Full wwPDB X-ray Structure Validation Report (i)

May 26, 2025 – 05:59 AM EDT

PDB ID	:	2NVY / pdb_00002nvy
Title	:	RNA Polymerase II form II in 150 mM Mn+2
Authors	:	Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on	:	2006-11-13
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

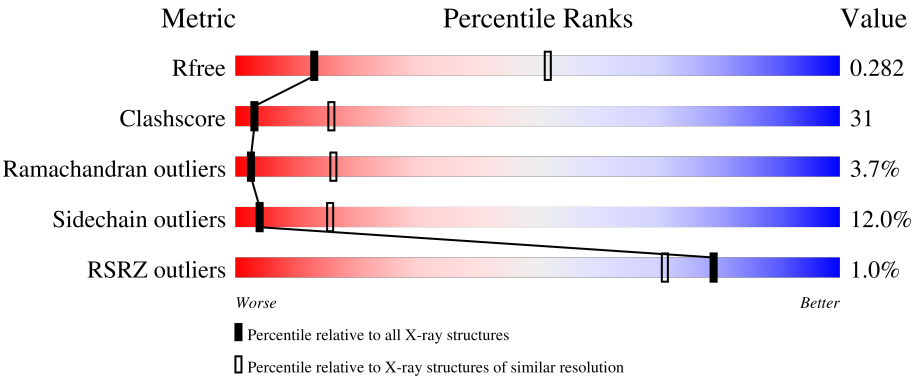
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	% 38% 36% 8% · 18%
2	B	1224	% 41% 42% 6% 11%
3	C	318	34% 39% 10% 16%
4	E	215	53% 40% 7%
5	F	155	21% 32% · 46%

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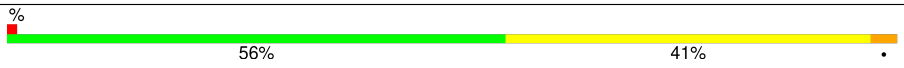
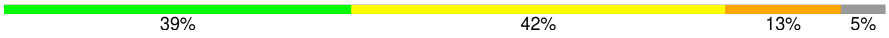
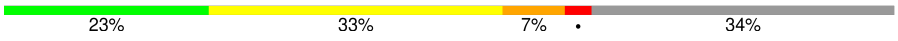
Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 28289 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11154	7023	1952	2118	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1094	Total	C	N	O	S	0	0	0
			8711	5525	1519	1614	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Zn	0	0
			2	2		
11	B	1	Total	Zn	0	0
			1	1		
11	C	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	J	1	Total	Zn	0	0
			1	1		
11	L	1	Total	Zn	0	0
			1	1		

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

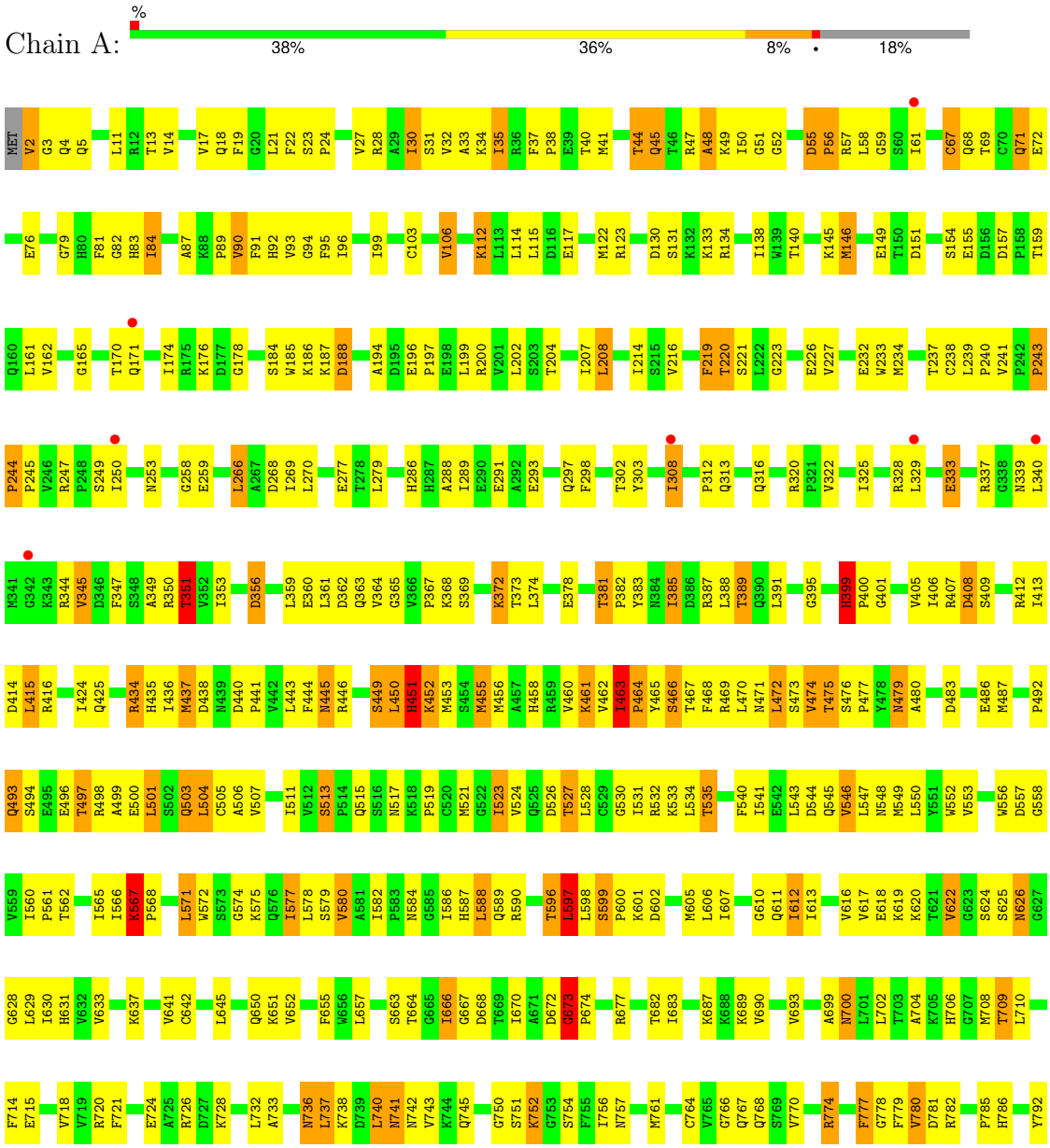
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	2	Total Mn 2 2	0	0

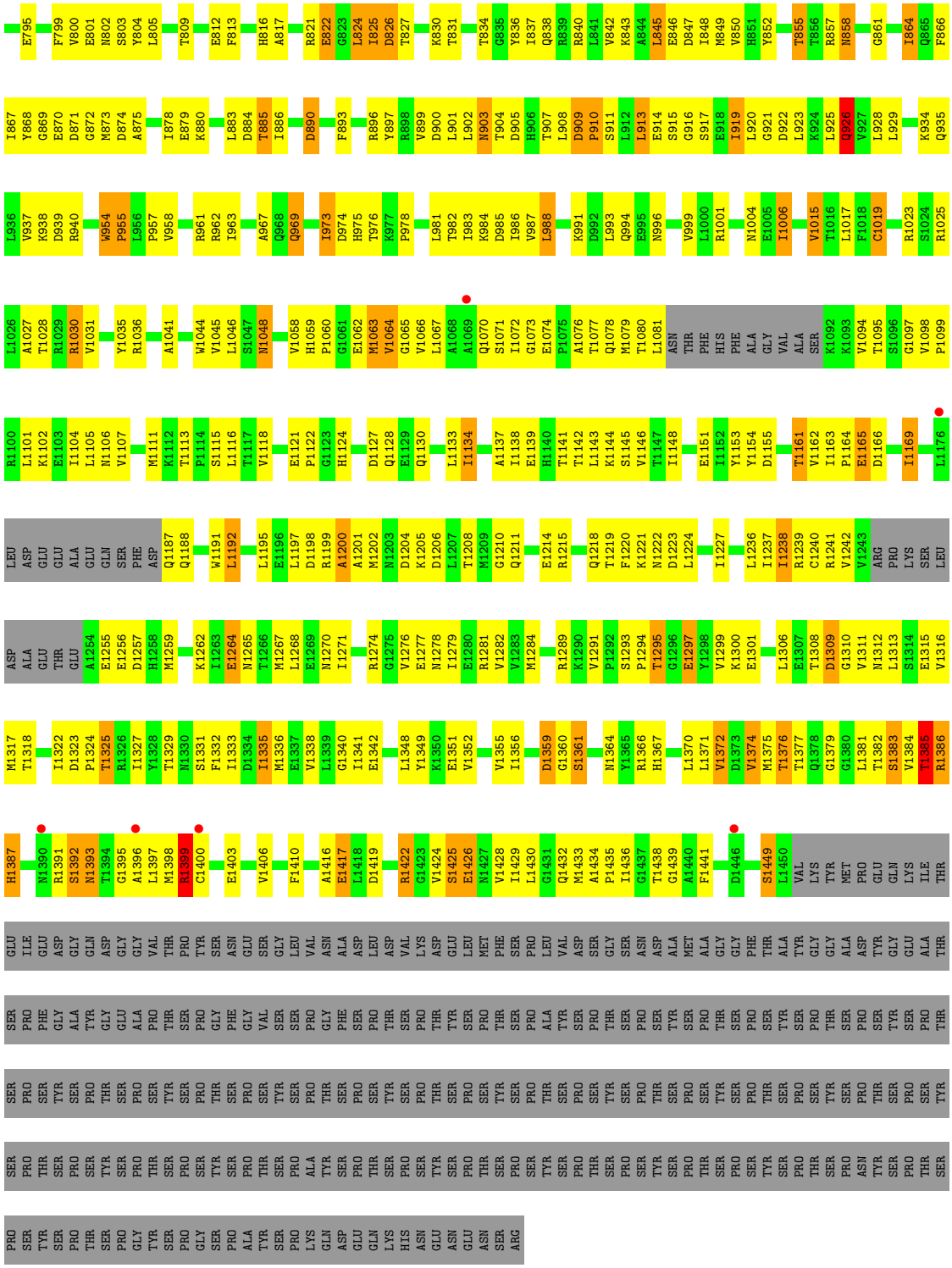
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase II largest subunit

