	1:80:A:HIS:HA	9	0.72
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	10	0.72
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	3	0.72
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	2	0.72
(2,3265)	1:84:A:VAL:HG11	1:84:A:VAL:H	11	0.72
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	11	0.72
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	7	0.72
(2,1884)	1:41:A:MET:HE2	1:46:A:HIS:HA	6	0.72
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	16	0.72
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	12	0.72
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	2	0.72
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	9	0.72
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	9	0.72
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	18	0.72
(2,1599)	1:4:A:MET:HE1	1:52:A:GLU:HA	2	0.72
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	7	0.72
(2,1512)	1:38:A:LEU:HD22	1:49:A:SER:HA	8	0.72
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	1	0.72
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	2	0.72
(2,1482)	1:11:A:LEU:HD11	1:11:A:LEU:H	6	0.72
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	8	0.72
(2,1190)	1:176:A:ILE:HG21	1:176:A:ILE:HA	14	0.72
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	2	0.72
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	7	0.72
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	12	0.72
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	1	0.72
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	5	0.72
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	11	0.72
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	4	0.72
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	12	0.72
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	17	0.72
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	9	0.72
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD22	9	0.71
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	17	0.71
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD22	20	0.71
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	3	0.71
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	13	0.71
(4,320)	1:151:A:MET:HE3	1:158:A:PHE:HB3	6	0.71
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	13	0.71
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	2	0.71
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	9	0.71
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD11	5	0.71
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	3	0.71
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	7	0.71
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	20	0.71
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	12	0.71
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	20	0.71
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	20	0.71
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	6	0.71
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	18	0.71
(2,3657)	1:63:A:LYS:HG2	1:62:A:LYS:HA	13	0.71
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	16	0.71
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	10	0.71
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	19	0.71
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	12	0.71
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	3	0.71
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	9	0.71
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	15	0.71
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	14	0.71
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	1	0.71
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	11	0.71
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	16	0.71
(2,1845)	1:110:A:LEU:HD12	1:176:A:ILE:HB	18	0.71
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	14	0.71
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	20	0.71
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE1	5	0.71
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	16	0.71
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	4	0.71
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	5	0.71
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	9	0.71
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	3	0.71
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	6	0.71
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	8	0.71
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	17	0.71
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	12	0.71
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	4	0.71
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	7	0.71
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	17	0.71
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	19	0.71
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	8	0.71
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	20	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	13	0.71
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	15	0.71
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	20	0.71
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	11	0.71
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	18	0.71
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	11	0.71
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	13	0.71
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	11	0.71
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	7	0.71
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	3	0.71
(2,35)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	11	0.71
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	8	0.7
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD23	2	0.7
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD23	3	0.7
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	16	0.7
(4,409)	1:4:A:MET:HE1	1:59:A:THR:HG23	5	0.7
(4,368)	1:20:A:ALA:HB3	1:22:A:ILE:HB	1	0.7
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	4	0.7
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	7	0.7
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	10	0.7
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	20	0.7
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	6	0.7
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	7	0.7
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	9	0.7
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	7	0.7
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE2	10	0.7
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE1	1	0.7
(2,3784)	1:37:A:LEU:HD13	1:41:A:MET:HE1	20	0.7
(2,3772)	1:151:A:MET:HE2	1:174:A:GLU:HG2	2	0.7
(2,3761)	1:117:A:MET:HE3	1:117:A:MET:HB2	12	0.7
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	8	0.7
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	14	0.7
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	9	0.7
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	16	0.7
(2,3570)	1:4:A:MET:HE2	1:52:A:GLU:HA	19	0.7
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	6	0.7
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	11	0.7
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	9	0.7
(2,3462)	1:168:A:ILE:HD13	1:175:A:PHE:HB3	18	0.7
(2,3416)	1:143:A:VAL:HG13	1:143:A:VAL:H	1	0.7
(2,3416)	1:143:A:VAL:HG11	1:143:A:VAL:H	4	0.7
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	17	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	1	0.7
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	4	0.7
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	10	0.7
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	6	0.7
(2,3265)	1:84:A:VAL:HG13	1:84:A:VAL:H	18	0.7
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	2	0.7
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	5	0.7
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	8	0.7
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	10	0.7
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	12	0.7
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	18	0.7
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	20	0.7
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	17	0.7
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	20	0.7
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	7	0.7
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	16	0.7
(2,1856)	1:22:A:ILE:HD12	1:14:A:VAL:HG22	7	0.7
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	3	0.7
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	4	0.7
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE1	16	0.7
(2,1823)	1:37:A:LEU:HD11	1:41:A:MET:HE1	17	0.7
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	1	0.7
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	6	0.7
(2,1807)	1:151:A:MET:HE2	1:174:A:GLU:HG2	16	0.7
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	8	0.7
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	12	0.7
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	13	0.7
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	3	0.7
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	15	0.7
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	15	0.7
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	18	0.7
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	20	0.7
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	18	0.7
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	15	0.7
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	16	0.7
(2,1377)	1:4:A:MET:HE2	1:55:A:HIS:HD2	20	0.7
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	1	0.7
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	11	0.7
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	6	0.7
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	10	0.7
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	12	0.7
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	1	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	10	0.7
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	6	0.7
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	16	0.7
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	7	0.7
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	10	0.7
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	19	0.7
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	4	0.7
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	17	0.7
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	2	0.7
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	15	0.7
(4,437)	1:178:A:VAL:HG23	1:177:A:LYS:HG2	19	0.69
(4,431)	1:37:A:LEU:HG	1:37:A:LEU:HD21	1	0.69
(4,332)	1:37:A:LEU:HD12	1:41:A:MET:HB2	19	0.69
(4,320)	1:151:A:MET:HE1	1:147:A:ASP:HB2	8	0.69
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	9	0.69
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	8	0.69
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	1	0.69
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	13	0.69
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	16	0.69
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	18	0.69
(4,95)	1:51:A:GLU:H	1:58:A:GLU:HG3	14	0.69
(2,3657)	1:63:A:LYS:HG3	1:62:A:LYS:HA	19	0.69
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	5	0.69
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	2	0.69
(2,3524)	1:13:A:LEU:HD11	1:18:A:ASN:HB2	5	0.69
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	13	0.69
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	10	0.69
(2,3346)	1:4:A:MET:HE2	1:55:A:HIS:HD2	20	0.69
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	1	0.69
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	13	0.69
(2,3265)	1:84:A:VAL:HG11	1:84:A:VAL:H	14	0.69
(2,3211)	1:151:A:MET:HE2	1:156:A:PHE:HZ	9	0.69
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	5	0.69
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	6	0.69
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	14	0.69
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	19	0.69
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	2	0.69
(2,1935)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	13	0.69
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	13	0.69
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	3	0.69
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	2	0.69
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	17	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1690)	1:63:A:LYS:HG2	1:62:A:LYS:HA	6	0.69
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	12	0.69
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	6	0.69
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	19	0.69
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	4	0.69
(2,1291)	1:84:A:VAL:HG11	1:84:A:VAL:H	7	0.69
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	9	0.69
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	18	0.69
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	4	0.69
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	14	0.69
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	9	0.69
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	14	0.69
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	14	0.69
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	14	0.69
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	4	0.69
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	12	0.69
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	1	0.69
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	10	0.69
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	16	0.69
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	3	0.69
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	3	0.68
(4,437)	1:178:A:VAL:HG23	1:177:A:LYS:HG2	2	0.68
(4,437)	1:178:A:VAL:HG23	1:177:A:LYS:HG2	5	0.68
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	11	0.68
(4,428)	1:108:A:LEU:HD12	1:107:A:ASP:HB2	4	0.68
(4,407)	1:178:A:VAL:HB	1:110:A:LEU:HD22	4	0.68
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	7	0.68
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	9	0.68
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	8	0.68
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	8	0.68
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	14	0.68
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	13	0.68
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	10	0.68
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	15	0.68
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	18	0.68
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	12	0.68
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD21	20	0.68
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	2	0.68
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	12	0.68
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	18	0.68
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	18	0.68
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	14	0.68
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	17	0.68
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	9	0.68
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	19	0.68
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	4	0.68
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	9	0.68
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	18	0.68
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	20	0.68
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	16	0.68
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	6	0.68
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	17	0.68
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	19	0.68
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	20	0.68
(2,1495)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	13	0.68
(2,1492)	1:167:A:LEU:HD23	1:123:A:HIS:HA	3	0.68
(2,1492)	1:167:A:LEU:HD22	1:123:A:HIS:HA	19	0.68
(2,1473)	1:110:A:LEU:HD11	1:110:A:LEU:H	14	0.68
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	1	0.68
(2,1378)	1:50:A:MET:HE1	1:67:A:PHE:HZ	14	0.68
(2,1297)	1:57:A:VAL:HG13	1:67:A:PHE:HB3	5	0.68
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	12	0.68
(2,1297)	1:57:A:VAL:HG13	1:67:A:PHE:HB3	13	0.68
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	2	0.68
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	3	0.68
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	19	0.68
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	16	0.68
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	16	0.68
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	11	0.68
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	13	0.68
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	4	0.68
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	6	0.68
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	8	0.68
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	9	0.68
(2,342)	1:41:A:MET:H	1:41:A:MET:HG2	16	0.68
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	1	0.68
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	3	0.68
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	6	0.68
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	18	0.68
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	15	0.68
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	18	0.68
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	16	0.67
(4,338)	1:111:A:LYS:HD3	1:104:A:LYS:HA	20	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,332)	1:37:A:LEU:HD11	1:41:A:MET:HB2	4	0.67
(4,332)	1:37:A:LEU:HD12	1:41:A:MET:HB2	13	0.67
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	1	0.67
(4,259)	1:117:A:MET:HE3	2:201:A:NAD:H2A	9	0.67
(4,227)	1:8:A:SER:HB3	1:55:A:HIS:HD2	15	0.67
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	9	0.67
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	16	0.67
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	15	0.67
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	1	0.67
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	5	0.67
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	8	0.67
(4,190)	1:60:A:ASN:H	1:73:A:LYS:H	17	0.67
(4,166)	1:171:A:VAL:H	1:168:A:ILE:HG13	2	0.67
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	6	0.67
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	13	0.67
(2,3964)	1:123:A:HIS:HB3	2:201:A:NAD:H6N	2	0.67
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	3	0.67
(2,3813)	1:56:A:ILE:HD12	1:11:A:LEU:HD11	11	0.67
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	13	0.67
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	15	0.67
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	16	0.67
(2,3784)	1:37:A:LEU:HD11	1:41:A:MET:HE1	2	0.67
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	19	0.67
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	14	0.67
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	1	0.67
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	12	0.67
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	6	0.67
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	8	0.67
(2,3462)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	4	0.67
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	19	0.67
(2,3459)	1:167:A:LEU:HD23	1:123:A:HIS:HA	11	0.67
(2,3416)	1:143:A:VAL:HG13	1:143:A:VAL:H	16	0.67
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	2	0.67
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	6	0.67
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	18	0.67
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	19	0.67
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	4	0.67
(2,3271)	1:57:A:VAL:HG13	1:67:A:PHE:HB3	5	0.67
(2,3271)	1:57:A:VAL:HG13	1:67:A:PHE:HB3	13	0.67
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	7	0.67
(2,2784)	1:53:A:LEU:HD22	1:53:A:LEU:H	6	0.67
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	10	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	19	0.67
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	4	0.67
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	17	0.67
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD12	20	0.67
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	19	0.67
(2,1865)	1:109:A:ILE:HD11	1:144:A:LEU:HD13	15	0.67
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	13	0.67
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	2	0.67
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	9	0.67
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	13	0.67
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	15	0.67
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	1	0.67
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	7	0.67
(2,1742)	1:110:A:LEU:HD11	1:173:A:ALA:HA	9	0.67
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	2	0.67
(2,1535)	1:22:A:ILE:HG21	1:44:A:LYS:HE3	16	0.67
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	17	0.67
(2,1412)	1:66:A:ALA:HB2	1:31:A:TRP:HZ3	12	0.67
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	19	0.67
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	3	0.67
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	18	0.67
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	11	0.67
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	17	0.67
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	18	0.67
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	4	0.67
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB3	5	0.67
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	9	0.67
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	5	0.67
(2,255)	1:168:A:ILE:HD12	1:157:A:ASP:H	17	0.67
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	8	0.67
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	12	0.67
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	19	0.67
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	20	0.67
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	17	0.67
(4,450)	1:97:A:LEU:HD23	1:124:A:LEU:HD23	17	0.66
(4,409)	1:4:A:MET:HE3	1:59:A:THR:HG23	17	0.66
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	20	0.66
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	15	0.66
(4,300)	1:97:A:LEU:HD23	1:175:A:PHE:HB3	17	0.66
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	10	0.66
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	11	0.66
(4,192)	1:176:A:ILE:HA	1:110:A:LEU:HD13	18	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	11	0.66
(4,70)	1:130:A:THR:H	2:201:A:NAD:H4D	2	0.66
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	8	0.66
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD12	14	0.66
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	8	0.66
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	19	0.66
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE2	11	0.66
(2,3784)	1:37:A:LEU:HD13	1:41:A:MET:HE3	3	0.66
(2,3772)	1:151:A:MET:HE3	1:174:A:GLU:HG2	7	0.66
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	15	0.66
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	2	0.66
(2,3466)	1:97:A:LEU:HD21	1:166:A:TRP:HB2	5	0.66
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	2	0.66
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	9	0.66
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	10	0.66
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	11	0.66
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	12	0.66
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	3	0.66
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	12	0.66
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	11	0.66
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	12	0.66
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD23	20	0.66
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	7	0.66
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	11	0.66
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	1	0.66
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	13	0.66
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	17	0.66
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	20	0.66
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD12	9	0.66
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	18	0.66
(2,1831)	1:142:A:VAL:HG23	1:143:A:VAL:HB	7	0.66
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	10	0.66
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	13	0.66
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	20	0.66
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	6	0.66
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	9	0.66
(2,1690)	1:63:A:LYS:HG2	1:62:A:LYS:HA	17	0.66
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	13	0.66
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	1	0.66
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	4	0.66
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	11	0.66
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	19	0.66
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	4	0.66
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	17	0.66
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	10	0.66
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	11	0.66
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	15	0.66
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	13	0.66
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	14	0.66
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	17	0.66
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	6	0.66
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	10	0.66
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	20	0.66
(2,339)	1:108:A:LEU:HD22	1:108:A:LEU:H	16	0.66
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	5	0.66
(2,122)	1:177:A:LYS:HG2	1:178:A:VAL:H	15	0.66
(2,67)	1:176:A:ILE:HG21	1:177:A:LYS:H	20	0.66
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	13	0.65
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	15	0.65
(4,292)	1:122:A:VAL:HG21	1:118:A:SER:H	5	0.65
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	19	0.65
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	2	0.65
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	18	0.65
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	17	0.65
(4,166)	1:171:A:VAL:H	1:168:A:ILE:HG13	7	0.65
(2,3813)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	1	0.65
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE1	10	0.65
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	16	0.65
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	4	0.65
(2,3657)	1:63:A:LYS:HG3	1:62:A:LYS:HA	11	0.65
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	7	0.65
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	9	0.65
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	11	0.65
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	13	0.65
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	19	0.65
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	6	0.65
(2,3466)	1:97:A:LEU:HD22	1:166:A:TRP:HB2	18	0.65
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	11	0.65
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	3	0.65
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	5	0.65
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	13	0.65
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	15	0.65
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	20	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	10	0.65
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	18	0.65
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	3	0.65
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	4	0.65
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD23	9	0.65
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	16	0.65
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	13	0.65
(2,2784)	1:53:A:LEU:HD22	1:53:A:LEU:H	16	0.65
(2,1859)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	8	0.65
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	20	0.65
(2,1847)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	9	0.65
(2,1840)	1:128:A:ILE:HG21	1:129:A:THR:HG21	20	0.65
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	5	0.65
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	4	0.65
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	11	0.65
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG12	6	0.65
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	16	0.65
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	2	0.65
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	3	0.65
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	5	0.65
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	10	0.65
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	13	0.65
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	14	0.65
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	18	0.65
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	20	0.65
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	19	0.65
(2,1473)	1:110:A:LEU:HD12	1:110:A:LEU:H	19	0.65
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	5	0.65
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	4	0.65
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	17	0.65
(2,1377)	1:4:A:MET:HE3	1:55:A:HIS:HD2	4	0.65
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	8	0.65
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	14	0.65
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	20	0.65
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	19	0.65
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	1	0.65
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	10	0.65
(2,948)	1:76:A:ALA:HB1	1:78:A:GLN:HE22	8	0.65
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	12	0.65
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	12	0.65
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	12	0.65
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	5	0.65
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	8	0.65
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	16	0.65
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	19	0.65
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	13	0.64
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	6	0.64
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	8	0.64
(4,384)	1:178:A:VAL:HA	1:110:A:LEU:HD11	1	0.64
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	5	0.64
(4,332)	1:37:A:LEU:HD12	1:41:A:MET:HB2	9	0.64
(4,325)	1:7:A:VAL:HG13	1:10:A:PHE:HB3	20	0.64
(4,311)	1:96:A:VAL:HG11	1:94:A:PRO:HA	5	0.64
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	11	0.64
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	16	0.64
(4,299)	1:168:A:ILE:HD12	1:152:A:ALA:HA	18	0.64
(4,278)	1:142:A:VAL:HG12	1:102:A:ALA:H	10	0.64
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	12	0.64
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	17	0.64
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	4	0.64
(4,222)	1:57:A:VAL:HG23	1:74:A:ILE:HB	6	0.64
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	6	0.64
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	2	0.64
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	13	0.64
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	14	0.64
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	2	0.64
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	19	0.64
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	5	0.64
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	10	0.64
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	17	0.64
(2,3466)	1:97:A:LEU:HD22	1:166:A:TRP:HB2	8	0.64
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	7	0.64
(2,3400)	1:38:A:LEU:HD23	1:39:A:ALA:H	8	0.64
(2,3346)	1:4:A:MET:HE3	1:55:A:HIS:HD2	4	0.64
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	8	0.64
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	10	0.64
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	17	0.64
(2,3265)	1:84:A:VAL:HG12	1:84:A:VAL:H	8	0.64
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD21	3	0.64
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	15	0.64
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	1	0.64
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	2	0.64
(2,1884)	1:41:A:MET:HE2	1:46:A:HIS:HA	18	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG22	11	0.64
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE1	1	0.64
(2,1823)	1:37:A:LEU:HD13	1:41:A:MET:HE1	20	0.64
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	14	0.64
(2,1690)	1:63:A:LYS:HG2	1:62:A:LYS:HA	13	0.64
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	6	0.64
(2,1601)	1:41:A:MET:HE2	1:10:A:PHE:HB3	19	0.64
(2,1566)	1:96:A:VAL:HG11	1:151:A:MET:HA	14	0.64
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	6	0.64
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	7	0.64
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	8	0.64
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	9	0.64
(2,1525)	1:38:A:LEU:HD23	1:38:A:LEU:HA	15	0.64
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	2	0.64
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	4	0.64
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	3	0.64
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	7	0.64
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	9	0.64
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	11	0.64
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	15	0.64
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	19	0.64
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	20	0.64
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	3	0.64
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	13	0.64
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	16	0.64
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	2	0.64
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	5	0.64
(2,561)	1:16:A:ARG:H	1:16:A:ARG:HB2	20	0.64
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	20	0.64
(2,342)	1:41:A:MET:H	1:41:A:MET:HG2	17	0.64
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	1	0.64
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	12	0.64
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	13	0.64
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	14	0.64
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	20	0.64
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	16	0.64
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG21	6	0.63
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	10	0.63
(4,332)	1:37:A:LEU:HD13	1:41:A:MET:HB2	2	0.63
(4,332)	1:37:A:LEU:HD11	1:41:A:MET:HB2	10	0.63
(4,332)	1:37:A:LEU:HD11	1:41:A:MET:HB2	11	0.63
(4,332)	1:37:A:LEU:HD11	1:41:A:MET:HB2	15	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,292)	1:122:A:VAL:HG22	1:118:A:SER:H	20	0.63
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	2	0.63
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	6	0.63
(4,278)	1:142:A:VAL:HG12	1:102:A:ALA:H	7	0.63
(4,227)	1:8:A:SER:HB3	1:55:A:HIS:HD2	10	0.63
(4,204)	1:173:A:ALA:HB1	1:111:A:LYS:HG3	11	0.63
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB2	15	0.63
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD22	2	0.63
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	20	0.63
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	3	0.63
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE3	4	0.63
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	3	0.63
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	10	0.63
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	17	0.63
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	8	0.63
(2,3466)	1:97:A:LEU:HD22	1:166:A:TRP:HB2	15	0.63
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	7	0.63
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	8	0.63
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	11	0.63
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	14	0.63
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	15	0.63
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	20	0.63
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	14	0.63
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	4	0.63
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	8	0.63
(2,2784)	1:53:A:LEU:HD21	1:53:A:LEU:H	2	0.63
(2,2509)	1:38:A:LEU:H	1:38:A:LEU:HG	16	0.63
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	12	0.63
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	3	0.63
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	4	0.63
(2,1846)	1:160:A:LEU:HD11	1:91:A:GLN:HB2	7	0.63
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	9	0.63
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	12	0.63
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	8	0.63
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	19	0.63
(2,1808)	1:13:A:LEU:HD22	1:13:A:LEU:HG	2	0.63
(2,1565)	1:22:A:ILE:HG22	1:41:A:MET:HB2	16	0.63
(2,1529)	1:144:A:LEU:HD22	1:145:A:SER:HB2	9	0.63
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	17	0.63
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	11	0.63
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	14	0.63
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	20	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1314)	1:142:A:VAL:HG11	1:103:A:GLU:HA	10	0.63
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	2	0.63
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	7	0.63
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	8	0.63
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	18	0.63
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	20	0.63
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	11	0.63
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	2	0.63
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	20	0.63
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	7	0.63
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	12	0.63
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	1	0.63
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	2	0.63
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	9	0.63
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	11	0.63
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HG3	5	0.62
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	2	0.62
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	10	0.62
(4,311)	1:143:A:VAL:HG12	1:178:A:VAL:HA	12	0.62
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	8	0.62
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	7	0.62
(4,203)	1:173:A:ALA:HB2	1:171:A:VAL:HB	16	0.62
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	13	0.62
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD21	5	0.62
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	7	0.62
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	12	0.62
(2,3813)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	9	0.62
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	7	0.62
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE1	14	0.62
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	1	0.62
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	15	0.62
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	3	0.62
(2,3532)	1:21:A:LEU:HD13	1:41:A:MET:HB2	20	0.62
(2,3514)	1:143:A:VAL:HG11	1:132:A:ARG:HA	2	0.62
(2,3514)	1:143:A:VAL:HG11	1:132:A:ARG:HA	9	0.62
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	2	0.62
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	4	0.62
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	9	0.62
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	10	0.62
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	20	0.62
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	4	0.62
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	13	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3481)	1:82:A:VAL:HG21	1:80:A:HIS:HA	2	0.62
(2,3378)	1:66:A:ALA:HB2	1:31:A:TRP:HZ3	12	0.62
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	2	0.62
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	7	0.62
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	19	0.62
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	11	0.62
(2,3265)	1:84:A:VAL:HG11	1:84:A:VAL:H	10	0.62
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	1	0.62
(2,2308)	1:108:A:LEU:HD21	1:108:A:LEU:H	18	0.62
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	5	0.62
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	8	0.62
(2,1884)	1:41:A:MET:HE3	1:46:A:HIS:HA	20	0.62
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG23	12	0.62
(2,1840)	1:128:A:ILE:HG21	1:129:A:THR:HG21	6	0.62
(2,1840)	1:128:A:ILE:HG23	1:129:A:THR:HG21	12	0.62
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	1	0.62
(2,1831)	1:142:A:VAL:HG23	1:143:A:VAL:HB	6	0.62
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	3	0.62
(2,1742)	1:110:A:LEU:HD12	1:173:A:ALA:HA	3	0.62
(2,1690)	1:63:A:LYS:HG3	1:62:A:LYS:HA	19	0.62
(2,1554)	1:38:A:LEU:HD21	1:50:A:MET:HG2	9	0.62
(2,1511)	1:82:A:VAL:HG21	1:80:A:HIS:HA	2	0.62
(2,1490)	1:167:A:LEU:HD12	1:166:A:TRP:HA	6	0.62
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	6	0.62
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	9	0.62
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	6	0.62
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	2	0.62
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	8	0.62
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	15	0.62
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	7	0.62
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	11	0.62
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	9	0.62
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	4	0.62
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	6	0.62
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	9	0.61
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	20	0.61
(4,449)	1:74:A:ILE:HD12	1:11:A:LEU:HD23	2	0.61
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	7	0.61
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	14	0.61
(4,415)	1:19:A:PRO:HB2	1:36:A:GLU:HG2	12	0.61
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	18	0.61
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	15	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,204)	1:173:A:ALA:HB2	1:111:A:LYS:HG2	8	0.61
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	7	0.61
(2,3964)	1:123:A:HIS:HB3	2:201:A:NAD:H6N	9	0.61
(2,3813)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	7	0.61
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	2	0.61
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	6	0.61
(2,3784)	1:37:A:LEU:HD11	1:41:A:MET:HE1	15	0.61
(2,3722)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	9	0.61
(2,3722)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	14	0.61
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	5	0.61
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	5	0.61
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	6	0.61
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	13	0.61
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	1	0.61
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	20	0.61
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	12	0.61
(2,3428)	1:108:A:LEU:HD12	2:201:A:NAD:H2A	19	0.61
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	6	0.61
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	9	0.61
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	5	0.61
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	18	0.61
(2,3265)	1:84:A:VAL:HG11	1:84:A:VAL:H	9	0.61
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	3	0.61
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	12	0.61
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	18	0.61
(2,1875)	1:5:A:VAL:HG22	1:5:A:VAL:HA	6	0.61
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD12	4	0.61
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	14	0.61
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	12	0.61
(2,1840)	1:128:A:ILE:HG21	1:129:A:THR:HG22	2	0.61
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	3	0.61
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE3	7	0.61
(2,1827)	1:21:A:LEU:HD22	1:21:A:LEU:HG	1	0.61
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	6	0.61
(2,1823)	1:37:A:LEU:HD11	1:41:A:MET:HE1	2	0.61
(2,1808)	1:13:A:LEU:HD22	1:13:A:LEU:HG	8	0.61
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	9	0.61
(2,1808)	1:13:A:LEU:HD23	1:13:A:LEU:HG	11	0.61
(2,1808)	1:13:A:LEU:HD22	1:13:A:LEU:HG	13	0.61
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	10	0.61
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	13	0.61
(2,1425)	1:56:A:ILE:HG21	1:65:A:PHE:HD1	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	8	0.61
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	13	0.61
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	9	0.61
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	16	0.61
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	7	0.61
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	20	0.61
(2,954)	1:56:A:ILE:HG22	1:57:A:VAL:H	10	0.61
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	14	0.61
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	15	0.61
(2,339)	1:108:A:LEU:HD22	1:108:A:LEU:H	2	0.61
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	11	0.61
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	18	0.61
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	6	0.61
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	18	0.61
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	12	0.6
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	18	0.6
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	14	0.6
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	20	0.6
(4,278)	1:142:A:VAL:HG12	1:102:A:ALA:H	11	0.6
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	10	0.6
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	10	0.6
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	17	0.6
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	4	0.6
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	13	0.6
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD21	6	0.6
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD23	19	0.6
(2,3839)	1:129:A:THR:HG21	1:129:A:THR:HA	6	0.6
(2,3813)	1:56:A:ILE:HD11	1:11:A:LEU:HD13	6	0.6
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	3	0.6
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	13	0.6
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	2	0.6
(2,3722)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	6	0.6
(2,3600)	1:42:A:LYS:HE2	1:39:A:ALA:HA	3	0.6
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	8	0.6
(2,3532)	1:21:A:LEU:HD12	1:41:A:MET:HB2	5	0.6
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	4	0.6
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	1	0.6
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	7	0.6
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	11	0.6
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	12	0.6
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	16	0.6
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	18	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	6	0.6
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	9	0.6
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	19	0.6
(2,3462)	1:168:A:ILE:HD11	1:175:A:PHE:HB3	13	0.6
(2,3416)	1:143:A:VAL:HG12	1:143:A:VAL:H	18	0.6
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	16	0.6
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	15	0.6
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	1	0.6
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG22	16	0.6
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG23	4	0.6
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	1	0.6
(2,1831)	1:142:A:VAL:HG23	1:143:A:VAL:HB	5	0.6
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	9	0.6
(2,1823)	1:37:A:LEU:HD13	1:41:A:MET:HE3	3	0.6
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	10	0.6
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	13	0.6
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	5	0.6
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	7	0.6
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	10	0.6
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	15	0.6
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	19	0.6
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	3	0.6
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	16	0.6
(2,1495)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	8	0.6
(2,1490)	1:167:A:LEU:HD12	1:166:A:TRP:HA	5	0.6
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	1	0.6
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	2	0.6
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	6	0.6
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	12	0.6
(2,1297)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	17	0.6
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	1	0.6
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	7	0.6
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	7	0.6
(2,602)	1:111:A:LYS:HB3	1:111:A:LYS:H	19	0.6
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	4	0.6
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	18	0.6
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	12	0.6
(2,305)	1:42:A:LYS:HA	1:46:A:HIS:H	14	0.6
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	2	0.6
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	7	0.6
(2,110)	1:171:A:VAL:H	1:168:A:ILE:HG21	10	0.6
(4,449)	1:74:A:ILE:HD12	1:11:A:LEU:HD23	7	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,449)	1:74:A:ILE:HD11	1:57:A:VAL:HG23	13	0.59
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	4	0.59
(4,410)	1:50:A:MET:HE3	1:54:A:LYS:HD2	5	0.59
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	17	0.59
(4,329)	1:142:A:VAL:HG21	1:103:A:GLU:HA	4	0.59
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	2	0.59
(4,292)	1:122:A:VAL:HG21	1:118:A:SER:H	8	0.59
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	1	0.59
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	4	0.59
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	2	0.59
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD11	5	0.59
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD21	11	0.59
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD23	13	0.59
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	11	0.59
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	20	0.59
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	3	0.59
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	15	0.59
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	2	0.59
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	10	0.59
(2,3470)	1:110:A:LEU:HD12	1:107:A:ASP:HA	15	0.59
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	12	0.59
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	16	0.59
(2,3265)	1:84:A:VAL:HG11	1:84:A:VAL:H	12	0.59
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD21	2	0.59
(2,1974)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	7	0.59
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	20	0.59
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	19	0.59
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE1	10	0.59
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	17	0.59
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB3	19	0.59
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	12	0.59
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	3	0.59
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	4	0.59
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	6	0.59
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	7	0.59
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	16	0.59
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	17	0.59
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	18	0.59
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	18	0.59
(2,1783)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	1	0.59
(2,1724)	1:149:A:LYS:HA	1:96:A:VAL:HG11	5	0.59
(2,1601)	1:41:A:MET:HE2	1:10:A:PHE:HB3	9	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1492)	1:167:A:LEU:HD22	1:123:A:HIS:HA	4	0.59
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	7	0.59
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	13	0.59
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	19	0.59
(2,1462)	1:14:A:VAL:HG23	1:14:A:VAL:H	13	0.59
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	2	0.59
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	8	0.59
(2,1388)	1:41:A:MET:HE2	1:41:A:MET:H	20	0.59
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	7	0.59
(2,948)	1:76:A:ALA:HB3	1:78:A:GLN:HE22	15	0.59
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	12	0.59
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	9	0.59
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	11	0.59
(2,305)	1:42:A:LYS:HA	1:46:A:HIS:H	16	0.59
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	10	0.59
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	18	0.59
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG21	9	0.58
(4,437)	1:178:A:VAL:HG23	1:177:A:LYS:HG2	3	0.58
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	20	0.58
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD11	4	0.58
(4,368)	1:20:A:ALA:HB1	1:22:A:ILE:HB	13	0.58
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	11	0.58
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	10	0.58
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	19	0.58
(4,332)	1:37:A:LEU:HD11	1:41:A:MET:HB2	12	0.58
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	6	0.58
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	9	0.58
(4,15)	1:177:A:LYS:H	1:96:A:VAL:HG21	3	0.58
(4,12)	1:175:A:PHE:HE1	1:168:A:ILE:HG23	2	0.58
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD22	7	0.58
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	15	0.58
(2,3784)	1:37:A:LEU:HD12	1:41:A:MET:HE3	11	0.58
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	7	0.58
(2,3657)	1:63:A:LYS:HG3	1:62:A:LYS:HA	9	0.58
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	7	0.58
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	18	0.58
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	8	0.58
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	14	0.58
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	7	0.58
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	18	0.58
(2,3470)	1:110:A:LEU:HD13	1:107:A:ASP:HA	9	0.58
(2,3459)	1:167:A:LEU:HD23	1:123:A:HIS:HA	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3415)	1:122:A:VAL:HG21	1:122:A:VAL:H	5	0.58
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	15	0.58
(2,3271)	1:57:A:VAL:HG12	1:67:A:PHE:HB3	17	0.58
(2,2784)	1:53:A:LEU:HD23	1:53:A:LEU:H	15	0.58
(2,1974)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	13	0.58
(2,1851)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	2	0.58
(2,1835)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	5	0.58
(2,1831)	1:142:A:VAL:HG23	1:143:A:VAL:HB	13	0.58
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	2	0.58
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	20	0.58
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	1	0.58
(2,1808)	1:13:A:LEU:HD23	1:13:A:LEU:HG	12	0.58
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	14	0.58
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	20	0.58
(2,1794)	1:117:A:MET:HE1	1:117:A:MET:HB2	20	0.58
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	12	0.58
(2,1690)	1:63:A:LYS:HG3	1:62:A:LYS:HA	11	0.58
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	17	0.58
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	1	0.58
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	9	0.58
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	10	0.58
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	15	0.58
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	16	0.58
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	19	0.58
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	2	0.58
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	10	0.58
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	18	0.58
(2,1276)	1:160:A:LEU:HD21	1:166:A:TRP:HE1	2	0.58
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	3	0.58
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	17	0.58
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	9	0.58
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	19	0.58
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	6	0.58
(4,332)	1:37:A:LEU:HD12	1:41:A:MET:HB2	1	0.57
(4,332)	1:37:A:LEU:HD12	1:41:A:MET:HB2	3	0.57
(4,332)	1:37:A:LEU:HD11	1:41:A:MET:HB2	14	0.57
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	16	0.57
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	17	0.57
(4,223)	1:13:A:LEU:HD12	1:10:A:PHE:HE1	5	0.57
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	7	0.57
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	13	0.57
(4,184)	1:105:A:ASN:H	1:136:A:MET:H	18	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	11	0.57
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	13	0.57
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	14	0.57
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	3	0.57
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	11	0.57
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	11	0.57
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	12	0.57
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	20	0.57
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	17	0.57
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	3	0.57
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	14	0.57
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	16	0.57
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	4	0.57
(2,3435)	1:14:A:VAL:HG13	1:10:A:PHE:HD1	5	0.57
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	18	0.57
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	1	0.57
(2,3182)	1:114:A:ILE:HD13	1:171:A:VAL:HB	5	0.57
(2,3177)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	13	0.57
(2,2308)	1:108:A:LEU:HD21	1:108:A:LEU:H	19	0.57
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	20	0.57
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	5	0.57
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	17	0.57
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	18	0.57
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	11	0.57
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	18	0.57
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	12	0.57
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE3	4	0.57
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	18	0.57
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG23	2	0.57
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	12	0.57
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	8	0.57
(2,1492)	1:167:A:LEU:HD21	1:123:A:HIS:HA	20	0.57
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	4	0.57
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	5	0.57
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	8	0.57
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	12	0.57
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	17	0.57
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	8	0.57
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	14	0.57
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	18	0.57
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	3	0.57
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	16	0.57
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	18	0.57
(2,339)	1:108:A:LEU:HD22	1:108:A:LEU:H	8	0.57
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	12	0.57
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	17	0.57
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	20	0.57
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HG3	2	0.56
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	12	0.56
(4,449)	1:57:A:VAL:HG21	1:74:A:ILE:HD11	4	0.56
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	1	0.56
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD12	13	0.56
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	18	0.56
(4,328)	1:122:A:VAL:HG13	1:113:A:GLY:HA2	13	0.56
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	17	0.56
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	8	0.56
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	18	0.56
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	3	0.56
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	3	0.56
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	7	0.56
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	15	0.56
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD3	14	0.56
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	19	0.56
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	2	0.56
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	8	0.56
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD23	16	0.56
(2,3843)	1:76:A:ALA:HB3	1:16:A:ARG:HA	15	0.56
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD11	13	0.56
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	10	0.56
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	9	0.56
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	4	0.56
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	1	0.56
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	12	0.56
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	20	0.56
(2,3470)	1:110:A:LEU:HD13	1:107:A:ASP:HA	14	0.56
(2,3415)	1:122:A:VAL:HG22	1:122:A:VAL:H	7	0.56
(2,3415)	1:122:A:VAL:HG22	1:122:A:VAL:H	17	0.56
(2,3265)	1:84:A:VAL:HG13	1:84:A:VAL:H	3	0.56
(2,2266)	1:153:A:ASP:H	1:95:A:ALA:HB1	6	0.56
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	14	0.56
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	5	0.56
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG23	19	0.56
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	13	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD12	7	0.56
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	8	0.56
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	9	0.56
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD13	11	0.56
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	15	0.56
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	20	0.56
(2,1813)	1:53:A:LEU:HD11	1:53:A:LEU:HG	12	0.56
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	19	0.56
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	16	0.56
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	18	0.56
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	18	0.56
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	2	0.56
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	6	0.56
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	7	0.56
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	14	0.56
(2,1391)	1:56:A:ILE:HB	1:57:A:VAL:H	5	0.56
(2,1276)	1:160:A:LEU:HD21	1:166:A:TRP:HE1	10	0.56
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	20	0.56
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	17	0.56
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	14	0.56
(2,948)	1:76:A:ALA:HB3	1:78:A:GLN:HE22	2	0.56
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	4	0.56
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	6	0.56
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	1	0.56
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	14	0.56
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	14	0.56
(2,305)	1:42:A:LYS:HA	1:46:A:HIS:H	17	0.56
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	10	0.56
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	14	0.56
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	11	0.56
(4,449)	1:74:A:ILE:HD11	1:57:A:VAL:HG23	1	0.55
(4,449)	1:74:A:ILE:HD12	1:11:A:LEU:HD21	8	0.55
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD13	1	0.55
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD13	12	0.55
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	2	0.55
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	6	0.55
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD3	17	0.55
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	14	0.55
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	14	0.55
(4,6)	1:65:A:PHE:HE1	1:74:A:ILE:HG23	4	0.55
(2,3839)	1:129:A:THR:HG21	1:129:A:THR:HA	20	0.55
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	1	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	13	0.55
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	5	0.55
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD11	7	0.55
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	16	0.55
(2,3772)	1:151:A:MET:HE2	1:174:A:GLU:HG2	16	0.55
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	19	0.55
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	7	0.55
(2,3570)	1:4:A:MET:HE3	1:52:A:GLU:HA	1	0.55
(2,3570)	1:4:A:MET:HE2	1:52:A:GLU:HA	18	0.55
(2,3454)	1:168:A:ILE:HD13	1:149:A:LYS:H	5	0.55
(2,3446)	1:74:A:ILE:HD12	1:67:A:PHE:HE1	5	0.55
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	5	0.55
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	6	0.55
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	7	0.55
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	10	0.55
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	13	0.55
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	15	0.55
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	19	0.55
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	3	0.55
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	5	0.55
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	10	0.55
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	12	0.55
(2,1823)	1:37:A:LEU:HD11	1:41:A:MET:HE1	15	0.55
(2,1819)	1:86:A:LEU:HD22	1:86:A:LEU:HG	13	0.55
(2,1813)	1:53:A:LEU:HD11	1:53:A:LEU:HG	8	0.55
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	14	0.55
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	16	0.55
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	20	0.55
(2,1808)	1:13:A:LEU:HD21	1:13:A:LEU:HG	5	0.55
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	2	0.55
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	20	0.55
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	3	0.55
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	11	0.55
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	18	0.55
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	5	0.55
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	19	0.55
(2,1314)	1:142:A:VAL:HG11	1:103:A:GLU:HA	3	0.55
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	1	0.55
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	15	0.55
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	18	0.55
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	5	0.55
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	12	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	4	0.54
(4,449)	1:57:A:VAL:HG21	1:74:A:ILE:HD11	16	0.54
(4,449)	1:74:A:ILE:HD11	1:57:A:VAL:HG23	20	0.54
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	17	0.54
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD12	9	0.54
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	4	0.54
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	6	0.54
(4,368)	1:20:A:ALA:HB1	1:22:A:ILE:HB	12	0.54
(4,338)	1:111:A:LYS:HD3	1:104:A:LYS:HA	3	0.54
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	4	0.54
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	12	0.54
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD11	1	0.54
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD11	7	0.54
(4,15)	1:177:A:LYS:H	1:96:A:VAL:HG21	16	0.54
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	14	0.54
(2,3788)	1:151:A:MET:HE1	1:151:A:MET:HG3	20	0.54
(2,3784)	1:37:A:LEU:HD13	1:41:A:MET:HE3	19	0.54
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	6	0.54
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	7	0.54
(2,3514)	1:143:A:VAL:HG11	1:132:A:ARG:HA	12	0.54
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	11	0.54
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	7	0.54
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	4	0.54
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	14	0.54
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	8	0.54
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	9	0.54
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	11	0.54
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	12	0.54
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	16	0.54
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	20	0.54
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	14	0.54
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	20	0.54
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	13	0.54
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	14	0.54
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD12	18	0.54
(2,1820)	1:142:A:VAL:HG11	1:142:A:VAL:HB	2	0.54
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	20	0.54
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	10	0.54
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	4	0.54
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	7	0.54
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	9	0.54
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	11	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	13	0.54
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	14	0.54
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	14	0.54
(2,1601)	1:41:A:MET:HE2	1:10:A:PHE:HB3	11	0.54
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	18	0.54
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	18	0.54
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	8	0.54
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	17	0.54
(2,539)	1:38:A:LEU:H	1:37:A:LEU:HB3	1	0.54
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	7	0.54
(2,16)	1:21:A:LEU:HD13	1:10:A:PHE:HE1	7	0.54
(4,449)	1:74:A:ILE:HD11	1:57:A:VAL:HG23	19	0.53
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG22	17	0.53
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	5	0.53
(4,368)	1:20:A:ALA:HB1	1:22:A:ILE:HB	11	0.53
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	16	0.53
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	10	0.53
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	1	0.53
(4,184)	1:64:A:ARG:H	1:12:A:SER:H	2	0.53
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	17	0.53
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB2	6	0.53
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	7	0.53
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	11	0.53
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	8	0.53
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD22	9	0.53
(2,3839)	1:129:A:THR:HG22	1:129:A:THR:HA	2	0.53
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD12	12	0.53
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	14	0.53
(2,3784)	1:37:A:LEU:HD13	1:41:A:MET:HE3	13	0.53
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	15	0.53
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	6	0.53
(2,3508)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	12	0.53
(2,3507)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	20	0.53
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	15	0.53
(2,3470)	1:110:A:LEU:HD13	1:107:A:ASP:HA	5	0.53
(2,3461)	1:168:A:ILE:HD12	1:156:A:PHE:HB2	17	0.53
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	1	0.53
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	17	0.53
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	1	0.53
(2,3270)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	20	0.53
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	4	0.53
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD12	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	11	0.53
(2,1814)	1:34:A:VAL:HG22	1:74:A:ILE:HB	16	0.53
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	8	0.53
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	1	0.53
(2,1794)	1:117:A:MET:HE1	1:117:A:MET:HB2	17	0.53
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	3	0.53
(2,1607)	1:73:A:LYS:HD2	1:33:A:PRO:HB2	20	0.53
(2,1490)	1:167:A:LEU:HD12	1:166:A:TRP:HA	2	0.53
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	4	0.53
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	11	0.53
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	10	0.53
(2,1276)	1:160:A:LEU:HD21	1:166:A:TRP:HE1	9	0.53
(2,1276)	1:160:A:LEU:HD21	1:166:A:TRP:HE1	19	0.53
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	13	0.53
(2,980)	1:165:A:VAL:H	1:91:A:GLN:HE22	19	0.53
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	3	0.53
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	12	0.53
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	6	0.53
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	7	0.53
(2,339)	1:108:A:LEU:HD21	1:108:A:LEU:H	11	0.53
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	8	0.53
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	4	0.53
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	10	0.53
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	19	0.52
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD21	14	0.52
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG23	3	0.52
(4,449)	1:74:A:ILE:HD11	1:11:A:LEU:HD21	5	0.52
(4,449)	1:74:A:ILE:HD11	1:11:A:LEU:HD21	14	0.52
(4,409)	1:4:A:MET:HE3	1:59:A:THR:HG23	18	0.52
(4,353)	1:165:A:VAL:HB	1:131:A:ALA:HA	17	0.52
(4,352)	1:36:A:GLU:HB3	1:42:A:LYS:HE3	7	0.52
(4,320)	1:151:A:MET:HE2	1:147:A:ASP:HB2	17	0.52
(4,303)	1:110:A:LEU:HD12	1:107:A:ASP:HA	15	0.52
(4,301)	1:97:A:LEU:HD23	1:156:A:PHE:HB2	9	0.52
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	10	0.52
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	11	0.52
(4,278)	1:142:A:VAL:HG12	1:102:A:ALA:H	4	0.52
(4,259)	1:117:A:MET:HE3	2:201:A:NAD:H2A	17	0.52
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	16	0.52
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	18	0.52
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	1	0.52
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,129)	1:13:A:LEU:HD21	1:18:A:ASN:H	5	0.52
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	3	0.52
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	10	0.52
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	3	0.52
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	9	0.52
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	17	0.52
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD23	5	0.52
(2,3832)	1:97:A:LEU:HD22	1:151:A:MET:HG3	2	0.52
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	8	0.52
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	14	0.52
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	20	0.52
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	11	0.52
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	14	0.52
(2,3527)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	4	0.52
(2,3409)	1:84:A:VAL:HG11	1:85:A:ASP:H	5	0.52
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	2	0.52
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	3	0.52
(2,1884)	1:41:A:MET:HE3	1:46:A:HIS:HA	17	0.52
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	6	0.52
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	19	0.52
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	8	0.52
(2,1849)	1:15:A:LEU:HD11	1:74:A:ILE:HD12	17	0.52
(2,1823)	1:37:A:LEU:HD12	1:41:A:MET:HE3	11	0.52
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	2	0.52
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	3	0.52
(2,1813)	1:53:A:LEU:HD11	1:53:A:LEU:HG	17	0.52
(2,1793)	1:53:A:LEU:HD12	1:53:A:LEU:HB2	6	0.52
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG21	16	0.52
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	14	0.52
(2,1555)	1:84:A:VAL:HG21	1:85:A:ASP:HB2	2	0.52
(2,1490)	1:167:A:LEU:HD13	1:166:A:TRP:HA	10	0.52
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	8	0.52
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	7	0.52
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	18	0.52
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	13	0.52
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD22	5	0.52
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	19	0.52
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	3	0.52
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	6	0.52
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG21	10	0.51
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG21	18	0.51
(4,446)	1:110:A:LEU:HD12	1:110:A:LEU:HG	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD11	4	0.51
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	11	0.51
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	14	0.51
(4,379)	1:50:A:MET:HA	1:39:A:ALA:HB3	7	0.51
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	12	0.51
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	13	0.51
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	3	0.51
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	7	0.51
(4,338)	1:111:A:LYS:HD3	1:104:A:LYS:HA	6	0.51
(4,338)	1:111:A:LYS:HD3	1:104:A:LYS:HA	18	0.51
(4,303)	1:110:A:LEU:HD13	1:107:A:ASP:HA	9	0.51
(4,300)	1:97:A:LEU:HD23	1:156:A:PHE:HB3	16	0.51
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	16	0.51
(4,39)	1:24:A:LEU:H	1:17:A:HIS:HB2	16	0.51
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	16	0.51
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD22	8	0.51
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	18	0.51
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	11	0.51
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	16	0.51
(2,3847)	1:41:A:MET:HE2	1:46:A:HIS:HA	12	0.51
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD12	5	0.51
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	11	0.51
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD22	2	0.51
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	11	0.51
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	13	0.51
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	16	0.51
(2,3788)	1:151:A:MET:HE2	1:151:A:MET:HG3	5	0.51
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	6	0.51
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	9	0.51
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	9	0.51
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	12	0.51
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	8	0.51
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	13	0.51
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG23	2	0.51
(2,3537)	1:96:A:VAL:HG11	1:151:A:MET:HA	14	0.51
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	13	0.51
(2,3462)	1:168:A:ILE:HD12	1:175:A:PHE:HB3	8	0.51
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	2	0.51
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	19	0.51
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	12	0.51
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	13	0.51
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	6	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	16	0.51
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	6	0.51
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	17	0.51
(2,2823)	1:74:A:ILE:H	1:37:A:LEU:HD22	5	0.51
(2,1877)	1:129:A:THR:HG21	1:129:A:THR:HA	6	0.51
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	10	0.51
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	16	0.51
(2,1834)	1:14:A:VAL:HG22	1:21:A:LEU:HG	20	0.51
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD12	1	0.51
(2,1824)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	16	0.51
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	5	0.51
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	16	0.51
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	19	0.51
(2,1819)	1:86:A:LEU:HD23	1:86:A:LEU:HG	20	0.51
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	1	0.51
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	15	0.51
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	18	0.51
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	3	0.51
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	13	0.51
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	7	0.51
(2,1690)	1:63:A:LYS:HG3	1:62:A:LYS:HA	9	0.51
(2,1541)	1:143:A:VAL:HG11	1:132:A:ARG:HA	2	0.51
(2,1541)	1:143:A:VAL:HG11	1:132:A:ARG:HA	9	0.51
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	12	0.51
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	19	0.51
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	8	0.51
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	6	0.51
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	12	0.51
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	17	0.51
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	2	0.51
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	4	0.51
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	18	0.51
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	9	0.51
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	19	0.51