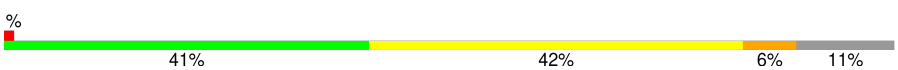
Chain A:

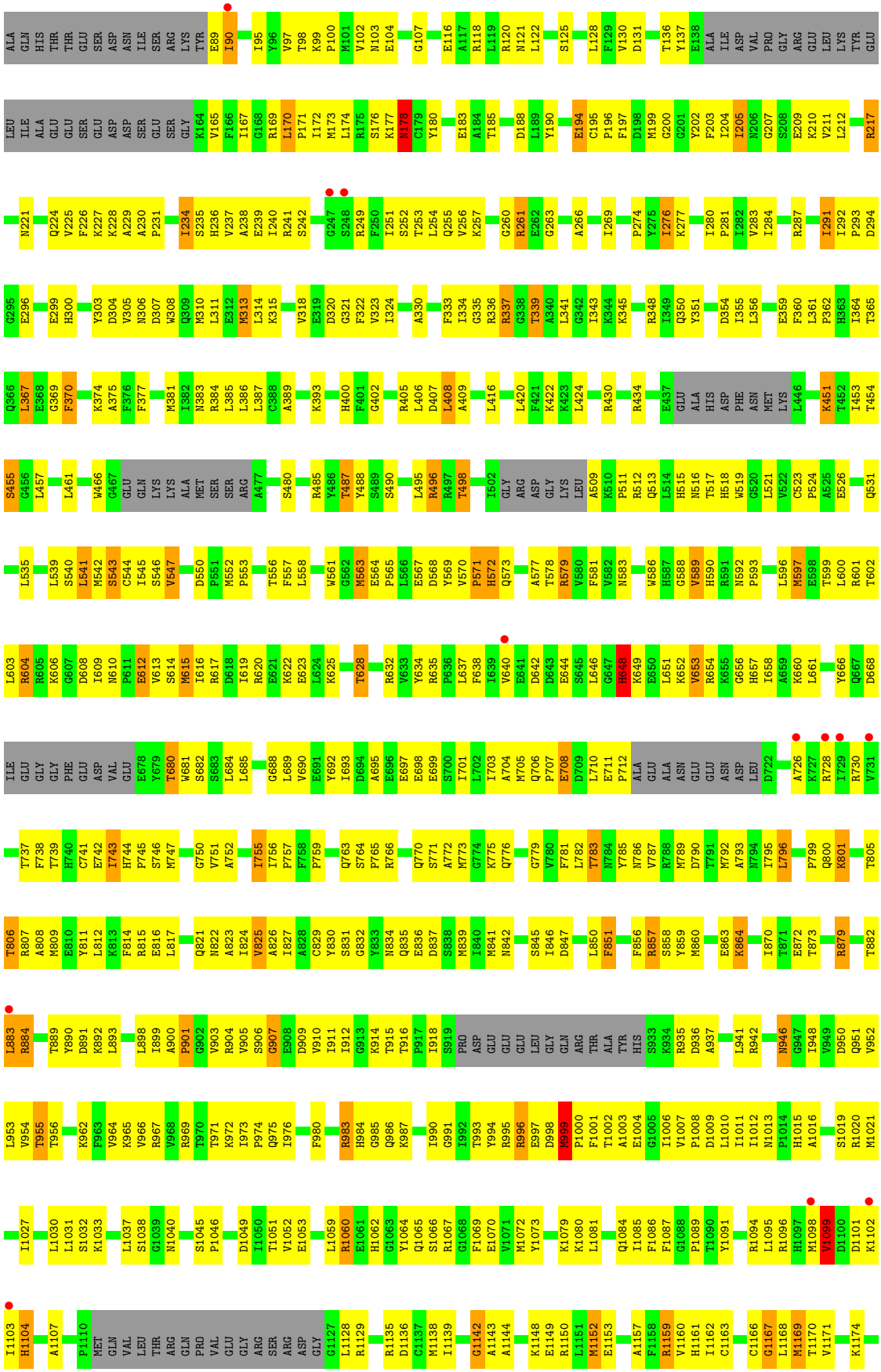


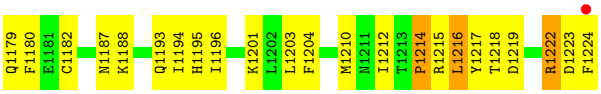


• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:

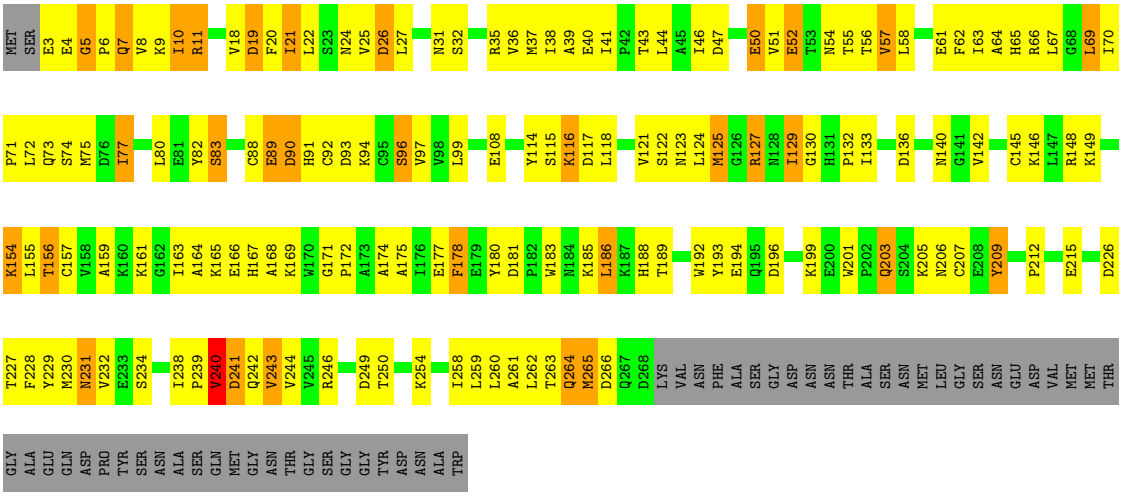






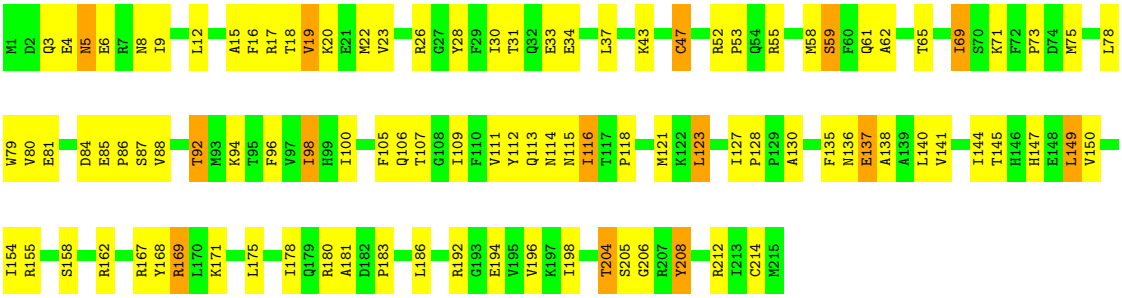
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:



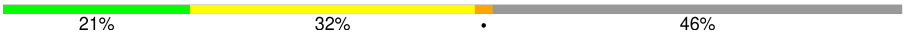
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

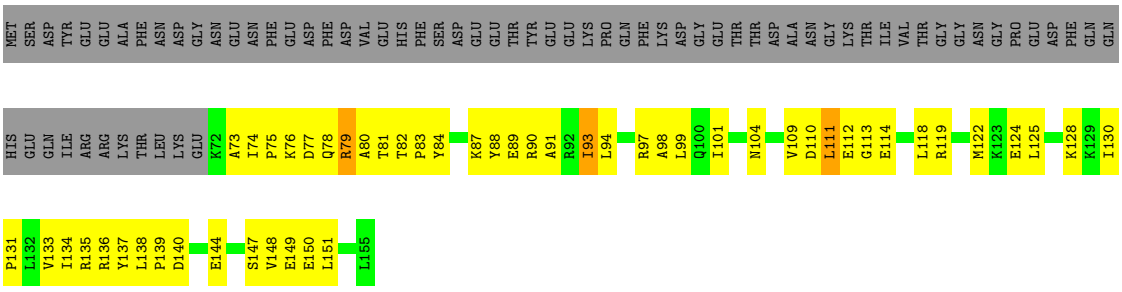
Chain E:



• Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

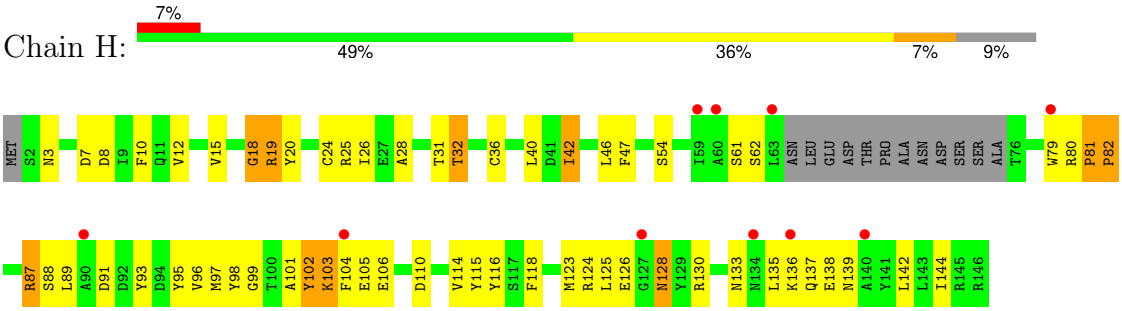
Chain F:





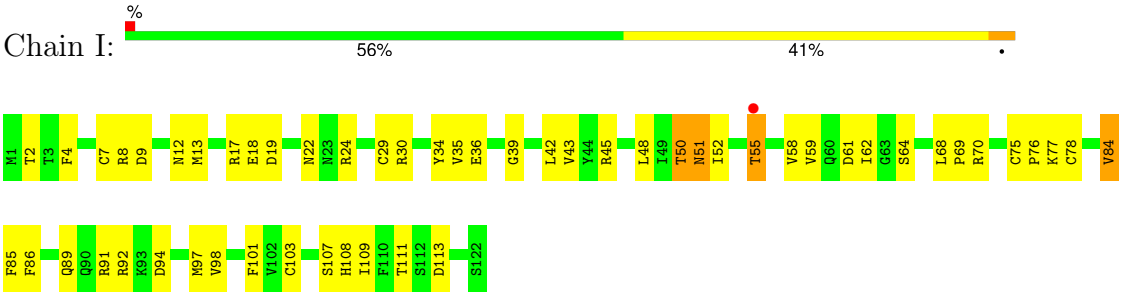
• Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



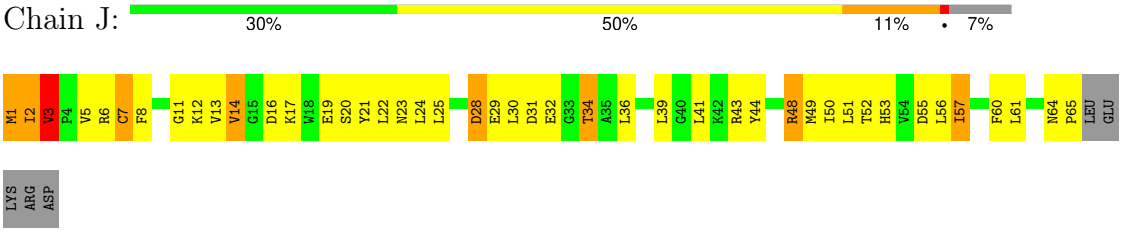
• Molecule 7: DNA-directed RNA polymerase II subunit 9

Chain I:



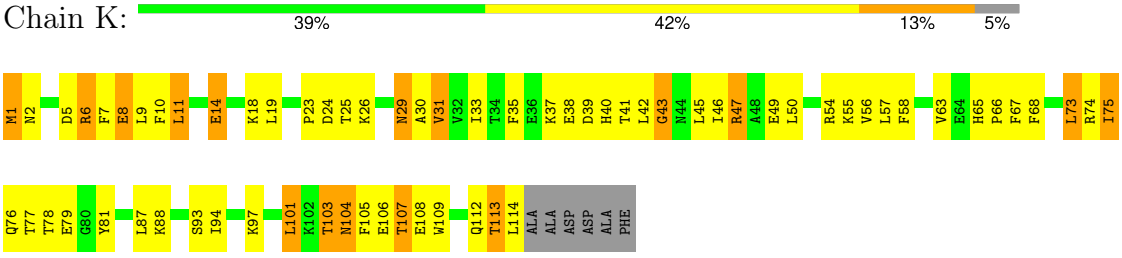
• Molecule 8: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



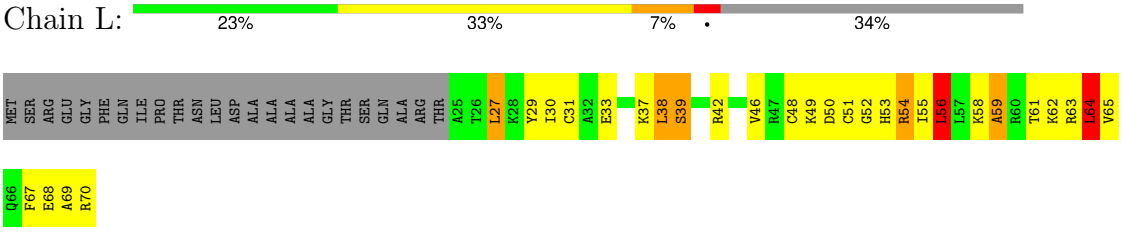
• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



• Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	118.04Å 218.91Å 369.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.40) 97.8 (40.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.249 , 0.323 0.229 , 0.282	Depositor DCC
R_{free} test set	1970 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	89.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	28289	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.74	1/11352 (0.0%)	1.03	34/15352 (0.2%)
2	B	0.72	0/8882	0.96	10/11976 (0.1%)
3	C	0.71	0/2133	0.96	7/2891 (0.2%)
4	E	0.73	1/1796 (0.1%)	1.06	7/2416 (0.3%)
5	F	0.73	0/691	0.99	2/933 (0.2%)
6	H	0.63	1/1086 (0.1%)	0.90	2/1470 (0.1%)
7	I	0.65	0/1016	0.91	1/1365 (0.1%)
8	J	0.73	0/541	1.06	1/727 (0.1%)
9	K	0.65	0/937	0.92	1/1265 (0.1%)
10	L	0.62	0/366	0.91	0/485
All	All	0.72	3/28800 (0.0%)	0.99	65/38880 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1449	SER	CB-OG	8.26	1.58	1.42
6	H	87	ARG	CA-C	6.01	1.55	1.52
4	E	128	PRO	CA-C	5.61	1.54	1.51