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB2	12	0.51
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD12	6	0.51
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	6	0.51
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	13	0.51
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	3	0.51
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	9	0.51
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	13	0.5
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG23	15	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,449)	1:74:A:ILE:HD11	1:57:A:VAL:HG23	17	0.5
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	6	0.5
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD13	18	0.5
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	10	0.5
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	8	0.5
(4,338)	1:111:A:LYS:HD3	1:104:A:LYS:HA	2	0.5
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	4	0.5
(4,303)	1:110:A:LEU:HD13	1:107:A:ASP:HA	14	0.5
(4,292)	1:122:A:VAL:HG22	1:118:A:SER:H	15	0.5
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	12	0.5
(4,202)	1:173:A:ALA:HA	1:150:A:GLY:HA3	11	0.5
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	19	0.5
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	4	0.5
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	17	0.5
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	4	0.5
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD23	14	0.5
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	8	0.5
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	14	0.5
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD21	2	0.5
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	6	0.5
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	8	0.5
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD21	15	0.5
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	16	0.5
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	19	0.5
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	3	0.5
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	16	0.5
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD11	1	0.5
(2,3784)	1:37:A:LEU:HD13	1:41:A:MET:HE1	9	0.5
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	11	0.5
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	11	0.5
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	17	0.5
(2,3676)	1:86:A:LEU:HD21	1:86:A:LEU:HA	13	0.5
(2,3676)	1:86:A:LEU:HD23	1:86:A:LEU:HA	18	0.5
(2,3514)	1:143:A:VAL:HG13	1:132:A:ARG:HA	20	0.5
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	2	0.5
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	9	0.5
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	18	0.5
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	8	0.5
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	20	0.5
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	7	0.5
(2,1897)	1:24:A:LEU:HG	1:24:A:LEU:HA	1	0.5
(2,1884)	1:41:A:MET:HE3	1:46:A:HIS:HA	16	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1874)	1:168:A:ILE:HD12	1:171:A:VAL:HG13	5	0.5
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	15	0.5
(2,1871)	1:97:A:LEU:HD22	1:151:A:MET:HG3	5	0.5
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	2	0.5
(2,1849)	1:15:A:LEU:HD13	1:74:A:ILE:HD11	12	0.5
(2,1846)	1:160:A:LEU:HD13	1:91:A:GLN:HB2	18	0.5
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	5	0.5
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	14	0.5
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	10	0.5
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	15	0.5
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	16	0.5
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD12	4	0.5
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	1	0.5
(2,1820)	1:142:A:VAL:HG11	1:142:A:VAL:HB	3	0.5
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	6	0.5
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	17	0.5
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	3	0.5
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	15	0.5
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	10	0.5
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	13	0.5
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	5	0.5
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG23	15	0.5
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	6	0.5
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	18	0.5
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	18	0.5
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	17	0.5
(2,1490)	1:167:A:LEU:HD12	1:166:A:TRP:HA	18	0.5
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	1	0.5
(2,1462)	1:14:A:VAL:HG22	1:14:A:VAL:H	20	0.5
(2,1459)	1:108:A:LEU:HD12	2:201:A:NAD:H2A	19	0.5
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	13	0.5
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	14	0.5
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	12	0.5
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	2	0.5
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	9	0.5
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	1	0.5
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	2	0.5
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	14	0.5
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	11	0.5
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	4	0.5
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	7	0.5
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	5	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:26:A:LEU:HD23	1:26:A:LEU:H	19	0.5
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	13	0.5
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	8	0.5
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	19	0.5
(2,29)	1:88:A:TYR:HD1	1:159:A:TYR:HD1	16	0.5
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD21	11	0.49
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG23	11	0.49
(4,446)	1:110:A:LEU:HD12	1:110:A:LEU:HG	2	0.49
(4,446)	1:110:A:LEU:HD11	1:110:A:LEU:HG	14	0.49
(4,446)	1:110:A:LEU:HD13	1:110:A:LEU:HG	15	0.49
(4,446)	1:110:A:LEU:HD12	1:110:A:LEU:HG	18	0.49
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	10	0.49
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	18	0.49
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD11	3	0.49
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	10	0.49
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	13	0.49
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	10	0.49
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD12	2	0.49
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD12	5	0.49
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG22	7	0.49
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	1	0.49
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	6	0.49
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	2	0.49
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	15	0.49
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	4	0.49
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	9	0.49
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	18	0.49
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD12	9	0.49
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	6	0.49
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD23	13	0.49
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD21	18	0.49
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	9	0.49
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	18	0.49
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD21	1	0.49
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	16	0.49
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	12	0.49
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	17	0.49
(2,3600)	1:42:A:LYS:HE2	1:39:A:ALA:HA	13	0.49
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	3	0.49
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	11	0.49
(2,3466)	1:97:A:LEU:HD22	1:166:A:TRP:HB2	17	0.49
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	4	0.49
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	10	0.49
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	17	0.49
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	4	0.49
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	6	0.49
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	10	0.49
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	11	0.49
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	5	0.49
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	8	0.49
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	9	0.49
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	11	0.49
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	16	0.49
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	9	0.49
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	6	0.49
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	19	0.49
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	19	0.49
(2,1872)	1:168:A:ILE:HD11	1:168:A:ILE:HG13	12	0.49
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	20	0.49
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	17	0.49
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	15	0.49
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	9	0.49
(2,1840)	1:128:A:ILE:HG23	1:129:A:THR:HG21	10	0.49
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD11	19	0.49
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	14	0.49
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	14	0.49
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	5	0.49
(2,1807)	1:151:A:MET:HE2	1:174:A:GLU:HG2	15	0.49
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	7	0.49
(2,1793)	1:53:A:LEU:HD12	1:53:A:LEU:HB2	18	0.49
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG23	17	0.49
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	19	0.49
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	1	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	2	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	6	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	8	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	9	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	10	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	12	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	13	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	16	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	17	0.49
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	18	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	20	0.49
(2,1531)	1:21:A:LEU:HD11	1:14:A:VAL:HA	3	0.49
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	2	0.49
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	10	0.49
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	20	0.49
(2,1462)	1:14:A:VAL:HG21	1:14:A:VAL:H	3	0.49
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	3	0.49
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	10	0.49
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	12	0.49
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	6	0.49
(2,1291)	1:84:A:VAL:HG11	1:84:A:VAL:H	5	0.49
(2,1291)	1:84:A:VAL:HG12	1:84:A:VAL:H	19	0.49
(2,1288)	1:167:A:LEU:HD23	1:167:A:LEU:HA	2	0.49
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	14	0.49
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	16	0.49
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	10	0.49
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	13	0.49
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	19	0.49
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	20	0.49
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB2	4	0.49
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	4	0.49
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	9	0.49
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	13	0.49
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	19	0.49
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	8	0.49
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	15	0.49
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	14	0.49
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	5	0.49
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	8	0.49
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	11	0.49
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	14	0.49
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	16	0.49
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	1	0.48
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	3	0.48
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	14	0.48
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	17	0.48
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	7	0.48
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD13	1	0.48
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD13	12	0.48
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD13	15	0.48
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	2	0.48
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	12	0.48
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	15	0.48
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG23	11	0.48
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG21	14	0.48
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG22	15	0.48
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	17	0.48
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	4	0.48
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	9	0.48
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	5	0.48
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	14	0.48
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	9	0.48
(4,278)	1:142:A:VAL:HG12	1:102:A:ALA:H	12	0.48
(4,204)	1:173:A:ALA:HB1	1:111:A:LYS:HG3	5	0.48
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	9	0.48
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	3	0.48
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	17	0.48
(4,95)	1:51:A:GLU:H	1:58:A:GLU:HG3	18	0.48
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	15	0.48
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	8	0.48
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	12	0.48
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	11	0.48
(2,3964)	1:123:A:HIS:HB3	2:201:A:NAD:H6N	20	0.48
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	10	0.48
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD23	7	0.48
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	9	0.48
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	17	0.48
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	6	0.48
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	20	0.48
(2,3832)	1:97:A:LEU:HD23	1:151:A:MET:HG3	11	0.48
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	11	0.48
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	13	0.48
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	9	0.48
(2,3798)	1:48:A:ILE:HD11	1:48:A:ILE:HG13	18	0.48
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	20	0.48
(2,3676)	1:86:A:LEU:HD21	1:86:A:LEU:HA	6	0.48
(2,3676)	1:86:A:LEU:HD23	1:86:A:LEU:HA	8	0.48
(2,3676)	1:86:A:LEU:HD23	1:86:A:LEU:HA	12	0.48
(2,3676)	1:86:A:LEU:HD21	1:86:A:LEU:HA	16	0.48
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	6	0.48
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	5	0.48
(2,3514)	1:143:A:VAL:HG11	1:132:A:ARG:HA	17	0.48
(2,3415)	1:122:A:VAL:HG22	1:122:A:VAL:H	19	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	18	0.48
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	5	0.48
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	15	0.48
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	3	0.48
(2,2521)	1:105:A:ASN:H	1:102:A:ALA:HB3	8	0.48
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG12	4	0.48
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	9	0.48
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	1	0.48
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	3	0.48
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	4	0.48
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	20	0.48
(2,1859)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	18	0.48
(2,1851)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	8	0.48
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	10	0.48
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	18	0.48
(2,1823)	1:37:A:LEU:HD13	1:41:A:MET:HE3	19	0.48
(2,1821)	1:143:A:VAL:HG22	1:143:A:VAL:HB	6	0.48
(2,1821)	1:143:A:VAL:HG22	1:143:A:VAL:HB	7	0.48
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	10	0.48
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	12	0.48
(2,1744)	1:109:A:ILE:HG21	1:109:A:ILE:HA	19	0.48
(2,1744)	1:109:A:ILE:HG21	1:109:A:ILE:HA	20	0.48
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	1	0.48
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	3	0.48
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	4	0.48
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	7	0.48
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	11	0.48
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	14	0.48
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	15	0.48
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	19	0.48
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	3	0.48
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	15	0.48
(2,1531)	1:21:A:LEU:HD11	1:14:A:VAL:HA	1	0.48
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	4	0.48
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	6	0.48
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	9	0.48
(2,1435)	1:15:A:LEU:HD23	1:15:A:LEU:H	5	0.48
(2,1435)	1:15:A:LEU:HD22	1:15:A:LEU:H	20	0.48
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	5	0.48
(2,1407)	1:95:A:ALA:HB3	1:95:A:ALA:H	19	0.48
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	16	0.48
(2,1377)	1:4:A:MET:HE1	1:55:A:HIS:HD2	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	18	0.48
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	7	0.48
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	12	0.48
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	18	0.48
(2,1281)	1:160:A:LEU:HD21	1:166:A:TRP:HD1	2	0.48
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	16	0.48
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	5	0.48
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	7	0.48
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	9	0.48
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	13	0.48
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	18	0.48
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	4	0.48
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	14	0.48
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	6	0.48
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	13	0.48
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	13	0.48
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	6	0.48
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	14	0.48
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	10	0.48
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	12	0.48
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	2	0.48
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	11	0.48
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	15	0.48
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	20	0.48
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	2	0.48
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	14	0.48
(2,203)	1:24:A:LEU:H	1:14:A:VAL:HG11	12	0.48
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	17	0.48
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	1	0.48
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	4	0.48
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	7	0.48
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	12	0.48
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	17	0.48
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	18	0.48
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	20	0.48
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	8	0.47
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	15	0.47
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	10	0.47
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	20	0.47
(4,446)	1:110:A:LEU:HD11	1:110:A:LEU:HG	5	0.47
(4,446)	1:110:A:LEU:HD12	1:110:A:LEU:HG	16	0.47
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	14	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	17	0.47
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	9	0.47
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	20	0.47
(4,415)	1:19:A:PRO:HB3	1:36:A:GLU:HG2	1	0.47
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD12	20	0.47
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	18	0.47
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	19	0.47
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	1	0.47
(4,311)	1:143:A:VAL:HG12	1:178:A:VAL:HA	9	0.47
(4,303)	1:110:A:LEU:HD13	1:107:A:ASP:HA	5	0.47
(4,301)	1:97:A:LEU:HD22	1:156:A:PHE:HB2	5	0.47
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	2	0.47
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	20	0.47
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB2	7	0.47
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	2	0.47
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	2	0.47
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	6	0.47
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	10	0.47
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	15	0.47
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	2	0.47
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	5	0.47
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	12	0.47
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	4	0.47
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	12	0.47
(2,3832)	1:97:A:LEU:HD23	1:151:A:MET:HG3	7	0.47
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD21	3	0.47
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	19	0.47
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	19	0.47
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	18	0.47
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	3	0.47
(2,3782)	1:143:A:VAL:HG22	1:143:A:VAL:HB	6	0.47
(2,3782)	1:143:A:VAL:HG22	1:143:A:VAL:HB	7	0.47
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	5	0.47
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	16	0.47
(2,3749)	1:44:A:LYS:HG3	1:21:A:LEU:HD22	20	0.47
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	19	0.47
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	13	0.47
(2,3676)	1:86:A:LEU:HD23	1:86:A:LEU:HA	14	0.47
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	13	0.47
(2,3527)	1:84:A:VAL:HG23	1:85:A:ASP:HB2	5	0.47
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	10	0.47
(2,3492)	1:96:A:VAL:HG11	1:96:A:VAL:HA	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3466)	1:97:A:LEU:HD21	1:166:A:TRP:HB2	2	0.47
(2,3459)	1:167:A:LEU:HD23	1:123:A:HIS:HA	2	0.47
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	13	0.47
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	17	0.47
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	4	0.47
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	12	0.47
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	16	0.47
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	18	0.47
(2,3391)	1:56:A:ILE:HG23	1:65:A:PHE:HD1	9	0.47
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	7	0.47
(2,3355)	1:41:A:MET:HE2	1:41:A:MET:H	5	0.47
(2,3346)	1:4:A:MET:HE1	1:55:A:HIS:HD2	12	0.47
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	8	0.47
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	7	0.47
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	10	0.47
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	17	0.47
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	1	0.47
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	2	0.47
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	3	0.47
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	8	0.47
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	11	0.47
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	19	0.47
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG22	5	0.47
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	6	0.47
(2,1859)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	9	0.47
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	14	0.47
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	15	0.47
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	17	0.47
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	15	0.47
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	17	0.47
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	18	0.47
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	14	0.47
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	19	0.47
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD12	17	0.47
(2,1823)	1:37:A:LEU:HD13	1:41:A:MET:HE3	13	0.47
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	1	0.47
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	2	0.47
(2,1821)	1:143:A:VAL:HG21	1:143:A:VAL:HB	5	0.47
(2,1821)	1:143:A:VAL:HG21	1:143:A:VAL:HB	16	0.47
(2,1821)	1:143:A:VAL:HG22	1:143:A:VAL:HB	19	0.47
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	8	0.47
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	10	0.47
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	6	0.47
(2,1813)	1:53:A:LEU:HD12	1:53:A:LEU:HG	6	0.47
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	4	0.47
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	1	0.47
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	3	0.47
(2,1744)	1:109:A:ILE:HG21	1:109:A:ILE:HA	9	0.47
(2,1744)	1:109:A:ILE:HG21	1:109:A:ILE:HA	15	0.47
(2,1710)	1:26:A:LEU:HD22	1:15:A:LEU:HA	19	0.47
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	14	0.47
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	1	0.47
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	12	0.47
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	13	0.47
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	16	0.47
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	18	0.47
(2,1490)	1:167:A:LEU:HD12	1:166:A:TRP:HA	9	0.47
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	11	0.47
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	5	0.47
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	3	0.47
(2,1424)	1:56:A:ILE:HG21	1:65:A:PHE:HE1	14	0.47
(2,1388)	1:41:A:MET:HE2	1:41:A:MET:H	17	0.47
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	19	0.47
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	8	0.47
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	5	0.47
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	15	0.47
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	19	0.47
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	16	0.47
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	8	0.47
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	18	0.47
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	6	0.47
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	7	0.47
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	6	0.47
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	5	0.47
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	16	0.47
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	16	0.47
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	18	0.47
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	10	0.47
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	20	0.47
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	20	0.47
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	16	0.47
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	5	0.47
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD21	18	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	9	0.47
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	12	0.47
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	2	0.47
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	6	0.47
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	13	0.47
(2,16)	1:21:A:LEU:HD13	1:10:A:PHE:HE1	20	0.47
(4,449)	1:74:A:ILE:HD13	1:57:A:VAL:HG23	12	0.46
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD12	3	0.46
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD12	4	0.46
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	11	0.46
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	12	0.46
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD12	16	0.46
(4,446)	1:110:A:LEU:HD12	1:110:A:LEU:HG	11	0.46
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	3	0.46
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	9	0.46
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	10	0.46
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG23	3	0.46
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD12	6	0.46
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG22	10	0.46
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	2	0.46
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	5	0.46
(4,204)	1:173:A:ALA:HB2	1:114:A:ILE:HG13	12	0.46
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	10	0.46
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	8	0.46
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	11	0.46
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	4	0.46
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	10	0.46
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD21	14	0.46
(2,3843)	1:76:A:ALA:HB1	1:16:A:ARG:HA	5	0.46
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	19	0.46
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	6	0.46
(2,3832)	1:97:A:LEU:HD23	1:151:A:MET:HG3	16	0.46
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	7	0.46
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	20	0.46
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	8	0.46
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	13	0.46
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	1	0.46
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	2	0.46
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	3	0.46
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	12	0.46
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	9	0.46
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	1	0.46
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	2	0.46
(2,3782)	1:143:A:VAL:HG21	1:143:A:VAL:HB	16	0.46
(2,3782)	1:143:A:VAL:HG22	1:143:A:VAL:HB	19	0.46
(2,3761)	1:117:A:MET:HE1	1:117:A:MET:HB2	20	0.46
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	4	0.46
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	13	0.46
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	6	0.46
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	15	0.46
(2,3570)	1:4:A:MET:HE2	1:52:A:GLU:HA	11	0.46
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	17	0.46
(2,3514)	1:143:A:VAL:HG11	1:132:A:ARG:HA	14	0.46
(2,3490)	1:48:A:ILE:HD13	1:53:A:LEU:HA	18	0.46
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	8	0.46
(2,3467)	1:11:A:LEU:HD12	1:38:A:LEU:HA	6	0.46
(2,3434)	1:15:A:LEU:HD12	1:65:A:PHE:HE1	20	0.46
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	8	0.46
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	19	0.46
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	9	0.46
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	11	0.46
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	18	0.46
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	3	0.46
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	20	0.46
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	18	0.46
(2,3177)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	4	0.46
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG12	3	0.46
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG12	11	0.46
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	13	0.46
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	17	0.46
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	7	0.46
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	9	0.46
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	11	0.46
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	18	0.46
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	19	0.46
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	17	0.46
(2,1877)	1:129:A:THR:HG21	1:129:A:THR:HA	20	0.46
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	9	0.46
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	3	0.46
(2,1859)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	2	0.46
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	2	0.46
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	6	0.46
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	19	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1827)	1:21:A:LEU:HD23	1:21:A:LEU:HG	2	0.46
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	5	0.46
(2,1827)	1:21:A:LEU:HD23	1:21:A:LEU:HG	9	0.46
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	3	0.46
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	8	0.46
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	10	0.46
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	12	0.46
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	20	0.46
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	15	0.46
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	1	0.46
(2,1819)	1:86:A:LEU:HD23	1:86:A:LEU:HG	5	0.46
(2,1819)	1:86:A:LEU:HD23	1:86:A:LEU:HG	6	0.46
(2,1819)	1:86:A:LEU:HD23	1:86:A:LEU:HG	7	0.46
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	19	0.46
(2,1793)	1:53:A:LEU:HD12	1:53:A:LEU:HB2	10	0.46
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	11	0.46
(2,1744)	1:109:A:ILE:HG21	1:109:A:ILE:HA	8	0.46
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	14	0.46
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	20	0.46
(2,1568)	1:32:A:ALA:HB1	1:32:A:ALA:HA	5	0.46
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	5	0.46
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	3	0.46
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	7	0.46
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	11	0.46
(2,1490)	1:167:A:LEU:HD13	1:166:A:TRP:HA	19	0.46
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	11	0.46
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	20	0.46
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	9	0.46
(2,1377)	1:4:A:MET:HE1	1:55:A:HIS:HD2	18	0.46
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	17	0.46
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	7	0.46
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	9	0.46
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	2	0.46
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	3	0.46
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	13	0.46
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	14	0.46
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	16	0.46
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	19	0.46
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	6	0.46
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	8	0.46
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	17	0.46
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	6	0.46
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	17	0.46
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	3	0.46
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	2	0.46
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	2	0.46
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	10	0.46
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	1	0.46
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	17	0.46
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	1	0.46
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	6	0.46
(2,405)	1:95:A:ALA:HB2	1:149:A:LYS:H	7	0.46
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	6	0.46
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	4	0.46
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	5	0.46
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	19	0.46
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	1	0.46
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	10	0.46
(2,32)	1:88:A:TYR:HE1	1:159:A:TYR:HD1	2	0.46
(2,19)	1:13:A:LEU:HA	1:17:A:HIS:HD2	16	0.46
(4,450)	1:97:A:LEU:HD22	1:124:A:LEU:HD23	16	0.45
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	7	0.45
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD12	9	0.45
(4,446)	1:110:A:LEU:HD12	1:110:A:LEU:HG	10	0.45
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	20	0.45
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD11	7	0.45
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	17	0.45
(4,320)	1:151:A:MET:HE1	1:147:A:ASP:HB2	3	0.45
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	13	0.45
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	1	0.45
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	3	0.45
(4,274)	1:124:A:LEU:HD21	1:156:A:PHE:HZ	9	0.45
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	18	0.45
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	4	0.45
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	4	0.45
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD11	15	0.45
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	2	0.45
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	10	0.45
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	17	0.45
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	10	0.45
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	16	0.45
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	4	0.45
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD21	16	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3821)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	8	0.45
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	15	0.45
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	19	0.45
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	3	0.45
(2,3782)	1:143:A:VAL:HG21	1:143:A:VAL:HB	5	0.45
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	8	0.45
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	10	0.45
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	20	0.45
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	14	0.45
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	1	0.45
(2,3676)	1:86:A:LEU:HD23	1:86:A:LEU:HA	4	0.45
(2,3676)	1:86:A:LEU:HD21	1:86:A:LEU:HA	7	0.45
(2,3570)	1:4:A:MET:HE3	1:52:A:GLU:HA	16	0.45
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	12	0.45
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	3	0.45
(2,3514)	1:143:A:VAL:HG12	1:132:A:ARG:HA	15	0.45
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	14	0.45
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	7	0.45
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	20	0.45
(2,3428)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	7	0.45
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	2	0.45
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	3	0.45
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	5	0.45
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	7	0.45
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	11	0.45
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	12	0.45
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	7	0.45
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	2	0.45
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	6	0.45
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	13	0.45
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	6	0.45
(2,3344)	1:41:A:MET:HE2	1:10:A:PHE:HD1	5	0.45
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	1	0.45
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	11	0.45
(2,3079)	1:118:A:SER:H	2:201:A:NAD:H51A	1	0.45
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	4	0.45
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	5	0.45
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	10	0.45
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	4	0.45
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	10	0.45
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	13	0.45
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	17	0.45
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	3	0.45
(2,1859)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	4	0.45
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	6	0.45
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	14	0.45
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	9	0.45
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	16	0.45
(2,1827)	1:21:A:LEU:HD23	1:21:A:LEU:HG	8	0.45
(2,1827)	1:21:A:LEU:HD23	1:21:A:LEU:HG	17	0.45
(2,1823)	1:37:A:LEU:HD13	1:41:A:MET:HE1	9	0.45
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	4	0.45
(2,1821)	1:143:A:VAL:HG22	1:143:A:VAL:HB	9	0.45
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	11	0.45
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	15	0.45
(2,1821)	1:143:A:VAL:HG22	1:143:A:VAL:HB	17	0.45
(2,1821)	1:143:A:VAL:HG22	1:143:A:VAL:HB	18	0.45
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	18	0.45
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	11	0.45
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	17	0.45
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	6	0.45
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	12	0.45
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	17	0.45
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	3	0.45
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	16	0.45
(2,1601)	1:41:A:MET:HE2	1:10:A:PHE:HB3	7	0.45
(2,1588)	1:152:A:ALA:HB2	1:149:A:LYS:HA	14	0.45
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	9	0.45
(2,1554)	1:38:A:LEU:HD21	1:50:A:MET:HG2	16	0.45
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	17	0.45
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	15	0.45
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	4	0.45
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	15	0.45
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	1	0.45
(2,1314)	1:142:A:VAL:HG11	1:103:A:GLU:HA	14	0.45
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	19	0.45
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	1	0.45
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	4	0.45
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	18	0.45
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	20	0.45
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	4	0.45
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	8	0.45
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	11	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	15	0.45
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	20	0.45
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	15	0.45
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	2	0.45
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	4	0.45
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	8	0.45
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	6	0.45
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	4	0.45
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	3	0.45
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	1	0.45
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	14	0.45
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	18	0.45
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	3	0.45
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	4	0.45
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	12	0.45
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	20	0.45
(2,30)	1:88:A:TYR:HD1	1:159:A:TYR:HE1	13	0.45
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	11	0.45
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	2	0.44
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	19	0.44
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	4	0.44
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	11	0.44
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	17	0.44
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	19	0.44
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG22	8	0.44
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	19	0.44
(4,368)	1:20:A:ALA:HB1	1:22:A:ILE:HB	10	0.44
(4,328)	1:122:A:VAL:HG12	1:113:A:GLY:HA2	14	0.44
(4,320)	1:151:A:MET:HE3	1:158:A:PHE:HB3	11	0.44
(4,129)	1:13:A:LEU:HD23	1:18:A:ASN:H	12	0.44
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD21	8	0.44
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	15	0.44
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	9	0.44
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	13	0.44
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	18	0.44
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	1	0.44
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	7	0.44
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD23	20	0.44
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	4	0.44
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	8	0.44
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	15	0.44
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	7	0.44
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	6	0.44
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	17	0.44
(2,3791)	1:142:A:VAL:HG23	1:143:A:VAL:HB	7	0.44
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	4	0.44
(2,3782)	1:143:A:VAL:HG22	1:143:A:VAL:HB	9	0.44
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	11	0.44
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	12	0.44
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	15	0.44
(2,3782)	1:143:A:VAL:HG22	1:143:A:VAL:HB	18	0.44
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	18	0.44
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	9	0.44
(2,3676)	1:86:A:LEU:HD23	1:86:A:LEU:HA	19	0.44
(2,3600)	1:42:A:LYS:HE2	1:39:A:ALA:HA	8	0.44
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	4	0.44
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	2	0.44
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	1	0.44
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	18	0.44
(2,3427)	1:165:A:VAL:HG13	2:201:A:NAD:H5N	7	0.44
(2,3415)	1:122:A:VAL:HG21	1:122:A:VAL:H	11	0.44
(2,3415)	1:122:A:VAL:HG22	1:122:A:VAL:H	18	0.44
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	4	0.44
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	10	0.44
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	16	0.44
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	19	0.44
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	7	0.44
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	8	0.44
(2,3399)	1:21:A:LEU:HD11	1:21:A:LEU:H	14	0.44
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	17	0.44
(2,3346)	1:4:A:MET:HE1	1:55:A:HIS:HD2	18	0.44
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	16	0.44
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	19	0.44
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	10	0.44
(2,2748)	1:86:A:LEU:HD11	1:87:A:GLY:H	13	0.44
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	8	0.44
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	16	0.44
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	6	0.44
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	8	0.44
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	13	0.44
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	2	0.44
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	6	0.44
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	11	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	15	0.44
(2,1877)	1:129:A:THR:HG22	1:129:A:THR:HA	2	0.44
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	13	0.44
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	1	0.44
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	11	0.44
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG22	10	0.44
(2,1856)	1:22:A:ILE:HD11	1:14:A:VAL:HG21	13	0.44
(2,1851)	1:56:A:ILE:HD12	1:11:A:LEU:HD13	5	0.44
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	7	0.44
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	7	0.44
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	8	0.44
(2,1827)	1:21:A:LEU:HD23	1:21:A:LEU:HG	7	0.44
(2,1827)	1:21:A:LEU:HD21	1:21:A:LEU:HG	13	0.44
(2,1821)	1:143:A:VAL:HG23	1:143:A:VAL:HB	14	0.44
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	3	0.44
(2,1819)	1:86:A:LEU:HD22	1:86:A:LEU:HG	4	0.44
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	18	0.44
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	15	0.44
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	15	0.44
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	19	0.44
(2,1744)	1:109:A:ILE:HG23	1:109:A:ILE:HA	11	0.44
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	16	0.44
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	18	0.44
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG21	4	0.44
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	10	0.44
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	11	0.44
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	8	0.44
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	14	0.44
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	7	0.44
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	17	0.44
(2,1426)	1:86:A:LEU:HD11	1:88:A:TYR:HD1	13	0.44
(2,1407)	1:95:A:ALA:HB3	1:95:A:ALA:H	7	0.44
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	8	0.44
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	11	0.44
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	15	0.44
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	16	0.44
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	17	0.44
(2,1211)	1:177:A:LYS:HD2	1:177:A:LYS:HA	11	0.44
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	6	0.44
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	10	0.44
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	8	0.44
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	12	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	19	0.44
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	20	0.44
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	1	0.44
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	19	0.44
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	16	0.44
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	1	0.44
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	4	0.44
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	8	0.44
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	18	0.44
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	4	0.44
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB1	2	0.44
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	20	0.44
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	7	0.44
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	13	0.44
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	13	0.44
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	3	0.44
(2,339)	1:108:A:LEU:HD23	1:108:A:LEU:H	6	0.44
(2,300)	1:153:A:ASP:H	1:95:A:ALA:HB1	6	0.44
(2,233)	1:21:A:LEU:HB2	1:21:A:LEU:H	1	0.44
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	6	0.44
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	8	0.44
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	9	0.44
(2,175)	1:53:A:LEU:HD22	1:56:A:ILE:H	6	0.44
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	7	0.44
(2,175)	1:53:A:LEU:HD22	1:56:A:ILE:H	16	0.44
(2,19)	1:13:A:LEU:HA	1:17:A:HIS:HD2	20	0.44
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	13	0.44
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HG3	20	0.43
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD12	6	0.43
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	13	0.43
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD11	15	0.43
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	8	0.43
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD13	18	0.43
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	19	0.43
(4,413)	1:144:A:LEU:HG	1:101:A:THR:HG22	19	0.43
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	20	0.43
(4,316)	1:37:A:LEU:HD22	1:8:A:SER:HB2	2	0.43
(4,311)	1:96:A:VAL:HG11	1:94:A:PRO:HA	10	0.43
(4,300)	1:97:A:LEU:HD23	1:156:A:PHE:HB3	11	0.43
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	18	0.43
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	1	0.43
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,259)	1:117:A:MET:HE2	2:201:A:NAD:H2A	20	0.43
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	1	0.43
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD2	8	0.43
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB2	4	0.43
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	10	0.43
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	2	0.43
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	7	0.43
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	20	0.43
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD21	11	0.43
(2,3836)	1:168:A:ILE:HD12	1:171:A:VAL:HG13	5	0.43
(2,3833)	1:168:A:ILE:HD11	1:168:A:ILE:HG13	12	0.43
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	20	0.43
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	20	0.43
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	8	0.43
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	10	0.43
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	1	0.43
(2,3782)	1:143:A:VAL:HG23	1:143:A:VAL:HB	14	0.43
(2,3782)	1:143:A:VAL:HG22	1:143:A:VAL:HB	17	0.43
(2,3781)	1:142:A:VAL:HG11	1:142:A:VAL:HB	2	0.43
(2,3742)	1:24:A:LEU:HD13	1:36:A:GLU:HG2	13	0.43
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG23	15	0.43
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG23	17	0.43
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	19	0.43
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	2	0.43
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	3	0.43
(2,3676)	1:86:A:LEU:HD21	1:86:A:LEU:HA	5	0.43
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	10	0.43
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	11	0.43
(2,3676)	1:86:A:LEU:HD22	1:86:A:LEU:HA	17	0.43
(2,3607)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	19	0.43
(2,3600)	1:42:A:LYS:HE2	1:39:A:ALA:HA	2	0.43
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE1	9	0.43
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE2	2	0.43
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	9	0.43
(2,3544)	1:66:A:ALA:HB3	1:66:A:ALA:HA	10	0.43
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	13	0.43
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	17	0.43
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	19	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	2	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	6	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	8	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	10	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	12	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	16	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	17	0.43
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	18	0.43
(2,3527)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	18	0.43
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	6	0.43
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	12	0.43
(2,3466)	1:97:A:LEU:HD22	1:166:A:TRP:HB2	20	0.43
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	1	0.43
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	7	0.43
(2,3439)	1:110:A:LEU:HD11	1:110:A:LEU:H	13	0.43
(2,3430)	1:128:A:ILE:HD13	1:127:A:ASP:H	14	0.43
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	1	0.43
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	6	0.43
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	8	0.43
(2,3411)	1:56:A:ILE:HG23	1:56:A:ILE:H	9	0.43
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	20	0.43
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	1	0.43
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	8	0.43
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	9	0.43
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	13	0.43
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	2	0.43
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	10	0.43
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	11	0.43
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	15	0.43
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	17	0.43
(2,3177)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	2	0.43
(2,3177)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	3	0.43
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD21	7	0.43
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	13	0.43
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	17	0.43
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	19	0.43
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	1	0.43
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	8	0.43
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	15	0.43
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	10	0.43
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	14	0.43
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	15	0.43
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	7	0.43
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	8	0.43
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	15	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	1	0.43
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	16	0.43
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	5	0.43
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	19	0.43
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	4	0.43
(2,1834)	1:14:A:VAL:HG23	1:21:A:LEU:HG	11	0.43
(2,1825)	1:38:A:LEU:HG	1:38:A:LEU:HD12	16	0.43
(2,1821)	1:143:A:VAL:HG22	1:143:A:VAL:HB	13	0.43
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	20	0.43
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	11	0.43
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	12	0.43
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	8	0.43
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	14	0.43
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	20	0.43
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	5	0.43
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	2	0.43
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	8	0.43
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	12	0.43
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	2	0.43
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	4	0.43
(2,1744)	1:109:A:ILE:HG23	1:109:A:ILE:HA	5	0.43
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	6	0.43
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	7	0.43
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	17	0.43
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	6	0.43
(2,1588)	1:152:A:ALA:HB2	1:149:A:LYS:HA	2	0.43
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	2	0.43
(2,1541)	1:143:A:VAL:HG11	1:132:A:ARG:HA	12	0.43
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	16	0.43
(2,1534)	1:151:A:MET:HE2	1:151:A:MET:HA	4	0.43
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	19	0.43
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	16	0.43
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	10	0.43
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	12	0.43
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	1	0.43
(2,1435)	1:15:A:LEU:HD22	1:15:A:LEU:H	4	0.43
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	3	0.43
(2,1388)	1:41:A:MET:HE2	1:41:A:MET:H	16	0.43
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	15	0.43
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	2	0.43
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	3	0.43
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	14	0.43
(2,1295)	1:57:A:VAL:HG11	1:57:A:VAL:HA	1	0.43
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	11	0.43
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	3	0.43
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	8	0.43
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	9	0.43
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	11	0.43
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	16	0.43
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	2	0.43
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	18	0.43
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	5	0.43
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	6	0.43
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	9	0.43
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	12	0.43
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	15	0.43
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	17	0.43
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	6	0.43
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	9	0.43
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	17	0.43
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	5	0.43
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	19	0.43
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	17	0.43
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	1	0.43
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	8	0.43
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	14	0.43
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD22	3	0.43
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	15	0.43
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD21	15	0.43
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD23	20	0.43
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	16	0.43
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	9	0.43
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	9	0.43
(2,29)	1:88:A:TYR:HD1	1:159:A:TYR:HD1	12	0.43
(2,19)	1:13:A:LEU:HA	1:17:A:HIS:HD2	7	0.43
(2,16)	1:21:A:LEU:HD13	1:10:A:PHE:HE1	8	0.43
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD12	8	0.42
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	1	0.42
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	2	0.42
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	2	0.42
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	5	0.42
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	8	0.42
(4,437)	1:178:A:VAL:HG21	1:177:A:LYS:HG2	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	13	0.42
(4,413)	1:108:A:LEU:HG	1:108:A:LEU:HD13	16	0.42
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	8	0.42
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	15	0.42
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	11	0.42
(4,311)	1:143:A:VAL:HG12	1:178:A:VAL:HA	14	0.42
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	15	0.42
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	17	0.42
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	3	0.42
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	5	0.42
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	6	0.42
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	12	0.42
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	14	0.42
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	16	0.42
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	19	0.42
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	13	0.42
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD22	3	0.42
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	3	0.42
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	1	0.42
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	12	0.42
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	8	0.42
(2,3811)	1:15:A:LEU:HD11	1:74:A:ILE:HD12	17	0.42
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	5	0.42
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	9	0.42
(2,3798)	1:48:A:ILE:HD12	1:48:A:ILE:HG13	13	0.42
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	14	0.42
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	16	0.42
(2,3797)	1:146:A:VAL:HG11	1:174:A:GLU:HG2	5	0.42
(2,3782)	1:143:A:VAL:HG22	1:143:A:VAL:HB	13	0.42
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	7	0.42
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	7	0.42
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	6	0.42
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	13	0.42
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	1	0.42
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	4	0.42
(2,3544)	1:66:A:ALA:HB3	1:66:A:ALA:HA	7	0.42
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	16	0.42
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	4	0.42
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	13	0.42
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	14	0.42
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	15	0.42
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	19	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	20	0.42
(2,3514)	1:143:A:VAL:HG11	1:132:A:ARG:HA	10	0.42
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	13	0.42
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	5	0.42
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	4	0.42
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	16	0.42
(2,3411)	1:56:A:ILE:HG21	1:56:A:ILE:H	14	0.42
(2,3411)	1:56:A:ILE:HG22	1:56:A:ILE:H	15	0.42
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	3	0.42
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	9	0.42
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	18	0.42
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	19	0.42
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	14	0.42
(2,3265)	1:84:A:VAL:HG11	1:84:A:VAL:H	7	0.42
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	1	0.42
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	6	0.42
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD21	1	0.42
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD21	16	0.42
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD11	16	0.42
(2,2738)	1:30:A:GLY:H	1:26:A:LEU:HD21	3	0.42
(2,2521)	1:105:A:ASN:H	1:102:A:ALA:HB3	15	0.42
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	12	0.42
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	17	0.42
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	2	0.42
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	4	0.42
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	2	0.42
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	5	0.42
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	9	0.42
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	14	0.42
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	16	0.42
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	19	0.42
(2,1872)	1:168:A:ILE:HD11	1:168:A:ILE:HG13	5	0.42
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	14	0.42
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	18	0.42
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	15	0.42
(2,1834)	1:14:A:VAL:HG22	1:21:A:LEU:HG	13	0.42
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	13	0.42
(2,1819)	1:86:A:LEU:HD22	1:86:A:LEU:HG	8	0.42
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	3	0.42
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	9	0.42
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	12	0.42
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	13	0.42
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	15	0.42
(2,1500)	1:11:A:LEU:HD13	1:38:A:LEU:HA	20	0.42
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	2	0.42
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	2	0.42
(2,1377)	1:4:A:MET:HE1	1:55:A:HIS:HD2	7	0.42
(2,1377)	1:4:A:MET:HE3	1:55:A:HIS:HD2	9	0.42
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	6	0.42
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	13	0.42
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	10	0.42
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	15	0.42
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	6	0.42
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	16	0.42
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	9	0.42
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	2	0.42
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	2	0.42
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	7	0.42
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	13	0.42
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	9	0.42
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	12	0.42
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	19	0.42
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	20	0.42
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	14	0.42
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	8	0.42
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	10	0.42
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	16	0.42
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	17	0.42
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	8	0.42
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	11	0.42
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	19	0.42
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	4	0.42
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	12	0.42
(2,118)	1:171:A:VAL:H	1:171:A:VAL:HG21	15	0.42
(2,16)	1:21:A:LEU:HD13	1:10:A:PHE:HE1	1	0.42
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	2	0.42
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	13	0.41
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	17	0.41
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	6	0.41
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG22	16	0.41
(4,325)	1:7:A:VAL:HG13	1:10:A:PHE:HB3	16	0.41
(4,320)	1:151:A:MET:HE3	1:158:A:PHE:HB3	2	0.41
(4,195)	1:114:A:ILE:HD11	1:117:A:MET:HE1	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	4	0.41
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	5	0.41
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	16	0.41
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD12	20	0.41
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	18	0.41
(2,3899)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	2	0.41
(2,3834)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	15	0.41
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	1	0.41
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	2	0.41
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	8	0.41
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	11	0.41
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	19	0.41
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	8	0.41
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	12	0.41
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	20	0.41
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	7	0.41
(2,3798)	1:48:A:ILE:HD11	1:48:A:ILE:HG13	11	0.41
(2,3798)	1:48:A:ILE:HD11	1:48:A:ILE:HG13	20	0.41
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	1	0.41
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	5	0.41
(2,3761)	1:117:A:MET:HE1	1:117:A:MET:HB2	17	0.41
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	5	0.41
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	11	0.41
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	17	0.41
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	13	0.41
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	2	0.41
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	11	0.41
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	19	0.41
(2,3666)	1:43:A:ALA:HB1	1:43:A:ALA:HA	18	0.41
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE3	3	0.41
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	8	0.41
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	11	0.41
(2,3544)	1:66:A:ALA:HB3	1:66:A:ALA:HA	18	0.41
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	1	0.41
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	3	0.41
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	7	0.41
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	11	0.41
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	5	0.41
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	10	0.41
(2,3482)	1:38:A:LEU:HD22	1:49:A:SER:HA	8	0.41
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	4	0.41
(2,3439)	1:110:A:LEU:HD11	1:110:A:LEU:H	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3428)	1:108:A:LEU:HD12	2:201:A:NAD:H2A	5	0.41
(2,3415)	1:122:A:VAL:HG23	1:122:A:VAL:H	12	0.41
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	4	0.41
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	12	0.41
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	13	0.41
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	13	0.41
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	15	0.41
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	3	0.41
(2,3346)	1:4:A:MET:HE1	1:55:A:HIS:HD2	7	0.41
(2,3346)	1:4:A:MET:HE3	1:55:A:HIS:HD2	9	0.41
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	17	0.41
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	19	0.41
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	20	0.41
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD11	17	0.41
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	7	0.41
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	7	0.41
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	10	0.41
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	2	0.41
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	3	0.41
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	12	0.41
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	17	0.41
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	15	0.41
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	8	0.41
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	11	0.41
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	17	0.41
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	11	0.41
(2,1834)	1:14:A:VAL:HG21	1:21:A:LEU:HG	12	0.41
(2,1827)	1:21:A:LEU:HD22	1:21:A:LEU:HG	6	0.41
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	7	0.41
(2,1819)	1:86:A:LEU:HD22	1:86:A:LEU:HG	12	0.41
(2,1819)	1:86:A:LEU:HD22	1:86:A:LEU:HG	18	0.41
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	11	0.41
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	17	0.41
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG21	9	0.41
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG21	20	0.41
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	5	0.41
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	20	0.41
(2,1744)	1:109:A:ILE:HG23	1:109:A:ILE:HA	1	0.41
(2,1744)	1:109:A:ILE:HG22	1:109:A:ILE:HA	13	0.41
(2,1744)	1:109:A:ILE:HG21	1:109:A:ILE:HA	17	0.41
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	2	0.41
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	11	0.41
(2,1699)	1:43:A:ALA:HB1	1:43:A:ALA:HA	18	0.41
(2,1599)	1:4:A:MET:HE1	1:52:A:GLU:HA	10	0.41
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	13	0.41
(2,1555)	1:84:A:VAL:HG21	1:85:A:ASP:HB2	15	0.41
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	3	0.41
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	18	0.41
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	15	0.41
(2,1377)	1:4:A:MET:HE3	1:55:A:HIS:HD2	16	0.41
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	2	0.41
(2,1314)	1:142:A:VAL:HG11	1:103:A:GLU:HA	8	0.41
(2,1311)	1:128:A:ILE:HG21	1:129:A:THR:H	17	0.41
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	12	0.41
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	14	0.41
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	7	0.41
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	7	0.41
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	15	0.41
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	1	0.41
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	5	0.41
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	13	0.41
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	16	0.41
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	18	0.41
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	19	0.41
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	4	0.41
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	20	0.41
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	12	0.41
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	17	0.41
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	4	0.41
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	12	0.41
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	3	0.41
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	6	0.41
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD21	2	0.41
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	12	0.41
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD23	13	0.41
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	2	0.41
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	15	0.41
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	8	0.41
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	1	0.41
(2,29)	1:88:A:TYR:HD1	1:159:A:TYR:HD1	14	0.41
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	20	0.4
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	13	0.4
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	3	0.4
(4,332)	1:37:A:LEU:HD12	1:41:A:MET:HB2	20	0.4
(4,259)	1:117:A:MET:HE3	2:201:A:NAD:H2A	10	0.4
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	15	0.4
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	19	0.4
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	19	0.4
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	17	0.4
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD23	16	0.4
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	9	0.4
(2,3824)	1:41:A:MET:HE1	1:11:A:LEU:HD12	5	0.4
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	14	0.4
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	2	0.4
(2,3811)	1:15:A:LEU:HD13	1:74:A:ILE:HD11	12	0.4
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	3	0.4
(2,3791)	1:142:A:VAL:HG23	1:143:A:VAL:HB	6	0.4
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	16	0.4
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	19	0.4
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	11	0.4
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	13	0.4
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	14	0.4
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	18	0.4
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	20	0.4
(2,3677)	1:15:A:LEU:HD22	1:15:A:LEU:HA	4	0.4
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	7	0.4
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	8	0.4
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	9	0.4
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	14	0.4
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	16	0.4
(2,3666)	1:43:A:ALA:HB1	1:43:A:ALA:HA	1	0.4
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	2	0.4
(2,3666)	1:43:A:ALA:HB1	1:43:A:ALA:HA	5	0.4
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	9	0.4
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	11	0.4
(2,3666)	1:43:A:ALA:HB1	1:43:A:ALA:HA	15	0.4
(2,3544)	1:66:A:ALA:HB3	1:66:A:ALA:HA	6	0.4
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	14	0.4
(2,3539)	1:32:A:ALA:HB1	1:32:A:ALA:HA	5	0.4
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	1	0.4
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	14	0.4
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	18	0.4
(2,3474)	1:146:A:VAL:HG12	1:96:A:VAL:HA	14	0.4
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	17	0.4
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	2	0.4
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	6	0.4
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	14	0.4
(2,3390)	1:56:A:ILE:HG23	1:65:A:PHE:HE1	9	0.4
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	11	0.4
(2,3346)	1:4:A:MET:HE3	1:55:A:HIS:HD2	16	0.4
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	7	0.4
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	12	0.4
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	13	0.4
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	18	0.4
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	4	0.4
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD23	14	0.4
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	13	0.4
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	3	0.4
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	4	0.4
(2,2425)	1:35:A:LYS:HB2	1:35:A:LYS:H	20	0.4
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	6	0.4
(2,2376)	1:95:A:ALA:HB2	1:149:A:LYS:H	7	0.4
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG23	16	0.4
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	8	0.4
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	2	0.4
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	7	0.4
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	13	0.4
(2,1861)	1:41:A:MET:HE1	1:11:A:LEU:HD12	5	0.4
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG22	1	0.4
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	7	0.4
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	19	0.4
(2,1831)	1:142:A:VAL:HG23	1:143:A:VAL:HB	10	0.4
(2,1827)	1:21:A:LEU:HD22	1:21:A:LEU:HG	4	0.4
(2,1824)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	11	0.4
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	11	0.4
(2,1807)	1:151:A:MET:HE3	1:174:A:GLU:HG2	5	0.4
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	10	0.4
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	17	0.4
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	19	0.4
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	7	0.4
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG21	16	0.4
(2,1699)	1:43:A:ALA:HB1	1:43:A:ALA:HA	1	0.4
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	2	0.4
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	3	0.4
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1699)	1:43:A:ALA:HB1	1:43:A:ALA:HA	5	0.4
(2,1699)	1:43:A:ALA:HB1	1:43:A:ALA:HA	10	0.4
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	13	0.4
(2,1699)	1:43:A:ALA:HB1	1:43:A:ALA:HA	15	0.4
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	7	0.4
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	10	0.4
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	12	0.4
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	9	0.4
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	20	0.4
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	18	0.4
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	20	0.4
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	3	0.4
(2,1221)	1:176:A:ILE:HG22	1:176:A:ILE:HB	5	0.4
(2,1221)	1:176:A:ILE:HG22	1:176:A:ILE:HB	6	0.4
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	8	0.4
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	20	0.4
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	5	0.4
(2,1156)	1:144:A:LEU:HD21	1:106:A:PHE:HE1	9	0.4
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	3	0.4
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	4	0.4
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	17	0.4
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	18	0.4
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	7	0.4
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	14	0.4
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	12	0.4
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD12	18	0.4
(2,521)	1:129:A:THR:HG22	1:129:A:THR:H	11	0.4
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	17	0.4
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	20	0.4
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	4	0.4
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	7	0.4
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	13	0.4
(2,405)	1:95:A:ALA:HB2	1:149:A:LYS:H	19	0.4
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	3	0.4
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	13	0.4
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	19	0.4
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	17	0.4
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	10	0.4
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	13	0.4
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	18	0.4
(2,29)	1:88:A:TYR:HD1	1:159:A:TYR:HD1	20	0.4
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	10	0.39
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	9	0.39
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD12	6	0.39
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	5	0.39
(4,368)	1:20:A:ALA:HB2	1:22:A:ILE:HB	15	0.39
(4,292)	1:122:A:VAL:HG23	1:118:A:SER:H	16	0.39
(4,259)	1:117:A:MET:HE3	2:201:A:NAD:H2A	13	0.39
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD11	9	0.39
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	18	0.39
(4,34)	1:24:A:LEU:H	1:22:A:ILE:HD13	19	0.39
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD23	18	0.39
(2,3863)	1:24:A:LEU:HA	1:24:A:LEU:HD21	1	0.39
(2,3847)	1:41:A:MET:HE2	1:46:A:HIS:HA	14	0.39
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	17	0.39
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	2	0.39
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	7	0.39
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	13	0.39
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	17	0.39
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	3	0.39
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	9	0.39
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	11	0.39
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD12	12	0.39
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	18	0.39
(2,3798)	1:48:A:ILE:HD13	1:48:A:ILE:HG13	4	0.39
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	1	0.39
(2,3781)	1:142:A:VAL:HG11	1:142:A:VAL:HB	3	0.39
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	6	0.39
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	17	0.39
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	1	0.39
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	3	0.39
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	6	0.39
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	8	0.39
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	10	0.39
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	3	0.39
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	6	0.39
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	17	0.39
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	3	0.39
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	4	0.39
(2,3666)	1:43:A:ALA:HB1	1:43:A:ALA:HA	10	0.39
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	12	0.39
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	13	0.39
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3607)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	2	0.39
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	12	0.39
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	16	0.39
(2,3527)	1:84:A:VAL:HG21	1:85:A:ASP:HB2	11	0.39
(2,3484)	1:124:A:LEU:HD11	1:167:A:LEU:HA	8	0.39
(2,3467)	1:11:A:LEU:HD12	1:38:A:LEU:HA	10	0.39
(2,3428)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	2	0.39
(2,3409)	1:84:A:VAL:HG11	1:85:A:ASP:H	7	0.39
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	10	0.39
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	11	0.39
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	15	0.39
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	19	0.39
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	14	0.39
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	9	0.39
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	9	0.39
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	16	0.39
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	15	0.39
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	19	0.39
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	19	0.39
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	1	0.39
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	14	0.39
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	1	0.39
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	15	0.39
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	17	0.39
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	8	0.39
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	4	0.39
(2,1872)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	7	0.39
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	17	0.39
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	20	0.39
(2,1827)	1:21:A:LEU:HD22	1:21:A:LEU:HG	11	0.39
(2,1827)	1:21:A:LEU:HD23	1:21:A:LEU:HG	12	0.39
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	7	0.39
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	10	0.39
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	9	0.39
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	12	0.39
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	4	0.39
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	7	0.39
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	12	0.39
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	16	0.39
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	6	0.39
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	10	0.39
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	3	0.39
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	4	0.39
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	20	0.39
(2,1720)	1:86:A:LEU:HA	1:84:A:VAL:HG13	1	0.39
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	12	0.39
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	14	0.39
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB2	19	0.39
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB2	20	0.39
(2,1692)	1:20:A:ALA:HB1	1:20:A:ALA:HA	3	0.39
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	8	0.39
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	4	0.39
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	3	0.39
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	18	0.39
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	18	0.39
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	3	0.39
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	10	0.39
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	7	0.39
(2,1377)	1:4:A:MET:HE1	1:55:A:HIS:HD2	13	0.39
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	8	0.39
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	2	0.39
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	11	0.39
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	14	0.39
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	17	0.39
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	18	0.39
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	19	0.39
(2,1211)	1:177:A:LYS:HD2	1:177:A:LYS:HA	9	0.39
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	10	0.39
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	4	0.39
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	7	0.39
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	9	0.39
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	10	0.39
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	3	0.39
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	10	0.39
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	11	0.39
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	16	0.39
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	15	0.39
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	7	0.39
(2,708)	1:113:A:GLY:H	1:109:A:ILE:HG21	6	0.39
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	5	0.39
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	10	0.39
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	15	0.39
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	7	0.39
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	16	0.39
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	3	0.39
(2,454)	1:35:A:LYS:HB2	1:35:A:LYS:H	20	0.39
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	18	0.39
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	9	0.39
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	16	0.39
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	17	0.39
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	5	0.39
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	7	0.39
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	4	0.39
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	9	0.39
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD21	14	0.39
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	9	0.39
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	11	0.38
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	8	0.38
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	19	0.38
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	11	0.38
(4,379)	1:50:A:MET:HA	1:39:A:ALA:HB3	3	0.38
(4,364)	1:4:A:MET:HE2	1:58:A:GLU:HG3	17	0.38
(4,299)	1:168:A:ILE:HD12	1:96:A:VAL:HA	7	0.38
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	12	0.38
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	11	0.38
(4,208)	1:14:A:VAL:HG21	1:11:A:LEU:HA	20	0.38
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	6	0.38
(4,15)	1:177:A:LYS:H	1:110:A:LEU:HD13	18	0.38
(4,6)	1:65:A:PHE:HE1	1:74:A:ILE:HG23	5	0.38
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD22	17	0.38
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD23	8	0.38
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	15	0.38
(2,3964)	1:123:A:HIS:HB3	2:201:A:NAD:H6N	4	0.38
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	13	0.38
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	20	0.38
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD22	18	0.38
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	6	0.38
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	6	0.38
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	17	0.38
(2,3791)	1:142:A:VAL:HG23	1:143:A:VAL:HB	5	0.38
(2,3790)	1:34:A:VAL:HG13	1:50:A:MET:HE3	7	0.38
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	14	0.38
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	10	0.38
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	20	0.38
(2,3769)	1:5:A:VAL:HG23	1:5:A:VAL:HB	2	0.38
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	8	0.38
(2,3769)	1:5:A:VAL:HG23	1:5:A:VAL:HB	12	0.38
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	15	0.38
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	18	0.38
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	4	0.38
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	1	0.38
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	5	0.38
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	1	0.38
(2,3677)	1:15:A:LEU:HD23	1:15:A:LEU:HA	12	0.38
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	15	0.38
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	6	0.38
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB2	7	0.38
(2,3666)	1:43:A:ALA:HB1	1:43:A:ALA:HA	16	0.38
(2,3666)	1:43:A:ALA:HB1	1:43:A:ALA:HA	17	0.38
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB2	19	0.38
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB2	20	0.38
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	15	0.38
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	20	0.38
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	17	0.38
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	8	0.38
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	18	0.38
(2,3439)	1:110:A:LEU:HD13	1:110:A:LEU:H	9	0.38
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	16	0.38
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	17	0.38
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	4	0.38
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	6	0.38
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	15	0.38
(2,3182)	1:114:A:ILE:HD13	1:171:A:VAL:HB	20	0.38
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD23	15	0.38
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	10	0.38
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	3	0.38
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	2	0.38
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	9	0.38
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	17	0.38
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	18	0.38
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	1	0.38
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG23	11	0.38
(2,1859)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	13	0.38
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	17	0.38
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	5	0.38
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	7	0.38
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	16	0.38
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	6	0.38
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	5	0.38
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD13	16	0.38
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	8	0.38
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	9	0.38
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	11	0.38
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	13	0.38
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	14	0.38
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	19	0.38
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	20	0.38
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD21	7	0.38
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD22	13	0.38
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	16	0.38
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	7	0.38
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	8	0.38
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	10	0.38
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	14	0.38
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	4	0.38
(2,1750)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	18	0.38
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	17	0.38
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	6	0.38
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB2	7	0.38
(2,1699)	1:43:A:ALA:HB1	1:43:A:ALA:HA	16	0.38
(2,1699)	1:43:A:ALA:HB1	1:43:A:ALA:HA	17	0.38
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	4	0.38
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	8	0.38
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	8	0.38
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	19	0.38
(2,1546)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	16	0.38
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	19	0.38
(2,1541)	1:143:A:VAL:HG13	1:132:A:ARG:HA	20	0.38
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	2	0.38
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	6	0.38
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	12	0.38
(2,1534)	1:151:A:MET:HE2	1:151:A:MET:HA	1	0.38
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	4	0.38
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	6	0.38
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	10	0.38
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	4	0.38
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	8	0.38
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	1	0.38
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	16	0.38
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	14	0.38
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	8	0.38
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	10	0.38
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	1	0.38
(2,1221)	1:176:A:ILE:HG22	1:176:A:ILE:HB	4	0.38
(2,1221)	1:176:A:ILE:HG22	1:176:A:ILE:HB	10	0.38
(2,1221)	1:176:A:ILE:HG22	1:176:A:ILE:HB	15	0.38
(2,1221)	1:176:A:ILE:HG22	1:176:A:ILE:HB	16	0.38
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	14	0.38
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	15	0.38
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	9	0.38
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	20	0.38
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	1	0.38
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD13	18	0.38
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	18	0.38
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	16	0.38
(2,584)	1:17:A:HIS:H	1:17:A:HIS:HD2	14	0.38
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	4	0.38
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	8	0.38
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	13	0.38
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	14	0.38
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	3	0.38
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	16	0.38
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	12	0.38
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	10	0.38
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	7	0.38
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	10	0.38
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	18	0.38
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	8	0.38
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	18	0.38
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	19	0.38
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	7	0.38
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	3	0.38
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	18	0.38
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	19	0.38
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	12	0.38
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	17	0.38
(4,447)	1:53:A:LEU:HD12	1:11:A:LEU:HD23	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	4	0.37
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	11	0.37
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	7	0.37
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	8	0.37
(4,415)	1:19:A:PRO:HB3	1:36:A:GLU:HG2	9	0.37
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	10	0.37
(4,167)	1:34:A:VAL:H	1:11:A:LEU:HB3	5	0.37
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB2	13	0.37
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	13	0.37
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	14	0.37
(2,3833)	1:168:A:ILE:HD11	1:168:A:ILE:HG13	5	0.37
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	5	0.37
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	13	0.37
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	1	0.37
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	3	0.37
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	8	0.37
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	14	0.37
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	2	0.37
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	12	0.37
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	15	0.37
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	18	0.37
(2,3759)	1:53:A:LEU:HD12	1:53:A:LEU:HB2	6	0.37
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	13	0.37
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	10	0.37
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	11	0.37
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	9	0.37
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG21	4	0.37
(2,3666)	1:43:A:ALA:HA	1:43:A:ALA:HB3	8	0.37
(2,3544)	1:66:A:ALA:HB1	1:66:A:ALA:HA	3	0.37
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	16	0.37
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	4	0.37
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	15	0.37
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	16	0.37
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	17	0.37
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	11	0.37
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	19	0.37
(2,3459)	1:167:A:LEU:HD22	1:123:A:HIS:HA	18	0.37
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	12	0.37
(2,3346)	1:4:A:MET:HE1	1:55:A:HIS:HD2	13	0.37
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	14	0.37
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	14	0.37
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	5	0.37
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	4	0.37
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	15	0.37
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	5	0.37
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	3	0.37
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	2	0.37
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	6	0.37
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	7	0.37
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	10	0.37
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD12	12	0.37
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	12	0.37
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	20	0.37
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	5	0.37
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	17	0.37
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	20	0.37
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	1	0.37
(2,1838)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	15	0.37
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	16	0.37
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	17	0.37
(2,1819)	1:86:A:LEU:HD22	1:86:A:LEU:HG	14	0.37
(2,1819)	1:86:A:LEU:HD22	1:86:A:LEU:HG	19	0.37
(2,1796)	1:76:A:ALA:HB2	1:15:A:LEU:HD12	16	0.37
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	12	0.37
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD22	1	0.37
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	3	0.37
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	5	0.37
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD22	12	0.37
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	14	0.37
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD22	17	0.37
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	20	0.37
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	13	0.37
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	20	0.37
(2,1699)	1:43:A:ALA:HA	1:43:A:ALA:HB3	8	0.37
(2,1692)	1:20:A:ALA:HB1	1:20:A:ALA:HA	10	0.37
(2,1692)	1:20:A:ALA:HB1	1:20:A:ALA:HA	11	0.37
(2,1692)	1:20:A:ALA:HB1	1:20:A:ALA:HA	13	0.37
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	16	0.37
(2,1599)	1:4:A:MET:HE2	1:52:A:GLU:HA	19	0.37
(2,1546)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	7	0.37
(2,1541)	1:143:A:VAL:HG11	1:132:A:ARG:HA	17	0.37
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	8	0.37
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	15	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	8	0.37
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	9	0.37
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	11	0.37
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	13	0.37
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	14	0.37
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	19	0.37
(2,1514)	1:124:A:LEU:HD11	1:167:A:LEU:HA	8	0.37
(2,1509)	1:151:A:MET:HE2	1:171:A:VAL:HA	8	0.37
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	19	0.37
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	11	0.37
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	1	0.37
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	5	0.37
(2,1380)	1:9:A:LYS:HB2	1:65:A:PHE:HE1	10	0.37
(2,1288)	1:167:A:LEU:HD23	1:167:A:LEU:HA	13	0.37
(2,1221)	1:176:A:ILE:HG22	1:176:A:ILE:HB	12	0.37
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	13	0.37
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	1	0.37
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	3	0.37
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	7	0.37
(2,874)	1:78:A:GLN:HG3	1:78:A:GLN:HE21	7	0.37
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	3	0.37
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	12	0.37
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	13	0.37
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	11	0.37
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	9	0.37
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	1	0.37
(2,521)	1:129:A:THR:HG23	1:129:A:THR:H	7	0.37
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	12	0.37
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	15	0.37
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	7	0.37
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	11	0.37
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	18	0.37
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	9	0.37
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	11	0.37
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	5	0.37
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	9	0.37
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	10	0.37
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	14	0.37
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	15	0.37
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	1	0.37
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	4	0.37
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	13	0.37
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	3	0.37
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	4	0.37
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	5	0.37
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	6	0.37
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	15	0.37
(4,451)	1:168:A:ILE:HD11	1:168:A:ILE:HG12	12	0.36
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	7	0.36
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	12	0.36
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	7	0.36
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	14	0.36
(4,432)	1:131:A:ALA:HB1	1:128:A:ILE:HB	6	0.36
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	1	0.36
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	3	0.36
(4,319)	1:26:A:LEU:HD22	1:14:A:VAL:HA	19	0.36
(4,300)	1:97:A:LEU:HD23	1:156:A:PHE:HB3	7	0.36
(4,299)	1:168:A:ILE:HD12	1:152:A:ALA:HA	1	0.36
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	18	0.36
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	8	0.36
(4,70)	1:130:A:THR:H	2:201:A:NAD:H4D	14	0.36
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	16	0.36
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	3	0.36
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD23	14	0.36
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	14	0.36
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	18	0.36
(2,3826)	1:11:A:LEU:HD13	1:11:A:LEU:HB3	10	0.36
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD21	15	0.36
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	10	0.36
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	10	0.36
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	18	0.36
(2,3794)	1:14:A:VAL:HG22	1:14:A:VAL:HB	20	0.36
(2,3791)	1:142:A:VAL:HG23	1:143:A:VAL:HB	13	0.36
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	6	0.36
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	7	0.36
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	8	0.36
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	9	0.36
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	5	0.36
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	6	0.36
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	8	0.36
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	9	0.36
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	12	0.36
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	14	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	1	0.36
(2,3769)	1:5:A:VAL:HG23	1:5:A:VAL:HB	7	0.36
(2,3769)	1:5:A:VAL:HG23	1:5:A:VAL:HB	9	0.36
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	9	0.36
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	20	0.36
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG21	9	0.36
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG21	20	0.36
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	12	0.36
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	3	0.36
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	16	0.36
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	19	0.36
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	6	0.36
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	13	0.36
(2,3659)	1:20:A:ALA:HB1	1:20:A:ALA:HA	3	0.36
(2,3600)	1:42:A:LYS:HE3	1:39:A:ALA:HA	15	0.36
(2,3544)	1:66:A:ALA:HB3	1:66:A:ALA:HA	5	0.36
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	3	0.36
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	7	0.36
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	9	0.36
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	12	0.36
(2,3371)	1:20:A:ALA:HB2	1:18:A:ASN:HD21	3	0.36
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	10	0.36
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	2	0.36
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	5	0.36
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	13	0.36
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	18	0.36
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD21	5	0.36
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD23	10	0.36
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	18	0.36
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	8	0.36
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	9	0.36
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	10	0.36
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	14	0.36
(2,2748)	1:86:A:LEU:HD11	1:87:A:GLY:H	20	0.36
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	20	0.36
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	7	0.36
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	10	0.36
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	18	0.36
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	17	0.36
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	8	0.36
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	18	0.36
(2,1874)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	1	0.36
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	3	0.36
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	14	0.36
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	15	0.36
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	4	0.36
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	17	0.36
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	8	0.36
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	9	0.36
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	13	0.36
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	9	0.36
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	10	0.36
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	4	0.36
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	2	0.36
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	4	0.36
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD21	8	0.36
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	9	0.36
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD22	10	0.36
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD22	11	0.36
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD22	15	0.36
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	3	0.36
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	6	0.36
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	15	0.36
(2,1750)	1:158:A:PHE:HB2	1:168:A:ILE:HG12	17	0.36
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	11	0.36
(2,1555)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	20	0.36
(2,1546)	1:48:A:ILE:HD11	1:53:A:LEU:HB2	1	0.36
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	2	0.36
(2,1546)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	4	0.36
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	9	0.36
(2,1546)	1:48:A:ILE:HD11	1:53:A:LEU:HB2	11	0.36
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	12	0.36
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	13	0.36
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	15	0.36
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	9	0.36
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	16	0.36
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	3	0.36
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	10	0.36
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	2	0.36
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	7	0.36
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	17	0.36
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	14	0.36
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	2	0.36
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	12	0.36
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	20	0.36
(2,1276)	1:160:A:LEU:HD21	1:166:A:TRP:HE1	4	0.36
(2,1221)	1:176:A:ILE:HG21	1:176:A:ILE:HB	9	0.36
(2,1211)	1:177:A:LYS:HD2	1:177:A:LYS:HA	2	0.36
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	2	0.36
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	18	0.36
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	9	0.36
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	20	0.36
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	10	0.36
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD13	17	0.36
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	5	0.36
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	16	0.36
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	19	0.36
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	15	0.36
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	17	0.36
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	19	0.36
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	5	0.36
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	9	0.36
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	9	0.36
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	9	0.36
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	8	0.36
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	12	0.36
(2,379)	1:156:A:PHE:H	1:168:A:ILE:HD11	5	0.36
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD23	2	0.36
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	12	0.36
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	17	0.36
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	6	0.36
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	20	0.36
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD23	7	0.36
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	6	0.36
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	13	0.36
(2,175)	1:53:A:LEU:HD21	1:56:A:ILE:H	2	0.36
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	10	0.36
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	11	0.36
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	5	0.36
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	7	0.36
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	12	0.36
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	14	0.36
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	19	0.36
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	17	0.36
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	6	0.36
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	19	0.35
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	9	0.35
(4,438)	1:108:A:LEU:HG	1:108:A:LEU:HD13	16	0.35
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	6	0.35
(4,430)	1:22:A:ILE:HG23	1:41:A:MET:HB3	18	0.35
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	9	0.35
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	3	0.35
(4,338)	1:111:A:LYS:HD3	1:104:A:LYS:HA	15	0.35
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	1	0.35
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	8	0.35
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	13	0.35
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	9	0.35
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	10	0.35
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	11	0.35
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	12	0.35
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	4	0.35
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	8	0.35
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	10	0.35
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD21	6	0.35
(2,3822)	1:53:A:LEU:HD13	1:53:A:LEU:HD22	10	0.35
(2,3822)	1:53:A:LEU:HD12	1:53:A:LEU:HD22	17	0.35
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	6	0.35
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	7	0.35
(2,3789)	1:22:A:ILE:HG22	1:44:A:LYS:HB3	3	0.35
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	2	0.35
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	9	0.35
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	11	0.35
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	14	0.35
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	17	0.35
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	18	0.35
(2,3783)	1:143:A:VAL:HG11	1:143:A:VAL:HB	20	0.35
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	15	0.35
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	18	0.35
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	19	0.35
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	19	0.35
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	1	0.35
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	15	0.35
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	18	0.35
(2,3677)	1:15:A:LEU:HD22	1:15:A:LEU:HA	20	0.35
(2,3600)	1:42:A:LYS:HE2	1:39:A:ALA:HA	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3600)	1:42:A:LYS:HE3	1:39:A:ALA:HA	6	0.35
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	19	0.35
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	2	0.35
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	6	0.35
(2,3484)	1:124:A:LEU:HD11	1:167:A:LEU:HA	10	0.35
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	10	0.35
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	12	0.35
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	8	0.35
(2,3439)	1:110:A:LEU:HD13	1:110:A:LEU:H	5	0.35
(2,3408)	1:7:A:VAL:HG11	1:7:A:VAL:H	5	0.35
(2,3408)	1:7:A:VAL:HG13	1:7:A:VAL:H	20	0.35
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	1	0.35
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	16	0.35
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	1	0.35
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	12	0.35
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	20	0.35
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	3	0.35
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	12	0.35
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	12	0.35
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	3	0.35
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	11	0.35
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	20	0.35
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	8	0.35
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	19	0.35
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	11	0.35
(2,1874)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	1	0.35
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD12	5	0.35
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	16	0.35
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	19	0.35
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	20	0.35
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	13	0.35
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	19	0.35
(2,1850)	1:97:A:LEU:HD12	1:124:A:LEU:HD23	4	0.35
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD12	12	0.35
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	10	0.35
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	10	0.35
(2,1838)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	18	0.35
(2,1832)	1:53:A:LEU:HD22	1:56:A:ILE:HB	6	0.35
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	14	0.35
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	17	0.35
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	18	0.35
(2,1819)	1:86:A:LEU:HD23	1:86:A:LEU:HG	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	9	0.35
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	1	0.35
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	3	0.35
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	5	0.35
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	2	0.35
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG23	5	0.35
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	2	0.35
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	16	0.35
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	15	0.35
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	9	0.35
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	11	0.35
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	19	0.35
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	1	0.35
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	10	0.35
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	2	0.35
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	4	0.35
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	7	0.35
(2,1692)	1:20:A:ALA:HB1	1:20:A:ALA:HA	12	0.35
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	14	0.35
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	18	0.35
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	6	0.35
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	10	0.35
(2,1541)	1:143:A:VAL:HG11	1:132:A:ARG:HA	14	0.35
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	7	0.35
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	11	0.35
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	13	0.35
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	4	0.35
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	6	0.35
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	12	0.35
(2,1459)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	7	0.35
(2,1412)	1:66:A:ALA:HB2	1:31:A:TRP:HZ3	18	0.35
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	5	0.35
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	20	0.35
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	3	0.35
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	5	0.35
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	18	0.35
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	1	0.35
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	4	0.35
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	5	0.35
(2,1274)	1:160:A:LEU:HD21	1:91:A:GLN:HE22	15	0.35
(2,1257)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	10	0.35
(2,1211)	1:177:A:LYS:HD2	1:177:A:LYS:HA	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1201)	1:144:A:LEU:HD23	1:144:A:LEU:HG	7	0.35
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	12	0.35
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	17	0.35
(2,1201)	1:144:A:LEU:HD23	1:144:A:LEU:HG	20	0.35
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	15	0.35
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	19	0.35
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	20	0.35
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	1	0.35
(2,775)	1:87:A:GLY:H	1:81:A:SER:HA	10	0.35
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	15	0.35
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	4	0.35
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB2	19	0.35
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	4	0.35
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	11	0.35
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	14	0.35
(2,521)	1:129:A:THR:HG23	1:129:A:THR:H	3	0.35
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	18	0.35
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	14	0.35
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	13	0.35
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	4	0.35
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	19	0.35
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	4	0.35
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	7	0.35
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	10	0.35
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD21	11	0.35
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	2	0.35
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	3	0.35
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	8	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	2	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	8	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	9	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	11	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	13	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	15	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	17	0.35
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	20	0.35
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	8	0.35
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	14	0.35
(2,19)	1:13:A:LEU:HA	1:17:A:HIS:HD2	2	0.35
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	4	0.35
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	14	0.34
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	1	0.34
(4,387)	1:83:A:GLU:HA	1:82:A:VAL:HG12	4	0.34
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	14	0.34
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	17	0.34
(4,379)	1:50:A:MET:HA	1:39:A:ALA:HB3	12	0.34
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	7	0.34
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	13	0.34
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	12	0.34
(4,325)	1:7:A:VAL:HG11	1:10:A:PHE:HB3	11	0.34
(4,292)	1:122:A:VAL:HG23	1:118:A:SER:H	6	0.34
(4,244)	1:51:A:GLU:HG2	1:72:A:GLU:H	1	0.34
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	1	0.34
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	17	0.34
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	1	0.34
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD23	17	0.34
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD23	3	0.34
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	7	0.34
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	19	0.34
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	12	0.34
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	14	0.34
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	13	0.34
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	15	0.34
(2,3804)	1:128:A:ILE:HG21	1:129:A:THR:HG21	20	0.34
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	3	0.34
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	3	0.34
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	8	0.34
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	12	0.34
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	20	0.34
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	2	0.34
(2,3783)	1:143:A:VAL:HG11	1:143:A:VAL:HB	4	0.34
(2,3783)	1:143:A:VAL:HG11	1:143:A:VAL:HB	8	0.34
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	15	0.34
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	18	0.34
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	17	0.34
(2,3772)	1:151:A:MET:HE2	1:174:A:GLU:HG2	15	0.34
(2,3759)	1:53:A:LEU:HD12	1:53:A:LEU:HB2	18	0.34
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD22	3	0.34
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD21	7	0.34
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD22	13	0.34
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	2	0.34
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	8	0.34
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3677)	1:15:A:LEU:HD21	1:15:A:LEU:HA	10	0.34
(2,3659)	1:20:A:ALA:HB1	1:20:A:ALA:HA	10	0.34
(2,3659)	1:20:A:ALA:HB1	1:20:A:ALA:HA	11	0.34
(2,3659)	1:20:A:ALA:HB1	1:20:A:ALA:HA	13	0.34
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	16	0.34
(2,3600)	1:42:A:LYS:HE3	1:39:A:ALA:HA	17	0.34
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE3	16	0.34
(2,3484)	1:124:A:LEU:HD11	1:167:A:LEU:HA	6	0.34
(2,3484)	1:124:A:LEU:HD12	1:167:A:LEU:HA	9	0.34
(2,3484)	1:124:A:LEU:HD12	1:167:A:LEU:HA	15	0.34
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	6	0.34
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	20	0.34
(2,3459)	1:167:A:LEU:HD22	1:123:A:HIS:HA	10	0.34
(2,3439)	1:110:A:LEU:HD11	1:110:A:LEU:H	10	0.34
(2,3428)	1:108:A:LEU:HD13	2:201:A:NAD:H2A	18	0.34
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	10	0.34
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	15	0.34
(2,3391)	1:56:A:ILE:HG21	1:65:A:PHE:HD1	14	0.34
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	12	0.34
(2,3384)	1:21:A:LEU:HD11	1:18:A:ASN:HD22	1	0.34
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	10	0.34
(2,3288)	1:142:A:VAL:HG11	1:103:A:GLU:HA	10	0.34
(2,3274)	1:57:A:VAL:HG13	1:66:A:ALA:HA	5	0.34
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	18	0.34
(2,3248)	1:160:A:LEU:HD21	1:91:A:GLN:HE22	15	0.34
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	3	0.34
(2,3196)	1:176:A:ILE:HG22	1:176:A:ILE:HB	6	0.34
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	7	0.34
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	20	0.34
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	8	0.34
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	2	0.34
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	18	0.34
(2,3156)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	2	0.34
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD23	6	0.34
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	8	0.34
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD23	11	0.34
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	12	0.34
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	2	0.34
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD11	6	0.34
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD11	7	0.34
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD11	18	0.34
(2,2376)	1:95:A:ALA:HB2	1:149:A:LYS:H	19	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	9	0.34
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	1	0.34
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG12	2	0.34
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	3	0.34
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	2	0.34
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	14	0.34
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	5	0.34
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	16	0.34
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	4	0.34
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	7	0.34
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	16	0.34
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	7	0.34
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	12	0.34
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	17	0.34
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	20	0.34
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	8	0.34
(2,1869)	1:97:A:LEU:HD22	1:96:A:VAL:HB	10	0.34
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	7	0.34
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	3	0.34
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	7	0.34
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	9	0.34
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD23	18	0.34
(2,1850)	1:97:A:LEU:HD12	1:124:A:LEU:HD23	19	0.34
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	14	0.34
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	4	0.34
(2,1838)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	2	0.34
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	12	0.34
(2,1838)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	14	0.34
(2,1838)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	20	0.34
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	5	0.34
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	8	0.34
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	13	0.34
(2,1820)	1:142:A:VAL:HG13	1:142:A:VAL:HB	12	0.34
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	10	0.34
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	15	0.34
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	20	0.34
(2,1804)	1:5:A:VAL:HG23	1:5:A:VAL:HB	2	0.34
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	8	0.34
(2,1804)	1:5:A:VAL:HG23	1:5:A:VAL:HB	12	0.34
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	14	0.34
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	15	0.34
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	2	0.34
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD21	6	0.34
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	2	0.34
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	18	0.34
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	9	0.34
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	5	0.34
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	17	0.34
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	20	0.34
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	3	0.34
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE1	9	0.34
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	12	0.34
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE3	14	0.34
(2,1563)	1:48:A:ILE:HG22	1:53:A:LEU:HB2	3	0.34
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	5	0.34
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	8	0.34
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	14	0.34
(2,1546)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	17	0.34
(2,1546)	1:48:A:ILE:HD11	1:53:A:LEU:HB2	18	0.34
(2,1546)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	20	0.34
(2,1541)	1:143:A:VAL:HG12	1:132:A:ARG:HA	15	0.34
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	19	0.34
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	7	0.34
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	9	0.34
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	11	0.34
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	13	0.34
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	17	0.34
(2,1531)	1:21:A:LEU:HD13	1:14:A:VAL:HA	16	0.34
(2,1521)	1:96:A:VAL:HG11	1:96:A:VAL:HA	5	0.34
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	7	0.34
(2,1405)	1:20:A:ALA:HB3	1:20:A:ALA:H	10	0.34
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	16	0.34
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	15	0.34
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	20	0.34
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	12	0.34
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	2	0.34
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	3	0.34
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	7	0.34
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	9	0.34
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	13	0.34
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	14	0.34
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	15	0.34
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	17	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	20	0.34
(2,1201)	1:144:A:LEU:HD22	1:144:A:LEU:HG	9	0.34
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	13	0.34
(2,1201)	1:144:A:LEU:HD23	1:144:A:LEU:HG	16	0.34
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	2	0.34
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	17	0.34
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	15	0.34
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	19	0.34
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	11	0.34
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	3	0.34
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	5	0.34
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	16	0.34
(2,567)	1:88:A:TYR:H	1:86:A:LEU:HB3	1	0.34
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	3	0.34
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	10	0.34
(2,521)	1:129:A:THR:HG21	1:129:A:THR:H	16	0.34
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	5	0.34
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	11	0.34
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	16	0.34
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	11	0.34
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	16	0.34
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	19	0.34
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD22	3	0.34
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	7	0.34
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	10	0.34
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	15	0.34
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	8	0.34
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	15	0.34
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	17	0.34
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	15	0.34
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	17	0.34
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	1	0.34
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	3	0.34
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	4	0.34
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	5	0.34
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	10	0.34
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	16	0.34
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	18	0.34
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	2	0.34
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	4	0.34
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	15	0.34
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	13	0.34
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	14	0.34
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	16	0.34
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	9	0.34
(4,451)	1:168:A:ILE:HD12	1:168:A:ILE:HG12	6	0.33
(4,451)	1:168:A:ILE:HD12	1:168:A:ILE:HG12	10	0.33
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD13	18	0.33
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	16	0.33
(4,430)	1:22:A:ILE:HB	1:22:A:ILE:HG23	5	0.33
(4,411)	1:172:A:PRO:HB2	1:114:A:ILE:HG12	13	0.33
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	16	0.33
(4,322)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	1	0.33
(4,259)	1:117:A:MET:HE3	2:201:A:NAD:H2A	19	0.33
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	20	0.33
(4,31)	1:24:A:LEU:H	1:24:A:LEU:HG	20	0.33
(2,3964)	1:123:A:HIS:HB3	2:201:A:NAD:H6N	18	0.33
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	20	0.33
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	4	0.33
(2,3833)	1:168:A:ILE:HD12	1:168:A:ILE:HG13	7	0.33
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	3	0.33
(2,3826)	1:11:A:LEU:HD13	1:11:A:LEU:HB3	14	0.33
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	18	0.33
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	7	0.33
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	2	0.33
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	19	0.33
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	19	0.33
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	3	0.33
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	5	0.33
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD12	7	0.33
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	9	0.33
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	10	0.33
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD13	11	0.33
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	15	0.33
(2,3785)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	15	0.33
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	1	0.33
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	10	0.33
(2,3783)	1:143:A:VAL:HG12	1:143:A:VAL:HB	12	0.33
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	16	0.33
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	19	0.33
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	16	0.33
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	17	0.33
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	18	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3749)	1:44:A:LYS:HG2	1:21:A:LEU:HD23	1	0.33
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD22	1	0.33
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	3	0.33
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	5	0.33
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD22	12	0.33
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	14	0.33
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD22	15	0.33
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD22	17	0.33
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	20	0.33
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	20	0.33
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG21	16	0.33
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	4	0.33
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	7	0.33
(2,3659)	1:20:A:ALA:HB1	1:20:A:ALA:HA	12	0.33
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	14	0.33
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	18	0.33
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE2	14	0.33
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	20	0.33
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	3	0.33
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	5	0.33
(2,3556)	1:28:A:ALA:HB3	1:28:A:ALA:HA	6	0.33
(2,3556)	1:28:A:ALA:HB3	1:28:A:ALA:HA	12	0.33
(2,3556)	1:28:A:ALA:HB2	1:28:A:ALA:HA	17	0.33
(2,3502)	1:21:A:LEU:HD11	1:14:A:VAL:HA	3	0.33
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	2	0.33
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	15	0.33
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	4	0.33
(2,3387)	1:21:A:LEU:HD21	1:10:A:PHE:HE1	11	0.33
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	13	0.33
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	14	0.33
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	20	0.33
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	1	0.33
(2,3196)	1:176:A:ILE:HG22	1:176:A:ILE:HB	5	0.33
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	8	0.33
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	11	0.33
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	14	0.33
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	17	0.33
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	19	0.33
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	7	0.33
(2,3175)	1:144:A:LEU:HD23	1:144:A:LEU:HG	7	0.33
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	12	0.33
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	17	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3175)	1:144:A:LEU:HD23	1:144:A:LEU:HG	20	0.33
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD22	2	0.33
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD23	9	0.33
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD21	20	0.33
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD12	11	0.33
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	15	0.33
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD13	20	0.33
(2,2738)	1:30:A:GLY:H	1:26:A:LEU:HD22	20	0.33
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	18	0.33
(2,2308)	1:108:A:LEU:HD22	1:108:A:LEU:H	16	0.33
(2,2255)	1:46:A:HIS:H	1:22:A:ILE:HG23	5	0.33
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	17	0.33
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	1	0.33
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	2	0.33
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	9	0.33
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	12	0.33
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	13	0.33
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	14	0.33
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	20	0.33
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	3	0.33
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	9	0.33
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	14	0.33
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	20	0.33
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	6	0.33
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	4	0.33
(2,1873)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	13	0.33
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	12	0.33
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	16	0.33
(2,1863)	1:11:A:LEU:HD13	1:11:A:LEU:HB3	10	0.33
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	3	0.33
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	7	0.33
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	10	0.33
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD23	13	0.33
(2,1850)	1:97:A:LEU:HD12	1:124:A:LEU:HD22	20	0.33
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	6	0.33
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	4	0.33
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	19	0.33
(2,1819)	1:86:A:LEU:HD21	1:86:A:LEU:HG	15	0.33
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	1	0.33
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	3	0.33
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	14	0.33
(2,1807)	1:151:A:MET:HE1	1:174:A:GLU:HG2	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1804)	1:5:A:VAL:HG23	1:5:A:VAL:HB	7	0.33
(2,1793)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	15	0.33
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	2	0.33
(2,1758)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	4	0.33
(2,1710)	1:26:A:LEU:HD21	1:15:A:LEU:HA	16	0.33
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	1	0.33
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	6	0.33
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	19	0.33
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	5	0.33
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	9	0.33
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE3	3	0.33
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	16	0.33
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	2	0.33
(2,1549)	1:37:A:LEU:HD13	1:41:A:MET:HG2	8	0.33
(2,1534)	1:151:A:MET:HA	1:151:A:MET:HE1	13	0.33
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	2	0.33
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	19	0.33
(2,1514)	1:124:A:LEU:HD11	1:167:A:LEU:HA	10	0.33
(2,1509)	1:151:A:MET:HE2	1:171:A:VAL:HA	18	0.33
(2,1487)	1:168:A:ILE:HD13	1:149:A:LYS:H	5	0.33
(2,1463)	1:57:A:VAL:HG23	1:67:A:PHE:HE1	6	0.33
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	19	0.33
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	20	0.33
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	1	0.33
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	4	0.33
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	6	0.33
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	7	0.33
(2,1405)	1:20:A:ALA:HB3	1:20:A:ALA:H	11	0.33
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	14	0.33
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	20	0.33
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	5	0.33
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	8	0.33
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	15	0.33
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	6	0.33
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	8	0.33
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	11	0.33
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	12	0.33
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	16	0.33
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	19	0.33
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	8	0.33
(2,1201)	1:144:A:LEU:HD22	1:144:A:LEU:HG	10	0.33
(2,1201)	1:144:A:LEU:HD22	1:144:A:LEU:HG	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1201)	1:144:A:LEU:HD22	1:144:A:LEU:HG	15	0.33
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	5	0.33
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	8	0.33
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	10	0.33
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	13	0.33
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	19	0.33
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	10	0.33
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	14	0.33
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	18	0.33
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	14	0.33
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	1	0.33
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	11	0.33
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	2	0.33
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	17	0.33
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	4	0.33
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	1	0.33
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	8	0.33
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	2	0.33
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	5	0.33
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	9	0.33
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	15	0.33
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	17	0.33
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	8	0.33
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	11	0.33
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	14	0.33
(2,175)	1:53:A:LEU:HD23	1:56:A:ILE:H	1	0.33
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	2	0.33
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	7	0.33
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	16	0.33
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	20	0.33
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	9	0.33
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	12	0.33
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	6	0.33
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	15	0.33
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	17	0.33
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	6	0.33
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	11	0.32
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	8	0.32
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	3	0.32
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	4	0.32
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	16	0.32
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,218)	1:172:A:PRO:HA	1:106:A:PHE:HE1	9	0.32
(4,208)	1:14:A:VAL:HG22	1:11:A:LEU:HA	18	0.32
(4,70)	1:130:A:THR:H	2:201:A:NAD:H4D	13	0.32
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	6	0.32
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	11	0.32
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	5	0.32
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	17	0.32
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	4	0.32
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	3	0.32
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	16	0.32
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	12	0.32
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	16	0.32
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	5	0.32
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	19	0.32
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	4	0.32
(2,3813)	1:56:A:ILE:HD13	1:11:A:LEU:HD11	2	0.32
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	8	0.32
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	1	0.32
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	13	0.32
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	14	0.32
(2,3783)	1:143:A:VAL:HG13	1:143:A:VAL:HB	3	0.32
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	20	0.32
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	11	0.32
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	13	0.32
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	10	0.32
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	12	0.32
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	2	0.32
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	6	0.32
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	9	0.32
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	20	0.32
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD21	8	0.32
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	9	0.32
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD22	10	0.32
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD22	11	0.32
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	5	0.32
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	19	0.32
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	2	0.32
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	5	0.32
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	4	0.32
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	1	0.32
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	2	0.32
(2,3556)	1:28:A:ALA:HB3	1:28:A:ALA:HA	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	8	0.32
(2,3556)	1:28:A:ALA:HB2	1:28:A:ALA:HA	13	0.32
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	14	0.32
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	15	0.32
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	16	0.32
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	19	0.32
(2,3502)	1:21:A:LEU:HD11	1:14:A:VAL:HA	1	0.32
(2,3490)	1:48:A:ILE:HD13	1:53:A:LEU:HA	1	0.32
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	13	0.32
(2,3459)	1:167:A:LEU:HD22	1:123:A:HIS:HA	15	0.32
(2,3387)	1:21:A:LEU:HD21	1:10:A:PHE:HE1	4	0.32
(2,3387)	1:21:A:LEU:HD21	1:10:A:PHE:HE1	6	0.32
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	9	0.32
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	1	0.32
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	2	0.32
(2,3196)	1:176:A:ILE:HG22	1:176:A:ILE:HB	4	0.32
(2,3196)	1:176:A:ILE:HG22	1:176:A:ILE:HB	16	0.32
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	18	0.32
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	3	0.32
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	4	0.32
(2,3175)	1:144:A:LEU:HD22	1:144:A:LEU:HG	9	0.32
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	13	0.32
(2,3175)	1:144:A:LEU:HD23	1:144:A:LEU:HG	16	0.32
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD11	4	0.32
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	12	0.32
(2,2198)	1:21:A:LEU:HB2	1:21:A:LEU:H	1	0.32
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	9	0.32
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	10	0.32
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	14	0.32
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	4	0.32
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	11	0.32
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	18	0.32
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	17	0.32
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	20	0.32
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	19	0.32
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	19	0.32
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	5	0.32
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	6	0.32
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	8	0.32
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	11	0.32
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	8	0.32
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	11	0.32
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	13	0.32
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD22	1	0.32
(2,1850)	1:97:A:LEU:HD12	1:124:A:LEU:HD22	6	0.32
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	8	0.32
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD22	15	0.32
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	3	0.32
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD12	5	0.32
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	11	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	2	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	3	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	4	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	5	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	6	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	8	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	13	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	16	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	17	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	19	0.32
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	20	0.32
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	1	0.32
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	3	0.32
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	12	0.32
(2,1839)	1:56:A:ILE:HG22	1:56:A:ILE:HG12	14	0.32
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	16	0.32
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	18	0.32
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	19	0.32
(2,1838)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	1	0.32
(2,1838)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	7	0.32
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	8	0.32
(2,1838)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	11	0.32
(2,1838)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	13	0.32
(2,1833)	1:14:A:VAL:HG22	1:14:A:VAL:HB	20	0.32
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	7	0.32
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	9	0.32
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	11	0.32
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	12	0.32
(2,1832)	1:53:A:LEU:HD22	1:56:A:ILE:HB	16	0.32
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	20	0.32
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	13	0.32
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	5	0.32
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	8	0.32
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	9	0.32
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	12	0.32
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	1	0.32
(2,1804)	1:5:A:VAL:HG23	1:5:A:VAL:HB	9	0.32
(2,1796)	1:76:A:ALA:HB1	1:15:A:LEU:HD12	10	0.32
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	1	0.32
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	4	0.32
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	18	0.32
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	8	0.32
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	9	0.32
(2,1692)	1:20:A:ALA:HB2	1:20:A:ALA:HA	15	0.32
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	4	0.32
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	15	0.32