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	673	GLY	CA-C-N	8.26	127.56	118.97
1	A	673	GLY	C-N-CA	8.26	127.56	118.97
1	A	244	PRO	N-CA-C	8.26	120.78	110.70
1	A	463	ILE	CA-C-N	8.11	129.98	119.84
1	A	463	ILE	C-N-CA	8.11	129.98	119.84
1	A	237	THR	N-CA-C	-7.89	104.26	114.04
4	E	127	ILE	CA-C-N	7.41	125.07	119.66
4	E	127	ILE	C-N-CA	7.41	125.07	119.66
6	H	3	ASN	N-CA-C	6.91	118.69	108.60
5	F	74	ILE	CA-C-N	6.69	126.67	119.78
5	F	74	ILE	C-N-CA	6.69	126.67	119.78
1	A	395	GLY	CA-C-N	6.67	126.36	119.56
1	A	395	GLY	C-N-CA	6.67	126.36	119.56
1	A	513	SER	CA-C-N	6.40	126.09	119.56
1	A	513	SER	C-N-CA	6.40	126.09	119.56
4	E	47	CYS	N-CA-C	6.26	119.61	109.40
2	B	107	GLY	N-CA-C	6.25	119.40	110.46
3	C	10	ILE	N-CA-C	6.15	117.68	109.37
1	A	864	ILE	N-CA-C	-6.13	105.84	111.67
2	B	1223	ASP	N-CA-C	-6.07	106.23	113.21
1	A	243	PRO	CA-C-N	6.06	126.62	120.38
1	A	243	PRO	C-N-CA	6.06	126.62	120.38
1	A	356	ASP	CA-C-N	6.03	126.14	119.87
1	A	356	ASP	C-N-CA	6.03	126.14	119.87
1	A	351	THR	CB-CA-C	-5.88	100.36	110.95
1	A	934	LYS	N-CA-C	-5.79	105.10	111.82
1	A	71	GLN	CB-CA-C	-5.77	108.28	115.89
3	C	243	VAL	N-CA-C	-5.68	104.79	110.30
3	C	5	GLY	CA-C-N	5.67	125.99	119.93
3	C	5	GLY	C-N-CA	5.67	125.99	119.93
9	K	14	GLU	N-CA-C	5.65	117.83	110.43
1	A	1019	CYS	N-CA-C	5.62	117.41	111.28
4	E	128	PRO	N-CA-C	5.62	115.86	110.47
3	C	7	GLN	N-CA-C	5.62	117.52	107.80
2	B	1142	GLY	N-CA-C	-5.57	107.42	115.27
4	E	208	TYR	N-CA-C	-5.52	100.77	109.50
1	A	546	VAL	N-CA-C	-5.44	105.41	110.53
1	A	1270	ASN	N-CA-C	5.43	117.28	111.36
7	I	29	CYS	N-CA-C	-5.41	102.51	110.52
1	A	1071	SER	N-CA-C	-5.39	106.55	113.23
1	A	802	ASN	N-CA-C	5.38	118.44	110.48
3	C	21	ILE	CB-CA-C	-5.38	105.12	111.09
6	H	102	TYR	N-CA-C	-5.34	106.63	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1422	ARG	N-CA-C	-5.33	106.01	112.88
1	A	333	GLU	N-CA-C	-5.28	107.01	113.50
1	A	227	VAL	CB-CA-C	-5.23	106.28	111.30
4	E	171	LYS	N-CA-C	-5.23	103.13	110.50
1	A	597	LEU	N-CA-C	-5.21	106.70	113.16
3	C	96	SER	N-CA-C	5.20	117.85	108.48
2	B	851	PHE	N-CA-C	5.17	118.88	112.47
1	A	954	TRP	CA-C-N	5.16	126.29	119.84
1	A	954	TRP	C-N-CA	5.16	126.29	119.84
2	B	387	LEU	N-CA-C	-5.12	106.29	112.54
2	B	999	MET	CA-C-N	-5.12	114.34	120.13
2	B	999	MET	C-N-CA	-5.12	114.34	120.13
8	J	3	VAL	CB-CA-C	-5.11	102.06	111.36
1	A	399	HIS	CA-C-N	-5.08	113.50	119.84
1	A	399	HIS	C-N-CA	-5.08	113.50	119.84
4	E	205	SER	N-CA-C	-5.07	102.28	110.14
2	B	832	GLY	N-CA-C	-5.07	108.33	114.92
1	A	909	ASP	CA-C-N	5.07	126.17	119.84
1	A	909	ASP	C-N-CA	5.07	126.17	119.84
2	B	178	ASN	N-CA-C	5.06	118.71	112.54
1	A	890	ASP	N-CA-C	-5.03	105.80	111.28
2	B	829	CYS	N-CA-C	-5.03	101.91	109.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11154	0	11225	742	0
2	B	8711	0	8737	588	0
3	C	2095	0	2051	172	0
4	E	1760	0	1788	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	679	0	701	56	0
6	H	1068	0	1040	84	0
7	I	997	0	955	42	0
8	J	532	0	542	65	0
9	K	919	0	929	87	0
10	L	364	0	388	37	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
All	All	28289	0	28356	1736	0

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 31.