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	19	0.32
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	13	0.32
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	20	0.32
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	6	0.32
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	9	0.32
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	13	0.32
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	19	0.32
(2,1532)	1:34:A:VAL:HG13	1:34:A:VAL:HA	1	0.32
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	8	0.32
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	15	0.32
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	16	0.32
(2,1514)	1:124:A:LEU:HD11	1:167:A:LEU:HA	6	0.32
(2,1514)	1:124:A:LEU:HD12	1:167:A:LEU:HA	9	0.32
(2,1514)	1:124:A:LEU:HD12	1:167:A:LEU:HA	15	0.32
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	8	0.32
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	2	0.32
(2,1405)	1:20:A:ALA:HB3	1:20:A:ALA:H	3	0.32
(2,1405)	1:20:A:ALA:HB3	1:20:A:ALA:H	12	0.32
(2,1405)	1:20:A:ALA:HB3	1:20:A:ALA:H	13	0.32
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	17	0.32
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	18	0.32
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	19	0.32
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	3	0.32
(2,1395)	1:39:A:ALA:HB3	1:40:A:LYS:H	13	0.32
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	19	0.32
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	2	0.32
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	16	0.32
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1201)	1:144:A:LEU:HD23	1:144:A:LEU:HG	1	0.32
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	4	0.32
(2,1201)	1:144:A:LEU:HD21	1:144:A:LEU:HG	19	0.32
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	2	0.32
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	13	0.32
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	1	0.32
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	4	0.32
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	14	0.32
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	5	0.32
(2,1053)	1:74:A:ILE:H	1:34:A:VAL:H	13	0.32
(2,1014)	1:160:A:LEU:H	1:89:A:GLU:H	13	0.32
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD12	7	0.32
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	9	0.32
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	3	0.32
(2,629)	1:44:A:LYS:H	1:42:A:LYS:HG3	17	0.32
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	8	0.32
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	3	0.32
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	17	0.32
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	19	0.32
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	10	0.32
(2,267)	1:21:A:LEU:H	1:18:A:ASN:HD21	3	0.32
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	8	0.32
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	3	0.32
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	12	0.32
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	14	0.32
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	13	0.32
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD13	13	0.32
(2,130)	1:173:A:ALA:HB1	1:173:A:ALA:H	6	0.32
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	20	0.32
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	3	0.32
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	8	0.32
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	10	0.32
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	18	0.32
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	15	0.32
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	3	0.31
(4,451)	1:168:A:ILE:HD12	1:168:A:ILE:HG12	5	0.31
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	16	0.31
(4,451)	1:168:A:ILE:HD12	1:168:A:ILE:HG12	20	0.31
(4,443)	1:48:A:ILE:HD12	1:38:A:LEU:HB2	12	0.31
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	11	0.31
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	11	0.31
(4,379)	1:50:A:MET:HA	1:39:A:ALA:HB3	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	6	0.31
(4,316)	1:37:A:LEU:HD23	1:8:A:SER:HB2	1	0.31
(4,311)	1:96:A:VAL:HG11	1:94:A:PRO:HA	7	0.31
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	10	0.31
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	14	0.31
(4,167)	1:34:A:VAL:H	1:54:A:LYS:HD3	7	0.31
(4,15)	1:177:A:LYS:H	1:96:A:VAL:HG21	5	0.31
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	9	0.31
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	16	0.31
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	5	0.31
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	7	0.31
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	8	0.31
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	11	0.31
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	3	0.31
(2,3832)	1:97:A:LEU:HD23	1:151:A:MET:HG3	14	0.31
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	5	0.31
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	6	0.31
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	8	0.31
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	11	0.31
(2,3826)	1:11:A:LEU:HD13	1:11:A:LEU:HB3	6	0.31
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	18	0.31
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	11	0.31
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	15	0.31
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	2	0.31
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	1	0.31
(2,3809)	1:176:A:ILE:HB	1:110:A:LEU:HD11	9	0.31
(2,3804)	1:128:A:ILE:HG23	1:129:A:THR:HG21	12	0.31
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD12	18	0.31
(2,3785)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	3	0.31
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	13	0.31
(2,3759)	1:53:A:LEU:HD12	1:53:A:LEU:HB2	10	0.31
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	4	0.31
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	5	0.31
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	2	0.31
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	16	0.31
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	6	0.31
(2,3679)	1:97:A:LEU:HD21	1:97:A:LEU:HA	9	0.31
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	6	0.31
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	17	0.31
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	19	0.31
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	20	0.31
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE3	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	9	0.31
(2,3556)	1:28:A:ALA:HB3	1:28:A:ALA:HA	10	0.31
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	11	0.31
(2,3556)	1:28:A:ALA:HB3	1:28:A:ALA:HA	18	0.31
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	20	0.31
(2,3531)	1:151:A:MET:HE2	1:175:A:PHE:HB3	5	0.31
(2,3484)	1:124:A:LEU:HD13	1:167:A:LEU:HA	17	0.31
(2,3479)	1:151:A:MET:HE2	1:171:A:VAL:HA	8	0.31
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	9	0.31
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	19	0.31
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	2	0.31
(2,3428)	1:108:A:LEU:HD13	2:201:A:NAD:H2A	6	0.31
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	11	0.31
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	13	0.31
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	2	0.31
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	2	0.31
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	7	0.31
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	15	0.31
(2,3384)	1:21:A:LEU:HD11	1:18:A:ASN:HD22	3	0.31
(2,3378)	1:66:A:ALA:HB2	1:31:A:TRP:HZ3	18	0.31
(2,3266)	1:53:A:LEU:HD11	1:67:A:PHE:HE1	6	0.31
(2,3266)	1:53:A:LEU:HD11	1:67:A:PHE:HE1	10	0.31
(2,3196)	1:176:A:ILE:HG22	1:176:A:ILE:HB	10	0.31
(2,3196)	1:176:A:ILE:HG22	1:176:A:ILE:HB	12	0.31
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	13	0.31
(2,3196)	1:176:A:ILE:HG22	1:176:A:ILE:HB	15	0.31
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	8	0.31
(2,3175)	1:144:A:LEU:HD22	1:144:A:LEU:HG	10	0.31
(2,3175)	1:144:A:LEU:HD22	1:144:A:LEU:HG	14	0.31
(2,3175)	1:144:A:LEU:HD22	1:144:A:LEU:HG	15	0.31
(2,2886)	1:178:A:VAL:H	1:144:A:LEU:HD23	3	0.31
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	11	0.31
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	6	0.31
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	17	0.31
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	6	0.31
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	2	0.31
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	5	0.31
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	6	0.31
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	10	0.31
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	13	0.31
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	19	0.31
(2,1886)	1:73:A:LYS:HG2	1:33:A:PRO:HB2	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	3	0.31
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	16	0.31
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	3	0.31
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	9	0.31
(2,1874)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	14	0.31
(2,1874)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	18	0.31
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	3	0.31
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	9	0.31
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	18	0.31
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	2	0.31
(2,1858)	1:109:A:ILE:HG21	1:109:A:ILE:HD11	10	0.31
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	19	0.31
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	6	0.31
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	10	0.31
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	5	0.31
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	5	0.31
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD21	9	0.31
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD23	12	0.31
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	16	0.31
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	9	0.31
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	16	0.31
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	9	0.31
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	11	0.31
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	14	0.31
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	13	0.31
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	15	0.31
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	17	0.31
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	3	0.31
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	5	0.31
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	7	0.31
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	18	0.31
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	19	0.31
(2,1796)	1:76:A:ALA:HB2	1:15:A:LEU:HD12	2	0.31
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	8	0.31
(2,1782)	1:108:A:LEU:HG	1:108:A:LEU:HD23	19	0.31
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	2	0.31
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	6	0.31
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	8	0.31
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	9	0.31
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	12	0.31
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	16	0.31
(2,1715)	1:84:A:VAL:HA	1:84:A:VAL:HG22	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	15	0.31
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	18	0.31
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	3	0.31
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	5	0.31
(2,1586)	1:28:A:ALA:HB3	1:28:A:ALA:HA	6	0.31
(2,1586)	1:28:A:ALA:HB3	1:28:A:ALA:HA	12	0.31
(2,1586)	1:28:A:ALA:HB2	1:28:A:ALA:HA	17	0.31
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	3	0.31
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	1	0.31
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	4	0.31
(2,1573)	1:66:A:ALA:HB3	1:66:A:ALA:HA	7	0.31
(2,1573)	1:66:A:ALA:HB3	1:66:A:ALA:HA	10	0.31
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	16	0.31
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	17	0.31
(2,1563)	1:48:A:ILE:HG23	1:53:A:LEU:HB2	12	0.31
(2,1541)	1:143:A:VAL:HG11	1:132:A:ARG:HA	10	0.31
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	4	0.31
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	5	0.31
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	5	0.31
(2,1532)	1:34:A:VAL:HG13	1:34:A:VAL:HA	18	0.31
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	20	0.31
(2,1463)	1:57:A:VAL:HG22	1:67:A:PHE:HE1	17	0.31
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	16	0.31
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	8	0.31
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	15	0.31
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	2	0.31
(2,1395)	1:39:A:ALA:HB3	1:40:A:LYS:H	4	0.31
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	6	0.31
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	7	0.31
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	9	0.31
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	11	0.31
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	9	0.31
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	13	0.31
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	14	0.31
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	16	0.31
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	20	0.31
(2,1288)	1:167:A:LEU:HD22	1:167:A:LEU:HA	15	0.31
(2,1276)	1:160:A:LEU:HD21	1:166:A:TRP:HE1	14	0.31
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	8	0.31
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	10	0.31
(2,1208)	1:114:A:ILE:HD13	1:171:A:VAL:HB	5	0.31
(2,1201)	1:144:A:LEU:HD23	1:144:A:LEU:HG	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1201)	1:144:A:LEU:HD22	1:144:A:LEU:HG	11	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	1	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	4	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	5	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	6	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	10	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	12	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	14	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	15	0.31
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	20	0.31
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	7	0.31
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	12	0.31
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	15	0.31
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	16	0.31
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	18	0.31
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	20	0.31
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	13	0.31
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	18	0.31
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	14	0.31
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	14	0.31
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	8	0.31
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	2	0.31
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	6	0.31
(2,629)	1:44:A:LYS:H	1:42:A:LYS:HG3	12	0.31
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	12	0.31
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	3	0.31
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	16	0.31
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	4	0.31
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	20	0.31
(2,266)	1:21:A:LEU:H	1:24:A:LEU:HD21	1	0.31
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	18	0.31
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	12	0.31
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	13	0.31
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	4	0.31
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	9	0.31
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	1	0.31
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	2	0.31
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	17	0.31
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD13	1	0.31
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	5	0.31
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	16	0.31
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	19	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	20	0.31
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	3	0.31
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	8	0.31
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	12	0.31
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	15	0.31
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	18	0.31
(2,32)	1:88:A:TYR:HE1	1:159:A:TYR:HD1	12	0.31
(2,21)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	15	0.31
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	2	0.31
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	12	0.31
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	14	0.31
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	5	0.31
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	20	0.31
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	15	0.3
(4,447)	1:160:A:LEU:HG	1:160:A:LEU:HD12	1	0.3
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	3	0.3
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	19	0.3
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	12	0.3
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	14	0.3
(4,426)	1:53:A:LEU:HD13	1:37:A:LEU:HG	18	0.3
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	7	0.3
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	10	0.3
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	2	0.3
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	6	0.3
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	11	0.3
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	11	0.3
(4,322)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	3	0.3
(4,319)	1:26:A:LEU:HD23	1:14:A:VAL:HA	2	0.3
(4,307)	1:26:A:LEU:HD23	1:15:A:LEU:HA	8	0.3
(4,307)	1:26:A:LEU:HD23	1:15:A:LEU:HA	18	0.3
(4,299)	1:168:A:ILE:HD11	1:96:A:VAL:HA	8	0.3
(4,208)	1:171:A:VAL:HG23	1:173:A:ALA:HA	6	0.3
(4,195)	1:114:A:ILE:HD11	1:117:A:MET:HE1	20	0.3
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	10	0.3
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB3	2	0.3
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	3	0.3
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	20	0.3
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	1	0.3
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	15	0.3
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	20	0.3
(4,4)	1:65:A:PHE:HD1	1:37:A:LEU:HD23	10	0.3
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	8	0.3
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	2	0.3
(2,3836)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	13	0.3
(2,3829)	1:109:A:ILE:HD11	1:101:A:THR:HG23	3	0.3
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	9	0.3
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	18	0.3
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	13	0.3
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	16	0.3
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	4	0.3
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	10	0.3
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	19	0.3
(2,3804)	1:128:A:ILE:HG21	1:129:A:THR:HG21	6	0.3
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	1	0.3
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	8	0.3
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	5	0.3
(2,3795)	1:14:A:VAL:HG22	1:21:A:LEU:HG	20	0.3
(2,3789)	1:22:A:ILE:HG22	1:44:A:LYS:HB3	1	0.3
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD12	6	0.3
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	11	0.3
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG22	16	0.3
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG23	5	0.3
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	8	0.3
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	15	0.3
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	17	0.3
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG12	19	0.3
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD21	6	0.3
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	18	0.3
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	10	0.3
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	18	0.3
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	19	0.3
(2,3677)	1:15:A:LEU:HD23	1:15:A:LEU:HA	5	0.3
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	1	0.3
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	9	0.3
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE3	12	0.3
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	12	0.3
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE3	14	0.3
(2,3514)	1:143:A:VAL:HG13	1:132:A:ARG:HA	4	0.3
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	5	0.3
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	17	0.3
(2,3490)	1:48:A:ILE:HD12	1:53:A:LEU:HA	7	0.3
(2,3490)	1:48:A:ILE:HD13	1:53:A:LEU:HA	11	0.3
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	17	0.3
(2,3428)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	14	0.3
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	17	0.3
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	19	0.3
(2,3196)	1:176:A:ILE:HG21	1:176:A:ILE:HB	9	0.3
(2,3175)	1:144:A:LEU:HD23	1:144:A:LEU:HG	1	0.3
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	4	0.3
(2,3175)	1:144:A:LEU:HD21	1:144:A:LEU:HG	19	0.3
(2,2949)	1:165:A:VAL:H	1:91:A:GLN:HE22	5	0.3
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	8	0.3
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	13	0.3
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	20	0.3
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG13	12	0.3
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	3	0.3
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	7	0.3
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	15	0.3
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	10	0.3
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	18	0.3
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	10	0.3
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	15	0.3
(2,1900)	1:24:A:LEU:HA	1:44:A:LYS:HE3	12	0.3
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	5	0.3
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	7	0.3
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	8	0.3
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	11	0.3
(2,1874)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	4	0.3
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	10	0.3
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	14	0.3
(2,1864)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	15	0.3
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	5	0.3
(2,1863)	1:11:A:LEU:HD13	1:11:A:LEU:HB3	14	0.3
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	18	0.3
(2,1858)	1:109:A:ILE:HG21	1:109:A:ILE:HD11	1	0.3
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	12	0.3
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	14	0.3
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	15	0.3
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	16	0.3
(2,1850)	1:97:A:LEU:HD13	1:124:A:LEU:HD21	11	0.3
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	6	0.3
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	18	0.3
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	1	0.3
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1839)	1:56:A:ILE:HG21	1:56:A:ILE:HG12	9	0.3
(2,1838)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	4	0.3
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	3	0.3
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	1	0.3
(2,1832)	1:53:A:LEU:HD21	1:56:A:ILE:HB	2	0.3
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	3	0.3
(2,1832)	1:53:A:LEU:HD23	1:56:A:ILE:HB	15	0.3
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	6	0.3
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	9	0.3
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	11	0.3
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	18	0.3
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	16	0.3
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	17	0.3
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	16	0.3
(2,1796)	1:76:A:ALA:HB1	1:15:A:LEU:HD12	18	0.3
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	17	0.3
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	5	0.3
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	11	0.3
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	13	0.3
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	14	0.3
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	18	0.3
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	6	0.3
(2,1709)	1:86:A:LEU:HD21	1:86:A:LEU:HA	13	0.3
(2,1709)	1:86:A:LEU:HD23	1:86:A:LEU:HA	18	0.3
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	3	0.3
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	6	0.3
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	7	0.3
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	10	0.3
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	12	0.3
(2,1686)	1:14:A:VAL:HG23	1:19:A:PRO:HA	20	0.3
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	7	0.3
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	12	0.3
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	9	0.3
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	7	0.3
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	1	0.3
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	2	0.3
(2,1586)	1:28:A:ALA:HB3	1:28:A:ALA:HA	4	0.3
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	8	0.3
(2,1586)	1:28:A:ALA:HB2	1:28:A:ALA:HA	13	0.3
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	14	0.3
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	15	0.3
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	19	0.3
(2,1573)	1:66:A:ALA:HB3	1:66:A:ALA:HA	18	0.3
(2,1532)	1:34:A:VAL:HG11	1:34:A:VAL:HA	14	0.3
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	6	0.3
(2,1459)	1:108:A:LEU:HD12	2:201:A:NAD:H2A	5	0.3
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	14	0.3
(2,1405)	1:20:A:ALA:HB1	1:20:A:ALA:H	9	0.3
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	1	0.3
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	12	0.3
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	14	0.3
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	16	0.3
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	17	0.3
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	18	0.3
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	6	0.3
(2,1201)	1:144:A:LEU:HD22	1:144:A:LEU:HG	6	0.3
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	3	0.3
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	11	0.3
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	17	0.3
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	19	0.3
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	11	0.3
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	4	0.3
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	1	0.3
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	12	0.3
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	20	0.3
(2,1075)	1:56:A:ILE:H	1:58:A:GLU:H	18	0.3
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	4	0.3
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	15	0.3
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	15	0.3
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	6	0.3
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	14	0.3
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	3	0.3
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	1	0.3
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	15	0.3
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	10	0.3
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	7	0.3
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	15	0.3
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	8	0.3
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB2	10	0.3
(2,438)	1:55:A:HIS:H	1:55:A:HIS:HB3	18	0.3
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	9	0.3
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	13	0.3
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	16	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	2	0.3
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	5	0.3
(2,187)	1:26:A:LEU:HD22	1:26:A:LEU:H	16	0.3
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	2	0.3
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	2	0.3
(2,120)	1:177:A:LYS:HB3	1:178:A:VAL:H	2	0.3
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	7	0.3
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	11	0.3
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	4	0.3
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	7	0.3
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	19	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	1	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	2	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	3	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	4	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	6	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	7	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	8	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	9	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	10	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	11	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	14	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	15	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	16	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	18	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	19	0.3
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	20	0.3
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	17	0.3
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	14	0.3
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	16	0.3
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	7	0.3
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	8	0.3
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	1	0.29
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	19	0.29
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	15	0.29
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	4	0.29
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	8	0.29
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	9	0.29
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	9	0.29
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	1	0.29
(4,426)	1:53:A:LEU:HD13	1:37:A:LEU:HG	10	0.29
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	7	0.29
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	2	0.29
(4,307)	1:38:A:LEU:HD11	1:50:A:MET:HA	1	0.29
(4,307)	1:38:A:LEU:HD13	1:50:A:MET:HA	9	0.29
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	3	0.29
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	3	0.29
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	16	0.29
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	14	0.29
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB3	3	0.29
(4,36)	1:76:A:ALA:H	1:11:A:LEU:HD23	1	0.29
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	2	0.29
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	16	0.29
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	9	0.29
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	10	0.29
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	14	0.29
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	17	0.29
(2,3829)	1:109:A:ILE:HD11	1:101:A:THR:HG23	11	0.29
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	10	0.29
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	14	0.29
(2,3827)	1:74:A:ILE:HD11	1:74:A:ILE:HG12	15	0.29
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	11	0.29
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	5	0.29
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	3	0.29
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	12	0.29
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	13	0.29
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	17	0.29
(2,3804)	1:128:A:ILE:HG21	1:129:A:THR:HG22	2	0.29
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	14	0.29
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	1	0.29
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	4	0.29
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	10	0.29
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	13	0.29
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	16	0.29
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG21	16	0.29
(2,3718)	1:158:A:PHE:HB3	1:168:A:ILE:HG12	4	0.29
(2,3710)	1:14:A:VAL:HG23	1:14:A:VAL:HA	13	0.29
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	8	0.29
(2,3659)	1:20:A:ALA:HB2	1:20:A:ALA:HA	15	0.29
(2,3600)	1:42:A:LYS:HE2	1:39:A:ALA:HA	20	0.29
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	7	0.29
(2,3556)	1:28:A:ALA:HB1	1:28:A:ALA:HA	7	0.29
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3508)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	16	0.29
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	1	0.29
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	4	0.29
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	11	0.29
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	3	0.29
(2,3484)	1:124:A:LEU:HD13	1:167:A:LEU:HA	5	0.29
(2,3461)	1:168:A:ILE:HD11	1:156:A:PHE:HB2	5	0.29
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	6	0.29
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	8	0.29
(2,3434)	1:15:A:LEU:HD11	1:65:A:PHE:HE1	3	0.29
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	17	0.29
(2,3409)	1:84:A:VAL:HG12	1:85:A:ASP:H	8	0.29
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	3	0.29
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	17	0.29
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	18	0.29
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	18	0.29
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	19	0.29
(2,3355)	1:41:A:MET:HE2	1:41:A:MET:H	20	0.29
(2,3266)	1:53:A:LEU:HD11	1:67:A:PHE:HE1	18	0.29
(2,3175)	1:144:A:LEU:HD23	1:144:A:LEU:HG	5	0.29
(2,3175)	1:144:A:LEU:HD22	1:144:A:LEU:HG	11	0.29
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG12	7	0.29
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	1	0.29
(2,2201)	1:21:A:LEU:H	1:22:A:ILE:HG21	20	0.29
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	6	0.29
(2,2123)	1:86:A:LEU:H	1:86:A:LEU:HB3	13	0.29
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD13	13	0.29
(2,2065)	1:171:A:VAL:H	1:168:A:ILE:HG21	7	0.29
(2,2041)	1:152:A:ALA:HB2	1:152:A:ALA:H	1	0.29
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	13	0.29
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	17	0.29
(2,2041)	1:152:A:ALA:HB2	1:152:A:ALA:H	19	0.29
(2,1974)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	18	0.29
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	6	0.29
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	1	0.29
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	15	0.29
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	18	0.29
(2,1874)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	11	0.29
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	13	0.29
(2,1864)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	17	0.29
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	15	0.29
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	18	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1857)	1:151:A:MET:HE1	1:171:A:VAL:HG12	2	0.29
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	14	0.29
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD21	14	0.29
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	10	0.29
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	20	0.29
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	5	0.29
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	10	0.29
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	12	0.29
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	15	0.29
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	7	0.29
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	11	0.29
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	20	0.29
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	1	0.29
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	2	0.29
(2,1822)	1:143:A:VAL:HG11	1:143:A:VAL:HB	8	0.29
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	14	0.29
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	15	0.29
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	17	0.29
(2,1822)	1:143:A:VAL:HG11	1:143:A:VAL:HB	20	0.29
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	13	0.29
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	8	0.29
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	17	0.29
(2,1796)	1:76:A:ALA:HB2	1:15:A:LEU:HD11	5	0.29
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	6	0.29
(2,1796)	1:76:A:ALA:HB2	1:15:A:LEU:HD12	14	0.29
(2,1794)	1:117:A:MET:HE1	1:117:A:MET:HB2	6	0.29
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	16	0.29
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	2	0.29
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG21	18	0.29
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	15	0.29
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	19	0.29
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	2	0.29
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	8	0.29
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	11	0.29
(2,1686)	1:14:A:VAL:HG23	1:19:A:PRO:HA	13	0.29
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	16	0.29
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	18	0.29
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	11	0.29
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE3	13	0.29
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	9	0.29
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	11	0.29
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1586)	1:28:A:ALA:HB3	1:28:A:ALA:HA	10	0.29
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	11	0.29
(2,1586)	1:28:A:ALA:HB3	1:28:A:ALA:HA	18	0.29
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	20	0.29
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	11	0.29
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	20	0.29
(2,1573)	1:66:A:ALA:HB3	1:66:A:ALA:HA	6	0.29
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	8	0.29
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	11	0.29
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	14	0.29
(2,1514)	1:124:A:LEU:HD13	1:167:A:LEU:HA	17	0.29
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	4	0.29
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	9	0.29
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	11	0.29
(2,1459)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	2	0.29
(2,1395)	1:39:A:ALA:HB2	1:40:A:LYS:H	10	0.29
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	12	0.29
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	12	0.29
(2,1377)	1:4:A:MET:HE3	1:55:A:HIS:HD2	2	0.29
(2,1301)	1:34:A:VAL:HG12	1:38:A:LEU:H	4	0.29
(2,1201)	1:144:A:LEU:HD22	1:144:A:LEU:HG	3	0.29
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	7	0.29
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	8	0.29
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	16	0.29
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	18	0.29
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	3	0.29
(2,1193)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	6	0.29
(2,1183)	1:165:A:VAL:HG11	2:201:A:NAD:H2N	2	0.29
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	6	0.29
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	5	0.29
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	16	0.29
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	6	0.29
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	8	0.29
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	18	0.29
(2,708)	1:113:A:GLY:H	1:109:A:ILE:HG21	3	0.29
(2,708)	1:113:A:GLY:H	1:109:A:ILE:HG21	7	0.29
(2,629)	1:44:A:LYS:H	1:42:A:LYS:HG3	16	0.29
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	10	0.29
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	17	0.29
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	20	0.29
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	10	0.29
(2,405)	1:95:A:ALA:HB1	1:149:A:LYS:H	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	4	0.29
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	12	0.29
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	3	0.29
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	1	0.29
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	17	0.29
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	18	0.29
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	19	0.29
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	4	0.29
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	18	0.29
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	1	0.29
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	16	0.29
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD13	17	0.29
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	3	0.29
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	10	0.29
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	13	0.29
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	1	0.29
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	20	0.29
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	12	0.29
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	13	0.29
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	17	0.29
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	3	0.29
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	8	0.29
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	14	0.29
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	1	0.29
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	3	0.29
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	19	0.29
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	14	0.29
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	17	0.29
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	2	0.28
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	13	0.28
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	2	0.28
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	3	0.28
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	5	0.28
(4,426)	1:53:A:LEU:HD13	1:37:A:LEU:HG	6	0.28
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	15	0.28
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	19	0.28
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	20	0.28
(4,409)	1:4:A:MET:HE1	1:59:A:THR:HG23	20	0.28
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	5	0.28
(4,395)	1:56:A:ILE:HG23	1:56:A:ILE:HA	14	0.28
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	13	0.28
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	18	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,371)	1:174:A:GLU:HB3	1:109:A:ILE:HA	16	0.28
(4,320)	1:151:A:MET:HE1	1:147:A:ASP:HB2	18	0.28
(4,319)	1:26:A:LEU:HD23	1:14:A:VAL:HA	10	0.28
(4,310)	1:21:A:LEU:HD13	1:10:A:PHE:HA	12	0.28
(4,307)	1:38:A:LEU:HD11	1:50:A:MET:HA	6	0.28
(4,307)	1:38:A:LEU:HD13	1:50:A:MET:HA	15	0.28
(4,307)	1:38:A:LEU:HD11	1:50:A:MET:HA	17	0.28
(4,278)	1:142:A:VAL:HG13	1:102:A:ALA:H	14	0.28
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	7	0.28
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	14	0.28
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB3	12	0.28
(4,103)	1:114:A:ILE:H	1:144:A:LEU:HA	1	0.28
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	13	0.28
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	14	0.28
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	17	0.28
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	4	0.28
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	6	0.28
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	13	0.28
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	15	0.28
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	18	0.28
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	19	0.28
(2,3836)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	1	0.28
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	17	0.28
(2,3829)	1:109:A:ILE:HD11	1:101:A:THR:HG23	1	0.28
(2,3827)	1:74:A:ILE:HD12	1:74:A:ILE:HG12	17	0.28
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	9	0.28
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	14	0.28
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	6	0.28
(2,3821)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	9	0.28
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	15	0.28
(2,3821)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	18	0.28
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	4	0.28
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	5	0.28
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	7	0.28
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	16	0.28
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	4	0.28
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	8	0.28
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD11	14	0.28
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	6	0.28
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD12	1	0.28
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	7	0.28
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	2	0.28
(2,3780)	1:86:A:LEU:HD12	1:86:A:LEU:HG	4	0.28
(2,3780)	1:86:A:LEU:HD13	1:86:A:LEU:HG	7	0.28
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	12	0.28
(2,3769)	1:5:A:VAL:HG22	1:5:A:VAL:HB	11	0.28
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	3	0.28
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG12	14	0.28
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	4	0.28
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	18	0.28
(2,3745)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	6	0.28
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	4	0.28
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	10	0.28
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD21	13	0.28
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	14	0.28
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	17	0.28
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	16	0.28
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	20	0.28
(2,3559)	1:102:A:ALA:HB1	2:201:A:NAD:H4B	11	0.28
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	13	0.28
(2,3514)	1:143:A:VAL:HG11	1:132:A:ARG:HA	18	0.28
(2,3508)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	5	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	2	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	3	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	5	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	10	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	12	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	13	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	14	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	18	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	19	0.28
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	20	0.28
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	10	0.28
(2,3484)	1:124:A:LEU:HD11	1:167:A:LEU:HA	12	0.28
(2,3484)	1:124:A:LEU:HD13	1:167:A:LEU:HA	20	0.28
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	5	0.28
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	3	0.28
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	15	0.28
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	3	0.28
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	9	0.28
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	16	0.28
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	5	0.28
(2,3387)	1:21:A:LEU:HD23	1:10:A:PHE:HE1	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3211)	1:151:A:MET:HE1	1:156:A:PHE:HZ	17	0.28
(2,3182)	1:114:A:ILE:HD13	1:171:A:VAL:HB	13	0.28
(2,3178)	1:24:A:LEU:HD13	1:36:A:GLU:HB2	12	0.28
(2,3175)	1:144:A:LEU:HD22	1:144:A:LEU:HG	6	0.28
(2,2918)	1:76:A:ALA:HB1	1:78:A:GLN:HE22	8	0.28
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	14	0.28
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	13	0.28
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	1	0.28
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	1	0.28
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD13	1	0.28
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	5	0.28
(2,2041)	1:152:A:ALA:HB2	1:152:A:ALA:H	8	0.28
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	16	0.28
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	18	0.28
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	8	0.28
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	6	0.28
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	9	0.28
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	10	0.28
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	14	0.28
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	15	0.28
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	17	0.28
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	18	0.28
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	19	0.28
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	1	0.28
(2,1863)	1:11:A:LEU:HD13	1:11:A:LEU:HB3	6	0.28
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	4	0.28
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	6	0.28
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	7	0.28
(2,1858)	1:109:A:ILE:HG22	1:109:A:ILE:HD11	11	0.28
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	16	0.28
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	3	0.28
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	19	0.28
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	10	0.28
(2,1841)	1:168:A:ILE:HG23	1:168:A:ILE:HB	18	0.28
(2,1838)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	5	0.28
(2,1822)	1:143:A:VAL:HG11	1:143:A:VAL:HB	4	0.28
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	10	0.28
(2,1822)	1:143:A:VAL:HG12	1:143:A:VAL:HB	12	0.28
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	16	0.28
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	11	0.28
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	19	0.28
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	7	0.28
(2,1737)	1:110:A:LEU:HA	1:110:A:LEU:HB3	10	0.28
(2,1709)	1:86:A:LEU:HD21	1:86:A:LEU:HA	6	0.28
(2,1709)	1:86:A:LEU:HD23	1:86:A:LEU:HA	8	0.28
(2,1709)	1:86:A:LEU:HD23	1:86:A:LEU:HA	12	0.28
(2,1709)	1:86:A:LEU:HD21	1:86:A:LEU:HA	16	0.28
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	1	0.28
(2,1686)	1:14:A:VAL:HG21	1:19:A:PRO:HA	14	0.28
(2,1590)	1:32:A:ALA:HB2	1:33:A:PRO:HD3	12	0.28
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	4	0.28
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	10	0.28
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	13	0.28
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	19	0.28
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	12	0.28
(2,1492)	1:167:A:LEU:HD22	1:123:A:HIS:HA	13	0.28
(2,1458)	1:165:A:VAL:HG13	2:201:A:NAD:H5N	7	0.28
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	17	0.28
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	1	0.28
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	1	0.28
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	6	0.28
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	8	0.28
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	6	0.28
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	2	0.28
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	10	0.28
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	13	0.28
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	15	0.28
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	7	0.28
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	17	0.28
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD11	14	0.28
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	15	0.28
(2,1211)	1:177:A:LYS:HD2	1:177:A:LYS:HA	16	0.28
(2,1200)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	9	0.28
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	17	0.28
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	4	0.28
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	5	0.28
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	19	0.28
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	8	0.28
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	11	0.28
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	12	0.28
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	14	0.28
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	18	0.28
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	6	0.28
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	10	0.28
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	5	0.28
(2,383)	1:20:A:ALA:H	1:19:A:PRO:HD3	1	0.28
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	15	0.28
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	3	0.28
(2,232)	1:109:A:ILE:H	1:102:A:ALA:H	20	0.28
(2,202)	1:24:A:LEU:H	1:24:A:LEU:HD21	1	0.28
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	4	0.28
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	6	0.28
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	8	0.28
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	10	0.28
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	12	0.28
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	13	0.28
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	14	0.28
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	16	0.28
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	3	0.28
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	20	0.28
(2,164)	1:86:A:LEU:H	1:86:A:LEU:HB3	13	0.28
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	2	0.28
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	3	0.28
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	20	0.28
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	5	0.28
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	1	0.28
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	12	0.28
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	16	0.28
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	20	0.28
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	18	0.28
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	8	0.28
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	20	0.28
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	5	0.28
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	9	0.28
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	13	0.28
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	1	0.28
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	3	0.28
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	8	0.28
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	12	0.28
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	2	0.28
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	4	0.28
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	6	0.28
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	9	0.28
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	11	0.28
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	18	0.28
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	14	0.28
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	8	0.27
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	9	0.27
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	17	0.27
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	16	0.27
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	7	0.27
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	17	0.27
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	14	0.27
(4,436)	1:34:A:VAL:HG11	1:35:A:LYS:HG3	18	0.27
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	4	0.27
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	7	0.27
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	9	0.27
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	11	0.27
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	13	0.27
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	16	0.27
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	6	0.27
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	18	0.27
(4,307)	1:26:A:LEU:HD23	1:15:A:LEU:HA	7	0.27
(4,307)	1:38:A:LEU:HD13	1:50:A:MET:HA	10	0.27
(4,307)	1:38:A:LEU:HD12	1:50:A:MET:HA	11	0.27
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	18	0.27
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	4	0.27
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	19	0.27
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	1	0.27
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	6	0.27
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	20	0.27
(2,3832)	1:97:A:LEU:HD22	1:151:A:MET:HG3	5	0.27
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	4	0.27
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	6	0.27
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	16	0.27
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG22	5	0.27
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	14	0.27
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	17	0.27
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	9	0.27
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	7	0.27
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	10	0.27
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	13	0.27
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	10	0.27
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD12	4	0.27
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3763)	1:76:A:ALA:HB2	1:15:A:LEU:HD12	16	0.27
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	1	0.27
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG11	11	0.27
(2,3748)	1:108:A:LEU:HG	1:108:A:LEU:HD23	19	0.27
(2,3718)	1:158:A:PHE:HB2	1:168:A:ILE:HG12	17	0.27
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	7	0.27
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD21	9	0.27
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	16	0.27
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	6	0.27
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	7	0.27
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	8	0.27
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	9	0.27
(2,3496)	1:38:A:LEU:HD23	1:38:A:LEU:HA	15	0.27
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	12	0.27
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	8	0.27
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	9	0.27
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	13	0.27
(2,3479)	1:151:A:MET:HE2	1:171:A:VAL:HA	18	0.27
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	3	0.27
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	18	0.27
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	20	0.27
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	8	0.27
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	11	0.27
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	14	0.27
(2,3404)	1:146:A:VAL:HG13	1:97:A:LEU:H	6	0.27
(2,3399)	1:21:A:LEU:HD13	1:21:A:LEU:H	20	0.27
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	4	0.27
(2,3346)	1:4:A:MET:HE3	1:55:A:HIS:HD2	2	0.27
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	8	0.27
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	10	0.27
(2,3175)	1:144:A:LEU:HD22	1:144:A:LEU:HG	3	0.27
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	1	0.27
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	4	0.27
(2,2308)	1:108:A:LEU:HD22	1:108:A:LEU:H	2	0.27
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	13	0.27
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	12	0.27
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	12	0.27
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	3	0.27
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	19	0.27
(2,1936)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	12	0.27
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	1	0.27
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	13	0.27
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	19	0.27
(2,1874)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	7	0.27
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	3	0.27
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	4	0.27
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	13	0.27
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	16	0.27
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD11	6	0.27
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	3	0.27
(2,1858)	1:109:A:ILE:HG21	1:109:A:ILE:HD11	5	0.27
(2,1858)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	13	0.27
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	12	0.27
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	10	0.27
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	17	0.27
(2,1844)	1:110:A:LEU:HD23	1:110:A:LEU:HB3	9	0.27
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	8	0.27
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	1	0.27
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	3	0.27
(2,1822)	1:143:A:VAL:HG13	1:143:A:VAL:HB	19	0.27
(2,1817)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	4	0.27
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	4	0.27
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	10	0.27
(2,1796)	1:76:A:ALA:HB1	1:15:A:LEU:HD11	15	0.27
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	7	0.27
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	16	0.27
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	15	0.27
(2,1709)	1:86:A:LEU:HD23	1:86:A:LEU:HA	14	0.27
(2,1686)	1:14:A:VAL:HG22	1:19:A:PRO:HA	17	0.27
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	16	0.27
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	3	0.27
(2,1599)	1:4:A:MET:HE1	1:52:A:GLU:HA	8	0.27
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	3	0.27
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	11	0.27
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	2	0.27
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	3	0.27
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	15	0.27
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	20	0.27
(2,1586)	1:28:A:ALA:HB1	1:28:A:ALA:HA	7	0.27
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	1	0.27
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	2	0.27
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	4	0.27
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	13	0.27
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	15	0.27
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	20	0.27
(2,1563)	1:48:A:ILE:HG23	1:53:A:LEU:HB2	2	0.27
(2,1555)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	6	0.27
(2,1535)	1:22:A:ILE:HG22	1:44:A:LYS:HE3	17	0.27
(2,1514)	1:124:A:LEU:HD13	1:167:A:LEU:HA	5	0.27
(2,1461)	1:128:A:ILE:HD13	1:127:A:ASP:H	14	0.27
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	3	0.27
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	9	0.27
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	16	0.27
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	9	0.27
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	12	0.27
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	15	0.27
(2,1426)	1:86:A:LEU:HD11	1:88:A:TYR:HD1	1	0.27
(2,1420)	1:22:A:ILE:HG23	1:10:A:PHE:HE1	4	0.27
(2,1420)	1:22:A:ILE:HG23	1:10:A:PHE:HE1	15	0.27
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	16	0.27
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	10	0.27
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	15	0.27
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	17	0.27
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	19	0.27
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	9	0.27
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	8	0.27
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	9	0.27
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	11	0.27
(2,1301)	1:34:A:VAL:HG12	1:38:A:LEU:H	6	0.27
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	9	0.27
(2,1301)	1:34:A:VAL:HG12	1:38:A:LEU:H	11	0.27
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	10	0.27
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	2	0.27
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD11	5	0.27
(2,1187)	1:176:A:ILE:HG21	1:106:A:PHE:HE1	12	0.27
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	14	0.27
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	5	0.27
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	18	0.27
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	16	0.27
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	20	0.27
(2,815)	1:102:A:ALA:H	1:101:A:THR:HG23	20	0.27
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD13	5	0.27
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD13	6	0.27
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD12	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	18	0.27
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	10	0.27
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	17	0.27
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	19	0.27
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	14	0.27
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	1	0.27
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	18	0.27
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	16	0.27
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD12	10	0.27
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	12	0.27
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	5	0.27
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	5	0.27
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	19	0.27
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	2	0.27
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	5	0.27
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	7	0.27
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	9	0.27
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	15	0.27
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	20	0.27
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	15	0.27
(2,120)	1:177:A:LYS:HB3	1:178:A:VAL:H	11	0.27
(2,33)	1:10:A:PHE:HD1	1:10:A:PHE:HZ	5	0.27
(2,16)	1:21:A:LEU:HD13	1:10:A:PHE:HE1	3	0.27
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	7	0.27
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	9	0.27
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	19	0.27
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	3	0.27
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	13	0.27
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	16	0.27
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	5	0.27
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	1	0.27
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	1	0.27
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	10	0.27
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	17	0.27
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	13	0.27
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	13	0.27
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	15	0.27
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	16	0.27
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	18	0.26
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD11	9	0.26
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	8	0.26
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	12	0.26
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	8	0.26
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	14	0.26
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	4	0.26
(4,307)	1:38:A:LEU:HD11	1:50:A:MET:HA	16	0.26
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	1	0.26
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	9	0.26
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	12	0.26
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB3	1	0.26
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB3	8	0.26
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	5	0.26
(4,40)	1:5:A:VAL:H	1:5:A:VAL:HB	10	0.26
(4,40)	1:5:A:VAL:H	1:5:A:VAL:HB	11	0.26
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	3	0.26
(2,3964)	1:123:A:HIS:HB3	2:201:A:NAD:H6N	8	0.26
(2,3959)	1:123:A:HIS:HB3	2:201:A:NAD:H5N	1	0.26
(2,3844)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	2	0.26
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	20	0.26
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	3	0.26
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	7	0.26
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD11	6	0.26
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	17	0.26
(2,3821)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	2	0.26
(2,3821)	1:144:A:LEU:HD13	1:109:A:ILE:HG21	4	0.26
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	11	0.26
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	17	0.26
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	2	0.26
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	3	0.26
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	5	0.26
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	6	0.26
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	13	0.26
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	16	0.26
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	16	0.26
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	2	0.26
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	15	0.26
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	17	0.26
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	18	0.26
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD11	19	0.26
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	3	0.26
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	6	0.26
(2,3769)	1:5:A:VAL:HG22	1:5:A:VAL:HB	10	0.26
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	19	0.26
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	4	0.26
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	1	0.26
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD22	2	0.26
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD22	3	0.26
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	12	0.26
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	15	0.26
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	18	0.26
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE2	15	0.26
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	6	0.26
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	14	0.26
(2,3490)	1:48:A:ILE:HD12	1:53:A:LEU:HA	5	0.26
(2,3490)	1:48:A:ILE:HD12	1:53:A:LEU:HA	16	0.26
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	17	0.26
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	12	0.26
(2,3409)	1:84:A:VAL:HG11	1:85:A:ASP:H	9	0.26
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	15	0.26
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	18	0.26
(2,3288)	1:142:A:VAL:HG11	1:103:A:GLU:HA	3	0.26
(2,3182)	1:114:A:ILE:HD13	1:171:A:VAL:HB	17	0.26
(2,2738)	1:30:A:GLY:H	1:26:A:LEU:HD23	16	0.26
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	16	0.26
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG12	18	0.26
(2,2148)	1:26:A:LEU:HD23	1:26:A:LEU:H	19	0.26
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD13	17	0.26
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	1	0.26
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	10	0.26
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	3	0.26
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	6	0.26
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	7	0.26
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	10	0.26
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	11	0.26
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	15	0.26
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	20	0.26
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	4	0.26
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	8	0.26
(2,1869)	1:97:A:LEU:HD23	1:96:A:VAL:HB	6	0.26
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	11	0.26
(2,1857)	1:151:A:MET:HE1	1:171:A:VAL:HG12	4	0.26
(2,1857)	1:151:A:MET:HE2	1:171:A:VAL:HG12	7	0.26
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	3	0.26
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1850)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	2	0.26
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	3	0.26
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	2	0.26
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD11	4	0.26
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	11	0.26
(2,1844)	1:110:A:LEU:HD23	1:110:A:LEU:HB3	12	0.26
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	14	0.26
(2,1844)	1:110:A:LEU:HD23	1:110:A:LEU:HB3	16	0.26
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	11	0.26
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	18	0.26
(2,1807)	1:151:A:MET:HE2	1:174:A:GLU:HG2	17	0.26
(2,1796)	1:76:A:ALA:HB2	1:15:A:LEU:HD11	1	0.26
(2,1796)	1:76:A:ALA:HB1	1:15:A:LEU:HD12	13	0.26
(2,1796)	1:76:A:ALA:HB2	1:15:A:LEU:HD11	17	0.26
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	6	0.26
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG21	14	0.26
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	12	0.26
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	15	0.26
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	5	0.26
(2,1640)	1:40:A:LYS:HE3	1:25:A:ASP:HB2	9	0.26
(2,1633)	1:42:A:LYS:HE2	1:39:A:ALA:HA	3	0.26
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE3	16	0.26
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE1	7	0.26
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	1	0.26
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	8	0.26
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	12	0.26
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	14	0.26
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	16	0.26
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	17	0.26
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	6	0.26
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	9	0.26
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	12	0.26
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	14	0.26
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	15	0.26
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	18	0.26
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	19	0.26
(2,1573)	1:66:A:ALA:HB1	1:66:A:ALA:HA	3	0.26
(2,1514)	1:124:A:LEU:HD11	1:167:A:LEU:HA	12	0.26
(2,1514)	1:124:A:LEU:HD13	1:167:A:LEU:HA	20	0.26
(2,1492)	1:167:A:LEU:HD23	1:123:A:HIS:HA	17	0.26
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	11	0.26
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1435)	1:15:A:LEU:HD23	1:15:A:LEU:H	12	0.26
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	18	0.26
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	6	0.26
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	8	0.26
(2,1378)	1:50:A:MET:HE3	1:67:A:PHE:HZ	3	0.26
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	18	0.26
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	7	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	1	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	3	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	4	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	7	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	14	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	16	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	18	0.26
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	19	0.26
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	9	0.26
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	10	0.26
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB3	20	0.26
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	4	0.26
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	10	0.26
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	16	0.26
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	2	0.26
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	2	0.26
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	13	0.26
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	15	0.26
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	19	0.26
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	10	0.26
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	19	0.26
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	4	0.26
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	5	0.26
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	17	0.26
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	7	0.26
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	9	0.26
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	12	0.26
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	15	0.26
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	12	0.26
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD13	8	0.26
(2,768)	1:30:A:GLY:H	1:26:A:LEU:HD21	3	0.26
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	9	0.26
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	16	0.26
(2,726)	1:20:A:ALA:HB2	1:23:A:GLY:H	3	0.26
(2,708)	1:113:A:GLY:H	1:109:A:ILE:HG21	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,708)	1:113:A:GLY:H	1:109:A:ILE:HG21	19	0.26
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	14	0.26
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	11	0.26
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	2	0.26
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	3	0.26
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	5	0.26
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	19	0.26
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	14	0.26
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	12	0.26
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	5	0.26
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	11	0.26
(2,289)	1:46:A:HIS:H	1:22:A:ILE:HG22	20	0.26
(2,206)	1:76:A:ALA:H	1:15:A:LEU:HD11	9	0.26
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	1	0.26
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	11	0.26
(2,145)	1:83:A:GLU:HB3	1:83:A:GLU:H	7	0.26
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	4	0.26
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD13	6	0.26
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	11	0.26
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	12	0.26
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	11	0.26
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	13	0.26
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	1	0.26
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	8	0.26
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	9	0.26
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	13	0.26
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	20	0.26
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	6	0.26
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	12	0.26
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	12	0.26
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	13	0.26
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	20	0.26
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	12	0.26
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	15	0.26
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	12	0.26
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	7	0.26
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	20	0.26
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	7	0.26
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	6	0.26
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	1	0.26
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	17	0.26
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,452)	1:59:A:THR:HB	1:59:A:THR:HG22	13	0.25
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	13	0.25
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	17	0.25
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	19	0.25
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	20	0.25
(4,443)	1:48:A:ILE:HD12	1:38:A:LEU:HB2	14	0.25
(4,426)	1:53:A:LEU:HD12	1:37:A:LEU:HG	17	0.25
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	2	0.25
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	13	0.25
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	15	0.25
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	12	0.25
(4,364)	1:4:A:MET:HE2	1:53:A:LEU:HB2	18	0.25
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	7	0.25
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	6	0.25
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	11	0.25
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	4	0.25
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	5	0.25
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	14	0.25
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	12	0.25
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	8	0.25
(2,3832)	1:97:A:LEU:HD23	1:151:A:MET:HG3	20	0.25
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	19	0.25
(2,3824)	1:41:A:MET:HE1	1:11:A:LEU:HD12	17	0.25
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	1	0.25
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	5	0.25
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	11	0.25
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	12	0.25
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	15	0.25
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	20	0.25
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	3	0.25
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	11	0.25
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	13	0.25
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	7	0.25
(2,3809)	1:110:A:LEU:HD13	1:176:A:ILE:HB	15	0.25
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	20	0.25
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	4	0.25
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	8	0.25
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	9	0.25
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	17	0.25
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	19	0.25
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	20	0.25
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	4	0.25
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	11	0.25
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	6	0.25
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	9	0.25
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	19	0.25
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD12	17	0.25
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	4	0.25
(2,3772)	1:151:A:MET:HE3	1:174:A:GLU:HG2	5	0.25
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	10	0.25
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	3	0.25
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	4	0.25
(2,3769)	1:5:A:VAL:HG22	1:5:A:VAL:HB	5	0.25
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	16	0.25
(2,3769)	1:5:A:VAL:HG21	1:5:A:VAL:HB	17	0.25
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	9	0.25
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	17	0.25
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	17	0.25
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	10	0.25
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	1	0.25
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	6	0.25
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	8	0.25
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	9	0.25
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	11	0.25
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	18	0.25
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD21	6	0.25
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	11	0.25
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	12	0.25
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE1	7	0.25
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	9	0.25
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE3	13	0.25
(2,3439)	1:110:A:LEU:HD11	1:110:A:LEU:H	14	0.25
(2,3434)	1:15:A:LEU:HD11	1:65:A:PHE:HE1	19	0.25
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	6	0.25
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	8	0.25
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	9	0.25
(2,2625)	1:29:A:ASN:H	1:29:A:ASN:HB3	9	0.25
(2,2625)	1:29:A:ASN:H	1:29:A:ASN:HB3	18	0.25
(2,2575)	1:111:A:LYS:HB2	1:111:A:LYS:H	8	0.25
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	13	0.25
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	10	0.25
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	14	0.25
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG11	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	11	0.25
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	18	0.25
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	15	0.25
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	19	0.25
(2,2123)	1:86:A:LEU:H	1:86:A:LEU:HB3	20	0.25
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	13	0.25
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	18	0.25
(2,2041)	1:152:A:ALA:HB2	1:152:A:ALA:H	2	0.25
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	2	0.25
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	15	0.25
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	11	0.25
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	17	0.25
(2,1889)	1:4:A:MET:HE1	1:4:A:MET:HA	3	0.25
(2,1881)	1:24:A:LEU:HD11	1:33:A:PRO:HD3	2	0.25
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	13	0.25
(2,1869)	1:97:A:LEU:HD21	1:96:A:VAL:HB	18	0.25
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	19	0.25
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	4	0.25
(2,1861)	1:41:A:MET:HE1	1:11:A:LEU:HD12	17	0.25
(2,1857)	1:151:A:MET:HE1	1:171:A:VAL:HG12	5	0.25
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	19	0.25
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	1	0.25
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG22	13	0.25
(2,1854)	1:22:A:ILE:HG23	1:14:A:VAL:HG21	16	0.25
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	14	0.25
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	8	0.25
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	2	0.25
(2,1844)	1:110:A:LEU:HD22	1:110:A:LEU:HB3	6	0.25
(2,1844)	1:110:A:LEU:HD23	1:110:A:LEU:HB3	13	0.25
(2,1844)	1:110:A:LEU:HD22	1:110:A:LEU:HB3	15	0.25
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	5	0.25
(2,1815)	1:86:A:LEU:HD21	1:86:A:LEU:HB2	10	0.25
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	6	0.25
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	9	0.25
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	12	0.25
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	15	0.25
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	8	0.25
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	3	0.25
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG23	11	0.25
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	15	0.25
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	1	0.25
(2,1709)	1:86:A:LEU:HD23	1:86:A:LEU:HA	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1709)	1:86:A:LEU:HD21	1:86:A:LEU:HA	7	0.25
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	4	0.25
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	5	0.25
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	19	0.25
(2,1587)	1:11:A:LEU:HG	1:11:A:LEU:HA	5	0.25
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	5	0.25
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	8	0.25
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	10	0.25
(2,1573)	1:66:A:ALA:HB3	1:66:A:ALA:HA	5	0.25
(2,1524)	1:82:A:VAL:HG11	1:82:A:VAL:HA	13	0.25
(2,1509)	1:151:A:MET:HE3	1:171:A:VAL:HA	20	0.25
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	8	0.25
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	14	0.25
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	15	0.25
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	10	0.25
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	3	0.25
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	16	0.25
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	1	0.25
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	2	0.25
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	4	0.25
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	10	0.25
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	11	0.25
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	15	0.25
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	18	0.25
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	11	0.25
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	5	0.25
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	6	0.25
(2,1301)	1:34:A:VAL:HG13	1:38:A:LEU:H	1	0.25
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	2	0.25
(2,1288)	1:167:A:LEU:HD22	1:167:A:LEU:HA	1	0.25
(2,1288)	1:167:A:LEU:HD22	1:167:A:LEU:HA	20	0.25
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	8	0.25
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	11	0.25
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	12	0.25
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	15	0.25
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	19	0.25
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	15	0.25
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	2	0.25
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	3	0.25
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	6	0.25
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	7	0.25
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	12	0.25
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	15	0.25
(2,1194)	1:176:A:ILE:HD12	1:114:A:ILE:HD13	6	0.25
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	16	0.25
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	1	0.25
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	3	0.25
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	10	0.25
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	12	0.25
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	13	0.25
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	15	0.25
(2,1131)	1:136:A:MET:H	1:105:A:ASN:HD22	2	0.25
(2,1131)	1:136:A:MET:H	1:105:A:ASN:HD22	3	0.25
(2,1075)	1:56:A:ILE:H	1:58:A:GLU:H	10	0.25
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	7	0.25
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	8	0.25
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	9	0.25
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	1	0.25
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	3	0.25
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	6	0.25
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	20	0.25
(2,985)	1:46:A:HIS:H	1:45:A:GLY:H	12	0.25
(2,985)	1:46:A:HIS:H	1:45:A:GLY:H	14	0.25
(2,752)	1:139:A:GLY:H	1:103:A:GLU:HA	20	0.25
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	16	0.25
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	5	0.25
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	20	0.25
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	3	0.25
(2,550)	1:102:A:ALA:HB1	1:105:A:ASN:H	9	0.25
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	8	0.25
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	11	0.25
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	13	0.25
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	14	0.25
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	19	0.25
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	20	0.25
(2,486)	1:58:A:GLU:H	1:58:A:GLU:HB3	15	0.25
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	8	0.25
(2,201)	1:24:A:LEU:H	1:24:A:LEU:HB2	3	0.25
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	18	0.25
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	1	0.25
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	6	0.25
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	15	0.25
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	4	0.25
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	14	0.25
(2,120)	1:177:A:LYS:HB3	1:178:A:VAL:H	9	0.25
(2,120)	1:177:A:LYS:HB3	1:178:A:VAL:H	16	0.25
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	17	0.25
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	4	0.25
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	6	0.25
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	5	0.25
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	19	0.25
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	5	0.25
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	15	0.25
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	17	0.25
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	18	0.25
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	19	0.25
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	9	0.25
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	10	0.25
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	1	0.25
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	17	0.25
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	20	0.25
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	2	0.25
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	4	0.25
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	12	0.25
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	18	0.25
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	12	0.25
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	4	0.25
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	7	0.25
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	11	0.25
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	14	0.25
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	4	0.25
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	1	0.25
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	3	0.25
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	16	0.25
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	1	0.25
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	4	0.25
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	18	0.25
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	5	0.25
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	12	0.25
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	19	0.25
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	7	0.25
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	9	0.25
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	11	0.25
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,452)	1:59:A:THR:HB	1:59:A:THR:HG22	5	0.24
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	7	0.24
(4,445)	1:14:A:VAL:HG12	1:11:A:LEU:HG	12	0.24
(4,442)	1:178:A:VAL:HG22	1:176:A:ILE:HB	17	0.24
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	4	0.24
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	15	0.24
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	20	0.24
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	6	0.24
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	20	0.24
(4,325)	1:7:A:VAL:HG13	1:10:A:PHE:HB3	15	0.24
(4,319)	1:26:A:LEU:HD23	1:14:A:VAL:HA	15	0.24
(4,311)	1:143:A:VAL:HG11	1:178:A:VAL:HA	4	0.24
(4,307)	1:38:A:LEU:HD13	1:50:A:MET:HA	2	0.24
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	12	0.24
(4,208)	1:14:A:VAL:HG21	1:11:A:LEU:HA	13	0.24
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB3	14	0.24
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	2	0.24
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	13	0.24
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	9	0.24
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	10	0.24
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	19	0.24
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD21	20	0.24
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD22	5	0.24
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	19	0.24
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	14	0.24
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	7	0.24
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	11	0.24
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	20	0.24
(2,3841)	1:76:A:ALA:HB3	1:76:A:ALA:H	15	0.24
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	3	0.24
(2,3836)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	4	0.24
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	9	0.24
(2,3836)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	14	0.24
(2,3836)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	18	0.24
(2,3823)	1:57:A:VAL:HG21	1:57:A:VAL:HB	8	0.24
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	19	0.24
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG22	10	0.24
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	6	0.24
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	10	0.24
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	8	0.24
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	9	0.24
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	15	0.24
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	14	0.24
(2,3810)	1:171:A:VAL:HG21	1:168:A:ILE:HD13	20	0.24
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	11	0.24
(2,3809)	1:176:A:ILE:HB	1:110:A:LEU:HD11	14	0.24
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	7	0.24
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	11	0.24
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	14	0.24
(2,3800)	1:56:A:ILE:HD11	1:56:A:ILE:HG12	6	0.24
(2,3800)	1:56:A:ILE:HD11	1:56:A:ILE:HG12	7	0.24
(2,3800)	1:56:A:ILE:HD11	1:56:A:ILE:HG12	9	0.24
(2,3800)	1:56:A:ILE:HD11	1:56:A:ILE:HG12	17	0.24
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	20	0.24
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	7	0.24
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	8	0.24
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	16	0.24
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	4	0.24
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	7	0.24
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	8	0.24
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	12	0.24
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	16	0.24
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	2	0.24
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG21	18	0.24
(2,3756)	1:144:A:LEU:HG	1:178:A:VAL:HG12	7	0.24
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	6	0.24
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	11	0.24
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	12	0.24
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	2	0.24
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	3	0.24
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	15	0.24
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD23	8	0.24
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD21	20	0.24
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	7	0.24
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	14	0.24
(2,3683)	1:84:A:VAL:HA	1:84:A:VAL:HG22	1	0.24
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	5	0.24
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	9	0.24
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE2	16	0.24
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE3	19	0.24
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	3	0.24
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	9	0.24
(2,3508)	1:21:A:LEU:HD12	1:44:A:LYS:HE2	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	12	0.24
(2,3495)	1:82:A:VAL:HG11	1:82:A:VAL:HA	13	0.24
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	15	0.24
(2,3490)	1:48:A:ILE:HD11	1:53:A:LEU:HA	19	0.24
(2,3479)	1:151:A:MET:HE1	1:171:A:VAL:HA	6	0.24
(2,3434)	1:15:A:LEU:HD12	1:65:A:PHE:HE1	5	0.24
(2,3434)	1:15:A:LEU:HD11	1:65:A:PHE:HE1	7	0.24
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	10	0.24
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	12	0.24
(2,3409)	1:84:A:VAL:HG11	1:85:A:ASP:H	12	0.24
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	1	0.24
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	5	0.24
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	5	0.24
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	5	0.24
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	8	0.24
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	3	0.24
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	15	0.24
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	2	0.24
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	17	0.24
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	3	0.24
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	8	0.24
(2,2785)	1:53:A:LEU:H	1:38:A:LEU:HD11	1	0.24
(2,2625)	1:29:A:ASN:H	1:29:A:ASN:HB3	1	0.24
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	5	0.24
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	5	0.24
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	6	0.24
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	15	0.24
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	19	0.24
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	9	0.24
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	13	0.24
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	16	0.24
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	1	0.24
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	5	0.24
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	20	0.24
(2,2266)	1:153:A:ASP:H	1:95:A:ALA:HB1	11	0.24
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	7	0.24
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	4	0.24
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	2	0.24
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	5	0.24
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	5	0.24
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	7	0.24
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	11	0.24
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	12	0.24
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	14	0.24
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	10	0.24
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	16	0.24
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD13	6	0.24
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	7	0.24
(2,1857)	1:151:A:MET:HE1	1:171:A:VAL:HG12	1	0.24
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	20	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	7	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	8	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	9	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	10	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	12	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	17	0.24
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	19	0.24
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	1	0.24
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	8	0.24
(2,1831)	1:142:A:VAL:HG23	1:143:A:VAL:HB	12	0.24
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	2	0.24
(2,1818)	1:86:A:LEU:HD12	1:86:A:LEU:HG	4	0.24
(2,1818)	1:86:A:LEU:HD13	1:86:A:LEU:HG	7	0.24
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	2	0.24
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	7	0.24
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	13	0.24
(2,1804)	1:5:A:VAL:HG22	1:5:A:VAL:HB	11	0.24
(2,1796)	1:76:A:ALA:HB1	1:15:A:LEU:HD11	7	0.24
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	11	0.24
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	8	0.24
(2,1754)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	14	0.24
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	20	0.24
(2,1709)	1:86:A:LEU:HD23	1:86:A:LEU:HA	19	0.24
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE2	14	0.24
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	6	0.24
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	8	0.24
(2,1576)	1:22:A:ILE:HG21	1:22:A:ILE:HA	16	0.24
(2,1565)	1:22:A:ILE:HG23	1:41:A:MET:HB2	3	0.24
(2,1534)	1:151:A:MET:HE3	1:151:A:MET:HA	7	0.24
(2,1524)	1:82:A:VAL:HG11	1:82:A:VAL:HA	17	0.24
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	18	0.24
(2,1459)	1:108:A:LEU:HD13	2:201:A:NAD:H2A	18	0.24
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	1	0.24
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	2	0.24
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	9	0.24
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	4	0.24
(2,1377)	1:4:A:MET:HE1	1:55:A:HIS:HD2	5	0.24
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	13	0.24
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	1	0.24
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	12	0.24
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	17	0.24
(2,1301)	1:34:A:VAL:HG12	1:38:A:LEU:H	17	0.24
(2,1288)	1:167:A:LEU:HD23	1:167:A:LEU:HA	3	0.24
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	3	0.24
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	4	0.24
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	13	0.24
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	16	0.24
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	17	0.24
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	18	0.24
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	1	0.24
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	5	0.24
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	8	0.24
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	13	0.24
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	17	0.24
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	19	0.24
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	20	0.24
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	7	0.24
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	19	0.24
(2,1155)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	17	0.24
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	4	0.24
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	10	0.24
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	16	0.24
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	13	0.24
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	8	0.24
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	12	0.24
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	10	0.24
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	19	0.24
(2,985)	1:46:A:HIS:H	1:45:A:GLY:H	16	0.24
(2,985)	1:46:A:HIS:H	1:45:A:GLY:H	17	0.24
(2,811)	1:14:A:VAL:HG21	1:22:A:ILE:H	5	0.24
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD11	12	0.24
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	4	0.24
(2,653)	1:29:A:ASN:H	1:29:A:ASN:HB3	9	0.24
(2,653)	1:29:A:ASN:H	1:29:A:ASN:HB3	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,550)	1:105:A:ASN:H	1:102:A:ALA:HB3	8	0.24
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	7	0.24
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	2	0.24
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	7	0.24
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	9	0.24
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	17	0.24
(2,486)	1:58:A:GLU:H	1:58:A:GLU:HB3	17	0.24
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	12	0.24
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	15	0.24
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	19	0.24
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	6	0.24
(2,412)	1:11:A:LEU:HD11	1:11:A:LEU:H	10	0.24
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	11	0.24
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	19	0.24
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	20	0.24
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	3	0.24
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	11	0.24
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	7	0.24
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	19	0.24
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	5	0.24
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	1	0.24
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	7	0.24
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	9	0.24
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD11	4	0.24
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD11	19	0.24
(2,120)	1:177:A:LYS:HB3	1:178:A:VAL:H	7	0.24
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	8	0.24
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	18	0.24
(2,21)	1:88:A:TYR:HE1	1:86:A:LEU:HD13	11	0.24
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	2	0.24
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	4	0.24
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	1	0.24
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	2	0.24
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	10	0.24
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	5	0.24
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	1	0.24
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	7	0.24
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	8	0.24
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	2	0.24
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	4	0.24
(1,84)	1:122:A:VAL:N	1:168:A:ILE:O	17	0.24
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	16	0.24
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	8	0.24
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	15	0.24
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	6	0.24
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	15	0.24
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	4	0.24
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	19	0.24
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	6	0.24
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	10	0.24
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	16	0.24
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	20	0.24
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	3	0.24
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	8	0.24
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	8	0.24
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	14	0.24
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	6	0.24
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	15	0.24
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	7	0.24
(4,453)	1:48:A:ILE:HG13	1:38:A:LEU:HA	11	0.23
(4,452)	1:59:A:THR:HB	1:59:A:THR:HG22	3	0.23
(4,452)	1:59:A:THR:HB	1:59:A:THR:HG22	4	0.23
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	20	0.23
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	4	0.23
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	3	0.23
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	18	0.23
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	19	0.23
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	5	0.23
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	15	0.23
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	19	0.23
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	19	0.23
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	9	0.23
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	19	0.23
(4,364)	1:4:A:MET:HE3	1:58:A:GLU:HG3	10	0.23
(4,300)	1:97:A:LEU:HD23	1:156:A:PHE:HB3	14	0.23
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	8	0.23
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	13	0.23
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	15	0.23
(4,254)	1:41:A:MET:HE2	1:14:A:VAL:H	20	0.23
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	16	0.23
(4,208)	1:14:A:VAL:HG22	1:11:A:LEU:HA	14	0.23
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD13	6	0.23
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	8	0.23
(4,9)	1:22:A:ILE:HD13	1:10:A:PHE:HD1	20	0.23
(4,6)	1:10:A:PHE:HD1	1:21:A:LEU:HD22	12	0.23
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	6	0.23
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	4	0.23
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	16	0.23
(2,3841)	1:76:A:ALA:HB1	1:76:A:ALA:H	1	0.23
(2,3841)	1:76:A:ALA:HB1	1:76:A:ALA:H	2	0.23
(2,3841)	1:76:A:ALA:HB1	1:76:A:ALA:H	17	0.23
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	11	0.23
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	7	0.23
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	13	0.23
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	16	0.23
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	15	0.23
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	16	0.23
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	3	0.23
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	20	0.23
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	4	0.23
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	6	0.23
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	4	0.23
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	1	0.23
(2,3800)	1:56:A:ILE:HD11	1:56:A:ILE:HG12	1	0.23
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	4	0.23
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	5	0.23
(2,3789)	1:22:A:ILE:HG22	1:44:A:LYS:HB3	18	0.23
(2,3781)	1:142:A:VAL:HG13	1:142:A:VAL:HB	12	0.23
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	1	0.23
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	2	0.23
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB3	7	0.23
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	9	0.23
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	11	0.23
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	13	0.23
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	14	0.23
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	19	0.23
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	20	0.23
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	5	0.23
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	7	0.23
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	9	0.23
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	20	0.23
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	5	0.23
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	7	0.23
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	6	0.23
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	11	0.23
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	4	0.23
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	19	0.23
(2,3575)	1:50:A:MET:HE1	1:50:A:MET:HG3	19	0.23
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE3	13	0.23
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	3	0.23
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	11	0.23
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	10	0.23
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	4	0.23
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	18	0.23
(2,3495)	1:82:A:VAL:HG11	1:82:A:VAL:HA	10	0.23
(2,3495)	1:82:A:VAL:HG11	1:82:A:VAL:HA	11	0.23
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	16	0.23
(2,3495)	1:82:A:VAL:HG11	1:82:A:VAL:HA	17	0.23
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	18	0.23
(2,3490)	1:48:A:ILE:HD13	1:53:A:LEU:HA	20	0.23
(2,3484)	1:124:A:LEU:HD12	1:167:A:LEU:HA	1	0.23
(2,3484)	1:124:A:LEU:HD13	1:167:A:LEU:HA	18	0.23
(2,3479)	1:151:A:MET:HE1	1:171:A:VAL:HA	4	0.23
(2,3479)	1:151:A:MET:HE1	1:171:A:VAL:HA	9	0.23
(2,3479)	1:151:A:MET:HE1	1:171:A:VAL:HA	11	0.23
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	11	0.23
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	4	0.23
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	5	0.23
(2,3372)	1:20:A:ALA:HB3	1:20:A:ALA:H	10	0.23
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	16	0.23
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	8	0.23
(2,3346)	1:4:A:MET:HE1	1:55:A:HIS:HD2	5	0.23
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	20	0.23
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	5	0.23
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	10	0.23
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	13	0.23
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	19	0.23
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	10	0.23
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	15	0.23
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	20	0.23
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	17	0.23
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	8	0.23
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	11	0.23
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	17	0.23
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	9	0.23
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	11	0.23
(2,2417)	1:36:A:GLU:H	1:36:A:GLU:HB3	13	0.23
(2,2376)	1:95:A:ALA:HB1	1:149:A:LYS:H	17	0.23
(2,2348)	1:156:A:PHE:H	1:168:A:ILE:HD12	3	0.23
(2,2308)	1:108:A:LEU:HD22	1:108:A:LEU:H	8	0.23
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	7	0.23
(2,2175)	1:57:A:VAL:HG22	1:66:A:ALA:H	4	0.23
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	16	0.23
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	5	0.23
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD21	18	0.23
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	8	0.23
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD13	6	0.23
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	19	0.23
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	3	0.23
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	17	0.23
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	9	0.23
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	14	0.23
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	16	0.23
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	20	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	2	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	3	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	4	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	9	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	10	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	13	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	15	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	16	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	17	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	18	0.23
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	19	0.23
(2,1874)	1:168:A:ILE:HD12	1:171:A:VAL:HG11	12	0.23
(2,1874)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	15	0.23
(2,1865)	1:109:A:ILE:HD13	1:144:A:LEU:HD12	8	0.23
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	3	0.23
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	19	0.23
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	8	0.23
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	18	0.23
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	4	0.23
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	6	0.23
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	11	0.23
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1848)	1:146:A:VAL:HG12	1:168:A:ILE:HD13	15	0.23
(2,1844)	1:110:A:LEU:HD23	1:110:A:LEU:HB3	1	0.23
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	18	0.23
(2,1839)	1:56:A:ILE:HG23	1:56:A:ILE:HG12	2	0.23
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	8	0.23
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	14	0.23
(2,1804)	1:5:A:VAL:HG22	1:5:A:VAL:HB	10	0.23
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	19	0.23
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	20	0.23
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	10	0.23
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG23	3	0.23
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	10	0.23
(2,1754)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	6	0.23
(2,1754)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	9	0.23
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	5	0.23
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	12	0.23
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	2	0.23
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	3	0.23
(2,1709)	1:86:A:LEU:HD21	1:86:A:LEU:HA	5	0.23
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	9	0.23
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	10	0.23
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	11	0.23
(2,1709)	1:86:A:LEU:HD22	1:86:A:LEU:HA	17	0.23
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	14	0.23
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE3	20	0.23
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	1	0.23
(2,1576)	1:22:A:ILE:HG22	1:22:A:ILE:HA	17	0.23
(2,1563)	1:48:A:ILE:HG23	1:53:A:LEU:HB2	1	0.23
(2,1536)	1:21:A:LEU:HD11	1:18:A:ASN:HB3	20	0.23
(2,1524)	1:82:A:VAL:HG13	1:82:A:VAL:HA	7	0.23
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	9	0.23
(2,1524)	1:82:A:VAL:HG11	1:82:A:VAL:HA	10	0.23
(2,1524)	1:82:A:VAL:HG11	1:82:A:VAL:HA	11	0.23
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	16	0.23
(2,1494)	1:168:A:ILE:HD12	1:156:A:PHE:HB2	17	0.23
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	10	0.23
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	13	0.23
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	14	0.23
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	17	0.23
(2,1410)	1:95:A:ALA:HB3	1:96:A:VAL:H	7	0.23
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	10	0.23
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	20	0.23
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	11	0.23
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	13	0.23
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	19	0.23
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	2	0.23
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	5	0.23
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	10	0.23
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	14	0.23
(2,1309)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	20	0.23
(2,1301)	1:34:A:VAL:HG12	1:38:A:LEU:H	16	0.23
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	6	0.23
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	7	0.23
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	20	0.23
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	9	0.23
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	14	0.23
(2,1222)	1:176:A:ILE:HD11	1:176:A:ILE:HB	18	0.23
(2,1218)	1:177:A:LYS:HG2	1:177:A:LYS:HA	2	0.23
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	9	0.23
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	11	0.23
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	14	0.23
(2,1172)	1:144:A:LEU:HD11	1:106:A:PHE:HE1	12	0.23
(2,1131)	1:136:A:MET:H	1:105:A:ASN:HD22	18	0.23
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	1	0.23
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	3	0.23
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	11	0.23
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	12	0.23
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	14	0.23
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	8	0.23
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	11	0.23
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	13	0.23
(2,977)	1:87:A:GLY:H	1:88:A:TYR:H	6	0.23
(2,943)	1:159:A:TYR:H	1:88:A:TYR:HD1	18	0.23
(2,935)	1:114:A:ILE:H	1:171:A:VAL:H	20	0.23
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	11	0.23
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	2	0.23
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD13	2	0.23
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD11	14	0.23
(2,726)	1:20:A:ALA:HB2	1:23:A:GLY:H	1	0.23
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	17	0.23
(2,653)	1:29:A:ASN:H	1:29:A:ASN:HB3	1	0.23
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	5	0.23
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,588)	1:17:A:HIS:H	1:16:A:ARG:HB2	19	0.23
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	1	0.23
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	4	0.23
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	11	0.23
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	15	0.23
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	18	0.23
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	20	0.23
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	2	0.23
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	5	0.23
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	10	0.23
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	18	0.23
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	2	0.23
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	5	0.23
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	11	0.23
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	13	0.23
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	15	0.23
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	18	0.23
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	11	0.23
(2,375)	1:156:A:PHE:H	1:156:A:PHE:HD1	9	0.23
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	8	0.23
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	5	0.23
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	14	0.23
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	8	0.23
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	16	0.23
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	20	0.23
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	4	0.23
(2,164)	1:86:A:LEU:H	1:86:A:LEU:HB3	20	0.23
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	11	0.23
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	11	0.23
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	9	0.23
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	2	0.23
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	16	0.23
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	16	0.23
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	2	0.23
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	5	0.23
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	10	0.23
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	3	0.23
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	7	0.23
(1,118)	1:168:A:ILE:N	1:122:A:VAL:O	1	0.23
(1,118)	1:168:A:ILE:N	1:122:A:VAL:O	15	0.23
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	4	0.23
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	4	0.23
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	14	0.23
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	13	0.23
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	19	0.23
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	14	0.23
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	19	0.23
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	12	0.23
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	20	0.23
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	1	0.23
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	10	0.23
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	13	0.23
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	14	0.23
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	15	0.23
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	8	0.23
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	10	0.23
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	11	0.23
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	14	0.23
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	19	0.23
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	4	0.23
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	17	0.23
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	6	0.23
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	7	0.23
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	12	0.23
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	20	0.23
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	16	0.23
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	1	0.23
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	9	0.23
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	1	0.23
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	2	0.23
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	3	0.23
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	3	0.23
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	5	0.23
(4,453)	1:48:A:ILE:HG13	1:38:A:LEU:HA	16	0.22
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	8	0.22
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	18	0.22
(4,451)	1:168:A:ILE:HD13	1:168:A:ILE:HG12	14	0.22
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	10	0.22
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	2	0.22
(4,410)	1:50:A:MET:HE3	1:54:A:LYS:HD3	2	0.22
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	1	0.22
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	2	0.22
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	18	0.22
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	7	0.22
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	13	0.22
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	20	0.22
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	1	0.22
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	3	0.22
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	8	0.22
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	11	0.22
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	14	0.22
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	15	0.22
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	17	0.22
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	8	0.22
(4,208)	1:14:A:VAL:HG22	1:11:A:LEU:HA	10	0.22
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	11	0.22
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	9	0.22
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	18	0.22
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	3	0.22
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	9	0.22
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	14	0.22
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	19	0.22
(2,3836)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	11	0.22
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	19	0.22
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	9	0.22
(2,3824)	1:41:A:MET:HE1	1:11:A:LEU:HD12	16	0.22
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	3	0.22
(2,3819)	1:151:A:MET:HE1	1:171:A:VAL:HG12	2	0.22
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	14	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	1	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	8	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	9	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	10	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	12	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG22	13	0.22
(2,3816)	1:22:A:ILE:HG23	1:14:A:VAL:HG21	16	0.22
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	17	0.22
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	2	0.22
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	5	0.22
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG22	13	0.22
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	16	0.22
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	19	0.22
(2,3813)	1:56:A:ILE:HD11	1:11:A:LEU:HD11	8	0.22
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	16	0.22
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	10	0.22
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	12	0.22
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	15	0.22
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	2	0.22
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	3	0.22
(2,3800)	1:56:A:ILE:HD12	1:56:A:ILE:HG12	4	0.22
(2,3800)	1:56:A:ILE:HD12	1:56:A:ILE:HG12	5	0.22
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	10	0.22
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	14	0.22
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	15	0.22
(2,3800)	1:56:A:ILE:HD13	1:56:A:ILE:HG12	18	0.22
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	9	0.22
(2,3795)	1:14:A:VAL:HG23	1:21:A:LEU:HG	11	0.22
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	9	0.22
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	16	0.22
(2,3765)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	18	0.22
(2,3760)	1:22:A:ILE:HB	1:22:A:ILE:HG23	5	0.22
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	7	0.22
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	16	0.22
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	13	0.22
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	16	0.22
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	19	0.22
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	12	0.22
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	17	0.22
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	10	0.22
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	16	0.22
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	2	0.22
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	8	0.22
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	9	0.22
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	17	0.22
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	15	0.22
(2,3570)	1:4:A:MET:HE3	1:52:A:GLU:HA	15	0.22
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE1	7	0.22
(2,3558)	1:152:A:ALA:HB2	1:149:A:LYS:HA	14	0.22
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	11	0.22
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	20	0.22
(2,3531)	1:151:A:MET:HE1	1:175:A:PHE:HB3	11	0.22
(2,3527)	1:84:A:VAL:HG21	1:85:A:ASP:HB2	8	0.22
(2,3509)	1:13:A:LEU:HD21	1:17:A:HIS:HB2	10	0.22
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	3	0.22
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	6	0.22
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	12	0.22
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	6	0.22
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	10	0.22
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	11	0.22
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	13	0.22
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	15	0.22
(2,3495)	1:82:A:VAL:HG13	1:82:A:VAL:HA	7	0.22
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	9	0.22
(2,3495)	1:82:A:VAL:HG11	1:82:A:VAL:HA	15	0.22
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	5	0.22
(2,3467)	1:11:A:LEU:HD12	1:38:A:LEU:HA	14	0.22
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	15	0.22
(2,3452)	1:168:A:ILE:HD13	1:156:A:PHE:HZ	11	0.22
(2,3439)	1:110:A:LEU:HD12	1:110:A:LEU:H	19	0.22
(2,3434)	1:15:A:LEU:HD11	1:65:A:PHE:HE1	1	0.22
(2,3434)	1:15:A:LEU:HD11	1:65:A:PHE:HE1	11	0.22
(2,3391)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	3	0.22
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	1	0.22
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	4	0.22
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	6	0.22
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	7	0.22
(2,3372)	1:20:A:ALA:HB3	1:20:A:ALA:H	11	0.22
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	14	0.22
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	20	0.22
(2,3345)	1:41:A:MET:HE1	1:10:A:PHE:HE1	1	0.22
(2,3345)	1:41:A:MET:HE2	1:10:A:PHE:HE1	20	0.22
(2,3265)	1:84:A:VAL:HG11	1:84:A:VAL:H	5	0.22
(2,3265)	1:84:A:VAL:HG12	1:84:A:VAL:H	19	0.22
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB3	20	0.22
(2,3182)	1:114:A:ILE:HD13	1:171:A:VAL:HB	14	0.22
(2,3182)	1:114:A:ILE:HD13	1:171:A:VAL:HB	19	0.22
(2,3167)	1:176:A:ILE:HD12	1:114:A:ILE:HD13	6	0.22
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	16	0.22
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	8	0.22
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	14	0.22
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	18	0.22
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	10	0.22
(2,2918)	1:76:A:ALA:HB3	1:78:A:GLN:HE22	15	0.22
(2,2657)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	9	0.22
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	8	0.22
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	7	0.22
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	16	0.22
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	12	0.22
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	3	0.22
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	5	0.22
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	8	0.22
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	14	0.22
(2,2210)	1:48:A:ILE:HD13	1:53:A:LEU:H	4	0.22
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	6	0.22
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	9	0.22
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	6	0.22
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD11	4	0.22
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	14	0.22
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	3	0.22
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	4	0.22
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	5	0.22
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	6	0.22
(2,2041)	1:152:A:ALA:HB3	1:152:A:ALA:H	9	0.22
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	1	0.22
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	8	0.22
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	14	0.22
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	16	0.22
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	1	0.22
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	6	0.22
(2,1898)	1:24:A:LEU:HA	1:24:A:LEU:HB3	20	0.22
(2,1880)	1:76:A:ALA:HB3	1:16:A:ARG:HA	15	0.22
(2,1869)	1:97:A:LEU:HD23	1:96:A:VAL:HB	5	0.22
(2,1861)	1:41:A:MET:HE1	1:11:A:LEU:HD12	16	0.22
(2,1857)	1:151:A:MET:HE1	1:171:A:VAL:HG12	17	0.22
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	2	0.22
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	14	0.22
(2,1854)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	18	0.22
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	4	0.22
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	6	0.22
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	13	0.22
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	17	0.22
(2,1800)	1:53:A:LEU:HD13	1:37:A:LEU:HG	10	0.22
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	12	0.22
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	14	0.22
(2,1800)	1:53:A:LEU:HD13	1:37:A:LEU:HG	18	0.22
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	19	0.22
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	7	0.22
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	3	0.22
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	12	0.22
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	14	0.22
(2,1599)	1:4:A:MET:HE2	1:52:A:GLU:HA	18	0.22
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE3	2	0.22
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE2	10	0.22
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE3	15	0.22
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE3	17	0.22
(2,1549)	1:37:A:LEU:HD12	1:41:A:MET:HG2	7	0.22
(2,1524)	1:82:A:VAL:HG11	1:82:A:VAL:HA	15	0.22
(2,1509)	1:151:A:MET:HE3	1:171:A:VAL:HA	14	0.22
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	5	0.22
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	12	0.22
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	11	0.22
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	13	0.22
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	15	0.22
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	12	0.22
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	16	0.22
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	13	0.22
(2,1294)	1:57:A:VAL:HG11	1:58:A:GLU:H	18	0.22
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	1	0.22
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	14	0.22
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	1	0.22
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	3	0.22
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD13	15	0.22
(2,1218)	1:177:A:LYS:HG2	1:177:A:LYS:HA	11	0.22
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	2	0.22
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	3	0.22
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	6	0.22
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	7	0.22
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	8	0.22
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	17	0.22
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	19	0.22
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	20	0.22
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	2	0.22
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	4	0.22
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	5	0.22
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	8	0.22
(2,1172)	1:144:A:LEU:HD11	1:106:A:PHE:HE1	9	0.22
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	4	0.22
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	16	0.22
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	20	0.22
(2,1155)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	12	0.22
(2,1131)	1:136:A:MET:H	1:105:A:ASN:HD22	19	0.22
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	6	0.22
(2,1067)	1:56:A:ILE:H	1:55:A:HIS:H	20	0.22
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	7	0.22
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	17	0.22
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	1	0.22
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD11	11	0.22
(2,780)	1:86:A:LEU:HD11	1:87:A:GLY:H	3	0.22
(2,692)	1:132:A:ARG:H	1:126:A:GLN:HE22	14	0.22
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	9	0.22
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	13	0.22
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	16	0.22
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	1	0.22
(2,594)	1:43:A:ALA:HB3	1:44:A:LYS:H	15	0.22
(2,550)	1:102:A:ALA:HB1	1:105:A:ASN:H	10	0.22
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	6	0.22
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	8	0.22
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	3	0.22
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	5	0.22
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	8	0.22
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	16	0.22
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	3	0.22
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	11	0.22
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	12	0.22
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	6	0.22
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	1	0.22
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	9	0.22
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	10	0.22
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	12	0.22
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	14	0.22
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	19	0.22
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	6	0.22
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	2	0.22
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	11	0.22
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	6	0.22
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	11	0.22
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	2	0.22
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	3	0.22
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	9	0.22
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	17	0.22
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	2	0.22
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	19	0.22
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD13	15	0.22
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	7	0.22
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	2	0.22
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	4	0.22
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	6	0.22
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	10	0.22
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	19	0.22
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	10	0.22
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	16	0.22
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	9	0.22
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	7	0.22
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	3	0.22
(1,112)	1:159:A:TYR:N	1:167:A:LEU:O	10	0.22
(1,112)	1:159:A:TYR:N	1:167:A:LEU:O	11	0.22
(1,112)	1:159:A:TYR:N	1:167:A:LEU:O	15	0.22
(1,112)	1:159:A:TYR:N	1:167:A:LEU:O	19	0.22
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	1	0.22
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	5	0.22
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	7	0.22
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	15	0.22
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	17	0.22
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	18	0.22
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	2	0.22
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	14	0.22
(1,92)	1:133:A:LYS:N	1:129:A:THR:O	14	0.22
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	16	0.22
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	2	0.22
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	3	0.22
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	9	0.22
(1,77)	1:112:A:ASP:H	1:108:A:LEU:O	5	0.22
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	12	0.22
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	17	0.22
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	18	0.22
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	13	0.22
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	18	0.22
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	7	0.22
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	11	0.22
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	2	0.22
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	5	0.22
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	9	0.22
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	5	0.22
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	17	0.22
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	5	0.22
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	8	0.22
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	2	0.22
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	8	0.22
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	18	0.22
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	9	0.22
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	11	0.22
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	15	0.22
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	19	0.22
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	2	0.22
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	7	0.22
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	11	0.22
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	13	0.22
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	15	0.22
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	17	0.22
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	19	0.22
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	20	0.22
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	10	0.22
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	12	0.22
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	13	0.22
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	14	0.22
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	19	0.22
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	9	0.22
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	13	0.22
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	17	0.22
(1,4)	1:8:A:SER:N	1:4:A:MET:O	15	0.22
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	7	0.21
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	10	0.21
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	16	0.21
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	19	0.21
(4,446)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	1	0.21
(4,445)	1:14:A:VAL:HG11	1:11:A:LEU:HG	2	0.21
(4,443)	1:48:A:ILE:HD12	1:38:A:LEU:HB2	5	0.21
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	1	0.21
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	13	0.21
(4,411)	1:84:A:VAL:HB	1:86:A:LEU:HB3	17	0.21
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	9	0.21
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	11	0.21
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	16	0.21
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	17	0.21
(4,395)	1:56:A:ILE:HG21	1:56:A:ILE:HA	8	0.21
(4,395)	1:56:A:ILE:HG22	1:56:A:ILE:HA	9	0.21
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	4	0.21
(4,379)	1:50:A:MET:HA	1:39:A:ALA:HB3	8	0.21
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	8	0.21
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	11	0.21
(4,307)	1:38:A:LEU:HD13	1:50:A:MET:HA	19	0.21
(4,307)	1:26:A:LEU:HD23	1:15:A:LEU:HA	20	0.21
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	14	0.21
(4,259)	1:117:A:MET:HE3	2:201:A:NAD:H2A	8	0.21
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	2	0.21
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	4	0.21
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	5	0.21
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	6	0.21
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	9	0.21
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	10	0.21
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	20	0.21
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	19	0.21
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	7	0.21
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	7	0.21
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	20	0.21
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD23	2	0.21
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	10	0.21
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	6	0.21
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	10	0.21
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	17	0.21
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	20	0.21
(2,3841)	1:76:A:ALA:HB1	1:76:A:ALA:H	14	0.21
(2,3841)	1:76:A:ALA:HB1	1:76:A:ALA:H	16	0.21
(2,3829)	1:109:A:ILE:HD11	1:101:A:THR:HG23	5	0.21
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	2	0.21
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	15	0.21
(2,3823)	1:57:A:VAL:HG23	1:57:A:VAL:HB	2	0.21
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	3	0.21
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	4	0.21
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	6	0.21
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	7	0.21
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG21	19	0.21
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	18	0.21
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	18	0.21
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	2	0.21
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	6	0.21
(2,3805)	1:168:A:ILE:HG23	1:168:A:ILE:HB	18	0.21
(2,3800)	1:56:A:ILE:HD11	1:56:A:ILE:HG12	8	0.21
(2,3800)	1:56:A:ILE:HD12	1:56:A:ILE:HG12	11	0.21
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	14	0.21
(2,3795)	1:14:A:VAL:HG21	1:21:A:LEU:HG	12	0.21
(2,3795)	1:14:A:VAL:HG22	1:21:A:LEU:HG	13	0.21
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	10	0.21
(2,3786)	1:38:A:LEU:HG	1:38:A:LEU:HD12	16	0.21
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	20	0.21
(2,3770)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	1	0.21
(2,3763)	1:76:A:ALA:HB2	1:15:A:LEU:HD12	2	0.21
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	8	0.21
(2,3763)	1:76:A:ALA:HB1	1:15:A:LEU:HD12	10	0.21
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	6	0.21
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG21	14	0.21
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	1	0.21
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	4	0.21
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	15	0.21
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	17	0.21
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	12	0.21
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	20	0.21
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	1	0.21
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	10	0.21
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	13	0.21
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	18	0.21
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	5	0.21
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	6	0.21
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	10	0.21
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	12	0.21
(2,3653)	1:14:A:VAL:HG23	1:19:A:PRO:HA	20	0.21
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	4	0.21
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	19	0.21
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	4	0.21
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	7	0.21
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	13	0.21
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	11	0.21
(2,3524)	1:13:A:LEU:HD13	1:18:A:ASN:HB2	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	9	0.21
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	11	0.21
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	13	0.21
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	17	0.21
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	8	0.21
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	9	0.21
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	14	0.21
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	19	0.21
(2,3495)	1:82:A:VAL:HG12	1:82:A:VAL:HA	5	0.21
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	6	0.21
(2,3430)	1:128:A:ILE:HD12	1:127:A:ASP:H	13	0.21
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	7	0.21
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	19	0.21
(2,3387)	1:21:A:LEU:HD22	1:10:A:PHE:HE1	8	0.21
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	2	0.21
(2,3372)	1:20:A:ALA:HB3	1:20:A:ALA:H	3	0.21
(2,3372)	1:20:A:ALA:HB3	1:20:A:ALA:H	12	0.21
(2,3372)	1:20:A:ALA:HB3	1:20:A:ALA:H	13	0.21
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	17	0.21
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	18	0.21
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	19	0.21
(2,3345)	1:41:A:MET:HE1	1:10:A:PHE:HE1	3	0.21
(2,3288)	1:142:A:VAL:HG13	1:103:A:GLU:HA	12	0.21
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	4	0.21
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	12	0.21
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	2	0.21
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	12	0.21
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	13	0.21
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	1	0.21
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	4	0.21
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	7	0.21
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	12	0.21
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	15	0.21
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	18	0.21
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	20	0.21
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	6	0.21
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	13	0.21
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	19	0.21
(2,2994)	1:84:A:VAL:H	1:83:A:GLU:H	9	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	1	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD22	6	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	13	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	15	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	18	0.21
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	19	0.21
(2,2680)	1:113:A:GLY:H	1:109:A:ILE:HG21	6	0.21
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	11	0.21
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	12	0.21
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	15	0.21
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	20	0.21
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	4	0.21
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	9	0.21
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	13	0.21
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	17	0.21
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG11	1	0.21
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	17	0.21
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	7	0.21
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	9	0.21
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	19	0.21
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	18	0.21
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	4	0.21
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	15	0.21
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD11	19	0.21
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	15	0.21
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	17	0.21
(2,1967)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	17	0.21
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	9	0.21
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	12	0.21
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	20	0.21
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	12	0.21
(2,1884)	1:41:A:MET:HE2	1:46:A:HIS:HA	12	0.21
(2,1871)	1:97:A:LEU:HD21	1:151:A:MET:HG3	4	0.21
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	17	0.21
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	2	0.21
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	9	0.21
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	12	0.21
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	18	0.21
(2,1857)	1:151:A:MET:HE3	1:171:A:VAL:HG12	12	0.21
(2,1844)	1:110:A:LEU:HD22	1:110:A:LEU:HB3	7	0.21
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	3	0.21
(2,1804)	1:5:A:VAL:HG22	1:5:A:VAL:HB	5	0.21
(2,1804)	1:5:A:VAL:HG21	1:5:A:VAL:HB	16	0.21
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	2	0.21
(2,1800)	1:53:A:LEU:HD13	1:37:A:LEU:HG	6	0.21
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	4	0.21
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	11	0.21
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	1	0.21
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	13	0.21
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE3	12	0.21
(2,1599)	1:4:A:MET:HE3	1:52:A:GLU:HA	1	0.21
(2,1594)	1:71:A:PHE:HB2	1:50:A:MET:HE1	18	0.21
(2,1524)	1:82:A:VAL:HG12	1:82:A:VAL:HA	5	0.21
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	6	0.21
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	19	0.21
(2,1514)	1:124:A:LEU:HD12	1:167:A:LEU:HA	1	0.21
(2,1514)	1:124:A:LEU:HD13	1:167:A:LEU:HA	18	0.21
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	2	0.21
(2,1474)	1:110:A:LEU:HD21	1:110:A:LEU:H	17	0.21
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	4	0.21
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	6	0.21
(2,1420)	1:22:A:ILE:HG23	1:10:A:PHE:HE1	19	0.21
(2,1417)	1:34:A:VAL:HG23	1:67:A:PHE:HZ	5	0.21
(2,1412)	1:66:A:ALA:HB2	1:31:A:TRP:HZ3	15	0.21
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	11	0.21
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	3	0.21
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	6	0.21
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	19	0.21
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	9	0.21
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	6	0.21
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	20	0.21
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	17	0.21
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	1	0.21
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	5	0.21
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	10	0.21
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	13	0.21
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	15	0.21
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	16	0.21
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	18	0.21
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	3	0.21
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	9	0.21
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	5	0.21
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	9	0.21
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	11	0.21
(2,1131)	1:136:A:MET:H	1:105:A:ASN:HD22	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	8	0.21
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	17	0.21
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	2	0.21
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	2	0.21
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	8	0.21
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	11	0.21
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	13	0.21
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	15	0.21
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	17	0.21
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD11	4	0.21
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD11	10	0.21
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD11	16	0.21
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	5	0.21
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	2	0.21
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	1	0.21
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	16	0.21
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	4	0.21
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	5	0.21
(2,594)	1:43:A:ALA:HB1	1:44:A:LYS:H	12	0.21
(2,550)	1:102:A:ALA:HB1	1:105:A:ASN:H	4	0.21
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	9	0.21
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	12	0.21
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	2	0.21
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	13	0.21
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	14	0.21