All (1736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:GLN:HB3	8:J:52:THR:CG2	1.63	1.25
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.66	1.21
1:A:672:ASP:HB2	1:A:736:ASN:ND2	1.60	1.15
1:A:855:THR:HG21	1:A:857:ARG:HE	0.98	1.14
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.27	1.14
1:A:672:ASP:CB	1:A:736:ASN:HD21	1.59	1.14
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.06	1.14
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.25	1.12
1:A:470:LEU:HD11	1:A:487:MET:HE1	1.21	1.10
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.24	1.09
3:C:148:ARG:NH1	8:J:64:ASN:HA	1.68	1.07
2:B:1081:LEU:HD12	2:B:1085:ILE:HD11	1.36	1.07
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.12	1.06
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.56	1.05
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.39	1.05
1:A:535:THR:HG21	1:A:617:VAL:H	1.24	1.02
1:A:774:ARG:HH11	1:A:774:ARG:HG3	1.25	1.02
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.02	1.02
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.35	1.01
1:A:855:THR:CG2	1:A:857:ARG:HE	1.74	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:MET:HE1	1:A:1436:ILE:HA	1.40	1.01
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.38	1.01
6:H:95:TYR:CE2	6:H:97:MET:HG3	1.96	1.01
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.90	1.00
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.24	1.00
1:A:470:LEU:HD11	1:A:487:MET:CE	1.94	0.97
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.00	0.97
6:H:130:ARG:HA	6:H:133:ASN:HB2	1.47	0.97
2:B:29:ASP:HB3	2:B:658:ILE:CD1	1.95	0.96
1:A:855:THR:HG21	1:A:857:ARG:NE	1.79	0.96
2:B:644:GLU:HG3	2:B:654:ARG:NH2	1.80	0.96
2:B:800:GLN:CB	8:J:52:THR:HG22	1.94	0.96
1:A:472:LEU:O	1:A:475:THR:HB	1.66	0.96
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.65	0.94
5:F:81:THR:HG22	5:F:136:ARG:NH1	1.84	0.93
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.48	0.93
2:B:542:MET:HG3	2:B:747:MET:HE3	1.51	0.92
2:B:824:ILE:HG12	8:J:48:ARG:NH1	1.83	0.92
1:A:470:LEU:CD1	1:A:487:MET:HE1	1.99	0.92
1:A:913:LEU:HD11	1:A:981:LEU:O	1.70	0.92
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.50	0.92
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.66	0.92
3:C:40:GLU:HA	3:C:163:ILE:HG23	1.51	0.92
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.33	0.92
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.11	0.91
1:A:869:GLY:O	4:E:204:THR:HG21	1.71	0.91
9:K:65:HIS:HD2	9:K:67:PHE:H	0.97	0.91
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.00	0.91
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.53	0.91
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.85	0.91
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.52	0.91
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.18	0.91
1:A:313:GLN:HG2	1:A:322:VAL:HB	1.52	0.90
1:A:672:ASP:HB2	1:A:736:ASN:HD21	0.77	0.90
9:K:65:HIS:CD2	9:K:67:PHE:H	1.88	0.90
3:C:166:GLU:HG2	10:L:70:ARG:HH12	1.37	0.90
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.08	0.88
1:A:55:ASP:H	1:A:56:PRO:HD2	1.36	0.87
2:B:1081:LEU:CD1	2:B:1085:ILE:HD11	2.03	0.87
5:F:81:THR:HB	5:F:144:GLU:OE1	1.74	0.87
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:558:LEU:HB3	2:B:563:MET:HE3	1.55	0.87
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.55	0.87
1:A:134:ARG:HD2	1:A:221:SER:O	1.75	0.87
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.39	0.87
7:I:4:PHE:HE1	7:I:13:MET:HE2	1.37	0.86
3:C:66:ARG:NH2	8:J:3:VAL:O	2.09	0.85
1:A:345:VAL:HG11	2:B:1128:LEU:O	1.74	0.85
1:A:519:PRO:HG2	1:A:624:SER:O	1.77	0.85
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.41	0.85
1:A:757:ASN:HA	2:B:1021:MET:HE1	1.59	0.85
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.89	0.85
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.59	0.85
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.07	0.84
1:A:1398:MET:HG3	1:A:1426:GLU:HG2	1.58	0.84
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.78	0.84
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.59	0.84
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.42	0.84
1:A:567:LYS:HB3	6:H:96:VAL:N	1.93	0.84
3:C:166:GLU:HG2	10:L:70:ARG:NH1	1.92	0.84
1:A:353:ILE:HD13	1:A:487:MET:CE	2.07	0.83
2:B:801:LYS:O	8:J:52:THR:HG23	1.77	0.83
2:B:324:ILE:HD11	2:B:333:PHE:HB2	1.58	0.83
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.41	0.83
1:A:302:THR:HG21	1:A:312:PRO:HG2	1.61	0.83
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.13	0.83
2:B:705:MET:CE	2:B:745:PRO:HB3	2.08	0.83
2:B:648:HIS:HE1	2:B:712:PRO:HD3	1.43	0.82
1:A:548:ASN:HD21	9:K:47:ARG:HH21	1.24	0.82
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.15	0.82
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.38	0.82
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.63	0.82
4:E:19:VAL:HG11	4:E:80:VAL:HG11	1.62	0.81
1:A:2:VAL:HG21	2:B:1157:ALA:O	1.80	0.81
2:B:899:ILE:HD13	2:B:905:VAL:HG11	1.63	0.81
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.15	0.81
2:B:35:SER:HA	2:B:811:TYR:HE2	1.43	0.81
3:C:54:ASN:OD1	3:C:56:THR:HG22	1.80	0.81
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.21	0.80
1:A:598:LEU:HD21	6:H:124:ARG:HB2	1.63	0.80
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.64	0.80
4:E:180:ARG:HH21	4:E:192:ARG:HB2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:VAL:HG13	1:A:822:GLU:HG3	1.63	0.80
1:A:535:THR:CG2	1:A:616:VAL:HA	2.11	0.79
3:C:32:SER:O	3:C:36:VAL:HG23	1.82	0.79
2:B:29:ASP:HB3	2:B:658:ILE:HD12	1.61	0.79
1:A:757:ASN:HA	2:B:1021:MET:CE	2.12	0.79
2:B:1065:GLN:HE21	2:B:1069:PHE:H	1.30	0.79
1:A:72:GLU:HB3	1:A:76:GLU:HB2	1.64	0.79
2:B:954:VAL:O	10:L:55:ILE:O	2.01	0.79
1:A:567:LYS:HB3	6:H:96:VAL:H	1.46	0.79
2:B:515:HIS:H	2:B:518:HIS:HD2	1.30	0.79
3:C:74:SER:HB2	3:C:238:ILE:HG13	1.63	0.79
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.65	0.78
1:A:535:THR:HG21	1:A:617:VAL:N	1.99	0.78
2:B:210:LYS:HE3	2:B:461:LEU:O	1.84	0.78
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.47	0.78
1:A:605:MET:HE1	1:A:612:ILE:HD12	1.66	0.78
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.14	0.78
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.18	0.78
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.14	0.77
5:F:81:THR:HG21	5:F:136:ARG:CD	2.14	0.77
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.14	0.77
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.66	0.77
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.67	0.77
7:I:4:PHE:CE1	7:I:13:MET:HE2	2.19	0.77
1:A:399:HIS:O	1:A:401:GLY:N	2.16	0.77
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.85	0.76
3:C:167:HIS:HD2	3:C:169:LYS:H	1.33	0.76
4:E:118:PRO:HA	4:E:121:MET:HB2	1.67	0.76
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.20	0.76
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.18	0.76
6:H:26:ILE:HD13	6:H:42:ILE:HD12	1.66	0.76
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.66	0.76
2:B:685:LEU:HD11	2:B:692:TYR:CE1	2.21	0.76
6:H:95:TYR:HE2	6:H:97:MET:CG	1.94	0.76
2:B:341:LEU:HD12	2:B:341:LEU:O	1.86	0.76
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.50	0.76
2:B:25:ILE:HD12	2:B:653:VAL:HB	1.67	0.75
2:B:43:LEU:HD11	2:B:811:TYR:O	1.84	0.75
2:B:1081:LEU:HD12	2:B:1085:ILE:CD1	2.15	0.75
1:A:494:SER:OG	1:A:497:THR:HB	1.87	0.75
1:A:911:SER:O	1:A:978:PRO:HB3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.67	0.75
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.67	0.75
1:A:984:LYS:O	1:A:988:LEU:HB2	1.85	0.75
6:H:81:PRO:CB	6:H:82:PRO:HD3	2.12	0.75
1:A:668:ASP:OD2	1:A:742:ASN:HB2	1.86	0.75
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.65	0.75
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.20	0.75
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.68	0.75
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.52	0.75
2:B:766:ARG:NH2	2:B:1020:ARG:HD2	2.01	0.75
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.69	0.74
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.50	0.74
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.16	0.74
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.69	0.74
1:A:848:ILE:HD11	1:A:1374:VAL:HG21	1.69	0.74
3:C:41:ILE:CG2	3:C:172:PRO:HG3	2.17	0.74
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.22	0.74
1:A:492:PRO:HG3	1:A:501:LEU:CD1	2.18	0.74
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.68	0.74
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.69	0.74
2:B:766:ARG:NH1	2:B:985:GLY:O	2.20	0.74
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.68	0.74
2:B:311:LEU:HB3	7:I:4:PHE:CZ	2.22	0.74
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.50	0.74
9:K:65:HIS:HD2	9:K:67:PHE:N	1.80	0.73
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.70	0.73
4:E:147:HIS:HD2	4:E:149:LEU:H	1.37	0.73
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.71	0.73
2:B:235:SER:OG	2:B:236:HIS:HD2	1.72	0.73
6:H:103:LYS:HZ2	6:H:114:VAL:HB	1.54	0.73
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.36	0.73
2:B:35:SER:HA	2:B:811:TYR:CE2	2.23	0.73
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.70	0.73
4:E:94:LYS:HG3	4:E:123:LEU:HD11	1.69	0.73
9:K:55:LYS:HB2	9:K:81:TYR:CD1	2.23	0.73
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.54	0.72
1:A:34:LYS:HA	1:A:83:HIS:HD2	1.53	0.72
1:A:499:ALA:O	1:A:503:GLN:HB2	1.89	0.72
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.55	0.72
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.51	0.72
1:A:899:VAL:HG12	1:A:929:LEU:HD13	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:986:GLN:HE21	2:B:987:LYS:N	1.87	0.72
4:E:147:HIS:CD2	4:E:149:LEU:H	2.08	0.72
8:J:24:LEU:O	8:J:30:LEU:HB2	1.89	0.72
2:B:680:THR:HG22	2:B:682:SER:N	2.05	0.72
1:A:548:ASN:ND2	9:K:47:ARG:HH21	1.85	0.72
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.71	0.72
3:C:93:ASP:O	3:C:127:ARG:NH2	2.21	0.72
1:A:33:ALA:O	1:A:83:HIS:HB3	1.90	0.71
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.72	0.71
2:B:845:SER:HB3	2:B:850:LEU:HD22	1.71	0.71
9:K:30:ALA:HB2	9:K:76:GLN:HG3	1.72	0.71
1:A:903:ASN:HD22	1:A:905:ASP:H	1.39	0.71
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.72	0.71
1:A:858:ASN:C	1:A:858:ASN:HD22	1.99	0.71
1:A:754:SER:H	1:A:757:ASN:HD22	1.38	0.71
1:A:761:MET:O	1:A:803:SER:HB2	1.90	0.71
1:A:579:SER:HB3	1:A:611:GLN:HA	1.71	0.71
2:B:238:ALA:HB2	2:B:385:LEU:HB2	1.73	0.70
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.06	0.70
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.72	0.70
6:H:10:PHE:O	6:H:54:SER:HA	1.91	0.70
1:A:1166:ASP:HA	1:A:1169:ILE:HG23	1.71	0.70
2:B:185:THR:HG23	2:B:188:ASP:OD2	1.90	0.70
1:A:774:ARG:HH11	1:A:774:ARG:CG	2.02	0.70
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.89	0.70
9:K:46:ILE:HG22	9:K:50:LEU:HD12	1.73	0.70
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.73	0.70
1:A:451:HIS:CE1	1:A:453:MET:HE2	2.27	0.70
1:A:548:ASN:HD21	9:K:47:ARG:NH2	1.89	0.70
1:A:374:LEU:HD23	2:B:1107:ALA:HB2	1.74	0.70
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.92	0.70
2:B:542:MET:HG3	2:B:747:MET:CE	2.20	0.70
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.57	0.69
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.74	0.69
3:C:22:LEU:HD11	9:K:101:LEU:HD11	1.75	0.69
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.04	0.69
2:B:914:LYS:HB3	2:B:937:ALA:O	1.93	0.69
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.75	0.69
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.27	0.69
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.74	0.69
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.57	0.69
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.74	0.69
2:B:205:ILE:HD12	2:B:461:LEU:HB3	1.74	0.69
5:F:109:VAL:HG12	5:F:110:ASP:N	2.07	0.69
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.74	0.68
1:A:567:LYS:CB	6:H:96:VAL:H	2.05	0.68
2:B:515:HIS:H	2:B:518:HIS:CD2	2.11	0.68
2:B:642:ASP:HB3	2:B:649:LYS:HE2	1.73	0.68
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.24	0.68
2:B:899:ILE:O	2:B:952:VAL:HG21	1.93	0.68
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.76	0.68
2:B:999:MET:HB3	2:B:1007:VAL:HG22	1.76	0.68
6:H:103:LYS:HA	6:H:115:TYR:HB2	1.76	0.68
1:A:44:THR:O	1:A:45:GLN:HB2	1.93	0.68
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.75	0.68
1:A:92:HIS:HD2	1:A:94:GLY:H	1.41	0.68
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.73	0.68
1:A:1434:ALA:HB3	1:A:1436:ILE:HG12	1.75	0.68
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.73	0.68
1:A:345:VAL:HG12	2:B:1150:ARG:HH22	1.59	0.68
2:B:1072:MET:HE1	2:B:1087:PHE:CE1	2.28	0.68
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.77	0.68
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.24	0.68
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.76	0.67
1:A:1329:THR:HG22	1:A:1335:ILE:HG13	1.77	0.67
4:E:112:TYR:CE1	4:E:115:ASN:HA	2.29	0.67
1:A:1383:SER:HB3	1:A:1387:HIS:NE2	2.09	0.67
2:B:324:ILE:CD1	2:B:333:PHE:HB2	2.25	0.67
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.30	0.67
2:B:1060:ARG:HB2	2:B:1066:SER:HB3	1.76	0.67
6:H:103:LYS:HG2	6:H:115:TYR:O	1.94	0.67
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.76	0.67
1:A:1063:MET:HG3	2:B:1139:ILE:HG22	1.76	0.67
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.77	0.67
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.25	0.66
2:B:996:ARG:NH2	3:C:174:ALA:O	2.27	0.66
2:B:1152:MET:HA	2:B:1152:MET:CE	2.25	0.66
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.31	0.66
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.25	0.66
7:I:111:THR:HG22	7:I:113:ASP:H	1.58	0.66
1:A:757:ASN:OD1	2:B:1021:MET:HE2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.30	0.66
3:C:18:VAL:HG12	3:C:18:VAL:O	1.96	0.66
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.77	0.66
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.78	0.66
1:A:1282:VAL:HG22	1:A:1308:THR:HG22	1.76	0.66
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.77	0.66
1:A:131:SER:HB2	1:A:223:GLY:HA2	1.77	0.66
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.77	0.66
7:I:59:VAL:HG12	7:I:61:ASP:H	1.59	0.66
1:A:302:THR:HG21	1:A:312:PRO:CG	2.25	0.66
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.78	0.66
1:A:1398:MET:HG3	1:A:1426:GLU:CG	2.24	0.65
9:K:6:ARG:O	9:K:9:LEU:HG	1.96	0.65
1:A:14:VAL:HB	1:A:1430:LEU:HD13	1.78	0.65
1:A:597:LEU:O	6:H:102:TYR:OH	2.14	0.65
3:C:261:ALA:O	3:C:265:MET:HB2	1.96	0.65
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.78	0.65
2:B:816:GLU:O	8:J:56:LEU:HD21	1.95	0.65
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.31	0.65
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.04	0.65
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.31	0.65
1:A:553:VAL:CG2	1:A:652:VAL:CG2	2.75	0.65
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.78	0.65
1:A:258:GLY:O	1:A:259:GLU:HG3	1.96	0.65
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.92	0.65
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.31	0.65
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.77	0.65
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.37	0.65
1:A:356:ASP:OD2	9:K:65:HIS:CE1	2.48	0.65
2:B:195:CYS:SG	2:B:783:THR:OG1	2.49	0.65
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.27	0.65
1:A:414:ASP:O	1:A:416:ARG:N	2.30	0.65
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.27	0.65
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.25	0.65
3:C:89:GLU:O	3:C:90:ASP:CB	2.45	0.65
1:A:785:PRO:HD2	1:A:786:HIS:HD2	1.62	0.64
2:B:805:THR:HG21	2:B:815:ARG:HE	1.63	0.64
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.43	0.64
2:B:311:LEU:HB3	7:I:4:PHE:HZ	1.63	0.64
1:A:1222:ASN:C	1:A:1224:LEU:H	2.03	0.64
2:B:994:TYR:HB2	2:B:999:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:MET:CE	1:A:1436:ILE:HA	2.21	0.64
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.32	0.64
2:B:884:ARG:O	2:B:936:ASP:HB3	1.98	0.64
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.79	0.64
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.33	0.64
2:B:276:ILE:HG21	2:B:280:ILE:CD1	2.27	0.64
5:F:118:LEU:O	5:F:122:MET:HG3	1.98	0.64
10:L:58:LYS:O	10:L:59:ALA:O	2.16	0.64
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.33	0.64
2:B:684:LEU:HD23	2:B:689:LEU:CD1	2.27	0.64
2:B:1212:ILE:O	2:B:1214:PRO:HD3	1.98	0.64
10:L:38:LEU:O	10:L:39:SER:HB3	1.97	0.64
1:A:1395:GLY:H	1:A:1398:MET:HE3	1.63	0.64
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.62	0.64
2:B:841:MET:O	2:B:993:THR:HA	1.98	0.64
10:L:61:THR:HB	10:L:63:ARG:HG2	1.80	0.64
10:L:33:GLU:HB2	10:L:53:HIS:CD2	2.33	0.64
1:A:626:ASN:O	1:A:631:HIS:HD2	1.82	0.63
5:F:75:PRO:O	5:F:77:ASP:O	2.16	0.63
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.63	0.63
1:A:49:LYS:HB3	1:A:55:ASP:HB2	1.80	0.63
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.79	0.63
1:A:1315:GLU:O	1:A:1318:THR:HG22	1.98	0.63
1:A:528:LEU:O	1:A:531:ILE:HG22	1.98	0.63
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.33	0.63
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.80	0.63
1:A:540:PHE:C	1:A:541:ILE:HD12	2.23	0.63
1:A:1199:ARG:HA	1:A:1202:MET:HB2	1.81	0.63
3:C:242:GLN:O	3:C:246:ARG:HG3	1.99	0.63
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.80	0.63