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	1	0.21
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	20	0.21
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	3	0.21
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	8	0.21
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	16	0.21
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	20	0.21
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	13	0.21
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	18	0.21
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	8	0.21
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	14	0.21
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	1	0.21
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	6	0.21
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	1	0.21
(2,342)	1:41:A:MET:H	1:41:A:MET:HG2	5	0.21
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	17	0.21
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	4	0.21
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	9	0.21
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	18	0.21
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	19	0.21
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	9	0.21
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	10	0.21
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	12	0.21
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	13	0.21
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	20	0.21
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	7	0.21
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	3	0.21
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	10	0.21
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	17	0.21
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	4	0.21
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	10	0.21
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	20	0.21
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	1	0.21
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	5	0.21
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	17	0.21
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	20	0.21
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	3	0.21
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	10	0.21
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	9	0.21
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	11	0.21
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	17	0.21
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	6	0.21
(1,118)	1:168:A:ILE:N	1:122:A:VAL:O	19	0.21
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	5	0.21
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	19	0.21
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	13	0.21
(1,114)	1:166:A:TRP:N	1:124:A:LEU:O	14	0.21
(1,112)	1:159:A:TYR:N	1:167:A:LEU:O	9	0.21
(1,112)	1:159:A:TYR:N	1:167:A:LEU:O	18	0.21
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	16	0.21
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	9	0.21
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	4	0.21
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	12	0.21
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	16	0.21
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	20	0.21
(1,92)	1:133:A:LYS:N	1:129:A:THR:O	2	0.21
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	10	0.21
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	12	0.21
(1,88)	1:131:A:ALA:N	1:127:A:ASP:O	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	7	0.21
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	8	0.21
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	11	0.21
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	14	0.21
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	17	0.21
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	18	0.21
(1,77)	1:112:A:ASP:H	1:108:A:LEU:O	20	0.21
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	5	0.21
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	9	0.21
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	13	0.21
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	1	0.21
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	4	0.21
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	14	0.21
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	6	0.21
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	5	0.21
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	16	0.21
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	17	0.21
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	3	0.21
(1,51)	1:60:A:ASN:H	1:56:A:ILE:O	17	0.21
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	13	0.21
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	14	0.21
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	20	0.21
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	10	0.21
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	13	0.21
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	15	0.21
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	2	0.21
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	7	0.21
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	12	0.21
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	17	0.21
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	17	0.21
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	8	0.21
(1,16)	1:14:A:VAL:N	1:10:A:PHE:O	1	0.21
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	2	0.21
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	7	0.21
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	15	0.21
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	17	0.21
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	4	0.21
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	10	0.21
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	16	0.21
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	20	0.21
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	16	0.21
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	11	0.2
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	6	0.2
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	10	0.2
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	2	0.2
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	3	0.2
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	4	0.2
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	7	0.2
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	10	0.2
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	12	0.2
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	14	0.2
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	20	0.2
(4,392)	1:8:A:SER:HB2	1:7:A:VAL:HB	16	0.2
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	3	0.2
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	16	0.2
(4,328)	1:171:A:VAL:HG12	1:113:A:GLY:HA2	5	0.2
(4,325)	1:7:A:VAL:HG13	1:10:A:PHE:HB3	1	0.2
(4,325)	1:7:A:VAL:HG11	1:10:A:PHE:HB3	3	0.2
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	17	0.2
(4,283)	1:142:A:VAL:HG13	1:103:A:GLU:H	9	0.2
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	17	0.2
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	7	0.2
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	13	0.2
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	19	0.2
(4,213)	1:143:A:VAL:HB	1:144:A:LEU:HA	18	0.2
(4,208)	1:14:A:VAL:HG22	1:11:A:LEU:HA	7	0.2
(4,208)	1:14:A:VAL:HG22	1:11:A:LEU:HA	9	0.2
(4,208)	1:14:A:VAL:HG22	1:11:A:LEU:HA	15	0.2
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	16	0.2
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	19	0.2
(4,198)	1:176:A:ILE:HD13	1:106:A:PHE:HE1	2	0.2
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	9	0.2
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	12	0.2
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	2	0.2
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	20	0.2
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	5	0.2
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	11	0.2
(2,3940)	1:134:A:VAL:HG11	2:201:A:NAD:H2N	7	0.2
(2,3940)	1:134:A:VAL:HG11	2:201:A:NAD:H2N	15	0.2
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	2	0.2
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	5	0.2
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	13	0.2
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	4	0.2
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	6	0.2
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	8	0.2
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	12	0.2
(2,3836)	1:168:A:ILE:HD11	1:171:A:VAL:HG11	7	0.2
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	2	0.2
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	8	0.2
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	17	0.2
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	2	0.2
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	9	0.2
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	12	0.2
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	18	0.2
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG22	1	0.2
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	7	0.2
(2,3819)	1:151:A:MET:HE1	1:171:A:VAL:HG12	4	0.2
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	2	0.2
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	15	0.2
(2,3800)	1:56:A:ILE:HD12	1:56:A:ILE:HG12	12	0.2
(2,3793)	1:53:A:LEU:HD22	1:56:A:ILE:HB	6	0.2
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	14	0.2
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	17	0.2
(2,3789)	1:22:A:ILE:HG22	1:44:A:LYS:HB3	19	0.2
(2,3785)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	18	0.2
(2,3763)	1:76:A:ALA:HB1	1:15:A:LEU:HD12	18	0.2
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	1	0.2
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	2	0.2
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	3	0.2
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	5	0.2
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG23	11	0.2
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	15	0.2
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	3	0.2
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	8	0.2
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	14	0.2
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	5	0.2
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	4	0.2
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	15	0.2
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	19	0.2
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	7	0.2
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	2	0.2
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	3	0.2
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	7	0.2
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	11	0.2
(2,3653)	1:14:A:VAL:HG23	1:19:A:PRO:HA	13	0.2
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	16	0.2
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	18	0.2
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	14	0.2
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	5	0.2
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	6	0.2
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	8	0.2
(2,3558)	1:152:A:ALA:HB2	1:149:A:LYS:HA	2	0.2
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	1	0.2
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	2	0.2
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	6	0.2
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	12	0.2
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	12	0.2
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	15	0.2
(2,3531)	1:151:A:MET:HE1	1:175:A:PHE:HB3	6	0.2
(2,3527)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	10	0.2
(2,3518)	1:128:A:ILE:HD13	1:128:A:ILE:HA	18	0.2
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	7	0.2
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	2	0.2
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	7	0.2
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	17	0.2
(2,3498)	1:38:A:LEU:HD23	1:47:A:GLY:HA2	12	0.2
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	19	0.2
(2,3490)	1:48:A:ILE:HD12	1:53:A:LEU:HA	4	0.2
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	9	0.2
(2,3430)	1:128:A:ILE:HD12	1:127:A:ASP:H	7	0.2
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	1	0.2
(2,3399)	1:21:A:LEU:HD13	1:21:A:LEU:H	1	0.2
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	8	0.2
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	14	0.2
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	8	0.2
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	15	0.2
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	11	0.2
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	14	0.2
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	18	0.2
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	18	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	1	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	3	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	4	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	5	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	10	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	14	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	15	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	19	0.2
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	20	0.2
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	16	0.2
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	1	0.2
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	4	0.2
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	5	0.2
(2,3127)	1:97:A:LEU:HD12	1:124:A:LEU:HD23	4	0.2
(2,3127)	1:97:A:LEU:HD12	1:124:A:LEU:HD23	19	0.2
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	4	0.2
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	9	0.2
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	12	0.2
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD22	16	0.2
(2,2852)	1:85:A:ASP:H	1:86:A:LEU:H	4	0.2
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	6	0.2
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	4	0.2
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	2	0.2
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	3	0.2
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	12	0.2
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	17	0.2
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	12	0.2
(2,2521)	1:105:A:ASN:H	1:102:A:ALA:HB3	17	0.2
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	4	0.2
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	10	0.2
(2,2308)	1:108:A:LEU:HD21	1:108:A:LEU:H	11	0.2
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	6	0.2
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	10	0.2
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	18	0.2
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	12	0.2
(2,2167)	1:24:A:LEU:H	1:14:A:VAL:HG11	11	0.2
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	9	0.2
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	18	0.2
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	19	0.2
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	20	0.2
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD13	15	0.2
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	8	0.2
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	1	0.2
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	7	0.2
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	19	0.2
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	4	0.2
(2,1889)	1:4:A:MET:HE1	1:4:A:MET:HA	14	0.2
(2,1871)	1:97:A:LEU:HD23	1:151:A:MET:HG3	18	0.2
(2,1869)	1:97:A:LEU:HD22	1:96:A:VAL:HB	4	0.2
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	9	0.2
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	1	0.2
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	2	0.2
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	15	0.2
(2,1861)	1:41:A:MET:HE1	1:11:A:LEU:HD12	20	0.2
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	3	0.2
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	4	0.2
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	17	0.2
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	19	0.2
(2,1828)	1:151:A:MET:HE1	1:151:A:MET:HG3	20	0.2
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	20	0.2
(2,1807)	1:151:A:MET:HE2	1:174:A:GLU:HG2	1	0.2
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	3	0.2
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	5	0.2
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	9	0.2
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	15	0.2
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	19	0.2
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	20	0.2
(2,1791)	1:144:A:LEU:HG	1:101:A:THR:HG22	19	0.2
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	18	0.2
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	10	0.2
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	13	0.2
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	14	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	2	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	4	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	6	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	7	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	8	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	9	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	11	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	16	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	17	0.2
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	19	0.2
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	8	0.2
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	16	0.2
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	18	0.2
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	10	0.2
(2,1563)	1:48:A:ILE:HG23	1:53:A:LEU:HB2	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	12	0.2
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	3	0.2
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	11	0.2
(2,1459)	1:108:A:LEU:HD13	2:201:A:NAD:H2A	6	0.2
(2,1459)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	14	0.2
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	3	0.2
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	8	0.2
(2,1420)	1:22:A:ILE:HG21	1:10:A:PHE:HE1	20	0.2
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	6	0.2
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	20	0.2
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	3	0.2
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	4	0.2
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	7	0.2
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	15	0.2
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	3	0.2
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	13	0.2
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	19	0.2
(2,1282)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	5	0.2
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	18	0.2
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	5	0.2
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	19	0.2
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	4	0.2
(2,1199)	1:176:A:ILE:HD11	1:176:A:ILE:HA	12	0.2
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	10	0.2
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	12	0.2
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	15	0.2
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	17	0.2
(2,1172)	1:144:A:LEU:HD11	1:106:A:PHE:HE1	2	0.2
(2,1172)	1:144:A:LEU:HD11	1:106:A:PHE:HE1	4	0.2
(2,1172)	1:144:A:LEU:HD11	1:106:A:PHE:HE1	8	0.2
(2,1172)	1:144:A:LEU:HD11	1:106:A:PHE:HE1	18	0.2
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	6	0.2
(2,1131)	1:136:A:MET:H	1:105:A:ASN:HD22	20	0.2
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	9	0.2
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	11	0.2
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	18	0.2
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	19	0.2
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	18	0.2
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	17	0.2
(2,974)	1:44:A:LYS:H	1:45:A:GLY:H	19	0.2
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	4	0.2
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	9	0.2
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	14	0.2
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	15	0.2
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	17	0.2
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	10	0.2
(2,866)	1:77:A:ASN:HD22	1:64:A:ARG:HA	5	0.2
(2,821)	1:97:A:LEU:H	1:97:A:LEU:HD11	17	0.2
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	12	0.2
(2,726)	1:20:A:ALA:HB2	1:23:A:GLY:H	13	0.2
(2,718)	1:91:A:GLN:HE21	1:89:A:GLU:HB2	13	0.2
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	7	0.2
(2,684)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	2	0.2
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	2	0.2
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	4	0.2
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	7	0.2
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	17	0.2
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	18	0.2
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	5	0.2
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	11	0.2
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	18	0.2
(2,594)	1:43:A:ALA:HB3	1:44:A:LYS:H	19	0.2
(2,594)	1:43:A:ALA:HB3	1:44:A:LYS:H	20	0.2
(2,549)	1:8:A:SER:H	1:6:A:LYS:HA	12	0.2
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	6	0.2
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	13	0.2
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	19	0.2
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	4	0.2
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	7	0.2
(2,472)	1:110:A:LEU:H	1:110:A:LEU:HA	17	0.2
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	2	0.2
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	4	0.2
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	7	0.2
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	9	0.2
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	11	0.2
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	16	0.2
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	20	0.2
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	19	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	3	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	5	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	11	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	13	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	17	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	18	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	19	0.2
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	20	0.2
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	6	0.2
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	6	0.2
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	8	0.2
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	13	0.2
(2,229)	1:43:A:ALA:H	1:42:A:LYS:HG3	14	0.2
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	15	0.2
(2,224)	1:81:A:SER:HA	1:82:A:VAL:H	15	0.2
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	15	0.2
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	18	0.2
(2,190)	1:13:A:LEU:H	1:13:A:LEU:HB3	12	0.2
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	4	0.2
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	6	0.2
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	7	0.2
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	10	0.2
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	11	0.2
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	18	0.2
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	20	0.2
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	18	0.2
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	20	0.2
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	10	0.2
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD11	14	0.2
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	8	0.2
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	17	0.2
(2,55)	1:34:A:VAL:H	1:73:A:LYS:HA	1	0.2
(1,117)	1:168:A:ILE:H	1:122:A:VAL:O	1	0.2
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	11	0.2
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	15	0.2
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	16	0.2
(1,111)	1:159:A:TYR:H	1:167:A:LEU:O	19	0.2
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	14	0.2
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	6	0.2
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	10	0.2
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	8	0.2
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	14	0.2
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	20	0.2
(1,92)	1:133:A:LYS:N	1:129:A:THR:O	6	0.2
(1,88)	1:131:A:ALA:N	1:127:A:ASP:O	19	0.2
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:112:A:ASP:H	1:108:A:LEU:O	14	0.2
(1,77)	1:112:A:ASP:H	1:108:A:LEU:O	17	0.2
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	6	0.2
(1,74)	1:110:A:LEU:N	1:106:A:PHE:O	15	0.2
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	5	0.2
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	17	0.2
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	1	0.2
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	6	0.2
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	12	0.2
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	20	0.2
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	1	0.2
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	6	0.2
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	12	0.2
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	13	0.2
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	5	0.2
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	1	0.2
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	3	0.2
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	10	0.2
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	19	0.2
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	20	0.2
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	14	0.2
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	8	0.2
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	14	0.2
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	1	0.2
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	4	0.2
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	14	0.2
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	1	0.2
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	2	0.2
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	3	0.2
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	9	0.2
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	11	0.2
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	13	0.2
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	15	0.2
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	19	0.2
(1,18)	1:15:A:LEU:N	1:11:A:LEU:O	3	0.2
(1,18)	1:15:A:LEU:N	1:11:A:LEU:O	20	0.2
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	16	0.2
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	5	0.2
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	8	0.2
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	17	0.2
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	20	0.2
(1,4)	1:8:A:SER:N	1:4:A:MET:O	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HG3	14	0.19
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	1	0.19
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	2	0.19
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	6	0.19
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	17	0.19
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	9	0.19
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	15	0.19
(4,439)	1:176:A:ILE:HG22	1:109:A:ILE:HB	6	0.19
(4,396)	1:34:A:VAL:HA	1:34:A:VAL:HG22	8	0.19
(4,387)	1:83:A:GLU:HA	1:82:A:VAL:HG12	15	0.19
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	15	0.19
(4,379)	1:50:A:MET:HA	1:39:A:ALA:HB3	20	0.19
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	5	0.19
(4,319)	1:26:A:LEU:HD23	1:14:A:VAL:HA	9	0.19
(4,311)	1:96:A:VAL:HG11	1:94:A:PRO:HA	2	0.19
(4,311)	1:143:A:VAL:HG12	1:178:A:VAL:HA	11	0.19
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	4	0.19
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	19	0.19
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	5	0.19
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	7	0.19
(4,227)	1:8:A:SER:HB3	1:65:A:PHE:HE1	18	0.19
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	17	0.19
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	2	0.19
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB2	11	0.19
(4,122)	1:111:A:LYS:H	1:109:A:ILE:HG22	8	0.19
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	16	0.19
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	1	0.19
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	19	0.19
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	11	0.19
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	1	0.19
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	4	0.19
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	15	0.19
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	16	0.19
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	19	0.19
(4,8)	1:22:A:ILE:HG23	1:10:A:PHE:HD1	4	0.19
(4,3)	1:65:A:PHE:HD1	1:15:A:LEU:HD23	10	0.19
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	3	0.19
(2,3913)	2:201:A:NAD:H51N	2:201:A:NAD:H2N	17	0.19
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	18	0.19
(2,3841)	1:76:A:ALA:HB1	1:76:A:ALA:H	5	0.19
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	9	0.19
(2,3841)	1:76:A:ALA:HB3	1:76:A:ALA:H	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3841)	1:76:A:ALA:HB2	1:76:A:ALA:H	11	0.19
(2,3841)	1:76:A:ALA:HB3	1:76:A:ALA:H	13	0.19
(2,3841)	1:76:A:ALA:HB3	1:76:A:ALA:H	18	0.19
(2,3837)	1:5:A:VAL:HG21	1:5:A:VAL:HA	2	0.19
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	7	0.19
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	8	0.19
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	7	0.19
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	9	0.19
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	10	0.19
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	18	0.19
(2,3829)	1:109:A:ILE:HD11	1:101:A:THR:HG23	13	0.19
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	1	0.19
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	11	0.19
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	13	0.19
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	15	0.19
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	19	0.19
(2,3824)	1:41:A:MET:HE1	1:11:A:LEU:HD12	20	0.19
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG23	11	0.19
(2,3821)	1:144:A:LEU:HD11	1:109:A:ILE:HG21	13	0.19
(2,3819)	1:151:A:MET:HE2	1:171:A:VAL:HG12	7	0.19
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	14	0.19
(2,3816)	1:22:A:ILE:HG21	1:14:A:VAL:HG23	18	0.19
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	20	0.19
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	10	0.19
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	19	0.19
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	5	0.19
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	8	0.19
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	18	0.19
(2,3777)	1:86:A:LEU:HD21	1:86:A:LEU:HB2	10	0.19
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	3	0.19
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	20	0.19
(2,3763)	1:76:A:ALA:HB2	1:15:A:LEU:HD11	5	0.19
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	6	0.19
(2,3763)	1:76:A:ALA:HB2	1:15:A:LEU:HD12	14	0.19
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG23	3	0.19
(2,3710)	1:14:A:VAL:HG22	1:14:A:VAL:HA	17	0.19
(2,3705)	1:7:A:VAL:HG11	1:7:A:VAL:HA	5	0.19
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	16	0.19
(2,3705)	1:7:A:VAL:HG13	1:7:A:VAL:HA	20	0.19
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	1	0.19
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	3	0.19
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	20	0.19
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	4	0.19
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	8	0.19
(2,3654)	1:96:A:VAL:HG22	1:96:A:VAL:HA	11	0.19
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	13	0.19
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	14	0.19
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	1	0.19
(2,3653)	1:14:A:VAL:HG21	1:19:A:PRO:HA	14	0.19
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	4	0.19
(2,3573)	1:71:A:PHE:HB3	1:50:A:MET:HE3	19	0.19
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	1	0.19
(2,3564)	1:108:A:LEU:HB3	1:111:A:LYS:HE2	10	0.19
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	5	0.19
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	9	0.19
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	10	0.19
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	14	0.19
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	15	0.19
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	18	0.19
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	19	0.19
(2,3531)	1:151:A:MET:HE1	1:175:A:PHE:HB3	9	0.19
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	2	0.19
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	8	0.19
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	15	0.19
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	16	0.19
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	19	0.19
(2,3502)	1:21:A:LEU:HD13	1:14:A:VAL:HA	16	0.19
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	1	0.19
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	12	0.19
(2,3479)	1:151:A:MET:HE3	1:171:A:VAL:HA	20	0.19
(2,3473)	1:146:A:VAL:HG23	1:96:A:VAL:HA	4	0.19
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	17	0.19
(2,3456)	1:167:A:LEU:HD13	1:123:A:HIS:HA	8	0.19
(2,3428)	1:108:A:LEU:HD11	2:201:A:NAD:H2A	8	0.19
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	20	0.19
(2,3399)	1:21:A:LEU:HD13	1:21:A:LEU:H	3	0.19
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	14	0.19
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	2	0.19
(2,3372)	1:20:A:ALA:HB1	1:20:A:ALA:H	9	0.19
(2,3288)	1:142:A:VAL:HG13	1:103:A:GLU:HA	18	0.19
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	7	0.19
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	19	0.19
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	7	0.19
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	11	0.19
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	17	0.19
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	18	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	1	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	2	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	3	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	4	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	6	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	7	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	8	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	9	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	10	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	11	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	12	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	13	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	14	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	15	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	16	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	17	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	18	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	19	0.19
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	20	0.19
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	2	0.19
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	4	0.19
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	5	0.19
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	8	0.19
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	3	0.19
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	6	0.19
(2,3166)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	11	0.19
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	12	0.19
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	16	0.19
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	17	0.19
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD23	18	0.19
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	3	0.19
(2,2918)	1:76:A:ALA:HB3	1:78:A:GLN:HE22	2	0.19
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	18	0.19
(2,2748)	1:86:A:LEU:HD11	1:87:A:GLY:H	10	0.19
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	8	0.19
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	19	0.19
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	10	0.19
(2,2506)	1:64:A:ARG:H	1:76:A:ALA:HB3	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	3	0.19
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	7	0.19
(2,2417)	1:36:A:GLU:H	1:36:A:GLU:HB3	4	0.19
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	12	0.19
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	19	0.19
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	8	0.19
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	10	0.19
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	15	0.19
(2,2189)	1:81:A:SER:HA	1:82:A:VAL:H	15	0.19
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	8	0.19
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD21	15	0.19
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD23	20	0.19
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	12	0.19
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	11	0.19
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	13	0.19
(2,1939)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	13	0.19
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	3	0.19
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	4	0.19
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	11	0.19
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	13	0.19
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD11	14	0.19
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	19	0.19
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	14	0.19
(2,1844)	1:110:A:LEU:HD21	1:110:A:LEU:HB3	20	0.19
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	5	0.19
(2,1830)	1:34:A:VAL:HG13	1:50:A:MET:HE2	13	0.19
(2,1805)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	1	0.19
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	4	0.19
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	7	0.19
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	11	0.19
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	13	0.19
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	16	0.19
(2,1792)	1:59:A:THR:HG21	1:58:A:GLU:HG2	1	0.19
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	4	0.19
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	13	0.19
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	1	0.19
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	3	0.19
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	6	0.19
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	8	0.19
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	10	0.19
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	14	0.19
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1747)	1:14:A:VAL:HB	1:14:A:VAL:HA	18	0.19
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	2	0.19
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	5	0.19
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	10	0.19
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	14	0.19
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	1	0.19
(2,1599)	1:4:A:MET:HE1	1:52:A:GLU:HA	14	0.19
(2,1549)	1:37:A:LEU:HD13	1:41:A:MET:HG2	6	0.19
(2,1541)	1:143:A:VAL:HG13	1:132:A:ARG:HA	4	0.19
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	1	0.19
(2,1524)	1:82:A:VAL:HG11	1:82:A:VAL:HA	4	0.19
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	14	0.19
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	2	0.19
(2,1474)	1:110:A:LEU:HD21	1:110:A:LEU:H	4	0.19
(2,1468)	1:22:A:ILE:HG22	1:10:A:PHE:HZ	12	0.19
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	1	0.19
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	7	0.19
(2,1438)	1:146:A:VAL:HG13	1:97:A:LEU:H	6	0.19
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	2	0.19
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	16	0.19
(2,1432)	1:38:A:LEU:HD13	1:39:A:ALA:H	7	0.19
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	13	0.19
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	17	0.19
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	13	0.19
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	15	0.19
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	9	0.19
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	11	0.19
(2,1301)	1:34:A:VAL:HG12	1:38:A:LEU:H	10	0.19
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	7	0.19
(2,1288)	1:167:A:LEU:HD22	1:167:A:LEU:HA	7	0.19
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	9	0.19
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	20	0.19
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	9	0.19
(2,1218)	1:177:A:LYS:HG2	1:177:A:LYS:HA	9	0.19
(2,1218)	1:177:A:LYS:HG2	1:177:A:LYS:HA	16	0.19
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	11	0.19
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	20	0.19
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	16	0.19
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	9	0.19
(2,1014)	1:160:A:LEU:H	1:89:A:GLU:H	15	0.19
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	1	0.19
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	5	0.19
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	10	0.19
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	16	0.19
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	3	0.19
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	6	0.19
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	10	0.19
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	19	0.19
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	13	0.19
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	16	0.19
(2,726)	1:20:A:ALA:HB2	1:23:A:GLY:H	12	0.19
(2,726)	1:20:A:ALA:HB2	1:23:A:GLY:H	20	0.19
(2,718)	1:91:A:GLN:HE21	1:89:A:GLU:HB2	5	0.19
(2,718)	1:91:A:GLN:HE21	1:89:A:GLU:HB2	17	0.19
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	19	0.19
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	11	0.19
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	15	0.19
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB1	4	0.19
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	11	0.19
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	3	0.19
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	6	0.19
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	8	0.19
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	11	0.19
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	12	0.19
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	19	0.19
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	6	0.19
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	8	0.19
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	9	0.19
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	10	0.19
(2,511)	1:128:A:ILE:HG21	1:129:A:THR:H	17	0.19
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	2	0.19
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	9	0.19
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	20	0.19
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	16	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	1	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	2	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	3	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	8	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	13	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	14	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	15	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	17	0.19
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	19	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	13	0.19
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	2	0.19
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	4	0.19
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	7	0.19
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	12	0.19
(2,268)	1:14:A:VAL:HG22	1:21:A:LEU:H	5	0.19
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	10	0.19
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	15	0.19
(2,224)	1:81:A:SER:HA	1:82:A:VAL:H	20	0.19
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	13	0.19
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	14	0.19
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	19	0.19
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	20	0.19
(2,137)	1:103:A:GLU:H	1:140:A:LYS:HB2	10	0.19
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	6	0.19
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	16	0.19
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	3	0.19
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	12	0.19
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	15	0.19
(2,61)	1:166:A:TRP:HE1	1:126:A:GLN:HB2	6	0.19
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	17	0.19
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	7	0.19
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	20	0.19
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	14	0.19
(2,13)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	18	0.19
(2,2)	1:159:A:TYR:HD1	1:94:A:PRO:HB3	20	0.19
(1,117)	1:168:A:ILE:H	1:122:A:VAL:O	19	0.19
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	9	0.19
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	20	0.19
(1,111)	1:159:A:TYR:H	1:167:A:LEU:O	9	0.19
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	2	0.19
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	16	0.19
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	4	0.19
(1,92)	1:133:A:LYS:N	1:129:A:THR:O	9	0.19
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	13	0.19
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	7	0.19
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	16	0.19
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	15	0.19
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	18	0.19
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	2	0.19
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	2	0.19
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	10	0.19
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	11	0.19
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	13	0.19
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	13	0.19
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	9	0.19
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	16	0.19
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	6	0.19
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	14	0.19
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	20	0.19
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	11	0.19
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	16	0.19
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	7	0.19
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	17	0.19
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	6	0.19
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	9	0.19
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	6	0.19
(1,2)	1:7:A:VAL:N	1:3:A:HIS:O	7	0.19
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	9	0.18
(4,443)	1:48:A:ILE:HD13	1:38:A:LEU:HB2	20	0.18
(4,442)	1:178:A:VAL:HG21	1:144:A:LEU:HG	3	0.18
(4,350)	1:6:A:LYS:HE2	1:44:A:LYS:HG3	8	0.18
(4,325)	1:7:A:VAL:HG13	1:10:A:PHE:HB3	4	0.18
(4,319)	1:26:A:LEU:HD23	1:14:A:VAL:HA	11	0.18
(4,307)	1:26:A:LEU:HD21	1:15:A:LEU:HA	12	0.18
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	5	0.18
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	2	0.18
(4,234)	1:53:A:LEU:HA	1:53:A:LEU:H	18	0.18
(4,208)	1:14:A:VAL:HG22	1:11:A:LEU:HA	11	0.18
(4,174)	1:97:A:LEU:H	1:152:A:ALA:H	12	0.18
(4,61)	1:37:A:LEU:H	1:24:A:LEU:HD12	1	0.18
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	17	0.18
(4,8)	1:22:A:ILE:HG23	1:10:A:PHE:HD1	13	0.18
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	7	0.18
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	14	0.18
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	4	0.18
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	1	0.18
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	15	0.18
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	18	0.18
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	5	0.18
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	14	0.18
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	17	0.18
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3841)	1:76:A:ALA:HB3	1:76:A:ALA:H	7	0.18
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	10	0.18
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	1	0.18
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	3	0.18
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	6	0.18
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD12	12	0.18
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	14	0.18
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	15	0.18
(2,3829)	1:109:A:ILE:HD11	1:101:A:THR:HG23	7	0.18
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	1	0.18
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	3	0.18
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	4	0.18
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD11	14	0.18
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	20	0.18
(2,3819)	1:151:A:MET:HE1	1:171:A:VAL:HG12	5	0.18
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	19	0.18
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	16	0.18
(2,3809)	1:176:A:ILE:HB	1:110:A:LEU:HD11	5	0.18
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	2	0.18
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	10	0.18
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	14	0.18
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	15	0.18
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	16	0.18
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	17	0.18
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	4	0.18
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	13	0.18
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	19	0.18
(2,3791)	1:142:A:VAL:HG23	1:143:A:VAL:HB	10	0.18
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	9	0.18
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	11	0.18
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	16	0.18
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	19	0.18
(2,3772)	1:151:A:MET:HE1	1:174:A:GLU:HG2	19	0.18
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD12	12	0.18
(2,3759)	1:53:A:LEU:HD11	1:53:A:LEU:HB2	15	0.18
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	10	0.18
(2,3710)	1:14:A:VAL:HG21	1:14:A:VAL:HA	14	0.18
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	17	0.18
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	3	0.18
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	6	0.18
(2,3654)	1:96:A:VAL:HG22	1:96:A:VAL:HA	7	0.18
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	10	0.18
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	12	0.18
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	16	0.18
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	19	0.18
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	20	0.18
(2,3653)	1:14:A:VAL:HG22	1:19:A:PRO:HA	17	0.18
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	20	0.18
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE3	2	0.18
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE2	10	0.18
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE3	15	0.18
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE3	17	0.18
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	8	0.18
(2,3503)	1:34:A:VAL:HG13	1:34:A:VAL:HA	1	0.18
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	5	0.18
(2,3503)	1:34:A:VAL:HG13	1:34:A:VAL:HA	18	0.18
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	20	0.18
(2,3495)	1:82:A:VAL:HG11	1:82:A:VAL:HA	4	0.18
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	14	0.18
(2,3490)	1:48:A:ILE:HD12	1:53:A:LEU:HA	14	0.18
(2,3484)	1:124:A:LEU:HD13	1:167:A:LEU:HA	19	0.18
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	12	0.18
(2,3470)	1:110:A:LEU:HD11	1:107:A:ASP:HA	19	0.18
(2,3430)	1:128:A:ILE:HD11	1:127:A:ASP:H	15	0.18
(2,3428)	1:108:A:LEU:HD12	2:201:A:NAD:H2A	20	0.18
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	2	0.18
(2,3424)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	13	0.18
(2,3424)	1:165:A:VAL:HG23	2:201:A:NAD:H5N	18	0.18
(2,3409)	1:84:A:VAL:HG11	1:85:A:ASP:H	10	0.18
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	2	0.18
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	3	0.18
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	5	0.18
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	8	0.18
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	15	0.18
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	16	0.18
(2,3382)	1:53:A:LEU:HD11	1:67:A:PHE:HZ	18	0.18
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	3	0.18
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	1	0.18
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	8	0.18
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	9	0.18
(2,3174)	1:24:A:LEU:HD11	1:32:A:ALA:HB2	16	0.18
(2,3168)	1:176:A:ILE:HB	1:176:A:ILE:HG12	5	0.18
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	2	0.18
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	7	0.18
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	3	0.18
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	7	0.18
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	10	0.18
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD23	13	0.18
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD22	15	0.18
(2,3127)	1:97:A:LEU:HD12	1:124:A:LEU:HD22	20	0.18
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD21	2	0.18
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	20	0.18
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	10	0.18
(2,2657)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	18	0.18
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	2	0.18
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	10	0.18
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	16	0.18
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	19	0.18
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	20	0.18
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	10	0.18
(2,2417)	1:36:A:GLU:H	1:36:A:GLU:HB3	2	0.18
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	4	0.18
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	5	0.18
(2,2367)	1:48:A:ILE:HG23	1:48:A:ILE:H	4	0.18
(2,2367)	1:48:A:ILE:HG23	1:48:A:ILE:H	7	0.18
(2,2367)	1:48:A:ILE:HG22	1:48:A:ILE:H	15	0.18
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	20	0.18
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	9	0.18
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	10	0.18
(2,2232)	1:21:A:LEU:H	1:24:A:LEU:HD23	7	0.18
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	6	0.18
(2,2189)	1:81:A:SER:HA	1:82:A:VAL:H	20	0.18
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	10	0.18
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	8	0.18
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	1	0.18
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	6	0.18
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	11	0.18
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD11	14	0.18
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	20	0.18
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	11	0.18
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	8	0.18
(2,2041)	1:152:A:ALA:HB2	1:152:A:ALA:H	14	0.18
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	4	0.18
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	4	0.18
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	7	0.18
(2,1958)	1:168:A:ILE:HD11	1:158:A:PHE:HE1	11	0.18
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	8	0.18
(2,1871)	1:97:A:LEU:HD21	1:151:A:MET:HG3	9	0.18
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	2	0.18
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	15	0.18
(2,1860)	1:57:A:VAL:HG21	1:57:A:VAL:HB	10	0.18
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	7	0.18
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	10	0.18
(2,1810)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	5	0.18
(2,1810)	1:21:A:LEU:HD12	1:21:A:LEU:HB3	20	0.18
(2,1800)	1:53:A:LEU:HD12	1:37:A:LEU:HG	17	0.18
(2,1796)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	20	0.18
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	4	0.18
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	15	0.18
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	7	0.18
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	18	0.18
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	19	0.18
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	4	0.18
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	15	0.18
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	8	0.18
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	14	0.18
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	17	0.18
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	20	0.18
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	4	0.18
(2,1474)	1:110:A:LEU:HD23	1:110:A:LEU:H	1	0.18
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	8	0.18
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	20	0.18
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	20	0.18
(2,1435)	1:15:A:LEU:HD21	1:15:A:LEU:H	9	0.18
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	1	0.18
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	14	0.18
(2,1407)	1:95:A:ALA:HB2	1:95:A:ALA:H	5	0.18
(2,1403)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	9	0.18
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	2	0.18
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	3	0.18
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	4	0.18
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	8	0.18
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	16	0.18
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	8	0.18
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	13	0.18
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	14	0.18
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	19	0.18
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	18	0.18
(2,1131)	1:136:A:MET:H	1:105:A:ASN:HD22	11	0.18
(2,1110)	1:76:A:ALA:H	1:75:A:ARG:H	2	0.18
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	20	0.18
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	1	0.18
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	2	0.18
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	3	0.18
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	7	0.18
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	11	0.18
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	14	0.18
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	18	0.18
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	10	0.18
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	16	0.18
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	18	0.18
(2,815)	1:102:A:ALA:H	1:101:A:THR:HG23	9	0.18
(2,726)	1:20:A:ALA:HB2	1:23:A:GLY:H	11	0.18
(2,718)	1:91:A:GLN:HE21	1:89:A:GLU:HB2	19	0.18
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	20	0.18
(2,673)	1:70:A:ASN:HD22	1:50:A:MET:HG3	3	0.18
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	1	0.18
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	7	0.18
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	9	0.18
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	12	0.18
(2,550)	1:105:A:ASN:H	1:102:A:ALA:HB3	15	0.18
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	14	0.18
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	1	0.18
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	15	0.18
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	11	0.18
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	10	0.18
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	14	0.18
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG11	18	0.18
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	10	0.18
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	6	0.18
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	9	0.18
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	10	0.18
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	14	0.18
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	16	0.18
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	1	0.18
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	18	0.18
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	18	0.18
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	2	0.18
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	14	0.18
(2,190)	1:13:A:LEU:H	1:13:A:LEU:HB3	5	0.18
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	12	0.18
(2,181)	1:66:A:ALA:H	1:67:A:PHE:HB3	15	0.18
(2,168)	1:39:A:ALA:H	1:41:A:MET:H	12	0.18
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	2	0.18
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	4	0.18
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	15	0.18
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	16	0.18
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	14	0.18
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	11	0.18
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	18	0.18
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	2	0.18
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	12	0.18
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	3	0.18
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	6	0.18
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	14	0.18
(1,111)	1:159:A:TYR:H	1:167:A:LEU:O	10	0.18
(1,111)	1:159:A:TYR:H	1:167:A:LEU:O	11	0.18
(1,108)	1:151:A:MET:N	1:148:A:ALA:O	5	0.18
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	15	0.18
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	14	0.18
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	3	0.18
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	11	0.18
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	10	0.18
(1,94)	1:134:A:VAL:N	1:130:A:THR:O	3	0.18
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	19	0.18
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	11	0.18
(1,83)	1:122:A:VAL:H	1:168:A:ILE:O	17	0.18
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	1	0.18
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	8	0.18
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	3	0.18
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	1	0.18
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	3	0.18
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	8	0.18
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	20	0.18
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	15	0.18
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	17	0.18
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	14	0.18
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	3	0.18
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	8	0.18
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	10	0.18
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	11	0.18
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	12	0.18
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	13	0.18
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	9	0.18
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	5	0.18
(1,24)	1:37:A:LEU:N	1:33:A:PRO:O	4	0.18
(1,24)	1:37:A:LEU:N	1:33:A:PRO:O	16	0.18
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	16	0.18
(1,17)	1:15:A:LEU:H	1:11:A:LEU:O	3	0.18
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	18	0.18
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	2	0.18
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	7	0.18
(4,453)	1:48:A:ILE:HG13	1:38:A:LEU:HA	2	0.17
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	15	0.17
(4,448)	1:110:A:LEU:HD22	1:144:A:LEU:HG	14	0.17
(4,440)	1:15:A:LEU:HD22	1:74:A:ILE:HB	14	0.17
(4,409)	1:4:A:MET:HE1	1:59:A:THR:HG23	2	0.17
(4,379)	1:50:A:MET:HA	1:35:A:LYS:HG2	13	0.17
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	11	0.17
(4,325)	1:7:A:VAL:HG13	1:10:A:PHE:HB3	18	0.17
(4,320)	1:151:A:MET:HE2	1:158:A:PHE:HB2	9	0.17
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	12	0.17
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	20	0.17
(4,198)	1:176:A:ILE:HD11	1:106:A:PHE:HE1	3	0.17
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	7	0.17
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	15	0.17
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	16	0.17
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	17	0.17
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD12	5	0.17
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	19	0.17
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	3	0.17
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	13	0.17
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	6	0.17
(2,3940)	1:134:A:VAL:HG11	2:201:A:NAD:H2N	10	0.17
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	11	0.17
(2,3920)	1:115:A:LYS:H	2:201:A:NAD:H8A	6	0.17
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	7	0.17
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	13	0.17
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	15	0.17
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	19	0.17
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	2	0.17
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	5	0.17
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	9	0.17
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	14	0.17
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	18	0.17
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	15	0.17
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	18	0.17
(2,3836)	1:168:A:ILE:HD12	1:171:A:VAL:HG11	12	0.17
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	16	0.17
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD12	5	0.17
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	16	0.17
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	20	0.17
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD12	8	0.17
(2,3824)	1:41:A:MET:HE3	1:11:A:LEU:HD11	10	0.17
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	9	0.17
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	17	0.17
(2,3819)	1:151:A:MET:HE1	1:171:A:VAL:HG12	1	0.17
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	8	0.17
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	20	0.17
(2,3814)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	1	0.17
(2,3813)	1:56:A:ILE:HD12	1:11:A:LEU:HD13	5	0.17
(2,3804)	1:128:A:ILE:HG23	1:129:A:THR:HG21	10	0.17
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	6	0.17
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	6	0.17
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	7	0.17
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	8	0.17
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	9	0.17
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	18	0.17
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	19	0.17
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	9	0.17
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	11	0.17
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	12	0.17
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	20	0.17
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	5	0.17
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	8	0.17
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	12	0.17
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	17	0.17
(2,3763)	1:76:A:ALA:HB1	1:15:A:LEU:HD11	15	0.17
(2,3761)	1:117:A:MET:HE1	1:117:A:MET:HB2	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	8	0.17
(2,3744)	1:57:A:VAL:HG12	1:57:A:VAL:HB	2	0.17
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	15	0.17
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	19	0.17
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	10	0.17
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	1	0.17
(2,3654)	1:96:A:VAL:HG22	1:96:A:VAL:HA	2	0.17
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	17	0.17
(2,3654)	1:96:A:VAL:HG21	1:96:A:VAL:HA	18	0.17
(2,3575)	1:50:A:MET:HE1	1:50:A:MET:HG3	13	0.17
(2,3575)	1:50:A:MET:HE2	1:50:A:MET:HG3	17	0.17
(2,3565)	1:71:A:PHE:HB2	1:50:A:MET:HE1	18	0.17
(2,3559)	1:102:A:ALA:HB1	2:201:A:NAD:H4B	7	0.17
(2,3547)	1:22:A:ILE:HG21	1:22:A:ILE:HA	16	0.17
(2,3518)	1:128:A:ILE:HD12	1:128:A:ILE:HA	13	0.17
(2,3518)	1:128:A:ILE:HD12	1:128:A:ILE:HA	17	0.17
(2,3509)	1:13:A:LEU:HD23	1:17:A:HIS:HB2	2	0.17
(2,3509)	1:13:A:LEU:HD21	1:17:A:HIS:HB2	14	0.17
(2,3503)	1:34:A:VAL:HG11	1:34:A:VAL:HA	14	0.17
(2,3473)	1:146:A:VAL:HG23	1:96:A:VAL:HA	8	0.17
(2,3409)	1:84:A:VAL:HG13	1:85:A:ASP:H	18	0.17
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	1	0.17
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	20	0.17
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	12	0.17
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	20	0.17
(2,3355)	1:41:A:MET:HE2	1:41:A:MET:H	17	0.17
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	2	0.17
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	17	0.17
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	1	0.17
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	2	0.17
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	4	0.17
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	17	0.17
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	9	0.17
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	10	0.17
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	12	0.17
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	15	0.17
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	17	0.17
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD22	1	0.17
(2,3127)	1:97:A:LEU:HD12	1:124:A:LEU:HD22	6	0.17
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	8	0.17
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	16	0.17
(2,2925)	1:57:A:VAL:H	1:53:A:LEU:HD23	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2657)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	11	0.17
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	2	0.17
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	3	0.17
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	13	0.17
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	1	0.17
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	6	0.17
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	13	0.17
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	14	0.17
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	15	0.17
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	1	0.17
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	3	0.17
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	14	0.17
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	3	0.17
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	11	0.17
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	9	0.17
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	18	0.17
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	13	0.17
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	11	0.17
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG12	14	0.17
(2,2232)	1:21:A:LEU:H	1:24:A:LEU:HD23	11	0.17
(2,2210)	1:48:A:ILE:HD12	1:53:A:LEU:H	8	0.17
(2,2192)	1:82:A:VAL:HB	1:82:A:VAL:H	15	0.17
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD21	2	0.17
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	12	0.17
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD23	13	0.17
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	16	0.17
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	17	0.17
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	1	0.17
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	2	0.17
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	14	0.17
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	17	0.17
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	16	0.17
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	5	0.17
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	1	0.17
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	2	0.17
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	6	0.17
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	13	0.17
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	20	0.17
(2,1889)	1:4:A:MET:HE1	1:4:A:MET:HA	6	0.17
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	19	0.17
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD12	8	0.17
(2,1861)	1:41:A:MET:HE3	1:11:A:LEU:HD11	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	11	0.17
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	17	0.17
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	11	0.17
(2,1828)	1:151:A:MET:HE2	1:151:A:MET:HG3	5	0.17
(2,1807)	1:151:A:MET:HE2	1:174:A:GLU:HG2	4	0.17
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	3	0.17
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	20	0.17
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	2	0.17
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	12	0.17
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	18	0.17
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	6	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	2	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	3	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	4	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	11	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	12	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	13	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	15	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	16	0.17
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	19	0.17
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	7	0.17
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	1	0.17
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	8	0.17
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	20	0.17
(2,1622)	1:73:A:LYS:HE3	1:25:A:ASP:HA	17	0.17
(2,1563)	1:48:A:ILE:HG23	1:53:A:LEU:HB2	16	0.17
(2,1555)	1:84:A:VAL:HG22	1:85:A:ASP:HB2	1	0.17
(2,1541)	1:143:A:VAL:HG11	1:132:A:ARG:HA	18	0.17
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	20	0.17
(2,1513)	1:26:A:LEU:HD13	1:32:A:ALA:HA	13	0.17
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	5	0.17
(2,1509)	1:151:A:MET:HE2	1:171:A:VAL:HA	16	0.17
(2,1509)	1:151:A:MET:HE3	1:171:A:VAL:HA	19	0.17
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	13	0.17
(2,1455)	1:165:A:VAL:HG23	2:201:A:NAD:H5N	18	0.17
(2,1432)	1:38:A:LEU:HD12	1:39:A:ALA:H	13	0.17
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	6	0.17
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	1	0.17
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	1	0.17
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	14	0.17
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	8	0.17
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	16	0.17
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	10	0.17
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	14	0.17
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	6	0.17
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	7	0.17
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	11	0.17
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	12	0.17
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	13	0.17
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	14	0.17
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	12	0.17
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	13	0.17
(2,1164)	1:131:A:ALA:HB1	1:132:A:ARG:H	17	0.17
(2,1155)	1:86:A:LEU:HD11	1:88:A:TYR:HE1	5	0.17
(2,1075)	1:56:A:ILE:H	1:58:A:GLU:H	5	0.17
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	6	0.17
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	12	0.17
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	13	0.17
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	19	0.17
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	1	0.17
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	8	0.17
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	14	0.17
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	5	0.17
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	12	0.17
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	10	0.17
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	18	0.17
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	11	0.17
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD12	9	0.17
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	8	0.17
(2,768)	1:30:A:GLY:H	1:26:A:LEU:HD22	20	0.17
(2,726)	1:20:A:ALA:HB2	1:23:A:GLY:H	10	0.17
(2,708)	1:113:A:GLY:H	1:109:A:ILE:HG21	16	0.17
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	5	0.17
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	5	0.17
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	7	0.17
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	19	0.17
(2,577)	1:96:A:VAL:H	1:148:A:ALA:HB2	1	0.17
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	8	0.17
(2,518)	1:111:A:LYS:HB3	1:112:A:ASP:H	8	0.17
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	5	0.17
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	3	0.17
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	13	0.17
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	3	0.17
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	7	0.17
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	2	0.17
(2,369)	1:57:A:VAL:HA	1:57:A:VAL:H	8	0.17
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	2	0.17
(2,309)	1:74:A:ILE:H	1:73:A:LYS:HG2	19	0.17
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	10	0.17
(2,184)	1:26:A:LEU:H	1:19:A:PRO:HA	19	0.17
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	9	0.17
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	13	0.17
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	3	0.17
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	9	0.17
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	10	0.17
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	12	0.17
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	14	0.17
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	18	0.17
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	8	0.17
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	8	0.17
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	7	0.17
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	9	0.17
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	13	0.17
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	18	0.17
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	13	0.17
(2,85)	1:152:A:ALA:HB2	1:152:A:ALA:H	19	0.17
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	8	0.17
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	9	0.17
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	5	0.17
(2,16)	1:21:A:LEU:HD12	1:10:A:PHE:HE1	16	0.17
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	16	0.17
(2,7)	1:168:A:ILE:HD11	1:158:A:PHE:HE1	11	0.17
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	14	0.17
(1,119)	1:171:A:VAL:H	1:114:A:ILE:O	16	0.17
(1,116)	1:167:A:LEU:N	1:159:A:TYR:O	18	0.17
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	1	0.17
(1,111)	1:159:A:TYR:H	1:167:A:LEU:O	15	0.17
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	12	0.17
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	5	0.17
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	6	0.17
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	6	0.17
(1,92)	1:133:A:LYS:N	1:129:A:THR:O	7	0.17
(1,89)	1:132:A:ARG:H	1:128:A:ILE:O	10	0.17
(1,87)	1:131:A:ALA:H	1:127:A:ASP:O	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	9	0.17
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	10	0.17
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	4	0.17
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	7	0.17
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	20	0.17
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	3	0.17
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	11	0.17
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	6	0.17