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.14	0.63
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.34	0.63
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.07	0.63
1:A:406:ILE:HG12	1:A:412:ARG:HG2	1.81	0.63
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.29	0.63
3:C:73:GLN:HE21	3:C:75:MET:H	1.46	0.63
3:C:166:GLU:CG	10:L:70:ARG:HH12	2.10	0.63
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	1.81	0.63
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.31	0.63
2:B:451:LYS:O	2:B:455:SER:HB2	1.97	0.63
1:A:903:ASN:HD22	1:A:903:ASN:C	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ILE:HG22	3:C:165:LYS:H	1.64	0.62
10:L:46:VAL:O	10:L:54:ARG:HA	1.99	0.62
1:A:477:PRO:HG3	1:A:521:MET:HG2	1.82	0.62
1:A:982:THR:O	1:A:985:ASP:HB2	1.98	0.62
4:E:19:VAL:HG22	4:E:140:LEU:HD13	1.81	0.62
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.81	0.62
1:A:901:LEU:HA	1:A:907:THR:HG23	1.80	0.62
3:C:40:GLU:HA	3:C:163:ILE:CG2	2.25	0.62
9:K:42:LEU:HG	9:K:46:ILE:HD11	1.78	0.62
9:K:55:LYS:CB	9:K:81:TYR:CD1	2.82	0.62
1:A:642:CYS:O	1:A:645:LEU:HB3	1.98	0.62
2:B:906:SER:HB2	2:B:946:ASN:HB2	1.82	0.62
2:B:1016:ALA:O	2:B:1020:ARG:HG2	2.00	0.62
1:A:89:PRO:HB3	1:A:208:LEU:HD12	1.81	0.62
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.25	0.62
1:A:1398:MET:CG	1:A:1426:GLU:HG2	2.28	0.62
5:F:111:LEU:C	5:F:113:GLY:H	2.07	0.62
9:K:55:LYS:CB	9:K:81:TYR:HD1	2.13	0.62
1:A:567:LYS:CG	6:H:96:VAL:H	2.12	0.62
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.81	0.62
1:A:1268:LEU:HD13	7:I:48:LEU:HD21	1.80	0.62
1:A:1062:GLU:O	1:A:1064:VAL:N	2.32	0.62
1:A:382:PRO:HD2	5:F:104:ASN:OD1	1.99	0.62
1:A:553:VAL:HG22	1:A:652:VAL:HG23	1.82	0.62
1:A:1289:ARG:O	1:A:1300:LYS:HA	2.00	0.62
9:K:1:MET:HG3	9:K:2:ASN:N	2.15	0.62
2:B:1222:ARG:H	2:B:1222:ARG:HD2	1.64	0.62
4:E:88:VAL:HG13	4:E:92:THR:HB	1.82	0.62
1:A:329:LEU:O	1:A:333:GLU:HG2	2.00	0.62
1:A:504:LEU:CD1	5:F:91:ALA:HB2	2.29	0.62
1:A:535:THR:HG21	1:A:616:VAL:HA	1.81	0.62
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.35	0.62
2:B:509:ALA:O	2:B:511:PRO:HD3	1.99	0.62
2:B:430:ARG:HB3	2:B:434:ARG:HD2	1.81	0.61
2:B:546:SER:HB2	2:B:612:GLU:HG3	1.80	0.61
2:B:1053:GLU:HA	2:B:1053:GLU:OE1	2.00	0.61
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.35	0.61
1:A:883:LEU:O	1:A:886:ILE:HG22	2.00	0.61
1:A:1222:ASN:O	1:A:1224:LEU:N	2.33	0.61
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.81	0.61
6:H:91:ASP:C	6:H:93:TYR:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:18:LYS:HZ2	9:K:38:GLU:HG2	1.65	0.61
1:A:23:SER:O	1:A:27:VAL:HG23	2.00	0.61
2:B:173:MET:HE1	2:B:409:ALA:CB	2.30	0.61
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.81	0.61
3:C:58:LEU:HD11	8:J:2:ILE:CD1	2.29	0.61
2:B:773:MET:CE	2:B:985:GLY:HA2	2.30	0.61
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.83	0.61
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.83	0.61
2:B:241:ARG:HG2	2:B:251:ILE:HG23	1.82	0.61
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.33	0.61
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.81	0.61
1:A:391:LEU:HD22	1:A:400:PRO:O	2.00	0.61
1:A:465:TYR:HA	9:K:2:ASN:HB3	1.82	0.61
1:A:720:ARG:NH2	1:A:721:PHE:CE2	2.69	0.61
1:A:1001:ARG:HB2	5:F:80:ALA:O	2.01	0.61
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.65	0.61
2:B:728:ARG:HD2	2:B:730:ARG:HE	1.64	0.61
2:B:237:VAL:HG22	2:B:257:LYS:HG2	1.82	0.61
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.82	0.61
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.12	0.61
3:C:265:MET:HE1	9:K:19:LEU:HB2	1.82	0.61
1:A:553:VAL:HG22	1:A:652:VAL:HG21	1.82	0.60
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.82	0.60
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.34	0.60
6:H:130:ARG:CA	6:H:133:ASN:HB2	2.26	0.60
1:A:3:GLY:O	1:A:5:GLN:N	2.34	0.60
2:B:190:TYR:OH	2:B:196:PRO:HG3	2.01	0.60
2:B:1065:GLN:HE21	2:B:1069:PHE:N	1.98	0.60
2:B:1166:CYS:O	2:B:1168:LEU:N	2.30	0.60
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.82	0.60
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.01	0.60
2:B:776:GLN:O	2:B:1095:LEU:HA	2.01	0.60
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.81	0.60
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.82	0.60
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.36	0.60
5:F:109:VAL:CG1	5:F:110:ASP:N	2.63	0.60
1:A:269:ILE:HD11	1:A:303:TYR:HB2	1.83	0.60
1:A:535:THR:HG22	1:A:616:VAL:HA	1.84	0.60
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.90	0.60
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.01	0.60
1:A:1398:MET:HA	1:A:1425:SER:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:SER:CB	2:B:946:ASN:HB2	2.32	0.60
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.83	0.60
9:K:113:THR:O	9:K:114:LEU:HB2	2.00	0.60
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.37	0.60
3:C:116:LYS:HG2	3:C:117:ASP:OD1	2.01	0.60
4:E:155:ARG:HD2	4:E:194:GLU:CD	2.27	0.60
6:H:101:ALA:HB1	6:H:103:LYS:HG3	1.82	0.60
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.34	0.60
2:B:1222:ARG:C	2:B:1224:PHE:H	2.10	0.60
3:C:121:VAL:O	3:C:121:VAL:HG12	2.01	0.60
2:B:172:ILE:CD1	2:B:178:ASN:HB3	2.31	0.60
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.37	0.60
3:C:58:LEU:HD11	8:J:2:ILE:HD11	1.84	0.60
4:E:65:THR:O	4:E:69:ILE:HG13	2.00	0.60
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.84	0.59
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.37	0.59
3:C:41:ILE:HG21	3:C:172:PRO:HG3	1.83	0.59
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.37	0.59
2:B:648:HIS:CE1	2:B:712:PRO:HD3	2.30	0.59
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.67	0.59
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.67	0.59
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.84	0.59
1:A:243:PRO:HB2	1:A:244:PRO:HD2	1.83	0.59
1:A:349:ALA:HB2	1:A:374:LEU:HD21	1.84	0.59
1:A:476:SER:N	1:A:477:PRO:HD2	2.16	0.59
1:A:587:HIS:HA	1:A:607:ILE:O	2.01	0.59
3:C:37:MET:HA	3:C:41:ILE:HD12	1.84	0.59
3:C:142:VAL:HG11	8:J:5:VAL:HG22	1.83	0.59
10:L:48:CYS:HB3	10:L:51:CYS:O	2.01	0.59
1:A:49:LYS:HD3	1:A:55:ASP:CG	2.27	0.59
1:A:523:ILE:CD1	1:A:622:VAL:HG22	2.32	0.59
1:A:1349:TYR:C	1:A:1349:TYR:CD2	2.81	0.59
3:C:241:ASP:CB	9:K:109:TRP:CE2	2.85	0.59
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.37	0.59
1:A:329:LEU:HB3	1:A:333:GLU:HB3	1.84	0.59
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.14	0.59
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.32	0.59
8:J:21:TYR:HB2	8:J:39:LEU:HD11	1.83	0.59
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.31	0.59
10:L:51:CYS:C	10:L:53:HIS:H	2.10	0.59
4:E:28:TYR:CZ	4:E:78:LEU:HG	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:PHE:HE1	1:A:792:TYR:CZ	2.19	0.59
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.36	0.59
9:K:8:GLU:O	9:K:37:LYS:HD2	2.02	0.59
1:A:313:GLN:HB2	1:A:320:ARG:HB3	1.85	0.59
1:A:493:GLN:NE2	1:A:493:GLN:HA	2.18	0.59
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.59
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.84	0.59
2:B:973:ILE:O	2:B:975:GLN:HG3	2.02	0.59
2:B:980:PHE:CE1	2:B:1094:ARG:HG3	2.37	0.59
4:E:9:ILE:HG21	4:E:43:LYS:HE3	1.84	0.59
4:E:28:TYR:CE1	4:E:75:MET:HE2	2.38	0.59
5:F:111:LEU:O	5:F:113:GLY:N	2.32	0.59
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.85	0.59
1:A:55:ASP:O	1:A:57:ARG:N	2.36	0.58
1:A:668:ASP:CG	1:A:742:ASN:HB2	2.27	0.58
1:A:1313:LEU:O	1:A:1317:MET:HB2	2.02	0.58
2:B:294:ASP:H	7:I:12:ASN:ND2	2.01	0.58
3:C:167:HIS:HD2	3:C:169:LYS:N	2.00	0.58
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.67	0.58
9:K:78:THR:HG22	9:K:79:GLU:N	2.16	0.58
1:A:353:ILE:HG21	1:A:487:MET:CE	2.21	0.58
2:B:586:TRP:NE1	2:B:588:GLY:O	2.36	0.58
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.36	0.58
2:B:531:GLN:CD	2:B:531:GLN:H	2.11	0.58
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.84	0.58
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.51	0.58
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.33	0.58
2:B:872:GLU:HG2	2:B:916:THR:OG1	2.03	0.58
2:B:950:ASP:OD2	2:B:969:ARG:HD3	2.02	0.58
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.19	0.58
1:A:479:ASN:C	1:A:479:ASN:HD22	2.12	0.58
1:A:567:LYS:HG2	6:H:96:VAL:H	1.68	0.58
2:B:130:VAL:HG12	2:B:131:ASP:H	1.68	0.58
2:B:276:ILE:HG23	2:B:337:ARG:HB2	1.85	0.58
2:B:120:ARG:HG3	2:B:955:THR:HG21	1.85	0.58
2:B:796:LEU:O	2:B:799:PRO:HD3	2.03	0.58
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.38	0.58
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.49	0.58
5:F:99:LEU:HG	5:F:99:LEU:O	2.03	0.58
6:H:82:PRO:HG2	9:K:54:ARG:HG2	1.86	0.58
1:A:1359:ASP:C	1:A:1361:SER:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:PHE:N	2:B:370:PHE:CD1	2.71	0.58