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	15	0.17
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	19	0.17
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	4	0.17
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	7	0.17
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	15	0.17
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	19	0.17
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	1	0.17
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	9	0.17
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	16	0.17
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	14	0.17
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	4	0.17
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	18	0.17
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	10	0.17
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	18	0.17
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	14	0.17
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	4	0.17
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	3	0.17
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	12	0.17
(1,4)	1:8:A:SER:N	1:4:A:MET:O	6	0.17
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	12	0.16
(4,442)	1:178:A:VAL:HG21	1:144:A:LEU:HG	2	0.16
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	1	0.16
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	5	0.16
(4,439)	1:176:A:ILE:HG21	1:177:A:LYS:HG2	12	0.16
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	16	0.16
(4,325)	1:7:A:VAL:HG11	1:10:A:PHE:HB3	7	0.16
(4,290)	1:53:A:LEU:HD22	1:56:A:ILE:H	6	0.16
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	7	0.16
(4,290)	1:53:A:LEU:HD22	1:56:A:ILE:H	16	0.16
(4,259)	1:117:A:MET:HE2	2:201:A:NAD:H2A	5	0.16
(4,227)	1:8:A:SER:HB3	1:65:A:PHE:HE1	2	0.16
(4,209)	1:76:A:ALA:HB1	1:16:A:ARG:H	15	0.16
(4,95)	1:41:A:MET:HG3	1:51:A:GLU:H	16	0.16
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	7	0.16
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	1	0.16
(4,8)	1:22:A:ILE:HG23	1:10:A:PHE:HD1	15	0.16
(2,3959)	1:123:A:HIS:HB3	2:201:A:NAD:H5N	5	0.16
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	3	0.16
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	18	0.16
(2,3900)	2:201:A:NAD:H5N	2:201:A:NAD:H6N	12	0.16
(2,3896)	2:201:A:NAD:H3D	2:201:A:NAD:H2N	15	0.16
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	6	0.16
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	8	0.16
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	9	0.16
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	11	0.16
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	16	0.16
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	20	0.16
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	6	0.16
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	8	0.16
(2,3836)	1:168:A:ILE:HD13	1:171:A:VAL:HG11	15	0.16
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD13	19	0.16
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD13	8	0.16
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	18	0.16
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD11	3	0.16
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	3	0.16
(2,3802)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	15	0.16
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	16	0.16
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	17	0.16
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	15	0.16
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	4	0.16
(2,3794)	1:14:A:VAL:HG23	1:14:A:VAL:HB	11	0.16
(2,3794)	1:14:A:VAL:HG21	1:14:A:VAL:HB	12	0.16
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	7	0.16
(2,3793)	1:53:A:LEU:HD22	1:56:A:ILE:HB	16	0.16
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	16	0.16
(2,3773)	1:34:A:VAL:HG13	1:37:A:LEU:HB3	1	0.16
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	14	0.16
(2,3770)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	4	0.16
(2,3770)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	6	0.16
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	15	0.16
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	18	0.16
(2,3763)	1:76:A:ALA:HB2	1:15:A:LEU:HD11	1	0.16
(2,3763)	1:76:A:ALA:HB1	1:15:A:LEU:HD12	13	0.16
(2,3763)	1:76:A:ALA:HB2	1:15:A:LEU:HD11	17	0.16
(2,3757)	1:144:A:LEU:HG	1:101:A:THR:HG22	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	6	0.16
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	10	0.16
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	17	0.16
(2,3654)	1:96:A:VAL:HG22	1:96:A:VAL:HA	15	0.16
(2,3575)	1:50:A:MET:HE2	1:50:A:MET:HG3	7	0.16
(2,3575)	1:50:A:MET:HE2	1:50:A:MET:HG3	15	0.16
(2,3547)	1:22:A:ILE:HG22	1:22:A:ILE:HA	17	0.16
(2,3509)	1:13:A:LEU:HD22	1:17:A:HIS:HB2	8	0.16
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	2	0.16
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	20	0.16
(2,3484)	1:124:A:LEU:HD11	1:167:A:LEU:HA	4	0.16
(2,3479)	1:151:A:MET:HE3	1:171:A:VAL:HA	14	0.16
(2,3445)	1:97:A:LEU:HD23	1:166:A:TRP:HE3	10	0.16
(2,3434)	1:15:A:LEU:HD12	1:65:A:PHE:HE1	13	0.16
(2,3424)	1:165:A:VAL:HG23	2:201:A:NAD:H5N	15	0.16
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	15	0.16
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	11	0.16
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	12	0.16
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	19	0.16
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	4	0.16
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	11	0.16
(2,3378)	1:66:A:ALA:HB2	1:31:A:TRP:HZ3	15	0.16
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	5	0.16
(2,3345)	1:41:A:MET:HE1	1:10:A:PHE:HE1	11	0.16
(2,3288)	1:142:A:VAL:HG13	1:103:A:GLU:HA	17	0.16
(2,3288)	1:142:A:VAL:HG13	1:103:A:GLU:HA	19	0.16
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	14	0.16
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	19	0.16
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	11	0.16
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	20	0.16
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	11	0.16
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD22	5	0.16
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD21	9	0.16
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD23	12	0.16
(2,2982)	1:160:A:LEU:H	1:89:A:GLU:H	13	0.16
(2,2852)	1:85:A:ASP:H	1:86:A:LEU:H	13	0.16
(2,2657)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	15	0.16
(2,2657)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	17	0.16
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	7	0.16
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	7	0.16
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	11	0.16
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	20	0.16
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	11	0.16
(2,2520)	1:8:A:SER:H	1:6:A:LYS:HA	4	0.16
(2,2417)	1:36:A:GLU:H	1:36:A:GLU:HB3	3	0.16
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	2	0.16
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	14	0.16
(2,2367)	1:48:A:ILE:HG23	1:48:A:ILE:H	3	0.16
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	11	0.16
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	13	0.16
(2,2234)	1:14:A:VAL:HG22	1:21:A:LEU:H	5	0.16
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	19	0.16
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	19	0.16
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	17	0.16
(2,2103)	1:84:A:VAL:HA	1:85:A:ASP:H	3	0.16
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	7	0.16
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	5	0.16
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	2	0.16
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	4	0.16
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	6	0.16
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	10	0.16
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	19	0.16
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	10	0.16
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	3	0.16
(2,1962)	1:110:A:LEU:HD13	1:106:A:PHE:HE1	5	0.16
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	10	0.16
(2,1962)	1:110:A:LEU:HD13	1:106:A:PHE:HE1	14	0.16
(2,1962)	1:110:A:LEU:HD12	1:106:A:PHE:HE1	15	0.16
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	18	0.16
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	11	0.16
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	14	0.16
(2,1932)	2:201:A:NAD:H3D	2:201:A:NAD:H2N	15	0.16
(2,1889)	1:4:A:MET:HE1	1:4:A:MET:HA	12	0.16
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	12	0.16
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	17	0.16
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	5	0.16
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	8	0.16
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	9	0.16
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	11	0.16
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	12	0.16
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	16	0.16
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	17	0.16
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	10	0.16
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	9	0.16
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	19	0.16
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	20	0.16
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	8	0.16
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	9	0.16
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	11	0.16
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	15	0.16
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	16	0.16
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	6	0.16
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	7	0.16
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	9	0.16
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	10	0.16
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	18	0.16
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	11	0.16
(2,1723)	1:38:A:LEU:HD13	1:50:A:MET:HA	12	0.16
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	18	0.16
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE1	7	0.16
(2,1591)	1:95:A:ALA:HB1	1:149:A:LYS:HA	6	0.16
(2,1588)	1:152:A:ALA:HB2	1:149:A:LYS:HA	5	0.16
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	1	0.16
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	2	0.16
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	3	0.16
(2,1524)	1:82:A:VAL:HG22	1:82:A:VAL:HA	8	0.16
(2,1514)	1:124:A:LEU:HD13	1:167:A:LEU:HA	19	0.16
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	7	0.16
(2,1509)	1:151:A:MET:HE2	1:171:A:VAL:HA	12	0.16
(2,1490)	1:167:A:LEU:HD13	1:166:A:TRP:HA	12	0.16
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	5	0.16
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	14	0.16
(2,1474)	1:110:A:LEU:HD21	1:110:A:LEU:H	16	0.16
(2,1455)	1:165:A:VAL:HG22	2:201:A:NAD:H5N	2	0.16
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	19	0.16
(2,1388)	1:41:A:MET:HE1	1:41:A:MET:H	9	0.16
(2,1378)	1:50:A:MET:HE2	1:67:A:PHE:HZ	6	0.16
(2,1339)	1:54:A:LYS:HA	1:67:A:PHE:HE1	20	0.16
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	2	0.16
(2,1321)	1:50:A:MET:HA	1:70:A:ASN:HD22	17	0.16
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	14	0.16
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	17	0.16
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	11	0.16
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	18	0.16
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	1	0.16
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	17	0.16
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	18	0.16
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	6	0.16
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	18	0.16
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	4	0.16
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	2	0.16
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	3	0.16
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	9	0.16
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	10	0.16
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	13	0.16
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	20	0.16
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	1	0.16
(2,1110)	1:76:A:ALA:H	1:75:A:ARG:H	19	0.16
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	5	0.16
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	19	0.16
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	16	0.16
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	8	0.16
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	9	0.16
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	20	0.16
(2,996)	1:164:A:GLY:H	1:91:A:GLN:HE22	5	0.16
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	18	0.16
(2,862)	1:76:A:ALA:H	1:74:A:ILE:HD11	9	0.16
(2,822)	1:148:A:ALA:H	1:96:A:VAL:HB	5	0.16
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	19	0.16
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD11	15	0.16
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	1	0.16
(2,772)	1:86:A:LEU:HG	1:87:A:GLY:H	12	0.16
(2,694)	1:77:A:ASN:HD22	1:64:A:ARG:H	6	0.16
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	4	0.16
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB1	6	0.16
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	16	0.16
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB1	18	0.16
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	20	0.16
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	13	0.16
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	9	0.16
(2,594)	1:43:A:ALA:HB2	1:44:A:LYS:H	2	0.16
(2,550)	1:102:A:ALA:HB1	1:105:A:ASN:H	7	0.16
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	10	0.16
(2,487)	1:57:A:VAL:HG21	1:58:A:GLU:H	7	0.16
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	6	0.16
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	9	0.16
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	11	0.16
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	15	0.16
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	19	0.16
(2,453)	1:34:A:VAL:HB	1:35:A:LYS:H	17	0.16
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	12	0.16
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	15	0.16
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	5	0.16
(2,268)	1:14:A:VAL:HG23	1:21:A:LEU:H	18	0.16
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	6	0.16
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	12	0.16
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG23	16	0.16
(2,236)	1:21:A:LEU:H	1:22:A:ILE:HG21	17	0.16
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	4	0.16
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	8	0.16
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	19	0.16
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	8	0.16
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	13	0.16
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	14	0.16
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	11	0.16
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	18	0.16
(2,96)	1:25:A:ASP:HB3	1:25:A:ASP:H	1	0.16
(2,91)	1:25:A:ASP:H	1:26:A:LEU:HG	11	0.16
(2,85)	1:152:A:ALA:HB2	1:152:A:ALA:H	1	0.16
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	17	0.16
(2,41)	1:96:A:VAL:HG11	1:148:A:ALA:H	9	0.16
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	16	0.16
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	14	0.16
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	18	0.16
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	2	0.16
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	5	0.16
(1,118)	1:168:A:ILE:N	1:122:A:VAL:O	9	0.16
(1,117)	1:168:A:ILE:H	1:122:A:VAL:O	15	0.16
(1,111)	1:159:A:TYR:H	1:167:A:LEU:O	18	0.16
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	15	0.16
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	3	0.16
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	11	0.16
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	5	0.16
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	19	0.16
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	11	0.16
(1,89)	1:132:A:ARG:H	1:128:A:ILE:O	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	13	0.16
(1,77)	1:112:A:ASP:H	1:108:A:LEU:O	1	0.16
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	2	0.16
(1,59)	1:77:A:ASN:H	1:64:A:ARG:O	3	0.16
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	7	0.16
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	9	0.16
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	12	0.16
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	6	0.16
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	10	0.16
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	8	0.16
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	3	0.16
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	8	0.16
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	11	0.16
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	12	0.16
(1,34)	1:42:A:LYS:N	1:38:A:LEU:O	5	0.16
(1,30)	1:40:A:LYS:N	1:36:A:GLU:O	13	0.16
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	10	0.16
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	3	0.16
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	19	0.16
(1,24)	1:37:A:LEU:N	1:33:A:PRO:O	2	0.16
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	6	0.16
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	3	0.16
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	11	0.16
(1,10)	1:11:A:LEU:N	1:7:A:VAL:O	18	0.16
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	1	0.16
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	5	0.16
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	16	0.16
(1,6)	1:9:A:LYS:N	1:5:A:VAL:O	2	0.16
(1,4)	1:8:A:SER:N	1:4:A:MET:O	11	0.16
(1,2)	1:7:A:VAL:N	1:3:A:HIS:O	12	0.16
(4,458)	1:50:A:MET:HE1	1:51:A:GLU:HA	2	0.15
(4,452)	1:92:A:VAL:HA	1:92:A:VAL:HG12	14	0.15
(4,448)	1:110:A:LEU:HD21	1:144:A:LEU:HG	9	0.15
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	5	0.15
(4,311)	1:143:A:VAL:HG12	1:178:A:VAL:HA	17	0.15
(4,307)	1:26:A:LEU:HD23	1:15:A:LEU:HA	13	0.15
(4,299)	1:168:A:ILE:HD12	1:152:A:ALA:HA	4	0.15
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	9	0.15
(4,259)	1:117:A:MET:HE1	2:201:A:NAD:H2A	16	0.15
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	18	0.15
(4,223)	1:13:A:LEU:HD12	1:10:A:PHE:HE1	12	0.15
(4,195)	1:114:A:ILE:HD11	1:117:A:MET:HE1	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	9	0.15
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	14	0.15
(4,61)	1:37:A:LEU:H	1:38:A:LEU:HD23	4	0.15
(4,61)	1:37:A:LEU:H	1:24:A:LEU:HD12	9	0.15
(4,37)	1:66:A:ALA:H	1:57:A:VAL:HG13	12	0.15
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	16	0.15
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	19	0.15
(4,7)	1:13:A:LEU:HD11	1:10:A:PHE:HE1	17	0.15
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD22	20	0.15
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	2	0.15
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	7	0.15
(2,3920)	1:115:A:LYS:H	2:201:A:NAD:H8A	3	0.15
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	10	0.15
(2,3884)	2:201:A:NAD:H1B	1:109:A:ILE:HD12	17	0.15
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	1	0.15
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	3	0.15
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	4	0.15
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	12	0.15
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	1	0.15
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	10	0.15
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	11	0.15
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	17	0.15
(2,3837)	1:5:A:VAL:HG22	1:5:A:VAL:HA	14	0.15
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	4	0.15
(2,3835)	1:168:A:ILE:HG23	1:168:A:ILE:HD11	13	0.15
(2,3832)	1:97:A:LEU:HD23	1:151:A:MET:HG3	1	0.15
(2,3825)	1:11:A:LEU:HD11	1:11:A:LEU:HB2	17	0.15
(2,3819)	1:151:A:MET:HE1	1:171:A:VAL:HG12	17	0.15
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	1	0.15
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	11	0.15
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	16	0.15
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	9	0.15
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	13	0.15
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	1	0.15
(2,3793)	1:53:A:LEU:HD21	1:56:A:ILE:HB	2	0.15
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	3	0.15
(2,3793)	1:53:A:LEU:HD23	1:56:A:ILE:HB	15	0.15
(2,3785)	1:142:A:VAL:HG13	1:103:A:GLU:HG2	8	0.15
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	17	0.15
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	2	0.15
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	3	0.15
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	6	0.15
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	7	0.15
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	15	0.15
(2,3770)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	2	0.15
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	5	0.15
(2,3770)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	7	0.15
(2,3770)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	9	0.15
(2,3770)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	11	0.15
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	19	0.15
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	7	0.15
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	8	0.15
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	10	0.15
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	14	0.15
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	7	0.15
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	2	0.15
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	16	0.15
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	18	0.15
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	20	0.15
(2,3679)	1:97:A:LEU:HD23	1:97:A:LEU:HA	2	0.15
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	9	0.15
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	10	0.15
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	12	0.15
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	13	0.15
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	16	0.15
(2,3575)	1:50:A:MET:HE2	1:50:A:MET:HG3	2	0.15
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	3	0.15
(2,3518)	1:128:A:ILE:HD13	1:128:A:ILE:HA	14	0.15
(2,3500)	1:144:A:LEU:HD23	1:145:A:SER:HB2	20	0.15
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	3	0.15
(2,3495)	1:82:A:VAL:HG22	1:82:A:VAL:HA	8	0.15
(2,3493)	1:142:A:VAL:HG23	1:178:A:VAL:HA	1	0.15
(2,3479)	1:151:A:MET:HE1	1:171:A:VAL:HA	2	0.15
(2,3478)	1:38:A:LEU:HD13	1:50:A:MET:HA	12	0.15
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	10	0.15
(2,3445)	1:97:A:LEU:HD21	1:166:A:TRP:HE3	6	0.15
(2,3409)	1:84:A:VAL:HG13	1:85:A:ASP:H	3	0.15
(2,3405)	1:56:A:ILE:HG21	1:57:A:VAL:H	14	0.15
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	4	0.15
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	7	0.15
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	13	0.15
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	4	0.15
(2,3288)	1:142:A:VAL:HG11	1:103:A:GLU:HA	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	3	0.15
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	15	0.15
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	5	0.15
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	7	0.15
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	9	0.15
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	16	0.15
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	7	0.15
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	13	0.15
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	14	0.15
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	19	0.15
(2,3159)	1:176:A:ILE:HG21	1:178:A:VAL:H	14	0.15
(2,3127)	1:97:A:LEU:HD13	1:124:A:LEU:HD21	11	0.15
(2,2853)	1:86:A:LEU:HD11	1:86:A:LEU:H	20	0.15
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	4	0.15
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	11	0.15
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	1	0.15
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB1	4	0.15
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	11	0.15
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	5	0.15
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	5	0.15
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	9	0.15
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	5	0.15
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	1	0.15
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	13	0.15
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	9	0.15
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	16	0.15
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	20	0.15
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	2	0.15
(2,2367)	1:48:A:ILE:HG23	1:48:A:ILE:H	6	0.15
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	19	0.15
(2,2296)	1:37:A:LEU:H	1:24:A:LEU:HD12	17	0.15
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	9	0.15
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD21	14	0.15
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	6	0.15
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	8	0.15
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	10	0.15
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	13	0.15
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	14	0.15
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	17	0.15
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	18	0.15
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	19	0.15
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	16	0.15
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	20	0.15
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	18	0.15
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	8	0.15
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	18	0.15
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	5	0.15
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	9	0.15
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	12	0.15
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	16	0.15
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	1	0.15
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	5	0.15
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	17	0.15
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	20	0.15
(2,1973)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	7	0.15
(2,1973)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	11	0.15
(2,1973)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	18	0.15
(2,1973)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	20	0.15
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	8	0.15
(2,1962)	1:110:A:LEU:HD13	1:106:A:PHE:HE1	9	0.15
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	17	0.15
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	20	0.15
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	1	0.15
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	8	0.15
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	9	0.15
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	12	0.15
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	15	0.15
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	16	0.15
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	16	0.15
(2,1809)	1:34:A:VAL:HG13	1:37:A:LEU:HB3	1	0.15
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	14	0.15
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	14	0.15
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	17	0.15
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	1	0.15
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	4	0.15
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	12	0.15
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	11	0.15
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	17	0.15
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	19	0.15
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	20	0.15
(2,1745)	1:34:A:VAL:HA	1:37:A:LEU:HD21	17	0.15
(2,1741)	1:173:A:ALA:HA	1:176:A:ILE:HD11	1	0.15
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1633)	1:42:A:LYS:HE2	1:39:A:ALA:HA	13	0.15
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	9	0.15
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	10	0.15
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE3	13	0.15
(2,1599)	1:4:A:MET:HE1	1:52:A:GLU:HA	3	0.15
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	3	0.15
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	16	0.15
(2,1455)	1:165:A:VAL:HG23	2:201:A:NAD:H5N	15	0.15
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	8	0.15
(2,1410)	1:95:A:ALA:HB2	1:96:A:VAL:H	12	0.15
(2,1410)	1:95:A:ALA:HB3	1:96:A:VAL:H	19	0.15
(2,1399)	1:86:A:LEU:HG	1:86:A:LEU:H	1	0.15
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	13	0.15
(2,1301)	1:34:A:VAL:HG11	1:38:A:LEU:H	5	0.15
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	11	0.15
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	2	0.15
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	3	0.15
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	4	0.15
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	13	0.15
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	19	0.15
(2,1274)	1:160:A:LEU:HD22	1:91:A:GLN:HE22	6	0.15
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	2	0.15
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	10	0.15
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	16	0.15
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	19	0.15
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	4	0.15
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	9	0.15
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	19	0.15
(2,1218)	1:177:A:LYS:HG2	1:177:A:LYS:HA	7	0.15
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	1	0.15
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	4	0.15
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	15	0.15
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	16	0.15
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	17	0.15
(2,1194)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	18	0.15
(2,1075)	1:56:A:ILE:H	1:58:A:GLU:H	17	0.15
(2,1066)	1:161:A:SER:H	2:201:A:NAD:H6N	12	0.15
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	2	0.15
(2,1021)	1:37:A:LEU:H	1:34:A:VAL:H	4	0.15
(2,1014)	1:160:A:LEU:H	1:89:A:GLU:H	3	0.15
(2,1012)	1:40:A:LYS:H	1:39:A:ALA:H	15	0.15
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	4	0.15
(2,969)	1:23:A:GLY:H	1:22:A:ILE:H	20	0.15
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	17	0.15
(2,908)	1:96:A:VAL:H	1:97:A:LEU:H	14	0.15
(2,810)	1:22:A:ILE:H	1:37:A:LEU:HD12	19	0.15
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	13	0.15
(2,708)	1:113:A:GLY:H	1:109:A:ILE:HG21	20	0.15
(2,681)	1:78:A:GLN:HE21	1:76:A:ALA:HA	1	0.15
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	2	0.15
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	6	0.15
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	3	0.15
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB1	10	0.15
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB1	13	0.15
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	14	0.15
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB3	17	0.15
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	9	0.15
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	10	0.15
(2,546)	1:114:A:ILE:HD11	1:114:A:ILE:H	17	0.15
(2,453)	1:34:A:VAL:HB	1:35:A:LYS:H	15	0.15
(2,445)	1:36:A:GLU:H	1:36:A:GLU:HB3	13	0.15
(2,431)	1:73:A:LYS:H	1:34:A:VAL:HG21	14	0.15
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	12	0.15
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	14	0.15
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	6	0.15
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	8	0.15
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	12	0.15
(2,268)	1:14:A:VAL:HG23	1:21:A:LEU:H	6	0.15
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	7	0.15
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	14	0.15
(2,198)	1:20:A:ALA:HA	1:24:A:LEU:H	20	0.15
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	12	0.15
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	1	0.15
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	6	0.15
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	18	0.15
(2,138)	1:83:A:GLU:H	1:85:A:ASP:H	19	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	3	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	4	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	5	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	6	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	7	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	9	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	15	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	16	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	17	0.15
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	19	0.15
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	9	0.15
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	5	0.15
(2,85)	1:152:A:ALA:HB2	1:152:A:ALA:H	8	0.15
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	16	0.15
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	18	0.15
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	9	0.15
(1,119)	1:171:A:VAL:H	1:114:A:ILE:O	20	0.15
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	10	0.15
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	15	0.15
(1,110)	1:153:A:ASP:N	1:149:A:LYS:O	13	0.15
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	18	0.15
(1,102)	1:144:A:LEU:N	1:99:A:HIS:O	2	0.15
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	9	0.15
(1,77)	1:112:A:ASP:H	1:108:A:LEU:O	10	0.15
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	18	0.15
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	19	0.15
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	7	0.15
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	12	0.15
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	16	0.15
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	18	0.15
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	3	0.15
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	14	0.15
(1,55)	1:74:A:ILE:H	1:32:A:ALA:O	18	0.15
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	5	0.15
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	15	0.15
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	7	0.15
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	10	0.15
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	2	0.15
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	6	0.15
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	15	0.15
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	18	0.15
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	6	0.15
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	9	0.15
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	17	0.15
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	19	0.15
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	1	0.15
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	20	0.15
(1,22)	1:32:A:ALA:N	1:74:A:ILE:O	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	4	0.15
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	16	0.15
(1,17)	1:15:A:LEU:H	1:11:A:LEU:O	20	0.15
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	19	0.15
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	10	0.15
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	15	0.15
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	9	0.15
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	13	0.15
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	18	0.14
(4,425)	1:34:A:VAL:HG21	1:35:A:LYS:HB2	12	0.14
(4,392)	1:8:A:SER:HB2	1:7:A:VAL:HB	1	0.14
(4,388)	1:107:A:ASP:HA	1:110:A:LEU:HD23	12	0.14
(4,307)	1:26:A:LEU:HD23	1:15:A:LEU:HA	4	0.14
(4,300)	1:97:A:LEU:HD23	1:156:A:PHE:HB3	20	0.14
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	11	0.14
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HZ	8	0.14
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	9	0.14
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	19	0.14
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	17	0.14
(4,61)	1:37:A:LEU:H	1:24:A:LEU:HD12	6	0.14
(4,59)	1:40:A:LYS:H	1:44:A:LYS:HE2	7	0.14
(4,41)	1:5:A:VAL:HG21	1:5:A:VAL:H	9	0.14
(4,41)	1:5:A:VAL:HG23	1:5:A:VAL:H	12	0.14
(4,25)	1:75:A:ARG:H	1:74:A:ILE:HG12	8	0.14
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	4	0.14
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	11	0.14
(2,3940)	1:134:A:VAL:HG11	2:201:A:NAD:H2N	19	0.14
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	16	0.14
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	20	0.14
(2,3918)	1:114:A:ILE:HD11	2:201:A:NAD:H8A	6	0.14
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	6	0.14
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	15	0.14
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	2	0.14
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	4	0.14
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	7	0.14
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	12	0.14
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	20	0.14
(2,3837)	1:5:A:VAL:HG23	1:5:A:VAL:HA	1	0.14
(2,3828)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	19	0.14
(2,3819)	1:151:A:MET:HE3	1:171:A:VAL:HG12	12	0.14
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD13	6	0.14
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3812)	1:56:A:ILE:HG21	1:11:A:LEU:HD11	9	0.14
(2,3811)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	1	0.14
(2,3809)	1:110:A:LEU:HD12	1:176:A:ILE:HB	18	0.14
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	10	0.14
(2,3802)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	18	0.14
(2,3802)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	20	0.14
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	16	0.14
(2,3794)	1:14:A:VAL:HG22	1:14:A:VAL:HB	13	0.14
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	19	0.14
(2,3770)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	8	0.14
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	10	0.14
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	3	0.14
(2,3763)	1:76:A:ALA:HB1	1:15:A:LEU:HD11	7	0.14
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	11	0.14
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	13	0.14
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	18	0.14
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	19	0.14
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	5	0.14
(2,3707)	1:11:A:LEU:HA	1:37:A:LEU:HD21	5	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	1	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	4	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	5	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	8	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	9	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	11	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	12	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	13	0.14
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	14	0.14
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	5	0.14
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	18	0.14
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	19	0.14
(2,3575)	1:50:A:MET:HE1	1:50:A:MET:HG3	4	0.14
(2,3575)	1:50:A:MET:HE3	1:50:A:MET:HG3	18	0.14
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	8	0.14
(2,3519)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	16	0.14
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	19	0.14
(2,3518)	1:128:A:ILE:HD12	1:128:A:ILE:HA	7	0.14
(2,3518)	1:128:A:ILE:HD11	1:128:A:ILE:HA	15	0.14
(2,3510)	1:144:A:LEU:HD23	1:106:A:PHE:HB2	12	0.14
(2,3509)	1:13:A:LEU:HD21	1:17:A:HIS:HB2	4	0.14
(2,3483)	1:26:A:LEU:HD13	1:32:A:ALA:HA	13	0.14
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3434)	1:15:A:LEU:HD12	1:65:A:PHE:HE1	2	0.14
(2,3434)	1:15:A:LEU:HD12	1:65:A:PHE:HE1	14	0.14
(2,3424)	1:165:A:VAL:HG23	2:201:A:NAD:H5N	19	0.14
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	5	0.14
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	7	0.14
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	8	0.14
(2,3405)	1:56:A:ILE:HG23	1:57:A:VAL:H	9	0.14
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	12	0.14
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	16	0.14
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	20	0.14
(2,3390)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	5	0.14
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	5	0.14
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	17	0.14
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	18	0.14
(2,3370)	1:152:A:ALA:HB3	1:158:A:PHE:HD1	14	0.14
(2,3362)	1:39:A:ALA:HB2	1:40:A:LYS:H	20	0.14
(2,3355)	1:41:A:MET:HE2	1:41:A:MET:H	16	0.14
(2,3345)	1:41:A:MET:HE1	1:10:A:PHE:HE1	9	0.14
(2,3288)	1:142:A:VAL:HG13	1:103:A:GLU:HA	15	0.14
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	16	0.14
(2,3248)	1:160:A:LEU:HD22	1:91:A:GLN:HE22	6	0.14
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	13	0.14
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD21	14	0.14
(2,3102)	1:136:A:MET:H	1:105:A:ASN:HD22	2	0.14
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	1	0.14
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	9	0.14
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	15	0.14
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	16	0.14
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	18	0.14
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	19	0.14
(2,2949)	1:165:A:VAL:H	1:91:A:GLN:HE22	8	0.14
(2,2887)	1:176:A:ILE:H	1:146:A:VAL:HG11	9	0.14
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	9	0.14
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	13	0.14
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	6	0.14
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	18	0.14
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	3	0.14
(2,2651)	1:78:A:GLN:HG3	1:78:A:GLN:HE22	1	0.14
(2,2651)	1:78:A:GLN:HG3	1:78:A:GLN:HE22	11	0.14
(2,2649)	1:70:A:ASN:HD22	1:50:A:MET:HB2	15	0.14
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	1	0.14
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	9	0.14
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	12	0.14
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	14	0.14
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	1	0.14
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	4	0.14
(2,2566)	1:43:A:ALA:HB3	1:44:A:LYS:H	15	0.14
(2,2521)	1:102:A:ALA:HB1	1:105:A:ASN:H	6	0.14
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	13	0.14
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	5	0.14
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	2	0.14
(2,2234)	1:14:A:VAL:HG23	1:21:A:LEU:H	18	0.14
(2,2216)	1:26:A:LEU:HD11	1:27:A:ASP:H	20	0.14
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	13	0.14
(2,2175)	1:57:A:VAL:HG21	1:66:A:ALA:H	8	0.14
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD22	4	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	4	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	5	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	7	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	9	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	12	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	15	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	16	0.14
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	20	0.14
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	7	0.14
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	2	0.14
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	3	0.14
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	5	0.14
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	9	0.14
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	17	0.14
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	10	0.14
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	3	0.14
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	12	0.14
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	19	0.14
(2,2106)	1:84:A:VAL:HB	1:85:A:ASP:H	5	0.14
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	2	0.14
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	2	0.14
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	15	0.14
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	2	0.14
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	15	0.14
(2,1973)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	8	0.14
(2,1973)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	9	0.14
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	19	0.14
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	2	0.14
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG23	15	0.14
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG23	16	0.14
(2,1860)	1:57:A:VAL:HG21	1:57:A:VAL:HB	4	0.14
(2,1860)	1:57:A:VAL:HG21	1:57:A:VAL:HB	18	0.14
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	4	0.14
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	6	0.14
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD12	9	0.14
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	2	0.14
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	9	0.14
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	10	0.14
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	14	0.14
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	15	0.14
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	16	0.14
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	17	0.14
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	2	0.14
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	14	0.14
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	2	0.14
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	3	0.14
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	6	0.14
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	15	0.14
(2,1805)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	4	0.14
(2,1805)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	6	0.14
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	15	0.14
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	18	0.14
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD12	5	0.14
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	10	0.14
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	20	0.14
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD22	5	0.14
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	11	0.14
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	17	0.14
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	5	0.14
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	6	0.14
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	7	0.14
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	11	0.14
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	12	0.14
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG23	17	0.14
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	3	0.14
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	5	0.14
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	6	0.14
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	14	0.14
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	17	0.14
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	20	0.14
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	9	0.14
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	10	0.14
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	13	0.14
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	14	0.14
(2,1723)	1:38:A:LEU:HD13	1:50:A:MET:HA	5	0.14
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	5	0.14
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	10	0.14
(2,1710)	1:26:A:LEU:HD23	1:15:A:LEU:HA	7	0.14
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	17	0.14
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	5	0.14
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	12	0.14
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	13	0.14
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	16	0.14
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	19	0.14
(2,1599)	1:4:A:MET:HE1	1:52:A:GLU:HA	6	0.14
(2,1599)	1:4:A:MET:HE1	1:52:A:GLU:HA	13	0.14
(2,1590)	1:32:A:ALA:HB2	1:33:A:PRO:HD3	18	0.14
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	4	0.14
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	11	0.14
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	20	0.14
(2,1514)	1:124:A:LEU:HD11	1:167:A:LEU:HA	4	0.14
(2,1509)	1:151:A:MET:HE1	1:171:A:VAL:HA	1	0.14
(2,1474)	1:110:A:LEU:HD23	1:110:A:LEU:H	6	0.14
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	7	0.14
(2,1474)	1:110:A:LEU:HD21	1:110:A:LEU:H	13	0.14
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	9	0.14
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	4	0.14
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	10	0.14
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	15	0.14
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	17	0.14
(2,1425)	1:56:A:ILE:HG22	1:65:A:PHE:HD1	20	0.14
(2,1420)	1:22:A:ILE:HG23	1:10:A:PHE:HE1	2	0.14
(2,1399)	1:86:A:LEU:HG	1:86:A:LEU:H	6	0.14
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	11	0.14
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	18	0.14
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	5	0.14
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	18	0.14
(2,1283)	1:117:A:MET:HE2	2:201:A:NAD:H2A	4	0.14
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	3	0.14
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	8	0.14
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	15	0.14
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	8	0.14
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	10	0.14
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	11	0.14
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	14	0.14
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	15	0.14
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	16	0.14
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	17	0.14
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	11	0.14
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	5	0.14
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	12	0.14
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	14	0.14
(2,1158)	1:165:A:VAL:HG21	1:165:A:VAL:H	18	0.14
(2,1158)	1:165:A:VAL:HG21	1:165:A:VAL:H	19	0.14
(2,1104)	1:18:A:ASN:H	1:27:A:ASP:H	17	0.14
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	11	0.14
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	17	0.14
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	3	0.14
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	13	0.14
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	15	0.14
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	20	0.14
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	7	0.14
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	13	0.14
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	7	0.14
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	11	0.14
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	14	0.14
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	18	0.14
(2,723)	1:20:A:ALA:HA	1:23:A:GLY:H	1	0.14
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	7	0.14
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	17	0.14
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	1	0.14
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	2	0.14
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	3	0.14
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	15	0.14
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	16	0.14
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG11	1	0.14
(2,431)	1:73:A:LYS:H	1:34:A:VAL:HG21	7	0.14
(2,431)	1:73:A:LYS:H	1:34:A:VAL:HG21	15	0.14
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	19	0.14
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	5	0.14
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	16	0.14
(2,297)	1:50:A:MET:H	1:50:A:MET:HB3	4	0.14
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	8	0.14
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	17	0.14
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	13	0.14
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	17	0.14
(2,205)	1:76:A:ALA:H	1:15:A:LEU:HB2	15	0.14
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	7	0.14
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	11	0.14
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	19	0.14
(2,187)	1:26:A:LEU:HD21	1:26:A:LEU:H	6	0.14
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	16	0.14
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	5	0.14
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	4	0.14
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	12	0.14
(2,134)	1:32:A:ALA:H	1:26:A:LEU:HD13	7	0.14
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	1	0.14
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	2	0.14
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	8	0.14
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	10	0.14
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	13	0.14
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	14	0.14
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	18	0.14
(2,129)	1:173:A:ALA:HA	1:173:A:ALA:H	20	0.14
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	6	0.14
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	12	0.14
(2,62)	1:178:A:VAL:H	1:177:A:LYS:H	11	0.14
(2,19)	1:13:A:LEU:HA	1:17:A:HIS:HD2	12	0.14
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	8	0.14
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	7	0.14
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	10	0.14
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	13	0.14
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	18	0.14
(1,118)	1:168:A:ILE:N	1:122:A:VAL:O	18	0.14
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	20	0.14
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	2	0.14
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	14	0.14
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	6	0.14
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	4	0.14
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	9	0.14
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	14	0.14
(1,55)	1:74:A:ILE:H	1:32:A:ALA:O	17	0.14
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	9	0.14
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	16	0.14
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	19	0.14
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	19	0.14
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	2	0.14
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	4	0.14
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	15	0.14
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	19	0.14
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	11	0.14
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	13	0.14
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	17	0.14
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	20	0.14
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	6	0.14
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	10	0.14
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	18	0.14
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	13	0.14
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	14	0.14
(1,4)	1:8:A:SER:N	1:4:A:MET:O	14	0.14
(1,4)	1:8:A:SER:N	1:4:A:MET:O	17	0.14
(1,1)	1:7:A:VAL:H	1:3:A:HIS:O	7	0.14
(4,459)	1:94:A:PRO:HA	1:151:A:MET:HB2	6	0.13
(4,443)	1:48:A:ILE:HD12	1:38:A:LEU:HB2	17	0.13
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	14	0.13
(4,442)	1:178:A:VAL:HG21	1:144:A:LEU:HG	19	0.13
(4,436)	1:34:A:VAL:HG12	1:35:A:LYS:HG3	15	0.13
(4,379)	1:50:A:MET:HA	1:39:A:ALA:HB3	1	0.13
(4,353)	1:143:A:VAL:HB	1:131:A:ALA:HA	2	0.13
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	8	0.13
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HE1	6	0.13
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HZ	9	0.13
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HZ	15	0.13
(4,259)	1:117:A:MET:HE3	2:201:A:NAD:H2A	18	0.13
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	6	0.13
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	8	0.13
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	12	0.13
(4,213)	1:165:A:VAL:HB	1:123:A:HIS:HA	16	0.13
(4,198)	1:176:A:ILE:HD13	1:106:A:PHE:HE1	11	0.13
(4,173)	1:52:A:GLU:H	1:58:A:GLU:H	13	0.13
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	18	0.13
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,65)	1:7:A:VAL:H	1:7:A:VAL:HB	1	0.13
(4,65)	1:7:A:VAL:H	1:7:A:VAL:HB	8	0.13
(4,41)	1:5:A:VAL:HG22	1:5:A:VAL:H	1	0.13
(4,41)	1:5:A:VAL:HG22	1:5:A:VAL:H	8	0.13
(4,41)	1:5:A:VAL:HG22	1:5:A:VAL:H	16	0.13
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD22	9	0.13
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	12	0.13
(3,20)	1:163:A:ASN:OD1	2:201:A:NAD:H71N	2	0.13
(2,3947)	1:165:A:VAL:HG21	2:201:A:NAD:H4N	18	0.13
(2,3937)	1:105:A:ASN:HD21	2:201:A:NAD:HO2A	20	0.13
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	15	0.13
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	17	0.13
(2,3918)	1:114:A:ILE:HD11	2:201:A:NAD:H8A	19	0.13
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	8	0.13
(2,3896)	2:201:A:NAD:H3D	2:201:A:NAD:H2N	10	0.13
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	17	0.13
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	3	0.13
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	3	0.13
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	13	0.13
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	15	0.13
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	19	0.13
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	7	0.13
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG23	15	0.13
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG23	16	0.13
(2,3837)	1:5:A:VAL:HG21	1:5:A:VAL:HA	12	0.13
(2,3826)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	20	0.13
(2,3825)	1:11:A:LEU:HD13	1:11:A:LEU:HB2	10	0.13
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	2	0.13
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	3	0.13
(2,3802)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	2	0.13
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	12	0.13
(2,3802)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	14	0.13
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	4	0.13
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	10	0.13
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	10	0.13
(2,3773)	1:34:A:VAL:HG13	1:37:A:LEU:HB3	18	0.13
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	14	0.13
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	16	0.13
(2,3770)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	17	0.13
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	6	0.13
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	15	0.13
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	11	0.13
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	15	0.13
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	16	0.13
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	8	0.13
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	14	0.13
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	17	0.13
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	20	0.13
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	7	0.13
(2,3575)	1:50:A:MET:HE1	1:50:A:MET:HG3	6	0.13
(2,3575)	1:50:A:MET:HE1	1:50:A:MET:HG3	10	0.13
(2,3570)	1:4:A:MET:HE1	1:52:A:GLU:HA	9	0.13
(2,3478)	1:38:A:LEU:HD13	1:50:A:MET:HA	5	0.13
(2,3474)	1:146:A:VAL:HG13	1:96:A:VAL:HA	16	0.13
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	1	0.13
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	6	0.13
(2,3468)	1:110:A:LEU:HD12	1:110:A:LEU:HA	1	0.13
(2,3459)	1:167:A:LEU:HD23	1:123:A:HIS:HA	9	0.13
(2,3409)	1:84:A:VAL:HG11	1:85:A:ASP:H	14	0.13
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	13	0.13
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	17	0.13
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	19	0.13
(2,3390)	1:56:A:ILE:HG21	1:65:A:PHE:HE1	14	0.13
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	1	0.13
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	6	0.13
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	11	0.13
(2,3362)	1:39:A:ALA:HB2	1:40:A:LYS:H	15	0.13
(2,3335)	1:16:A:ARG:HD2	1:12:A:SER:H	4	0.13
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	3	0.13
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	5	0.13
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	12	0.13
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	15	0.13
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	2	0.13
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	9	0.13
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	6	0.13
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	15	0.13
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	17	0.13
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	19	0.13
(2,3211)	1:151:A:MET:HE3	1:156:A:PHE:HZ	5	0.13
(2,3180)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	8	0.13
(2,3102)	1:136:A:MET:H	1:105:A:ASN:HD22	3	0.13
(2,3036)	1:161:A:SER:H	2:201:A:NAD:H6N	14	0.13
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	10	0.13
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	11	0.13
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	14	0.13
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	7	0.13
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	4	0.13
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	9	0.13
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	11	0.13
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	16	0.13
(2,2722)	1:139:A:GLY:H	1:103:A:GLU:HA	13	0.13
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	8	0.13
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	18	0.13
(2,2651)	1:78:A:GLN:HG3	1:78:A:GLN:HE22	3	0.13
(2,2651)	1:78:A:GLN:HG3	1:78:A:GLN:HE22	10	0.13
(2,2651)	1:78:A:GLN:HG3	1:78:A:GLN:HE22	12	0.13
(2,2651)	1:78:A:GLN:HG3	1:78:A:GLN:HE22	14	0.13
(2,2649)	1:70:A:ASN:HD22	1:50:A:MET:HB2	11	0.13
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	5	0.13
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	20	0.13
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	16	0.13
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	17	0.13
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	5	0.13
(2,2566)	1:43:A:ALA:HB1	1:44:A:LYS:H	12	0.13
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	18	0.13
(2,2566)	1:43:A:ALA:HB3	1:44:A:LYS:H	19	0.13
(2,2550)	1:86:A:LEU:H	1:88:A:TYR:H	7	0.13
(2,2506)	1:64:A:ARG:H	1:76:A:ALA:HB1	4	0.13
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	6	0.13
(2,2367)	1:48:A:ILE:HG21	1:48:A:ILE:H	14	0.13
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	5	0.13
(2,2268)	1:83:A:GLU:HA	1:84:A:VAL:H	2	0.13
(2,2232)	1:21:A:LEU:H	1:24:A:LEU:HD21	12	0.13
(2,2210)	1:48:A:ILE:HD12	1:53:A:LEU:H	14	0.13
(2,2210)	1:48:A:ILE:HD11	1:53:A:LEU:H	18	0.13
(2,2210)	1:48:A:ILE:HD12	1:53:A:LEU:H	19	0.13
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	5	0.13
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	7	0.13
(2,2175)	1:57:A:VAL:HG21	1:66:A:ALA:H	19	0.13
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	1	0.13
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	2	0.13
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	11	0.13
(2,2151)	1:13:A:LEU:H	1:13:A:LEU:HB3	12	0.13
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	12	0.13
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	13	0.13
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	17	0.13
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	19	0.13
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	9	0.13
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	1	0.13
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	8	0.13
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	10	0.13
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	19	0.13
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	3	0.13
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	12	0.13
(2,2010)	1:34:A:VAL:H	1:73:A:LYS:HA	6	0.13
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	12	0.13
(2,1962)	1:110:A:LEU:HD11	1:106:A:PHE:HE1	16	0.13
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	6	0.13
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	9	0.13
(2,1934)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	16	0.13
(2,1932)	2:201:A:NAD:H3D	2:201:A:NAD:H2N	10	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	1	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	2	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	3	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	5	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	9	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	10	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	12	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	15	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	16	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	18	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	19	0.13
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	20	0.13
(2,1880)	1:76:A:ALA:HB1	1:16:A:ARG:HA	5	0.13
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	7	0.13
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	13	0.13
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	18	0.13
(2,1867)	1:109:A:ILE:HD11	1:101:A:THR:HG23	12	0.13
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	3	0.13
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	10	0.13
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	15	0.13
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	2	0.13
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	5	0.13
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG22	13	0.13
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG21	19	0.13
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	19	0.13
(2,1842)	1:11:A:LEU:HD22	1:11:A:LEU:HB2	2	0.13
(2,1842)	1:11:A:LEU:HD22	1:11:A:LEU:HB2	20	0.13
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	6	0.13
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	7	0.13
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	8	0.13
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	18	0.13
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	19	0.13
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG23	3	0.13
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	11	0.13
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	4	0.13
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	7	0.13
(2,1805)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	2	0.13
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	5	0.13
(2,1805)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	7	0.13
(2,1805)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	9	0.13
(2,1805)	1:21:A:LEU:HD23	1:21:A:LEU:HB3	11	0.13
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	19	0.13
(2,1798)	1:34:A:VAL:HG22	1:74:A:ILE:HD12	18	0.13
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD12	3	0.13
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD12	4	0.13
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	11	0.13
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	12	0.13
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD12	16	0.13
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD21	18	0.13
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	9	0.13
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	16	0.13
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	20	0.13
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	2	0.13
(2,1752)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	13	0.13
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	5	0.13
(2,1745)	1:34:A:VAL:HA	1:37:A:LEU:HD21	15	0.13
(2,1723)	1:38:A:LEU:HD13	1:50:A:MET:HA	13	0.13
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	1	0.13
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	12	0.13
(2,1640)	1:40:A:LYS:HE2	1:25:A:ASP:HB2	20	0.13
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	18	0.13
(2,1599)	1:4:A:MET:HE2	1:52:A:GLU:HA	11	0.13
(2,1590)	1:32:A:ALA:HB2	1:33:A:PRO:HD3	15	0.13
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	7	0.13
(2,1511)	1:82:A:VAL:HG21	1:80:A:HIS:HA	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1482)	1:11:A:LEU:HD12	1:11:A:LEU:H	12	0.13
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	19	0.13
(2,1455)	1:165:A:VAL:HG23	2:201:A:NAD:H5N	19	0.13
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	2	0.13
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	5	0.13
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	10	0.13
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	16	0.13
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	19	0.13
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	15	0.13
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	1	0.13
(2,1279)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	5	0.13
(2,1276)	1:160:A:LEU:HD21	1:166:A:TRP:HE1	17	0.13
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	5	0.13
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	4	0.13
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	20	0.13
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	2	0.13
(2,1258)	1:14:A:VAL:HG12	1:14:A:VAL:H	7	0.13
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	2	0.13
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	11	0.13
(2,1255)	1:176:A:ILE:HD11	1:173:A:ALA:HB3	12	0.13
(2,1158)	1:165:A:VAL:HG21	1:165:A:VAL:H	15	0.13
(2,1110)	1:76:A:ALA:H	1:75:A:ARG:H	16	0.13
(2,1099)	1:100:A:GLY:H	1:166:A:TRP:H	7	0.13
(2,1071)	1:86:A:LEU:H	1:88:A:TYR:H	9	0.13
(2,1026)	1:84:A:VAL:H	1:85:A:ASP:H	5	0.13
(2,1025)	1:84:A:VAL:H	1:83:A:GLU:H	3	0.13
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	18	0.13
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	9	0.13
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	11	0.13
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	17	0.13
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	19	0.13
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	11	0.13
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	15	0.13
(2,948)	1:76:A:ALA:HB3	1:78:A:GLN:HE22	14	0.13
(2,904)	1:92:A:VAL:H	1:92:A:VAL:HA	13	0.13
(2,867)	1:78:A:GLN:HE22	1:76:A:ALA:HA	3	0.13
(2,815)	1:101:A:THR:HG21	1:102:A:ALA:H	8	0.13
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	8	0.13
(2,723)	1:20:A:ALA:HA	1:23:A:GLY:H	3	0.13
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	8	0.13
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	10	0.13
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	11	0.13
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	12	0.13
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	15	0.13
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	20	0.13
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	7	0.13
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	8	0.13
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	14	0.13
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	16	0.13
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	18	0.13
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	20	0.13
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	10	0.13
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	1	0.13
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	11	0.13
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	12	0.13
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	14	0.13
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	18	0.13
(2,537)	1:38:A:LEU:H	1:53:A:LEU:HD11	15	0.13
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	17	0.13
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	4	0.13
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	17	0.13
(2,431)	1:73:A:LYS:H	1:34:A:VAL:HG21	4	0.13
(2,431)	1:73:A:LYS:H	1:34:A:VAL:HG21	11	0.13
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	17	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	3	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	7	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	9	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	10	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	11	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	13	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	14	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	15	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	17	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	18	0.13
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	19	0.13
(2,224)	1:81:A:SER:HA	1:82:A:VAL:H	4	0.13
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	4	0.13
(2,198)	1:20:A:ALA:HA	1:24:A:LEU:H	3	0.13
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	4	0.13
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	5	0.13
(2,196)	1:24:A:LEU:H	1:19:A:PRO:HA	12	0.13
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	11	0.13
(2,154)	1:97:A:LEU:H	1:96:A:VAL:HB	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	3	0.13
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	7	0.13
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	10	0.13
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	11	0.13
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	15	0.13
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	20	0.13
(2,54)	1:34:A:VAL:H	1:74:A:ILE:HG22	5	0.13
(2,54)	1:34:A:VAL:H	1:74:A:ILE:HG22	15	0.13
(2,43)	1:96:A:VAL:HG21	1:148:A:ALA:H	15	0.13
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	20	0.13
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	6	0.13
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	13	0.13
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	8	0.13
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	4	0.13
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	11	0.13
(1,115)	1:167:A:LEU:H	1:159:A:TYR:O	20	0.13
(1,104)	1:147:A:ASP:N	1:175:A:PHE:O	8	0.13
(1,97)	1:136:A:MET:H	1:132:A:ARG:O	4	0.13
(1,91)	1:133:A:LYS:H	1:129:A:THR:O	6	0.13
(1,89)	1:132:A:ARG:H	1:128:A:ILE:O	11	0.13
(1,88)	1:131:A:ALA:N	1:127:A:ASP:O	14	0.13
(1,88)	1:131:A:ALA:N	1:127:A:ASP:O	20	0.13
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	8	0.13
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	4	0.13
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	12	0.13
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	17	0.13
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	2	0.13
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	6	0.13
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	11	0.13
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	12	0.13
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	15	0.13
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	12	0.13
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	1	0.13
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	16	0.13
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	2	0.13
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	11	0.13
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	15	0.13
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	5	0.13
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	7	0.13
(1,24)	1:37:A:LEU:N	1:33:A:PRO:O	1	0.13
(1,24)	1:37:A:LEU:N	1:33:A:PRO:O	18	0.13
(1,9)	1:11:A:LEU:H	1:7:A:VAL:O	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:11:A:LEU:H	1:7:A:VAL:O	7	0.13
(1,9)	1:11:A:LEU:H	1:7:A:VAL:O	14	0.13
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	17	0.13
(1,2)	1:7:A:VAL:N	1:3:A:HIS:O	1	0.13
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	8	0.12
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	13	0.12
(4,319)	1:26:A:LEU:HD21	1:14:A:VAL:HA	16	0.12
(4,311)	1:143:A:VAL:HG13	1:178:A:VAL:HA	1	0.12
(4,307)	1:26:A:LEU:HD22	1:15:A:LEU:HA	3	0.12
(4,257)	1:66:A:ALA:HB2	1:66:A:ALA:H	10	0.12
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	2	0.12
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	16	0.12
(4,209)	1:76:A:ALA:HB3	1:16:A:ARG:H	10	0.12
(4,204)	1:173:A:ALA:HB3	1:111:A:LYS:HG3	10	0.12
(4,198)	1:176:A:ILE:HD13	1:106:A:PHE:HE1	6	0.12
(4,198)	1:176:A:ILE:HD11	1:106:A:PHE:HE1	18	0.12
(4,126)	1:21:A:LEU:HD13	1:14:A:VAL:H	5	0.12
(4,121)	1:111:A:LYS:H	1:110:A:LEU:HB2	6	0.12
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	4	0.12
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	11	0.12
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	12	0.12
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	13	0.12
(4,69)	1:37:A:LEU:H	1:53:A:LEU:HD11	20	0.12
(4,65)	1:6:A:LYS:HB3	1:7:A:VAL:H	14	0.12
(4,61)	1:37:A:LEU:H	1:38:A:LEU:HD23	15	0.12
(4,61)	1:37:A:LEU:H	1:38:A:LEU:HD23	18	0.12
(4,41)	1:5:A:VAL:HG22	1:5:A:VAL:H	3	0.12
(4,41)	1:5:A:VAL:HG21	1:5:A:VAL:H	7	0.12
(4,41)	1:5:A:VAL:HG23	1:5:A:VAL:H	10	0.12
(4,41)	1:5:A:VAL:HG22	1:5:A:VAL:H	17	0.12
(4,1)	1:67:A:PHE:HD1	1:37:A:LEU:HD21	8	0.12
(2,3959)	1:123:A:HIS:HB3	2:201:A:NAD:H5N	12	0.12
(2,3947)	1:165:A:VAL:HG21	2:201:A:NAD:H4N	15	0.12
(2,3940)	1:134:A:VAL:HG11	2:201:A:NAD:H2N	9	0.12
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	4	0.12
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	8	0.12
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	9	0.12
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	10	0.12
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	19	0.12
(2,3924)	1:109:A:ILE:HD11	2:201:A:NAD:H2A	3	0.12
(2,3924)	1:109:A:ILE:HD11	2:201:A:NAD:H2A	6	0.12
(2,3924)	1:109:A:ILE:HD11	2:201:A:NAD:H2A	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3920)	1:115:A:LYS:H	2:201:A:NAD:H8A	1	0.12
(2,3884)	2:201:A:NAD:H1B	1:109:A:ILE:HD12	20	0.12
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	10	0.12
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	13	0.12
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	18	0.12
(2,3861)	1:24:A:LEU:HG	1:24:A:LEU:HA	1	0.12
(2,3842)	1:34:A:VAL:HG21	1:74:A:ILE:H	4	0.12
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	1	0.12
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	8	0.12
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	9	0.12
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	13	0.12
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	18	0.12
(2,3837)	1:5:A:VAL:HG23	1:5:A:VAL:HA	8	0.12
(2,3825)	1:11:A:LEU:HD11	1:11:A:LEU:HB2	8	0.12
(2,3825)	1:11:A:LEU:HD11	1:11:A:LEU:HB2	12	0.12
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	2	0.12
(2,3810)	1:171:A:VAL:HG22	1:168:A:ILE:HD13	9	0.12
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	8	0.12
(2,3802)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	13	0.12
(2,3796)	1:14:A:VAL:HG11	1:11:A:LEU:HG	17	0.12
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	19	0.12
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	20	0.12
(2,3789)	1:22:A:ILE:HG22	1:44:A:LYS:HB3	4	0.12
(2,3775)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	12	0.12
(2,3775)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	17	0.12
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	6	0.12
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	9	0.12
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	11	0.12
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	12	0.12
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	15	0.12
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	18	0.12
(2,3770)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	12	0.12
(2,3770)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	13	0.12
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	9	0.12
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	11	0.12
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	19	0.12
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	4	0.12
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	9	0.12
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	12	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	2	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	3	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	11	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	12	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	13	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	15	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	16	0.12
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	19	0.12
(2,3690)	1:24:A:LEU:HA	1:24:A:LEU:HD13	3	0.12
(2,3688)	1:96:A:VAL:HG11	1:94:A:PRO:HA	18	0.12
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	1	0.12
(2,3594)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	17	0.12
(2,3575)	1:50:A:MET:HE1	1:50:A:MET:HG3	1	0.12
(2,3575)	1:50:A:MET:HE1	1:50:A:MET:HG3	5	0.12
(2,3559)	1:102:A:ALA:HB1	2:201:A:NAD:H4B	3	0.12
(2,3519)	1:48:A:ILE:HD11	1:53:A:LEU:HB2	1	0.12
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	2	0.12
(2,3519)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	4	0.12
(2,3519)	1:48:A:ILE:HD13	1:53:A:LEU:HB2	7	0.12
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	9	0.12
(2,3519)	1:48:A:ILE:HD11	1:53:A:LEU:HB2	11	0.12
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	12	0.12
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	13	0.12
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	15	0.12
(2,3518)	1:128:A:ILE:HD12	1:128:A:ILE:HA	3	0.12
(2,3518)	1:128:A:ILE:HD13	1:128:A:ILE:HA	19	0.12
(2,3516)	1:142:A:VAL:HG12	1:109:A:ILE:HA	19	0.12
(2,3500)	1:144:A:LEU:HD21	1:145:A:SER:HB2	19	0.12
(2,3481)	1:82:A:VAL:HG21	1:80:A:HIS:HA	15	0.12
(2,3481)	1:82:A:VAL:HG21	1:80:A:HIS:HA	17	0.12
(2,3478)	1:38:A:LEU:HD13	1:50:A:MET:HA	13	0.12
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	3	0.12
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	18	0.12
(2,3468)	1:110:A:LEU:HD12	1:110:A:LEU:HA	4	0.12
(2,3468)	1:110:A:LEU:HD12	1:110:A:LEU:HA	7	0.12
(2,3467)	1:11:A:LEU:HD13	1:38:A:LEU:HA	12	0.12
(2,3437)	1:57:A:VAL:HG21	1:57:A:VAL:H	18	0.12
(2,3434)	1:15:A:LEU:HD12	1:65:A:PHE:HE1	16	0.12
(2,3434)	1:15:A:LEU:HD11	1:65:A:PHE:HE1	17	0.12
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	6	0.12
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	11	0.12
(2,3382)	1:53:A:LEU:HD13	1:67:A:PHE:HZ	9	0.12
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	6	0.12
(2,3379)	1:66:A:ALA:HB3	1:77:A:ASN:HD21	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	1	0.12
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	2	0.12
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	3	0.12
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	16	0.12
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	7	0.12
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	13	0.12
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	2	0.12
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	7	0.12
(2,3362)	1:39:A:ALA:HB2	1:40:A:LYS:H	3	0.12
(2,3362)	1:39:A:ALA:HB2	1:40:A:LYS:H	5	0.12
(2,3362)	1:39:A:ALA:HB2	1:40:A:LYS:H	8	0.12
(2,3362)	1:39:A:ALA:HB3	1:40:A:LYS:H	13	0.12
(2,3295)	1:50:A:MET:HA	1:70:A:ASN:HD22	12	0.12
(2,3295)	1:50:A:MET:HA	1:70:A:ASN:HD22	20	0.12
(2,3288)	1:142:A:VAL:HG11	1:103:A:GLU:HA	8	0.12
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	2	0.12
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	9	0.12
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	14	0.12
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	17	0.12
(2,3257)	1:117:A:MET:HE2	2:201:A:NAD:H2A	18	0.12
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	9	0.12
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	10	0.12
(2,3253)	1:160:A:LEU:HD21	1:164:A:GLY:HA3	15	0.12
(2,3232)	1:142:A:VAL:HG21	1:106:A:PHE:HE1	8	0.12
(2,3230)	1:176:A:ILE:HD11	1:173:A:ALA:HB2	4	0.12
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	1	0.12
(2,3167)	1:176:A:ILE:HD13	1:114:A:ILE:HD13	18	0.12
(2,3036)	1:161:A:SER:H	2:201:A:NAD:H6N	4	0.12
(2,3036)	1:161:A:SER:H	2:201:A:NAD:H6N	15	0.12
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	12	0.12
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	20	0.12
(2,2832)	1:77:A:ASN:H	1:77:A:ASN:HD22	5	0.12
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	19	0.12
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	1	0.12
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	7	0.12
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	12	0.12
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	13	0.12
(2,2738)	1:30:A:GLY:H	1:26:A:LEU:HD21	19	0.12
(2,2722)	1:139:A:GLY:H	1:103:A:GLU:HA	5	0.12
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	6	0.12
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	9	0.12
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2649)	1:70:A:ASN:HD22	1:50:A:MET:HB2	5	0.12
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	3	0.12
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB1	6	0.12
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB1	10	0.12
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	16	0.12
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB1	18	0.12
(2,2620)	1:170:A:PHE:H	1:168:A:ILE:HG13	4	0.12
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	12	0.12
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	13	0.12
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	7	0.12
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	10	0.12
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	20	0.12
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	10	0.12
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	11	0.12
(2,2566)	1:43:A:ALA:HB3	1:44:A:LYS:H	20	0.12
(2,2520)	1:8:A:SER:H	1:6:A:LYS:HA	16	0.12
(2,2492)	1:129:A:THR:HG21	1:129:A:THR:H	19	0.12
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	12	0.12
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	14	0.12
(2,2254)	1:6:A:LYS:H	1:5:A:VAL:HG11	8	0.12
(2,2234)	1:14:A:VAL:HG23	1:21:A:LEU:H	6	0.12
(2,2212)	1:53:A:LEU:H	1:48:A:ILE:HG12	8	0.12
(2,2210)	1:48:A:ILE:HD12	1:53:A:LEU:H	10	0.12
(2,2210)	1:48:A:ILE:HD13	1:53:A:LEU:H	20	0.12
(2,2192)	1:82:A:VAL:HB	1:82:A:VAL:H	4	0.12
(2,2192)	1:82:A:VAL:HB	1:82:A:VAL:H	7	0.12
(2,2192)	1:82:A:VAL:HB	1:82:A:VAL:H	14	0.12
(2,2189)	1:81:A:SER:HA	1:82:A:VAL:H	4	0.12
(2,2175)	1:57:A:VAL:HG21	1:66:A:ALA:H	2	0.12
(2,2175)	1:57:A:VAL:HG22	1:66:A:ALA:H	10	0.12
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD23	7	0.12
(2,2164)	1:24:A:LEU:H	1:24:A:LEU:HB2	3	0.12
(2,2151)	1:13:A:LEU:H	1:13:A:LEU:HB3	5	0.12
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	13	0.12
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	4	0.12
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	6	0.12
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	7	0.12
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	10	0.12
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	11	0.12
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	18	0.12
(2,2132)	1:56:A:ILE:HD11	1:56:A:ILE:H	10	0.12
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	6	0.12
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	7	0.12
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	9	0.12
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	14	0.12
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	7	0.12
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	11	0.12
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	13	0.12
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	3	0.12
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	6	0.12
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	7	0.12
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	13	0.12
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	18	0.12
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	20	0.12
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	3	0.12
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	4	0.12
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	16	0.12
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	19	0.12
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	14	0.12
(2,2010)	1:34:A:VAL:H	1:73:A:LYS:HA	14	0.12
(2,1973)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	16	0.12
(2,1966)	1:57:A:VAL:HG12	1:67:A:PHE:HE1	18	0.12
(2,1964)	1:15:A:LEU:HD11	1:65:A:PHE:HD1	1	0.12
(2,1960)	1:65:A:PHE:HE1	1:15:A:LEU:HD21	5	0.12
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	4	0.12
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	6	0.12
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	7	0.12
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	8	0.12
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	11	0.12
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	13	0.12
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	14	0.12
(2,1924)	2:201:A:NAD:H51N	2:201:A:NAD:H52N	17	0.12
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	1	0.12
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	4	0.12
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	8	0.12
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	9	0.12
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	12	0.12
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	8	0.12
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	11	0.12
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	16	0.12
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	18	0.12
(2,1853)	1:21:A:LEU:HD13	1:14:A:VAL:HG23	18	0.12
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1833)	1:14:A:VAL:HG23	1:14:A:VAL:HB	11	0.12
(2,1833)	1:14:A:VAL:HG21	1:14:A:VAL:HB	12	0.12
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG23	6	0.12
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	20	0.12
(2,1810)	1:21:A:LEU:HD12	1:21:A:LEU:HB3	1	0.12
(2,1809)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	10	0.12
(2,1809)	1:34:A:VAL:HG13	1:37:A:LEU:HB3	18	0.12
(2,1805)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	8	0.12
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	10	0.12
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	7	0.12
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD12	9	0.12
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	13	0.12
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	19	0.12
(2,1729)	1:41:A:MET:HA	1:22:A:ILE:HB	7	0.12
(2,1723)	1:38:A:LEU:HD11	1:50:A:MET:HA	7	0.12
(2,1723)	1:38:A:LEU:HD13	1:50:A:MET:HA	20	0.12
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	6	0.12
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	13	0.12
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	17	0.12
(2,1687)	1:96:A:VAL:HG21	1:96:A:VAL:HA	5	0.12
(2,1601)	1:41:A:MET:HE3	1:10:A:PHE:HB3	14	0.12
(2,1599)	1:4:A:MET:HE3	1:52:A:GLU:HA	16	0.12
(2,1590)	1:32:A:ALA:HB2	1:33:A:PRO:HD3	2	0.12
(2,1588)	1:152:A:ALA:HB2	1:149:A:LYS:HA	19	0.12
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	10	0.12
(2,1511)	1:82:A:VAL:HG21	1:80:A:HIS:HA	17	0.12
(2,1509)	1:151:A:MET:HE2	1:171:A:VAL:HA	10	0.12
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	18	0.12
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	14	0.12
(2,1440)	1:37:A:LEU:HD12	1:37:A:LEU:H	2	0.12
(2,1440)	1:37:A:LEU:HD11	1:37:A:LEU:H	4	0.12
(2,1440)	1:37:A:LEU:HD11	1:37:A:LEU:H	5	0.12
(2,1440)	1:37:A:LEU:HD12	1:37:A:LEU:H	18	0.12
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	12	0.12
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	16	0.12
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	18	0.12
(2,1432)	1:38:A:LEU:HD12	1:39:A:ALA:H	3	0.12
(2,1432)	1:38:A:LEU:HD11	1:39:A:ALA:H	11	0.12
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	7	0.12
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	1	0.12
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	9	0.12
(2,1308)	1:13:A:LEU:HD11	1:13:A:LEU:HA	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	12	0.12
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	16	0.12
(2,1259)	1:171:A:VAL:HA	1:171:A:VAL:HG11	5	0.12
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	18	0.12
(2,1219)	1:177:A:LYS:HA	1:178:A:VAL:HG21	2	0.12
(2,1208)	1:114:A:ILE:HD13	1:171:A:VAL:HB	20	0.12
(2,1207)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	9	0.12
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	7	0.12
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	11	0.12
(2,1110)	1:76:A:ALA:H	1:75:A:ARG:H	8	0.12
(2,1099)	1:100:A:GLY:H	1:166:A:TRP:H	14	0.12
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	8	0.12
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	1	0.12
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	9	0.12
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	15	0.12
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	16	0.12
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	18	0.12
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	19	0.12
(2,1001)	1:177:A:LYS:H	1:145:A:SER:H	9	0.12
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	12	0.12
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	16	0.12
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	5	0.12
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	9	0.12
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	19	0.12
(2,904)	1:92:A:VAL:H	1:92:A:VAL:HA	5	0.12
(2,904)	1:92:A:VAL:H	1:92:A:VAL:HA	14	0.12
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	4	0.12
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	6	0.12
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	14	0.12
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	19	0.12
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	4	0.12
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	4	0.12
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	11	0.12
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	19	0.12
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	20	0.12
(2,639)	1:173:A:ALA:HB1	1:174:A:GLU:H	15	0.12
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	6	0.12
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	2	0.12
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	4	0.12
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	6	0.12
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	9	0.12
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	15	0.12
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	3	0.12
(2,458)	1:35:A:LYS:H	1:34:A:VAL:HG12	7	0.12
(2,453)	1:34:A:VAL:HB	1:35:A:LYS:H	12	0.12
(2,431)	1:73:A:LYS:H	1:34:A:VAL:HG21	13	0.12
(2,409)	1:11:A:LEU:H	1:11:A:LEU:HG	5	0.12
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	9	0.12
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	4	0.12
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	20	0.12
(2,303)	1:84:A:VAL:H	1:83:A:GLU:HB3	17	0.12
(2,300)	1:153:A:ASP:H	1:95:A:ALA:HB1	11	0.12
(2,268)	1:14:A:VAL:HG21	1:21:A:LEU:H	15	0.12
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	10	0.12
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	17	0.12
(2,212)	1:74:A:ILE:HD11	1:75:A:ARG:H	19	0.12
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	1	0.12
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	3	0.12
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	9	0.12
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	13	0.12
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	14	0.12
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	20	0.12
(2,184)	1:26:A:LEU:H	1:19:A:PRO:HA	15	0.12
(2,171)	1:56:A:ILE:H	1:55:A:HIS:HB3	3	0.12
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	7	0.12
(2,161)	1:86:A:LEU:HA	1:86:A:LEU:H	17	0.12
(2,144)	1:82:A:VAL:HB	1:83:A:GLU:H	17	0.12
(2,142)	1:83:A:GLU:HB2	1:83:A:GLU:H	18	0.12
(2,127)	1:92:A:VAL:H	1:91:A:GLN:HG3	1	0.12
(2,121)	1:177:A:LYS:HD2	1:178:A:VAL:H	11	0.12
(2,99)	1:140:A:LYS:H	1:103:A:GLU:HA	3	0.12
(2,96)	1:25:A:ASP:HB3	1:25:A:ASP:H	5	0.12
(2,85)	1:152:A:ALA:HB2	1:152:A:ALA:H	2	0.12
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	6	0.12
(2,43)	1:96:A:VAL:HG21	1:148:A:ALA:H	11	0.12
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	2	0.12
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	6	0.12
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	14	0.12
(1,126)	1:177:A:LYS:N	1:145:A:SER:O	15	0.12
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	1	0.12
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	17	0.12
(1,122)	1:175:A:PHE:N	1:172:A:PRO:O	20	0.12
(1,121)	1:175:A:PHE:H	1:172:A:PRO:O	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:175:A:PHE:H	1:172:A:PRO:O	3	0.12
(1,119)	1:171:A:VAL:H	1:114:A:ILE:O	14	0.12
(1,110)	1:153:A:ASP:N	1:149:A:LYS:O	9	0.12
(1,110)	1:153:A:ASP:N	1:149:A:LYS:O	10	0.12
(1,106)	1:150:A:GLY:N	1:147:A:ASP:O	11	0.12
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	18	0.12
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	20	0.12
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	9	0.12
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	13	0.12
(1,97)	1:136:A:MET:H	1:132:A:ARG:O	5	0.12
(1,97)	1:136:A:MET:H	1:132:A:ARG:O	14	0.12
(1,94)	1:134:A:VAL:N	1:130:A:THR:O	18	0.12
(1,92)	1:133:A:LYS:N	1:129:A:THR:O	8	0.12
(1,92)	1:133:A:LYS:N	1:129:A:THR:O	12	0.12
(1,91)	1:133:A:LYS:H	1:129:A:THR:O	2	0.12
(1,91)	1:133:A:LYS:H	1:129:A:THR:O	9	0.12
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	4	0.12
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	5	0.12
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	7	0.12
(1,88)	1:131:A:ALA:N	1:127:A:ASP:O	6	0.12
(1,86)	1:124:A:LEU:N	1:166:A:TRP:O	18	0.12
(1,85)	1:124:A:LEU:H	1:166:A:TRP:O	5	0.12
(1,82)	1:114:A:ILE:N	1:171:A:VAL:O	9	0.12
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	3	0.12
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	19	0.12
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	8	0.12
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	14	0.12
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	16	0.12
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	16	0.12
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	8	0.12
(1,56)	1:74:A:ILE:N	1:32:A:ALA:O	4	0.12
(1,55)	1:74:A:ILE:H	1:32:A:ALA:O	1	0.12
(1,55)	1:74:A:ILE:H	1:32:A:ALA:O	8	0.12
(1,48)	1:58:A:GLU:N	1:54:A:LYS:O	3	0.12
(1,45)	1:57:A:VAL:H	1:53:A:LEU:O	2	0.12
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	9	0.12
(1,39)	1:54:A:LYS:H	1:50:A:MET:O	8	0.12
(1,39)	1:54:A:LYS:H	1:50:A:MET:O	10	0.12
(1,39)	1:54:A:LYS:H	1:50:A:MET:O	19	0.12
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	4	0.12
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	6	0.12
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	13	0.12
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	14	0.12
(1,21)	1:32:A:ALA:H	1:74:A:ILE:O	5	0.12
(1,15)	1:14:A:VAL:H	1:10:A:PHE:O	5	0.12
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	20	0.12
(4,442)	1:178:A:VAL:HG21	1:144:A:LEU:HG	5	0.11
(4,425)	1:34:A:VAL:HG21	1:35:A:LYS:HB2	8	0.11
(4,385)	1:15:A:LEU:HA	1:14:A:VAL:HG11	1	0.11
(4,379)	1:50:A:MET:HA	1:35:A:LYS:HG2	14	0.11
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	1	0.11
(4,328)	1:122:A:VAL:HG13	1:113:A:GLY:HA2	1	0.11
(4,311)	1:143:A:VAL:HG12	1:178:A:VAL:HA	19	0.11
(4,303)	1:110:A:LEU:HD11	1:107:A:ASP:HA	19	0.11
(4,297)	1:168:A:ILE:HD13	1:114:A:ILE:H	17	0.11
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HZ	2	0.11
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HZ	18	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	3	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	7	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	9	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	10	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	11	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	13	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	14	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	15	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	17	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	18	0.11
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	19	0.11
(4,213)	1:165:A:VAL:HB	1:123:A:HIS:HA	2	0.11
(4,198)	1:176:A:ILE:HD11	1:106:A:PHE:HE1	7	0.11
(4,198)	1:176:A:ILE:HD11	1:106:A:PHE:HE1	14	0.11
(4,198)	1:176:A:ILE:HD11	1:106:A:PHE:HE1	19	0.11
(4,166)	1:171:A:VAL:H	1:124:A:LEU:HD11	15	0.11
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	2	0.11
(4,69)	1:57:A:VAL:H	1:56:A:ILE:HG12	6	0.11
(4,65)	1:6:A:LYS:HB3	1:7:A:VAL:H	3	0.11
(4,65)	1:7:A:VAL:H	1:7:A:VAL:HB	9	0.11
(4,61)	1:37:A:LEU:H	1:38:A:LEU:HD23	10	0.11
(4,61)	1:37:A:LEU:H	1:38:A:LEU:HD23	20	0.11
(4,41)	1:5:A:VAL:HG23	1:5:A:VAL:H	2	0.11
(4,41)	1:5:A:VAL:HG22	1:5:A:VAL:H	4	0.11
(4,41)	1:5:A:VAL:HG23	1:5:A:VAL:H	5	0.11
(4,41)	1:5:A:VAL:HG23	1:5:A:VAL:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,41)	1:5:A:VAL:HG22	1:5:A:VAL:H	13	0.11
(4,41)	1:5:A:VAL:HG21	1:5:A:VAL:H	14	0.11
(4,41)	1:5:A:VAL:HG21	1:5:A:VAL:H	15	0.11
(4,23)	1:39:A:ALA:H	1:42:A:LYS:HB2	7	0.11
(4,8)	1:22:A:ILE:HG23	1:10:A:PHE:HD1	2	0.11
(4,8)	1:22:A:ILE:HG23	1:10:A:PHE:HD1	6	0.11
(2,3952)	1:165:A:VAL:HG11	2:201:A:NAD:H5N	18	0.11
(2,3935)	1:102:A:ALA:HB1	2:201:A:NAD:HO3A	18	0.11
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	3	0.11
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	4	0.11
(2,3903)	2:201:A:NAD:H6N	1:165:A:VAL:HG12	19	0.11
(2,3898)	2:201:A:NAD:H1D	2:201:A:NAD:H6N	4	0.11
(2,3884)	2:201:A:NAD:H1B	1:109:A:ILE:HD12	9	0.11
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	2	0.11
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	6	0.11
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	11	0.11
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	15	0.11
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	4	0.11
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	5	0.11
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	10	0.11
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG23	11	0.11
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	12	0.11
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	17	0.11
(2,3829)	1:109:A:ILE:HD11	1:101:A:THR:HG23	4	0.11
(2,3820)	1:109:A:ILE:HG21	1:109:A:ILE:HD11	1	0.11
(2,3820)	1:109:A:ILE:HG21	1:109:A:ILE:HD11	10	0.11
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	12	0.11
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	14	0.11
(2,3820)	1:109:A:ILE:HG23	1:109:A:ILE:HD11	19	0.11
(2,3815)	1:21:A:LEU:HD13	1:14:A:VAL:HG22	20	0.11
(2,3812)	1:56:A:ILE:HG23	1:11:A:LEU:HD11	17	0.11
(2,3802)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	1	0.11
(2,3802)	1:24:A:LEU:HD21	1:24:A:LEU:HB3	3	0.11
(2,3802)	1:24:A:LEU:HD22	1:24:A:LEU:HB3	7	0.11
(2,3802)	1:24:A:LEU:HD23	1:24:A:LEU:HB3	11	0.11
(2,3796)	1:14:A:VAL:HG12	1:11:A:LEU:HG	12	0.11
(2,3785)	1:142:A:VAL:HG11	1:103:A:GLU:HG2	17	0.11
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	10	0.11
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	13	0.11
(2,3775)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	2	0.11
(2,3775)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	14	0.11
(2,3775)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	7	0.11
(2,3773)	1:34:A:VAL:HG11	1:37:A:LEU:HB3	13	0.11
(2,3764)	1:160:A:LEU:HG	1:160:A:LEU:HD13	14	0.11
(2,3764)	1:160:A:LEU:HG	1:160:A:LEU:HD13	17	0.11
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	4	0.11
(2,3763)	1:76:A:ALA:HB3	1:15:A:LEU:HD11	19	0.11
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	2	0.11
(2,3726)	1:44:A:LYS:HE2	1:22:A:ILE:HG22	18	0.11
(2,3722)	1:16:A:ARG:HD3	1:76:A:ALA:HB1	1	0.11
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	1	0.11
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	3	0.11
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	5	0.11
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	10	0.11
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	20	0.11
(2,3712)	1:109:A:ILE:HG22	1:109:A:ILE:HA	10	0.11
(2,3712)	1:109:A:ILE:HG22	1:109:A:ILE:HA	12	0.11
(2,3712)	1:109:A:ILE:HG21	1:109:A:ILE:HA	19	0.11
(2,3712)	1:109:A:ILE:HG21	1:109:A:ILE:HA	20	0.11
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	6	0.11
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	7	0.11
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	9	0.11
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	10	0.11
(2,3708)	1:173:A:ALA:HA	1:176:A:ILE:HD11	18	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	2	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	5	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	6	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	8	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	9	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	11	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	12	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	13	0.11
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	16	0.11
(2,3679)	1:97:A:LEU:HD21	1:97:A:LEU:HA	17	0.11
(2,3575)	1:50:A:MET:HE3	1:50:A:MET:HG3	20	0.11
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	2	0.11
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	10	0.11
(2,3514)	1:143:A:VAL:HG12	1:132:A:ARG:HA	1	0.11
(2,3509)	1:13:A:LEU:HD23	1:17:A:HIS:HB2	11	0.11
(2,3479)	1:151:A:MET:HE1	1:171:A:VAL:HA	5	0.11
(2,3479)	1:151:A:MET:HE2	1:171:A:VAL:HA	16	0.11
(2,3479)	1:151:A:MET:HE3	1:171:A:VAL:HA	19	0.11
(2,3478)	1:38:A:LEU:HD11	1:50:A:MET:HA	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3478)	1:38:A:LEU:HD13	1:50:A:MET:HA	20	0.11
(2,3473)	1:146:A:VAL:HG22	1:96:A:VAL:HA	13	0.11
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	15	0.11
(2,3473)	1:146:A:VAL:HG21	1:96:A:VAL:HA	17	0.11
(2,3473)	1:146:A:VAL:HG23	1:96:A:VAL:HA	20	0.11
(2,3468)	1:110:A:LEU:HD12	1:110:A:LEU:HA	3	0.11
(2,3468)	1:110:A:LEU:HD12	1:110:A:LEU:HA	17	0.11
(2,3446)	1:74:A:ILE:HD12	1:67:A:PHE:HE1	15	0.11
(2,3414)	1:146:A:VAL:HG13	1:146:A:VAL:H	9	0.11
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	2	0.11
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	3	0.11
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	9	0.11
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	18	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	2	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	3	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	8	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	9	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	12	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	14	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	15	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	16	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	19	0.11
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	20	0.11
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	14	0.11
(2,3362)	1:39:A:ALA:HB2	1:40:A:LYS:H	9	0.11
(2,3362)	1:39:A:ALA:HB2	1:40:A:LYS:H	19	0.11
(2,3345)	1:41:A:MET:HE2	1:10:A:PHE:HE1	16	0.11
(2,3335)	1:16:A:ARG:HD2	1:12:A:SER:H	17	0.11
(2,3302)	1:82:A:VAL:HA	1:83:A:GLU:H	2	0.11
(2,3295)	1:50:A:MET:HA	1:70:A:ASN:HD22	3	0.11
(2,3288)	1:142:A:VAL:HG13	1:103:A:GLU:HA	2	0.11
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	1	0.11
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	4	0.11
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	7	0.11
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	8	0.11
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	13	0.11
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	19	0.11
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	20	0.11
(2,3266)	1:53:A:LEU:HD13	1:67:A:PHE:HE1	9	0.11
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	3	0.11
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	8	0.11
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	12	0.11
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	15	0.11
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	19	0.11
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	6	0.11
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	7	0.11
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	11	0.11
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	12	0.11
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	13	0.11
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	14	0.11
(2,3233)	1:171:A:VAL:HG11	1:171:A:VAL:H	5	0.11
(2,3231)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	10	0.11
(2,3197)	1:176:A:ILE:HD11	1:176:A:ILE:HB	16	0.11
(2,3184)	1:92:A:VAL:HG21	1:92:A:VAL:H	20	0.11
(2,3182)	1:114:A:ILE:HD13	1:171:A:VAL:HB	2	0.11
(2,3180)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	3	0.11
(2,3180)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	10	0.11
(2,3180)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	13	0.11
(2,3180)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	20	0.11
(2,3173)	1:176:A:ILE:HD11	1:176:A:ILE:HA	9	0.11
(2,3173)	1:176:A:ILE:HD11	1:176:A:ILE:HA	11	0.11
(2,3173)	1:176:A:ILE:HD11	1:176:A:ILE:HA	14	0.11
(2,3127)	1:97:A:LEU:HD11	1:124:A:LEU:HD23	2	0.11
(2,3102)	1:136:A:MET:H	1:105:A:ASN:HD22	18	0.11
(2,3102)	1:136:A:MET:H	1:105:A:ASN:HD22	19	0.11
(2,3036)	1:161:A:SER:H	2:201:A:NAD:H6N	6	0.11
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	2	0.11
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	4	0.11
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	13	0.11
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	17	0.11
(2,2980)	1:40:A:LYS:H	1:39:A:ALA:H	1	0.11
(2,2980)	1:40:A:LYS:H	1:39:A:ALA:H	4	0.11
(2,2980)	1:40:A:LYS:H	1:39:A:ALA:H	17	0.11
(2,2887)	1:176:A:ILE:H	1:146:A:VAL:HG11	2	0.11
(2,2887)	1:176:A:ILE:H	1:146:A:VAL:HG11	11	0.11
(2,2887)	1:176:A:ILE:H	1:146:A:VAL:HG11	15	0.11
(2,2887)	1:176:A:ILE:H	1:146:A:VAL:HG11	16	0.11
(2,2841)	1:78:A:GLN:HE22	1:77:A:ASN:H	11	0.11
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	15	0.11
(2,2757)	1:59:A:THR:H	1:76:A:ALA:HA	17	0.11
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	3	0.11
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	5	0.11
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	19	0.11
(2,2722)	1:139:A:GLY:H	1:103:A:GLU:HA	4	0.11
(2,2680)	1:113:A:GLY:H	1:109:A:ILE:HG21	3	0.11
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	2	0.11
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	7	0.11
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	13	0.11
(2,2649)	1:70:A:ASN:HD22	1:50:A:MET:HB2	4	0.11
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB1	13	0.11
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB2	14	0.11
(2,2632)	1:29:A:ASN:H	1:28:A:ALA:HB3	17	0.11
(2,2627)	1:29:A:ASN:H	1:29:A:ASN:HD22	6	0.11
(2,2597)	1:44:A:LYS:H	1:21:A:LEU:HA	6	0.11
(2,2597)	1:44:A:LYS:H	1:21:A:LEU:HA	19	0.11
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	6	0.11
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	18	0.11
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	3	0.11
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	15	0.11
(2,2574)	1:111:A:LYS:HB3	1:111:A:LYS:H	2	0.11
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	6	0.11
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	8	0.11
(2,2566)	1:43:A:ALA:HB2	1:44:A:LYS:H	9	0.11
(2,2550)	1:86:A:LEU:H	1:88:A:TYR:H	4	0.11
(2,2526)	1:7:A:VAL:HG11	1:8:A:SER:H	20	0.11
(2,2492)	1:129:A:THR:HG22	1:129:A:THR:H	11	0.11
(2,2429)	1:35:A:LYS:H	1:34:A:VAL:HG12	20	0.11
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	3	0.11
(2,2401)	1:73:A:LYS:H	1:73:A:LYS:HB3	7	0.11
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	19	0.11
(2,2308)	1:108:A:LEU:HD23	1:108:A:LEU:H	6	0.11
(2,2305)	1:173:A:ALA:HB1	1:176:A:ILE:H	4	0.11
(2,2305)	1:173:A:ALA:HB1	1:176:A:ILE:H	14	0.11
(2,2269)	1:84:A:VAL:HA	1:84:A:VAL:H	5	0.11
(2,2269)	1:84:A:VAL:HA	1:84:A:VAL:H	17	0.11
(2,2216)	1:26:A:LEU:HD13	1:27:A:ASP:H	7	0.11
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	9	0.11
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	10	0.11
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	14	0.11
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	15	0.11
(2,2192)	1:82:A:VAL:HB	1:82:A:VAL:H	13	0.11
(2,2189)	1:81:A:SER:HA	1:82:A:VAL:H	14	0.11
(2,2166)	1:24:A:LEU:H	1:24:A:LEU:HD21	11	0.11
(2,2148)	1:26:A:LEU:HD21	1:26:A:LEU:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	13	0.11
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	14	0.11
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	2	0.11
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	3	0.11
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	4	0.11
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	11	0.11
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	15	0.11
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	16	0.11
(2,2130)	1:56:A:ILE:H	1:56:A:ILE:HB	20	0.11
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	5	0.11
(2,2122)	1:86:A:LEU:HB2	1:86:A:LEU:H	11	0.11
(2,2098)	1:83:A:GLU:HB2	1:83:A:GLU:H	17	0.11
(2,2090)	1:32:A:ALA:H	1:26:A:LEU:HD13	7	0.11
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	4	0.11
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	17	0.11
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	4	0.11
(2,2075)	1:178:A:VAL:H	1:177:A:LYS:H	17	0.11
(2,2067)	1:91:A:GLN:H	1:159:A:TYR:HD1	15	0.11
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	10	0.11
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	12	0.11
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	7	0.11
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	9	0.11
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	13	0.11
(2,2047)	1:25:A:ASP:H	1:26:A:LEU:HG	18	0.11
(2,2018)	1:166:A:TRP:HE1	1:126:A:GLN:HB2	6	0.11
(2,2010)	1:34:A:VAL:H	1:73:A:LYS:HA	2	0.11
(2,2010)	1:34:A:VAL:H	1:73:A:LYS:HA	4	0.11
(2,2010)	1:34:A:VAL:H	1:73:A:LYS:HA	15	0.11
(2,1989)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	8	0.11
(2,1989)	1:142:A:VAL:HG21	1:106:A:PHE:HD1	15	0.11
(2,1964)	1:15:A:LEU:HD11	1:65:A:PHE:HD1	11	0.11
(2,1964)	1:15:A:LEU:HD11	1:65:A:PHE:HD1	20	0.11
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	3	0.11
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	5	0.11
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	10	0.11
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG23	11	0.11
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	17	0.11
(2,1876)	1:129:A:THR:HB	1:129:A:THR:HG22	19	0.11
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	20	0.11
(2,1863)	1:11:A:LEU:HD11	1:11:A:LEU:HB3	20	0.11
(2,1860)	1:57:A:VAL:HG21	1:57:A:VAL:HB	6	0.11
(2,1860)	1:57:A:VAL:HG21	1:57:A:VAL:HB	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1860)	1:57:A:VAL:HG21	1:57:A:VAL:HB	14	0.11
(2,1860)	1:57:A:VAL:HG21	1:57:A:VAL:HB	16	0.11
(2,1852)	1:57:A:VAL:HG12	1:74:A:ILE:HD13	8	0.11
(2,1849)	1:15:A:LEU:HD12	1:74:A:ILE:HD12	20	0.11
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG23	4	0.11
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	9	0.11
(2,1810)	1:21:A:LEU:HD12	1:21:A:LEU:HB3	3	0.11
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	14	0.11
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	16	0.11
(2,1805)	1:21:A:LEU:HD21	1:21:A:LEU:HB3	17	0.11
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	2	0.11
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD12	6	0.11
(2,1797)	1:160:A:LEU:HG	1:160:A:LEU:HD13	19	0.11
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	1	0.11
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	3	0.11
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	4	0.11
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	15	0.11
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	17	0.11
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	1	0.11
(2,1746)	1:32:A:ALA:HB1	1:33:A:PRO:HD3	3	0.11
(2,1733)	1:7:A:VAL:HA	1:7:A:VAL:HB	12	0.11
(2,1723)	1:38:A:LEU:HD13	1:50:A:MET:HA	3	0.11
(2,1723)	1:38:A:LEU:HD13	1:50:A:MET:HA	8	0.11
(2,1723)	1:38:A:LEU:HD11	1:50:A:MET:HA	18	0.11
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	15	0.11
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	16	0.11
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	20	0.11
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	1	0.11
(2,1625)	1:52:A:GLU:HG2	1:47:A:GLY:HA2	17	0.11
(2,1603)	1:71:A:PHE:HB3	1:50:A:MET:HE3	19	0.11
(2,1591)	1:95:A:ALA:HB1	1:149:A:LYS:HA	15	0.11
(2,1563)	1:48:A:ILE:HG23	1:53:A:LEU:HB2	11	0.11
(2,1549)	1:37:A:LEU:HD13	1:41:A:MET:HG2	18	0.11
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	5	0.11
(2,1540)	1:56:A:ILE:HG21	1:56:A:ILE:HA	17	0.11
(2,1474)	1:110:A:LEU:HD21	1:110:A:LEU:H	9	0.11
(2,1474)	1:110:A:LEU:HD21	1:110:A:LEU:H	12	0.11
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	4	0.11
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	11	0.11
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	12	0.11
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	19	0.11
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1440)	1:37:A:LEU:HD12	1:37:A:LEU:H	3	0.11
(2,1440)	1:37:A:LEU:HD12	1:37:A:LEU:H	6	0.11
(2,1440)	1:37:A:LEU:HD12	1:37:A:LEU:H	7	0.11
(2,1440)	1:37:A:LEU:HD13	1:37:A:LEU:H	8	0.11
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	6	0.11
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	9	0.11
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	11	0.11
(2,1424)	1:56:A:ILE:HG22	1:65:A:PHE:HE1	16	0.11
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	3	0.11
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	5	0.11
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	8	0.11
(2,1348)	1:83:A:GLU:HA	1:84:A:VAL:H	14	0.11
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	15	0.11
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	17	0.11
(2,1314)	1:142:A:VAL:HG13	1:103:A:GLU:HA	13	0.11
(2,1308)	1:13:A:LEU:HD11	1:13:A:LEU:HA	17	0.11
(2,1308)	1:13:A:LEU:HD11	1:13:A:LEU:HA	20	0.11
(2,1275)	1:160:A:LEU:HD21	1:161:A:SER:H	12	0.11
(2,1256)	1:173:A:ALA:HB3	1:110:A:LEU:HD12	2	0.11
(2,1206)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	18	0.11
(2,1203)	1:24:A:LEU:HD13	1:36:A:GLU:HG3	1	0.11
(2,1172)	1:144:A:LEU:HD11	1:106:A:PHE:HE1	19	0.11
(2,1080)	1:21:A:LEU:H	1:22:A:ILE:H	5	0.11
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	5	0.11
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	12	0.11
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	15	0.11
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	16	0.11
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	6	0.11
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	11	0.11
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	14	0.11
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	6	0.11
(2,979)	1:96:A:VAL:H	1:95:A:ALA:H	7	0.11
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	2	0.11
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	8	0.11
(2,950)	1:76:A:ALA:H	1:76:A:ALA:HA	2	0.11
(2,950)	1:76:A:ALA:H	1:76:A:ALA:HA	14	0.11
(2,950)	1:76:A:ALA:H	1:76:A:ALA:HA	18	0.11
(2,942)	1:114:A:ILE:H	1:170:A:PHE:HD1	2	0.11
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	2	0.11
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	17	0.11
(2,693)	1:126:A:GLN:HE22	1:166:A:TRP:HB2	2	0.11
(2,676)	1:70:A:ASN:HD22	1:50:A:MET:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,660)	1:29:A:ASN:H	1:28:A:ALA:HB2	15	0.11
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	8	0.11
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	19	0.11
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	17	0.11
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	8	0.11
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	11	0.11
(2,628)	1:44:A:LYS:HB3	1:44:A:LYS:H	17	0.11
(2,550)	1:102:A:ALA:HB1	1:105:A:ASN:H	12	0.11
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	5	0.11
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	8	0.11
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	17	0.11
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	19	0.11
(2,538)	1:38:A:LEU:HA	1:38:A:LEU:H	20	0.11
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	4	0.11
(2,473)	1:110:A:LEU:H	1:110:A:LEU:HB3	16	0.11
(2,468)	1:51:A:GLU:H	1:50:A:MET:HB2	19	0.11
(2,445)	1:36:A:GLU:H	1:36:A:GLU:HB3	4	0.11
(2,439)	1:55:A:HIS:H	1:54:A:LYS:HB2	4	0.11
(2,413)	1:11:A:LEU:H	1:11:A:LEU:HA	5	0.11
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	3	0.11
(2,382)	1:20:A:ALA:HA	1:20:A:ALA:H	1	0.11
(2,342)	1:41:A:MET:H	1:41:A:MET:HG2	20	0.11
(2,268)	1:14:A:VAL:HG21	1:21:A:LEU:H	2	0.11
(2,268)	1:14:A:VAL:HG22	1:21:A:LEU:H	8	0.11
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	4	0.11
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	5	0.11
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	7	0.11
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	3	0.11
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	5	0.11
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	6	0.11
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	11	0.11
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	12	0.11
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	19	0.11
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	20	0.11
(2,224)	1:81:A:SER:HA	1:82:A:VAL:H	14	0.11
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	10	0.11
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	15	0.11
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	16	0.11
(2,148)	1:85:A:ASP:H	1:85:A:ASP:HB3	20	0.11
(2,99)	1:140:A:LYS:H	1:103:A:GLU:HA	2	0.11
(2,85)	1:152:A:ALA:HB3	1:152:A:ALA:H	4	0.11
(2,65)	1:177:A:LYS:H	1:177:A:LYS:HD2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:178:A:VAL:H	1:177:A:LYS:H	5	0.11
(2,62)	1:178:A:VAL:H	1:177:A:LYS:H	9	0.11
(2,62)	1:178:A:VAL:H	1:177:A:LYS:H	12	0.11
(2,62)	1:178:A:VAL:H	1:177:A:LYS:H	16	0.11
(2,61)	1:166:A:TRP:HE1	1:126:A:GLN:HB2	14	0.11
(2,54)	1:34:A:VAL:H	1:74:A:ILE:HG21	12	0.11
(2,42)	1:148:A:ALA:H	1:148:A:ALA:HB1	5	0.11
(2,42)	1:148:A:ALA:H	1:148:A:ALA:HB1	9	0.11
(2,42)	1:148:A:ALA:H	1:148:A:ALA:HB1	19	0.11
(2,42)	1:148:A:ALA:H	1:148:A:ALA:HB1	20	0.11
(2,20)	1:3:A:HIS:HD2	1:3:A:HIS:HB2	13	0.11
(2,14)	1:34:A:VAL:HG23	1:67:A:PHE:HE1	12	0.11
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	1	0.11
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	11	0.11
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	20	0.11
(1,119)	1:171:A:VAL:H	1:114:A:ILE:O	10	0.11
(1,118)	1:168:A:ILE:N	1:122:A:VAL:O	14	0.11
(1,103)	1:147:A:ASP:H	1:175:A:PHE:O	8	0.11
(1,101)	1:144:A:LEU:H	1:99:A:HIS:O	2	0.11
(1,98)	1:136:A:MET:N	1:132:A:ARG:O	10	0.11
(1,97)	1:136:A:MET:H	1:132:A:ARG:O	20	0.11
(1,89)	1:132:A:ARG:H	1:128:A:ILE:O	14	0.11
(1,89)	1:132:A:ARG:H	1:128:A:ILE:O	19	0.11
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	2	0.11
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	14	0.11
(1,80)	1:113:A:GLY:N	1:109:A:ILE:O	16	0.11
(1,78)	1:112:A:ASP:N	1:108:A:LEU:O	8	0.11
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	10	0.11
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	17	0.11
(1,72)	1:109:A:ILE:N	1:105:A:ASN:O	19	0.11
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	4	0.11
(1,71)	1:109:A:ILE:H	1:105:A:ASN:O	10	0.11
(1,59)	1:77:A:ASN:H	1:64:A:ARG:O	17	0.11
(1,55)	1:74:A:ILE:H	1:32:A:ALA:O	5	0.11
(1,46)	1:57:A:VAL:N	1:53:A:LEU:O	17	0.11
(1,40)	1:54:A:LYS:N	1:50:A:MET:O	16	0.11
(1,39)	1:54:A:LYS:H	1:50:A:MET:O	1	0.11
(1,36)	1:43:A:ALA:N	1:39:A:ALA:O	20	0.11
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	12	0.11
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	14	0.11
(1,26)	1:38:A:LEU:N	1:34:A:VAL:O	18	0.11
(1,12)	1:12:A:SER:N	1:8:A:SER:O	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:10:A:PHE:N	1:6:A:LYS:O	19	0.11
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	18	0.11
(1,5)	1:9:A:LYS:H	1:5:A:VAL:O	2	0.11
(1,4)	1:8:A:SER:N	1:4:A:MET:O	19	0.11
(4,442)	1:178:A:VAL:HG22	1:144:A:LEU:HG	16	0.1
(4,425)	1:34:A:VAL:HG21	1:35:A:LYS:HB2	17	0.1
(4,335)	1:146:A:VAL:HG12	1:158:A:PHE:HB3	18	0.1
(4,290)	1:53:A:LEU:HD23	1:56:A:ILE:H	3	0.1
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HZ	5	0.1
(4,270)	1:110:A:LEU:HG	1:106:A:PHE:HZ	10	0.1
(4,235)	1:20:A:ALA:HA	1:20:A:ALA:H	20	0.1
(4,221)	1:14:A:VAL:HG22	1:14:A:VAL:HA	19	0.1
(4,208)	1:14:A:VAL:HG23	1:11:A:LEU:HA	5	0.1
(4,198)	1:176:A:ILE:HD11	1:106:A:PHE:HE1	13	0.1
(4,164)	1:87:A:GLY:H	1:162:A:ASN:HB3	19	0.1
(4,70)	1:130:A:THR:H	2:201:A:NAD:H4D	1	0.1
(4,30)	1:24:A:LEU:H	1:22:A:ILE:HB	3	0.1
(3,20)	1:163:A:ASN:OD1	2:201:A:NAD:H71N	6	0.1
(2,3963)	1:123:A:HIS:HB2	2:201:A:NAD:H6N	1	0.1
(2,3924)	1:109:A:ILE:HD11	2:201:A:NAD:H2A	7	0.1
(2,3920)	1:115:A:LYS:H	2:201:A:NAD:H8A	10	0.1
(2,3864)	1:24:A:LEU:HA	1:44:A:LYS:HE3	7	0.1
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	3	0.1
(2,3838)	1:129:A:THR:HB	1:129:A:THR:HG22	19	0.1
(2,3825)	1:11:A:LEU:HD13	1:11:A:LEU:HB2	14	0.1
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB2	17	0.1
(2,3779)	1:96:A:VAL:HG11	1:95:A:ALA:HB3	19	0.1
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	2	0.1
(2,3774)	1:21:A:LEU:HD11	1:21:A:LEU:HB3	13	0.1
(2,3772)	1:151:A:MET:HE2	1:174:A:GLU:HG2	17	0.1
(2,3764)	1:160:A:LEU:HG	1:160:A:LEU:HD13	10	0.1
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	6	0.1
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	14	0.1
(2,3720)	1:90:A:LYS:HE3	1:90:A:LYS:HD3	17	0.1
(2,3703)	1:110:A:LEU:HA	1:110:A:LEU:HB3	18	0.1
(2,3535)	1:21:A:LEU:HD11	1:18:A:ASN:HB2	4	0.1
(2,3519)	1:48:A:ILE:HD12	1:53:A:LEU:HB2	6	0.1
(2,3479)	1:151:A:MET:HE2	1:171:A:VAL:HA	12	0.1
(2,3468)	1:110:A:LEU:HD11	1:110:A:LEU:HA	9	0.1
(2,3405)	1:56:A:ILE:HG22	1:57:A:VAL:H	1	0.1
(2,3376)	1:95:A:ALA:HB3	1:96:A:VAL:H	7	0.1
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3376)	1:95:A:ALA:HB2	1:96:A:VAL:H	20	0.1
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	4	0.1
(2,3375)	1:48:A:ILE:HG13	1:48:A:ILE:H	10	0.1
(2,3371)	1:20:A:ALA:HB3	1:18:A:ASN:HD21	17	0.1
(2,3362)	1:39:A:ALA:HB3	1:40:A:LYS:H	4	0.1
(2,3302)	1:82:A:VAL:HA	1:83:A:GLU:H	13	0.1
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	10	0.1
(2,3269)	1:34:A:VAL:HG21	1:34:A:VAL:H	18	0.1
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	4	0.1
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	16	0.1
(2,3256)	1:160:A:LEU:HD21	1:160:A:LEU:HB2	17	0.1
(2,3234)	1:171:A:VAL:HA	1:171:A:VAL:HG11	1	0.1
(2,3197)	1:176:A:ILE:HD11	1:176:A:ILE:HB	4	0.1
(2,3197)	1:176:A:ILE:HD11	1:176:A:ILE:HB	7	0.1
(2,3197)	1:176:A:ILE:HD11	1:176:A:ILE:HB	10	0.1
(2,3184)	1:92:A:VAL:HG21	1:92:A:VAL:H	7	0.1
(2,3184)	1:92:A:VAL:HG21	1:92:A:VAL:H	10	0.1
(2,3184)	1:92:A:VAL:HG21	1:92:A:VAL:H	13	0.1
(2,3180)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	2	0.1
(2,3180)	1:114:A:ILE:HD11	1:114:A:ILE:HG21	9	0.1
(2,3173)	1:176:A:ILE:HD11	1:176:A:ILE:HA	2	0.1
(2,3173)	1:176:A:ILE:HD11	1:176:A:ILE:HA	6	0.1
(2,3173)	1:176:A:ILE:HD11	1:176:A:ILE:HA	20	0.1
(2,3157)	1:176:A:ILE:HG21	1:176:A:ILE:H	14	0.1
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	5	0.1
(2,2987)	1:38:A:LEU:H	1:37:A:LEU:H	7	0.1
(2,2980)	1:40:A:LYS:H	1:39:A:ALA:H	5	0.1
(2,2980)	1:40:A:LYS:H	1:39:A:ALA:H	16	0.1
(2,2949)	1:165:A:VAL:H	1:91:A:GLN:HE22	14	0.1
(2,2822)	1:74:A:ILE:H	1:73:A:LYS:HB2	1	0.1
(2,2822)	1:74:A:ILE:H	1:73:A:LYS:HB2	18	0.1
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	2	0.1
(2,2756)	1:59:A:THR:HG21	1:59:A:THR:H	15	0.1
(2,2748)	1:86:A:LEU:HD11	1:87:A:GLY:H	5	0.1
(2,2680)	1:113:A:GLY:H	1:109:A:ILE:HG21	7	0.1
(2,2664)	1:132:A:ARG:H	1:126:A:GLN:HE22	20	0.1
(2,2657)	1:126:A:GLN:HE21	1:166:A:TRP:HB2	8	0.1
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	9	0.1
(2,2595)	1:14:A:VAL:HG12	1:14:A:VAL:H	19	0.1
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	4	0.1
(2,2593)	1:14:A:VAL:H	1:11:A:LEU:HA	18	0.1
(2,2520)	1:8:A:SER:H	1:6:A:LYS:HA	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2520)	1:8:A:SER:H	1:6:A:LYS:HA	17	0.1
(2,2520)	1:8:A:SER:H	1:6:A:LYS:HA	20	0.1
(2,2492)	1:129:A:THR:HG21	1:129:A:THR:H	17	0.1
(2,2360)	1:28:A:ALA:H	1:27:A:ASP:HB3	17	0.1
(2,2221)	1:168:A:ILE:HD12	1:157:A:ASP:H	20	0.1
(2,2212)	1:53:A:LEU:H	1:48:A:ILE:HG12	1	0.1
(2,2210)	1:48:A:ILE:HD12	1:53:A:LEU:H	5	0.1
(2,2197)	1:109:A:ILE:H	1:102:A:ALA:H	12	0.1
(2,2169)	1:76:A:ALA:H	1:15:A:LEU:HB2	20	0.1
(2,2142)	1:66:A:ALA:H	1:67:A:PHE:HB3	12	0.1
(2,2132)	1:56:A:ILE:HD11	1:56:A:ILE:H	15	0.1
(2,2078)	1:177:A:LYS:HG2	1:178:A:VAL:H	16	0.1
(2,2077)	1:177:A:LYS:HD2	1:178:A:VAL:H	14	0.1
(2,2052)	1:25:A:ASP:HB3	1:25:A:ASP:H	9	0.1
(2,2010)	1:34:A:VAL:H	1:73:A:LYS:HA	12	0.1
(2,1984)	1:106:A:PHE:HD1	1:106:A:PHE:HE1	6	0.1
(2,1984)	1:106:A:PHE:HD1	1:106:A:PHE:HE1	10	0.1
(2,1984)	1:106:A:PHE:HD1	1:106:A:PHE:HE1	14	0.1
(2,1984)	1:106:A:PHE:HD1	1:106:A:PHE:HE1	15	0.1
(2,1964)	1:15:A:LEU:HD11	1:65:A:PHE:HD1	4	0.1
(2,1879)	1:34:A:VAL:HG21	1:74:A:ILE:H	16	0.1
(2,1866)	1:109:A:ILE:HD13	1:109:A:ILE:HG12	2	0.1
(2,1842)	1:11:A:LEU:HD21	1:11:A:LEU:HB2	1	0.1
(2,1829)	1:22:A:ILE:HG22	1:44:A:LYS:HB3	3	0.1
(2,1811)	1:48:A:ILE:HG12	1:48:A:ILE:HG21	19	0.1
(2,1805)	1:21:A:LEU:HD22	1:21:A:LEU:HB3	13	0.1
(2,1779)	1:83:A:GLU:HB2	1:86:A:LEU:HD23	10	0.1
(2,1778)	1:57:A:VAL:HG12	1:57:A:VAL:HB	14	0.1
(2,1776)	1:22:A:ILE:HB	1:22:A:ILE:HG22	16	0.1
(2,1745)	1:34:A:VAL:HA	1:37:A:LEU:HD21	12	0.1
(2,1733)	1:7:A:VAL:HA	1:7:A:VAL:HB	6	0.1
(2,1733)	1:7:A:VAL:HA	1:7:A:VAL:HB	7	0.1
(2,1713)	1:146:A:VAL:HG11	1:146:A:VAL:HA	14	0.1
(2,1687)	1:96:A:VAL:HG21	1:96:A:VAL:HA	8	0.1
(2,1540)	1:56:A:ILE:HG23	1:56:A:ILE:HA	14	0.1
(2,1474)	1:110:A:LEU:HD22	1:110:A:LEU:H	10	0.1
(2,1447)	1:146:A:VAL:HG13	1:146:A:VAL:H	8	0.1
(2,1440)	1:37:A:LEU:HD12	1:37:A:LEU:H	13	0.1
(2,1440)	1:37:A:LEU:HD13	1:37:A:LEU:H	17	0.1
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	2	0.1
(2,1433)	1:21:A:LEU:HD11	1:21:A:LEU:H	13	0.1
(2,1432)	1:38:A:LEU:HD12	1:39:A:ALA:H	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1432)	1:38:A:LEU:HD12	1:39:A:ALA:H	5	0.1
(2,1399)	1:86:A:LEU:HG	1:86:A:LEU:H	17	0.1
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	3	0.1
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	4	0.1
(2,1328)	1:82:A:VAL:HA	1:83:A:GLU:H	14	0.1
(2,1296)	1:57:A:VAL:HG13	1:65:A:PHE:HB3	1	0.1
(2,1211)	1:177:A:LYS:HD2	1:177:A:LYS:HA	15	0.1
(2,1207)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	2	0.1
(2,1207)	1:109:A:ILE:HG13	1:114:A:ILE:HD11	17	0.1
(2,1110)	1:76:A:ALA:H	1:75:A:ARG:H	4	0.1
(2,1110)	1:76:A:ALA:H	1:75:A:ARG:H	5	0.1
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	7	0.1
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	11	0.1
(2,1019)	1:52:A:GLU:H	1:53:A:LEU:H	14	0.1
(2,1018)	1:38:A:LEU:H	1:37:A:LEU:H	10	0.1
(2,956)	1:58:A:GLU:H	1:57:A:VAL:H	16	0.1
(2,950)	1:76:A:ALA:H	1:76:A:ALA:HA	10	0.1
(2,950)	1:76:A:ALA:H	1:76:A:ALA:HA	13	0.1
(2,811)	1:14:A:VAL:HG23	1:22:A:ILE:H	2	0.1
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	16	0.1
(2,809)	1:22:A:ILE:H	1:22:A:ILE:HG12	19	0.1
(2,673)	1:70:A:ASN:HD22	1:50:A:MET:HG3	16	0.1
(2,673)	1:70:A:ASN:HD22	1:50:A:MET:HG3	20	0.1
(2,655)	1:29:A:ASN:H	1:29:A:ASN:HD22	2	0.1
(2,647)	1:14:A:VAL:H	1:13:A:LEU:HB2	6	0.1
(2,453)	1:34:A:VAL:HB	1:35:A:LYS:H	3	0.1
(2,445)	1:36:A:GLU:H	1:36:A:GLU:HB3	2	0.1
(2,439)	1:55:A:HIS:H	1:54:A:LYS:HB2	8	0.1
(2,431)	1:73:A:LYS:H	1:34:A:VAL:HG21	12	0.1
(2,393)	1:57:A:VAL:H	1:67:A:PHE:HE1	14	0.1
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	1	0.1
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	4	0.1
(2,391)	1:28:A:ALA:H	1:27:A:ASP:HB3	6	0.1
(2,305)	1:42:A:LYS:HA	1:46:A:HIS:H	5	0.1
(2,243)	1:53:A:LEU:H	1:53:A:LEU:HD11	11	0.1
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	16	0.1
(2,227)	1:82:A:VAL:HB	1:82:A:VAL:H	18	0.1
(2,197)	1:24:A:LEU:HA	1:24:A:LEU:H	2	0.1
(2,96)	1:25:A:ASP:HB3	1:25:A:ASP:H	2	0.1
(2,62)	1:178:A:VAL:H	1:177:A:LYS:H	15	0.1
(2,42)	1:148:A:ALA:H	1:148:A:ALA:HB1	17	0.1
(1,125)	1:177:A:LYS:H	1:145:A:SER:O	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:171:A:VAL:H	1:114:A:ILE:O	9	0.1
(1,90)	1:132:A:ARG:N	1:128:A:ILE:O	8	0.1
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	5	0.1
(1,73)	1:110:A:LEU:H	1:106:A:PHE:O	13	0.1
(1,64)	1:99:A:HIS:N	1:144:A:LEU:O	3	0.1
(1,60)	1:77:A:ASN:N	1:64:A:ARG:O	20	0.1
(1,59)	1:77:A:ASN:H	1:64:A:ARG:O	12	0.1
(1,54)	1:66:A:ALA:N	1:75:A:ARG:O	8	0.1
(1,39)	1:54:A:LYS:H	1:50:A:MET:O	20	0.1
(1,29)	1:40:A:LYS:H	1:36:A:GLU:O	7	0.1
(1,24)	1:37:A:LEU:N	1:33:A:PRO:O	11	0.1
(1,7)	1:10:A:PHE:H	1:6:A:LYS:O	1	0.1

10 Dihedral-angle violation analysis [i](#)

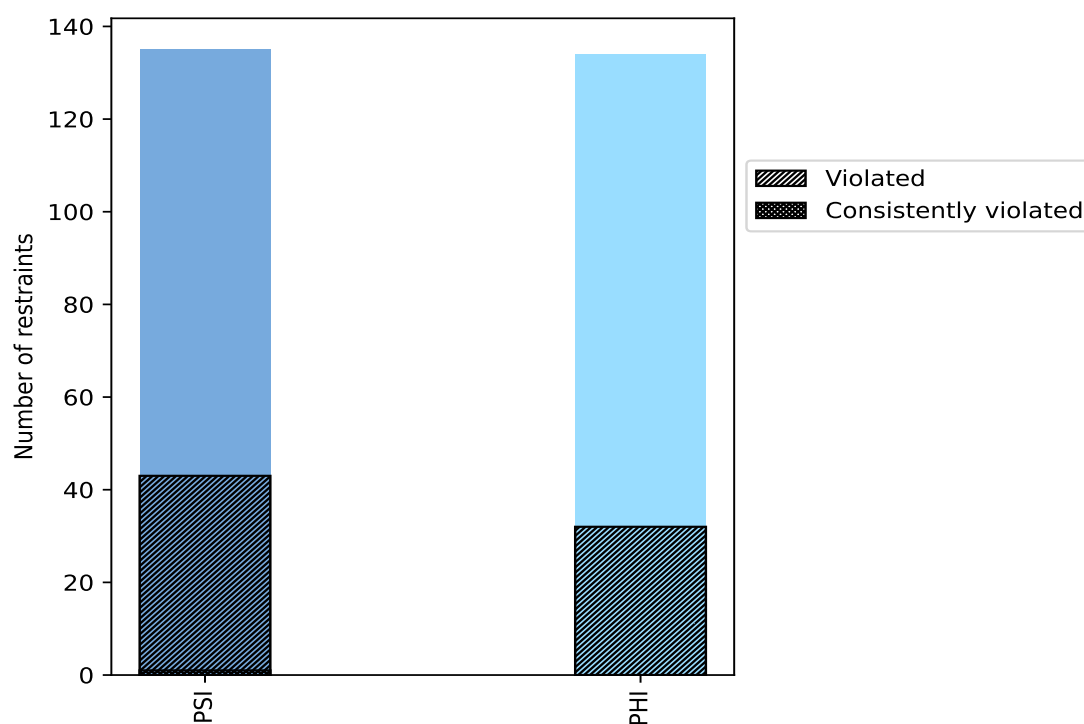
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	135	50.2	43	31.9	16.0	1	0.7	0.4
PHI	134	49.8	32	23.9	11.9	0	0.0	0.0
Total	269	100.0	75	27.9	27.9	1	0.4	0.4

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



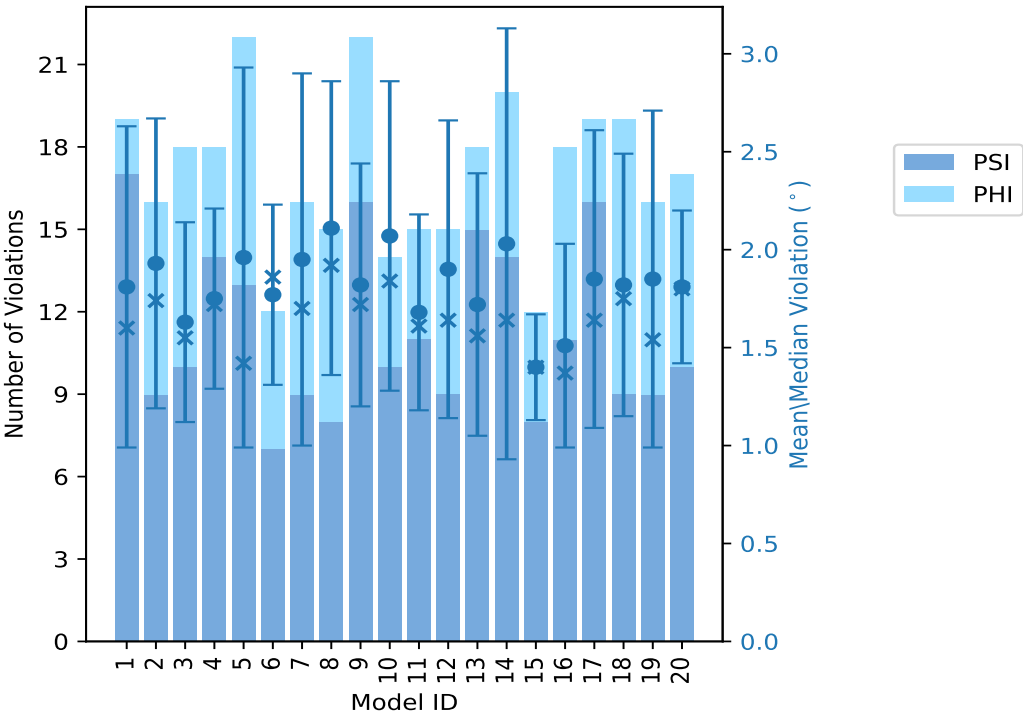
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	17	2	19	1.81	4.13	0.82	1.6
2	9	7	16	1.93	3.25	0.74	1.74
3	10	8	18	1.63	2.57	0.51	1.55
4	14	4	18	1.75	2.54	0.46	1.72
5	13	9	22	1.96	4.43	0.97	1.42
6	7	5	12	1.77	2.57	0.46	1.86
7	9	7	16	1.95	3.98	0.95	1.7
8	8	7	15	2.11	3.6	0.75	1.92
9	16	6	22	1.82	3.36	0.62	1.72
10	10	4	14	2.07	3.51	0.79	1.84
11	11	4	15	1.68	2.57	0.5	1.61
12	9	6	15	1.9	3.69	0.76	1.64
13	15	3	18	1.72	3.47	0.67	1.56
14	14	6	20	2.03	4.91	1.1	1.64
15	8	4	12	1.4	2.01	0.27	1.4
16	11	7	18	1.51	2.86	0.52	1.37
17	16	3	19	1.85	4.12	0.76	1.64
18	9	10	19	1.82	3.76	0.67	1.75
19	9	7	16	1.85	3.93	0.86	1.54
20	10	7	17	1.81	2.41	0.39	1.8

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
10	11	21	1	5.0
8	6	14	2	10.0
7	5	12	3	15.0
1	0	1	4	20.0
1	2	3	5	25.0
3	3	6	6	30.0
2	1	3	7	35.0
3	1	4	8	40.0
0	1	1	9	45.0
1	0	1	10	50.0
2	0	2	11	55.0

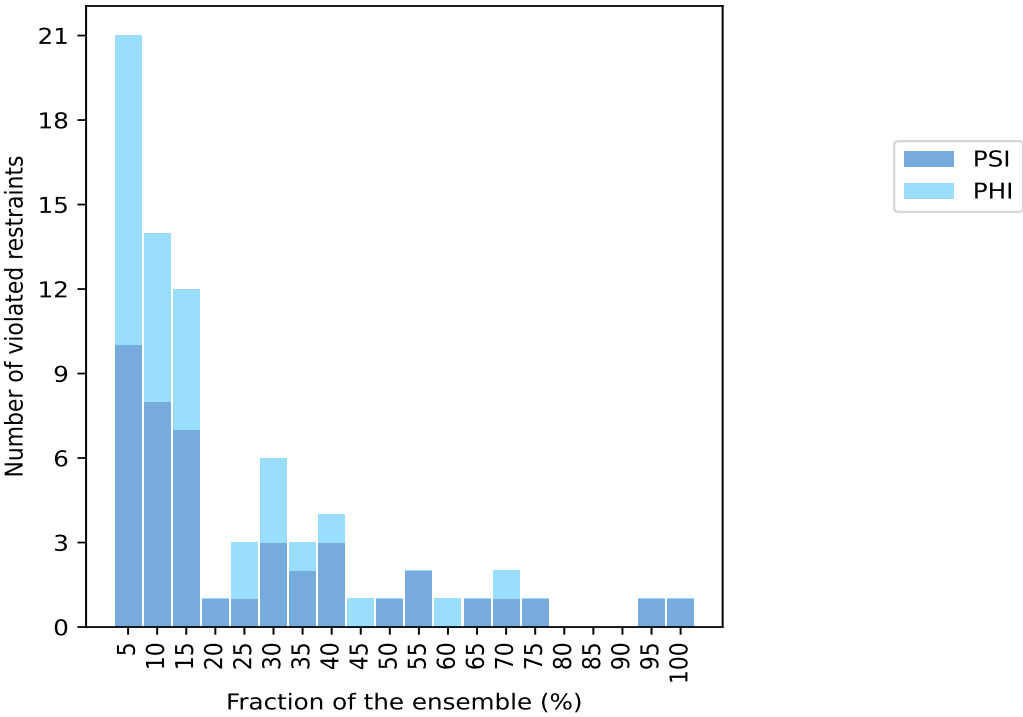
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	1	1	12	60.0
1	0	1	13	65.0
1	1	2	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
1	0	1	19	95.0
1	0	1	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

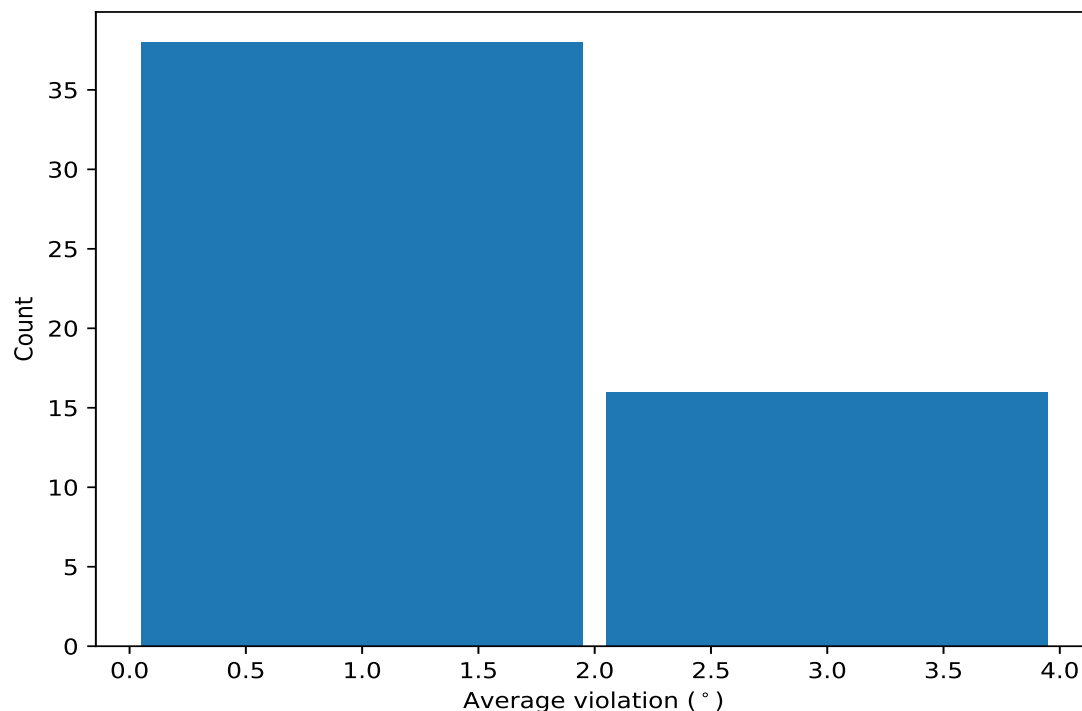


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	20	2.21	0.53	2.12
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	19	1.9	0.48	1.79
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	15	1.7	0.38	1.67
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	14	2.46	1.01	2.24
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	14	1.68	0.5	1.81
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	13	2.45	0.9	2.57
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	12	1.57	0.45	1.44
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	11	2.03	0.47	1.96
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	11	1.83	0.54	1.55
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	10	1.32	0.36	1.15
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	9	1.32	0.37	1.19
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	8	2.65	1.21	2.17
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	8	1.6	0.47	1.5
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	8	1.52	0.42	1.44
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	8	1.3	0.35	1.2
(1,82)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:ILE:N	7	2.92	1.24	2.86
(1,109)	1:60:A:ASN:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	7	2.33	0.8	2.24
(1,195)	1:138:A:HIS:N	1:138:A:HIS:CA	1:138:A:HIS:C	1:139:A:GLY:N	7	2.19	0.47	2.08
(1,158)	1:104:A:LYS:C	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	6	2.42	0.46	2.46
(1,138)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASN:N	6	2.36	0.74	2.1

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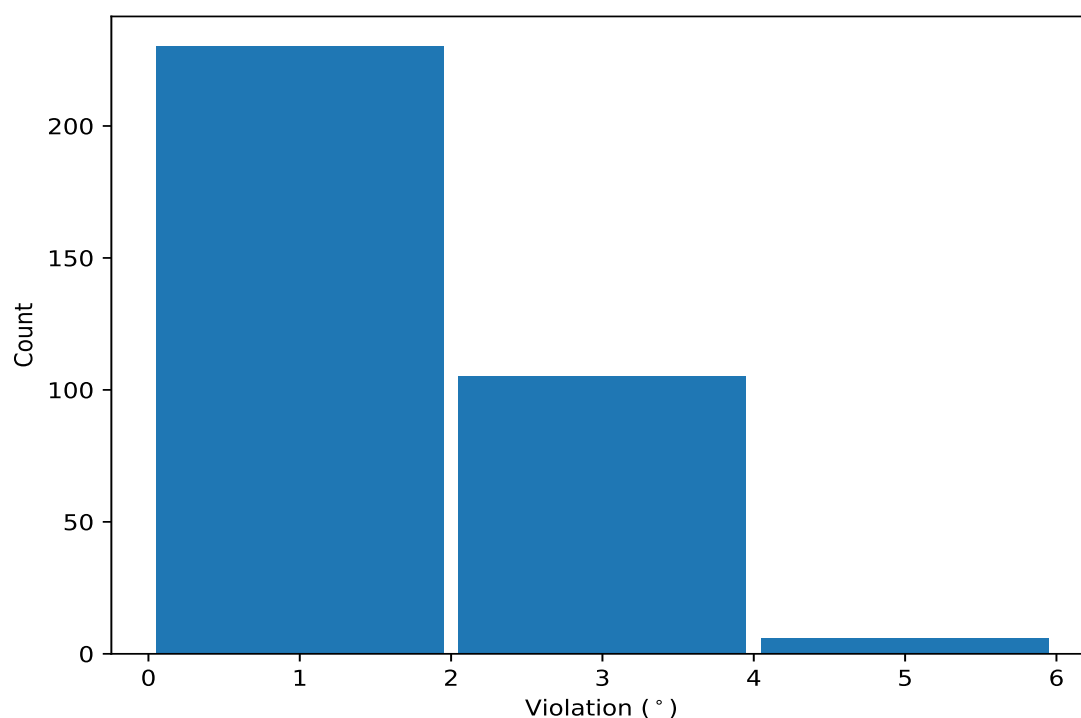
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,231)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:SER:N	6	2.28	0.9	2.21
(1,154)	1:102:A:ALA:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	6	1.62	0.42	1.65
(1,58)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:VAL:N	6	1.59	0.32	1.74
(1,39)	1:22:A:ILE:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	6	1.19	0.09	1.23
(1,139)	1:76:A:ALA:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	5	2.36	0.79	2.26
(1,212)	1:150:A:GLY:C	1:151:A:MET:N	1:151:A:MET:CA	1:151:A:MET:C	5	1.59	0.28	1.67
(1,201)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:SER:N	5	1.58	0.61	1.14
(1,34)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:LEU:N	4	1.41	0.14	1.36
(1,83)	1:47:A:GLY:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	3	2.42	0.42	2.42
(1,50)	1:29:A:ASN:N	1:29:A:ASN:CA	1:29:A:ASN:C	1:30:A:GLY:N	3	2.38	0.26	2.48
(1,207)	1:148:A:ALA:N	1:148:A:ALA:CA	1:148:A:ALA:C	1:149:A:LYS:N	3	2.27	1.53	1.21
(1,206)	1:147:A:ASP:C	1:148:A:ALA:N	1:148:A:ALA:CA	1:148:A:ALA:C	3	1.61	0.18	1.65
(1,173)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	3	1.6	0.25	1.61
(1,81)	1:46:A:HIS:C	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	3	1.54	0.19	1.41
(1,80)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:GLY:N	3	1.46	0.4	1.24
(1,18)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:LEU:N	3	1.38	0.28	1.44
(1,230)	1:159:A:TYR:C	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	3	1.32	0.32	1.1
(1,41)	1:23:A:GLY:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	3	1.29	0.25	1.14
(1,191)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:ARG:N	3	1.2	0.04	1.19
(1,22)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:LEU:N	3	1.15	0.09	1.2
(1,107)	1:59:A:THR:C	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	2	2.68	0.42	2.68
(1,112)	1:62:A:LYS:N	1:62:A:LYS:CA	1:62:A:LYS:C	1:63:A:LYS:N	2	1.73	0.72	1.73
(1,223)	1:156:A:PHE:N	1:156:A:PHE:CA	1:156:A:PHE:C	1:157:A:ASP:N	2	1.57	0.05	1.57
(1,226)	1:157:A:ASP:C	1:158:A:PHE:N	1:158:A:PHE:CA	1:158:A:PHE:C	2	1.56	0.03	1.56
(1,147)	1:94:A:PRO:N	1:94:A:PRO:CA	1:94:A:PRO:C	1:95:A:ALA:N	2	1.56	0.07	1.56
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:ILE:N	2	1.4	0.17	1.4
(1,145)	1:93:A:PRO:N	1:93:A:PRO:CA	1:93:A:PRO:C	1:94:A:PRO:N	2	1.35	0.0	1.35
(1,79)	1:43:A:ALA:C	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	2	1.31	0.05	1.31
(1,266)	1:94:A:PRO:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	2	1.3	0.0	1.3
(1,221)	1:155:A:GLY:N	1:155:A:GLY:CA	1:155:A:GLY:C	1:156:A:PHE:N	2	1.27	0.06	1.27
(1,105)	1:58:A:GLU:C	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	2	1.14	0.1	1.14
(1,159)	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	1:106:A:PHE:N	2	1.09	0.01	1.09
(1,228)	1:158:A:PHE:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	2	1.04	0.01	1.04
(1,4)	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	1:6:A:LYS:N	2	1.02	0.01	1.02

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	14	4.91
(1,82)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:ILE:N	14	4.63
(1,207)	1:148:A:ALA:N	1:148:A:ALA:CA	1:148:A:ALA:C	1:149:A:LYS:N	5	4.43
(1,82)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:ILE:N	5	4.26
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	1	4.13
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	17	4.12
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	7	3.98
(1,109)	1:60:A:ASN:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	19	3.93
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	1	3.85
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	7	3.81
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	18	3.76
(1,82)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:ILE:N	12	3.69
(1,138)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASN:N	8	3.6
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	10	3.51
(1,231)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:SER:N	13	3.47
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	10	3.47
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	9	3.36
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	7	3.36
(1,139)	1:76:A:ALA:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	8	3.28
(1,139)	1:76:A:ALA:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	2	3.25
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	19	3.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,195)	1:138:A:HIS:N	1:138:A:HIS:CA	1:138:A:HIS:C	1:139:A:GLY:N	5	3.18
(1,231)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:SER:N	9	3.15
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	19	3.11
(1,138)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASN:N	2	3.09
(1,107)	1:59:A:THR:C	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	10	3.09
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	12	3.07
(1,240)	1:164:A:GLY:C	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	5	3.01
(1,158)	1:104:A:LYS:C	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	2	3.01
(1,83)	1:47:A:GLY:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	14	2.93
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	8	2.91
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	12	2.9
(1,82)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:ILE:N	16	2.86
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	14	2.84
(1,231)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:SER:N	2	2.82
(1,158)	1:104:A:LYS:C	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	16	2.8
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	14	2.79
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	17	2.76
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	17	2.72
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	5	2.7
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	8	2.67
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	19	2.65
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	18	2.64
(1,50)	1:29:A:ASN:N	1:29:A:ASN:CA	1:29:A:ASN:C	1:30:A:GLY:N	10	2.64
(1,109)	1:60:A:ASN:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	7	2.63
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	17	2.59
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	8	2.57
(1,158)	1:104:A:LYS:C	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	11	2.57
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	3	2.57
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	6	2.57
(1,201)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:SER:N	8	2.55
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	4	2.54
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	13	2.54
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	2	2.52
(1,50)	1:29:A:ASN:N	1:29:A:ASN:CA	1:29:A:ASN:C	1:30:A:GLY:N	9	2.48
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	11	2.48
(1,112)	1:62:A:LYS:N	1:62:A:LYS:CA	1:62:A:LYS:C	1:63:A:LYS:N	18	2.45
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	4	2.45
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	4	2.42
(1,83)	1:47:A:GLY:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	5	2.42
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	1	2.41
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	20	2.41
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	20	2.41
(1,195)	1:138:A:HIS:N	1:138:A:HIS:CA	1:138:A:HIS:C	1:139:A:GLY:N	6	2.4
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	11	2.37
(1,154)	1:102:A:ALA:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	3	2.37
(1,109)	1:60:A:ASN:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	17	2.37
(1,158)	1:104:A:LYS:C	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	3	2.35
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	14	2.35
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	5	2.33
(1,144)	1:92:A:VAL:C	1:93:A:PRO:N	1:93:A:PRO:CA	1:93:A:PRO:C	9	2.32
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	14	2.32

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	9	2.3
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	10	2.29
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	3	2.27
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	20	2.27
(1,139)	1:76:A:ALA:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	18	2.26
(1,107)	1:59:A:THR:C	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	18	2.26
(1,109)	1:60:A:ASN:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	9	2.24
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	13	2.22
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	13	2.22
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	4	2.21
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	11	2.2
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	12	2.2
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	20	2.18
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	3	2.17
(1,158)	1:104:A:LYS:C	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	18	2.15
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	20	2.15
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	13	2.15
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	13	2.14
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	10	2.14
(1,195)	1:138:A:HIS:N	1:138:A:HIS:CA	1:138:A:HIS:C	1:139:A:GLY:N	13	2.13
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	9	2.13
(1,109)	1:60:A:ASN:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	12	2.12
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	8	2.12
(1,138)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASN:N	18	2.11
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	6	2.11
(1,138)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASN:N	13	2.1
(1,195)	1:138:A:HIS:N	1:138:A:HIS:CA	1:138:A:HIS:C	1:139:A:GLY:N	4	2.08
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	19	2.08
(1,82)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:ILE:N	17	2.07
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	12	2.06
(1,195)	1:138:A:HIS:N	1:138:A:HIS:CA	1:138:A:HIS:C	1:139:A:GLY:N	2	2.06
(1,201)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:SER:N	20	2.05
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	1	2.03
(1,50)	1:29:A:ASN:N	1:29:A:ASN:CA	1:29:A:ASN:C	1:30:A:GLY:N	18	2.03
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	5	2.02
(1,109)	1:60:A:ASN:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	6	2.02
(1,80)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:GLY:N	20	2.02
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	15	2.01
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	4	2.0
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	6	1.96
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	10	1.95
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	17	1.94
(1,232)	1:160:A:LEU:C	1:161:A:SER:N	1:161:A:SER:CA	1:161:A:SER:C	7	1.92
(1,212)	1:150:A:GLY:C	1:151:A:MET:N	1:151:A:MET:CA	1:151:A:MET:C	3	1.92
(1,58)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:VAL:N	8	1.92
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	16	1.92
(1,195)	1:138:A:HIS:N	1:138:A:HIS:CA	1:138:A:HIS:C	1:139:A:GLY:N	1	1.91
(1,173)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	9	1.91
(1,83)	1:47:A:GLY:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	12	1.91
(1,82)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:ILE:N	20	1.91
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	11	1.91

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	14	1.9
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	4	1.9
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	9	1.9
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	6	1.89
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	18	1.89
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	2	1.89
(1,229)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:LEU:N	14	1.88
(1,58)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:VAL:N	4	1.84
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	7	1.84
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	1	1.83
(1,212)	1:150:A:GLY:C	1:151:A:MET:N	1:151:A:MET:CA	1:151:A:MET:C	4	1.82
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	6	1.82
(1,206)	1:147:A:ASP:C	1:148:A:ALA:N	1:148:A:ALA:CA	1:148:A:ALA:C	7	1.8
(1,81)	1:46:A:HIS:C	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	20	1.8
(1,58)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:VAL:N	3	1.8
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	5	1.79
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	2	1.79
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	16	1.79
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	1	1.79
(1,230)	1:159:A:TYR:C	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	8	1.77
(1,154)	1:102:A:ALA:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	19	1.77
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	18	1.75
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	14	1.74
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	9	1.74
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	10	1.74
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	7	1.73
(1,154)	1:102:A:ALA:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	11	1.73
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	9	1.73
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	17	1.71
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	9	1.71
(1,219)	1:154:A:GLY:N	1:154:A:GLY:CA	1:154:A:GLY:C	1:155:A:GLY:N	17	1.7
(1,58)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:VAL:N	2	1.69
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	7	1.68
(1,18)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:LEU:N	11	1.68
(1,212)	1:150:A:GLY:C	1:151:A:MET:N	1:151:A:MET:CA	1:151:A:MET:C	19	1.67
(1,138)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASN:N	1	1.67
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	3	1.67
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	7	1.66
(1,206)	1:147:A:ASP:C	1:148:A:ALA:N	1:148:A:ALA:CA	1:148:A:ALA:C	8	1.65
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	12	1.64
(1,41)	1:23:A:GLY:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	20	1.64
(1,34)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:LEU:N	15	1.64
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	17	1.64
(1,147)	1:94:A:PRO:N	1:94:A:PRO:CA	1:94:A:PRO:C	1:95:A:ALA:N	4	1.63
(1,136)	1:75:A:ARG:N	1:75:A:ARG:CA	1:75:A:ARG:C	1:76:A:ALA:N	20	1.63
(1,223)	1:156:A:PHE:N	1:156:A:PHE:CA	1:156:A:PHE:C	1:157:A:ASP:N	17	1.62
(1,173)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	1	1.61
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	11	1.61
(1,158)	1:104:A:LYS:C	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	19	1.61
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	11	1.61
(1,231)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:SER:N	20	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,139)	1:76:A:ALA:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	13	1.6
(1,138)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:ASN:N	9	1.6
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	1	1.6
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	4	1.59
(1,226)	1:157:A:ASP:C	1:158:A:PHE:N	1:158:A:PHE:CA	1:158:A:PHE:C	18	1.58
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	9	1.58
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	4	1.58
(1,195)	1:138:A:HIS:N	1:138:A:HIS:CA	1:138:A:HIS:C	1:139:A:GLY:N	15	1.57
(1,154)	1:102:A:ALA:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	16	1.57
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	1	1.57
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	3	1.57
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	5	1.56
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:ILE:N	1	1.56
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	15	1.55
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	10	1.55
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	14	1.55
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	8	1.55
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	1	1.54
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	12	1.54
(1,226)	1:157:A:ASP:C	1:158:A:PHE:N	1:158:A:PHE:CA	1:158:A:PHE:C	20	1.53
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	3	1.53
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	13	1.53
(1,223)	1:156:A:PHE:N	1:156:A:PHE:CA	1:156:A:PHE:C	1:157:A:ASP:N	4	1.52
(1,231)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:SER:N	10	1.51
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	18	1.51
(1,146)	1:93:A:PRO:C	1:94:A:PRO:N	1:94:A:PRO:CA	1:94:A:PRO:C	6	1.51
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	8	1.51
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	6	1.5
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	15	1.5
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	17	1.49
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	19	1.48
(1,147)	1:94:A:PRO:N	1:94:A:PRO:CA	1:94:A:PRO:C	1:95:A:ALA:N	14	1.48
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	17	1.46
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	4	1.45
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	2	1.44
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	18	1.44
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	5	1.44
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	2	1.44
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	14	1.44
(1,18)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:LEU:N	16	1.44
(1,139)	1:76:A:ALA:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	9	1.43
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	5	1.41
(1,81)	1:46:A:HIS:C	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	16	1.41
(1,25)	1:15:A:LEU:C	1:16:A:ARG:N	1:16:A:ARG:CA	1:16:A:ARG:C	5	1.41
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	15	1.4
(1,177)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:THR:N	5	1.4
(1,157)	1:104:A:LYS:N	1:104:A:LYS:CA	1:104:A:LYS:C	1:105:A:ASN:N	15	1.4
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	9	1.4
(1,81)	1:46:A:HIS:C	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	5	1.4
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	16	1.39
(1,34)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:LEU:N	17	1.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	12	1.38
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	16	1.37
(1,206)	1:147:A:ASP:C	1:148:A:ALA:N	1:148:A:ALA:CA	1:148:A:ALA:C	14	1.37
(1,244)	1:166:A:TRP:C	1:167:A:LEU:N	1:167:A:LEU:CA	1:167:A:LEU:C	18	1.36
(1,108)	1:60:A:ASN:N	1:60:A:ASN:CA	1:60:A:ASN:C	1:61:A:SER:N	16	1.36
(1,79)	1:43:A:ALA:C	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	5	1.36
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	12	1.36
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	15	1.36
(1,145)	1:93:A:PRO:N	1:93:A:PRO:CA	1:93:A:PRO:C	1:94:A:PRO:N	5	1.35
(1,145)	1:93:A:PRO:N	1:93:A:PRO:CA	1:93:A:PRO:C	1:94:A:PRO:N	20	1.35
(1,74)	1:41:A:MET:N	1:41:A:MET:CA	1:41:A:MET:C	1:42:A:LYS:N	16	1.35
(1,251)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:VAL:N	5	1.33
(1,221)	1:155:A:GLY:N	1:155:A:GLY:CA	1:155:A:GLY:C	1:156:A:PHE:N	9	1.33
(1,34)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:LEU:N	10	1.33
(1,241)	1:165:A:VAL:N	1:165:A:VAL:CA	1:165:A:VAL:C	1:166:A:TRP:N	11	1.32
(1,266)	1:94:A:PRO:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	4	1.3
(1,266)	1:94:A:PRO:C	1:95:A:ALA:N	1:95:A:ALA:CA	1:95:A:ALA:C	13	1.3
(1,212)	1:150:A:GLY:C	1:151:A:MET:N	1:151:A:MET:CA	1:151:A:MET:C	20	1.3
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	1	1.29
(1,173)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	19	1.29
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	10	1.29
(1,34)	1:20:A:ALA:N	1:20:A:ALA:CA	1:20:A:ALA:C	1:21:A:LEU:N	9	1.29
(1,39)	1:22:A:ILE:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	16	1.28
(1,38)	1:22:A:ILE:N	1:22:A:ILE:CA	1:22:A:ILE:C	1:23:A:GLY:N	2	1.28
(1,39)	1:22:A:ILE:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	2	1.27
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	20	1.26
(1,79)	1:43:A:ALA:C	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	20	1.26
(1,191)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:ARG:N	14	1.25
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	19	1.24
(1,105)	1:58:A:GLU:C	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	8	1.24
(1,80)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:GLY:N	17	1.24
(1,39)	1:22:A:ILE:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	10	1.23
(1,36)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:ILE:N	3	1.23
(1,22)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:LEU:N	11	1.23
(1,212)	1:150:A:GLY:C	1:151:A:MET:N	1:151:A:MET:CA	1:151:A:MET:C	12	1.22
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	13	1.22
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	1	1.22
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	1	1.22
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	11	1.22
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	16	1.22
(1,39)	1:22:A:ILE:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	6	1.22
(1,221)	1:155:A:GLY:N	1:155:A:GLY:CA	1:155:A:GLY:C	1:156:A:PHE:N	16	1.21
(1,207)	1:148:A:ALA:N	1:148:A:ALA:CA	1:148:A:ALA:C	1:149:A:LYS:N	9	1.21
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	3	1.21
(1,58)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:VAL:N	12	1.21
(1,154)	1:102:A:ALA:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	18	1.2
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	19	1.2
(1,22)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:LEU:N	7	1.2
(1,243)	1:166:A:TRP:N	1:166:A:TRP:CA	1:166:A:TRP:C	1:167:A:LEU:N	17	1.19
(1,222)	1:155:A:GLY:C	1:156:A:PHE:N	1:156:A:PHE:CA	1:156:A:PHE:C	4	1.19
(1,191)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:ARG:N	7	1.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	8	1.19
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	3	1.19
(1,114)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:ARG:N	19	1.19
(1,19)	1:12:A:SER:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	7	1.19
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	13	1.18
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	10	1.18
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	15	1.18
(1,207)	1:148:A:ALA:N	1:148:A:ALA:CA	1:148:A:ALA:C	1:149:A:LYS:N	11	1.17
(1,235)	1:162:A:ASN:N	1:162:A:ASN:CA	1:162:A:ASN:C	1:163:A:ASN:N	6	1.16
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	5	1.16
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	17	1.16
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	2	1.16
(1,191)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:ARG:N	13	1.15
(1,201)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:SER:N	1	1.14
(1,41)	1:23:A:GLY:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	3	1.14
(1,201)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:SER:N	3	1.13
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	8	1.13
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	19	1.13
(1,205)	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	1:148:A:ALA:N	9	1.12
(1,231)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:SER:N	19	1.11
(1,80)	1:44:A:LYS:N	1:44:A:LYS:CA	1:44:A:LYS:C	1:45:A:GLY:N	14	1.11
(1,230)	1:159:A:TYR:C	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	6	1.1
(1,204)	1:146:A:VAL:C	1:147:A:ASP:N	1:147:A:ASP:CA	1:147:A:ASP:C	12	1.1
(1,202)	1:144:A:LEU:C	1:145:A:SER:N	1:145:A:SER:CA	1:145:A:SER:C	7	1.1
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	2	1.1
(1,159)	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	1:106:A:PHE:N	18	1.1
(1,41)	1:23:A:GLY:C	1:24:A:LEU:N	1:24:A:LEU:CA	1:24:A:LEU:C	5	1.1
(1,230)	1:159:A:TYR:C	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	18	1.09
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	11	1.09
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:GLN:N	12	1.09
(1,58)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:VAL:N	5	1.09
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	9	1.09
(1,39)	1:22:A:ILE:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	15	1.09
(1,159)	1:105:A:ASN:N	1:105:A:ASN:CA	1:105:A:ASN:C	1:106:A:PHE:N	11	1.08
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	3	1.08
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	5	1.07
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	3	1.07
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	14	1.07
(1,168)	1:109:A:ILE:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	16	1.07
(1,154)	1:102:A:ALA:C	1:103:A:GLU:N	1:103:A:GLU:CA	1:103:A:GLU:C	2	1.07
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	1	1.07
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	7	1.07
(1,43)	1:24:A:LEU:C	1:25:A:ASP:N	1:25:A:ASP:CA	1:25:A:ASP:C	15	1.06
(1,28)	1:17:A:HIS:N	1:17:A:HIS:CA	1:17:A:HIS:C	1:18:A:ASN:N	16	1.06
(1,228)	1:158:A:PHE:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	18	1.05
(1,201)	1:144:A:LEU:N	1:144:A:LEU:CA	1:144:A:LEU:C	1:145:A:SER:N	15	1.05
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	7	1.05
(1,228)	1:158:A:PHE:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	14	1.04
(1,141)	1:91:A:GLN:N	1:91:A:GLN:CA	1:91:A:GLN:C	1:92:A:VAL:N	16	1.04
(1,105)	1:58:A:GLU:C	1:59:A:THR:N	1:59:A:THR:CA	1:59:A:THR:C	3	1.04
(1,86)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:MET:N	17	1.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,264)	1:176:A:ILE:C	1:177:A:LYS:N	1:177:A:LYS:CA	1:177:A:LYS:C	18	1.03
(1,109)	1:60:A:ASN:C	1:61:A:SER:N	1:61:A:SER:CA	1:61:A:SER:C	14	1.03
(1,39)	1:22:A:ILE:C	1:23:A:GLY:N	1:23:A:GLY:CA	1:23:A:GLY:C	14	1.03
(1,4)	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	1:6:A:LYS:N	4	1.03
(1,220)	1:154:A:GLY:C	1:155:A:GLY:N	1:155:A:GLY:CA	1:155:A:GLY:C	17	1.02
(1,102)	1:57:A:VAL:N	1:57:A:VAL:CA	1:57:A:VAL:C	1:58:A:GLU:N	13	1.02
(1,90)	1:51:A:GLU:N	1:51:A:GLU:CA	1:51:A:GLU:C	1:52:A:GLU:N	13	1.02
(1,22)	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1:15:A:LEU:N	19	1.02
(1,4)	1:5:A:VAL:N	1:5:A:VAL:CA	1:5:A:VAL:C	1:6:A:LYS:N	16	1.02
(1,236)	1:162:A:ASN:C	1:163:A:ASN:N	1:163:A:ASN:CA	1:163:A:ASN:C	9	1.01
(1,112)	1:62:A:LYS:N	1:62:A:LYS:CA	1:62:A:LYS:C	1:63:A:LYS:N	13	1.01
(1,82)	1:47:A:GLY:N	1:47:A:GLY:CA	1:47:A:GLY:C	1:48:A:ILE:N	1	1.01
(1,18)	1:12:A:SER:N	1:12:A:SER:CA	1:12:A:SER:C	1:13:A:LEU:N	4	1.01
(1,124)	1:69:A:GLU:N	1:69:A:GLU:CA	1:69:A:GLU:C	1:70:A:ASN:N	13	1.0