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.86	0.58
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.86	0.58
1:A:1199:ARG:HG3	1:A:1236:LEU:CD1	2.31	0.58
3:C:18:VAL:O	3:C:19:ASP:C	2.46	0.58
10:L:30:ILE:HG13	10:L:59:ALA:HB2	1.86	0.58
1:A:626:ASN:O	1:A:631:HIS:CD2	2.57	0.58
2:B:593:PRO:O	2:B:596:LEU:N	2.37	0.58
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.19	0.58
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.85	0.58
8:J:53:HIS:HE1	8:J:55:ASP:OD1	1.85	0.58
10:L:30:ILE:HG22	10:L:31:CYS:N	2.19	0.58
2:B:239:GLU:HG3	2:B:255:GLN:HG2	1.85	0.58
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.18	0.58
2:B:602:THR:O	2:B:606:LYS:HG3	2.04	0.58
10:L:38:LEU:O	10:L:39:SER:CB	2.51	0.58
1:A:493:GLN:CA	1:A:493:GLN:HE21	2.17	0.57
1:A:1107:VAL:HG12	1:A:1333:ILE:HD11	1.84	0.57
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.34	0.57
2:B:36:ALA:HA	2:B:39:ARG:CZ	2.34	0.57
2:B:228:LYS:O	2:B:261:ARG:NH2	2.36	0.57
7:I:70:ARG:HG2	7:I:84:VAL:HG23	1.87	0.57
2:B:235:SER:HA	2:B:261:ARG:NH2	2.19	0.57
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.87	0.57
10:L:51:CYS:HB3	10:L:53:HIS:NE2	2.19	0.57
2:B:701:ILE:HB	2:B:739:THR:OG1	2.04	0.57
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.86	0.57
2:B:1072:MET:HE1	2:B:1087:PHE:CZ	2.40	0.57
6:H:103:LYS:NZ	6:H:114:VAL:HB	2.18	0.57
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.86	0.57
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.39	0.57
4:E:78:LEU:HD23	4:E:107:THR:HB	1.86	0.57
4:E:180:ARG:HH21	4:E:192:ARG:CB	2.16	0.57
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.86	0.57
1:A:689:LYS:O	1:A:693:VAL:HG23	2.04	0.57
1:A:34:LYS:HA	1:A:83:HIS:CD2	2.37	0.57
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.85	0.57
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.85	0.57
5:F:83:PRO:HD2	5:F:84:TYR:HD1	1.69	0.57
6:H:103:LYS:CE	6:H:114:VAL:HB	2.35	0.57
9:K:1:MET:HG3	9:K:2:ASN:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.87	0.57
1:A:286:HIS:C	1:A:288:ALA:H	2.13	0.57
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.87	0.57
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.40	0.57
8:J:6:ARG:HG2	8:J:13:VAL:HA	1.87	0.57
1:A:347:PHE:H	2:B:1107:ALA:HA	1.70	0.57
1:A:471:ASN:O	1:A:474:VAL:HG12	2.05	0.57
1:A:579:SER:HA	1:A:582:ILE:HD12	1.87	0.57
1:A:1102:LYS:O	1:A:1106:ASN:HB2	2.05	0.57
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.87	0.57
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.20	0.57
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.86	0.57
2:B:1079:LYS:CA	3:C:27:LEU:HD21	2.35	0.57
4:E:12:LEU:HG	4:E:58:MET:HE1	1.87	0.57
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.86	0.56
4:E:94:LYS:O	4:E:98:ILE:HB	2.05	0.56
1:A:337:ARG:HA	1:A:340:LEU:HB2	1.85	0.56
1:A:975:HIS:H	6:H:136:LYS:HZ1	1.52	0.56
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.05	0.56
2:B:54:PHE:HE2	2:B:170:LEU:HD21	1.71	0.56
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.40	0.56
1:A:1063:MET:HG3	2:B:1139:ILE:CG2	2.35	0.56
1:A:1396:ALA:HB2	1:A:1417:GLU:OE1	2.05	0.56
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.40	0.56
1:A:1116:LEU:HD13	1:A:1311:VAL:HA	1.86	0.56
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.40	0.56
7:I:103:CYS:O	7:I:107:SER:HA	2.05	0.56
8:J:6:ARG:HD3	8:J:11:GLY:O	2.06	0.56
1:A:446:ARG:HB2	1:A:487:MET:SD	2.46	0.56
1:A:850:VAL:O	1:A:1060:PRO:HA	2.06	0.56
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.87	0.56
2:B:242:SER:OG	2:B:362:PRO:HD2	2.05	0.56
1:A:40:THR:HG22	1:A:41:MET:HG3	1.88	0.56
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.45	0.56
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.88	0.56
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.21	0.56
9:K:29:ASN:HB3	9:K:77:THR:O	2.05	0.56
1:A:824:LEU:CD2	2:B:765:PRO:HB3	2.35	0.56
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.04	0.56
2:B:63:ILE:HD13	2:B:95:ILE:HD11	1.88	0.56
2:B:408:LEU:HD23	2:B:409:ALA:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:772:ALA:O	2:B:775:LYS:HB2	2.05	0.56
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	1.87	0.56
1:A:1208:THR:HB	1:A:1211:GLN:H	1.71	0.56
2:B:361:LEU:HD21	2:B:381:MET:HE1	1.86	0.56
2:B:997:GLU:CG	3:C:39:ALA:HB2	2.36	0.56
4:E:22:MET:O	4:E:26:ARG:HG3	2.06	0.56
6:H:12:VAL:HA	6:H:28:ALA:HA	1.87	0.56
3:C:124:LEU:O	3:C:127:ARG:HG3	2.06	0.56
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.71	0.56
1:A:219:PHE:CD1	1:A:219:PHE:C	2.84	0.56
1:A:1341:ILE:HD12	1:A:1379:GLY:CA	2.36	0.56
2:B:890:TYR:CD2	2:B:893:LEU:HD11	2.41	0.56
3:C:19:ASP:HA	3:C:231:ASN:HA	1.87	0.56
3:C:209:TYR:N	3:C:209:TYR:CD1	2.74	0.56
3:C:246:ARG:HA	3:C:249:ASP:HB3	1.87	0.56
1:A:96:ILE:HG22	1:A:176:LYS:HD2	1.89	0.55
1:A:738:LYS:HA	6:H:19:ARG:HH22	1.70	0.55
1:A:785:PRO:HD2	1:A:786:HIS:CD2	2.41	0.55
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.39	0.55
1:A:903:ASN:O	1:A:905:ASP:N	2.38	0.55
1:A:1115:SER:HA	1:A:1308:THR:O	2.07	0.55
2:B:705:MET:CE	2:B:742:GLU:HG3	2.36	0.55
1:A:451:HIS:CG	1:A:1074:GLU:HG3	2.41	0.55
1:A:503:GLN:NE2	5:F:90:ARG:HH21	2.04	0.55
1:A:1295:THR:HB	1:A:1297:GLU:OE1	2.06	0.55
1:A:1376:THR:HG23	4:E:212:ARG:NH2	2.19	0.55
2:B:25:ILE:CD1	2:B:658:ILE:HD11	2.37	0.55
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.36	0.55
1:A:847:ASP:OD1	1:A:847:ASP:N	2.31	0.55
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.88	0.55
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.88	0.55
1:A:84:ILE:HG22	1:A:241:VAL:CG2	2.37	0.55
1:A:458:HIS:HE1	1:A:474:VAL:HG21	1.70	0.55
1:A:843:LYS:NZ	1:A:1386:ARG:HB3	2.21	0.55
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.41	0.55
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.86	0.55
3:C:209:TYR:N	3:C:209:TYR:HD1	2.05	0.55
7:I:55:THR:O	7:I:58:VAL:HG23	2.06	0.55
8:J:8:PHE:HB2	8:J:48:ARG:NH2	2.20	0.55
1:A:809:THR:O	1:A:813:PHE:N	2.35	0.55
2:B:558:LEU:CB	2:B:563:MET:HE3	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:685:LEU:HD11	2:B:692:TYR:CZ	2.41	0.55
1:A:92:HIS:CD2	1:A:94:GLY:H	2.21	0.55
1:A:572:TRP:HE3	1:A:572:TRP:H	1.53	0.55
1:A:774:ARG:HG3	1:A:774:ARG:NH1	2.06	0.55
2:B:336:ARG:HG2	2:B:348:ARG:CD	2.37	0.55
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.71	0.55
5:F:114:GLU:CD	5:F:119:ARG:HG2	2.32	0.55
6:H:103:LYS:HE2	6:H:116:TYR:CZ	2.42	0.55
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.88	0.55
1:A:469:ARG:NH2	2:B:991:GLY:O	2.39	0.55
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.89	0.55
1:A:852:TYR:CD2	5:F:136:ARG:HD3	2.42	0.55
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.87	0.55
2:B:995:ARG:HD3	9:K:6:ARG:HH12	1.71	0.55
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.65	0.55
5:F:76:LYS:O	5:F:79:ARG:HD3	2.06	0.55
5:F:101:ILE:HD11	5:F:124:GLU:OE1	2.07	0.55
1:A:35:ILE:HB	1:A:83:HIS:O	2.06	0.55
1:A:914:GLU:C	1:A:916:GLY:H	2.15	0.55
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.87	0.55
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.70	0.55
8:J:8:PHE:HB2	8:J:48:ARG:HH21	1.71	0.55
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.88	0.55
2:B:999:MET:HE2	2:B:1011:ILE:HD12	1.90	0.55
9:K:56:VAL:HG22	9:K:77:THR:HG22	1.89	0.55
1:A:115:LEU:O	1:A:122:MET:HE2	2.06	0.54
1:A:527:THR:CG2	1:A:650:GLN:HA	2.37	0.54
1:A:535:THR:O	1:A:575:LYS:HE3	2.07	0.54
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.89	0.54
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.42	0.54
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.89	0.54
9:K:42:LEU:HG	9:K:46:ILE:CD1	2.36	0.54
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.43	0.54
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.42	0.54
2:B:955:THR:HG23	10:L:55:ILE:HA	1.90	0.54
3:C:71:PRO:HG3	8:J:13:VAL:HG21	1.88	0.54
8:J:7:CYS:HA	8:J:49:MET:HG2	1.89	0.54
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.90	0.54
2:B:104:GLU:HG3	10:L:54:ARG:NH1	2.23	0.54
2:B:652:LYS:HE3	2:B:688:GLY:O	2.08	0.54
4:E:19:VAL:O	4:E:23:VAL:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:103:LYS:HD3	6:H:114:VAL:HB	1.89	0.54
7:I:78:CYS:SG	7:I:103:CYS:SG	3.06	0.54
8:J:32:GLU:CD	8:J:32:GLU:H	2.14	0.54
1:A:31:SER:CB	1:A:83:HIS:HB2	2.38	0.54
1:A:589:GLN:HB2	1:A:961:ARG:NH2	2.23	0.54
3:C:263:THR:C	3:C:265:MET:H	2.16	0.54
4:E:61:GLN:HG3	4:E:105:PHE:CE2	2.42	0.54
1:A:92:HIS:CD2	1:A:92:HIS:C	2.86	0.54
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.89	0.54
1:A:935:GLN:HG3	1:A:1023:ARG:HD3	1.89	0.54
2:B:1180:PHE:O	2:B:1188:LYS:HA	2.08	0.54
3:C:239:PRO:O	3:C:242:GLN:HB2	2.08	0.54
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.89	0.54
2:B:521:LEU:CD2	2:B:635:ARG:HD3	2.37	0.54
2:B:903:VAL:HG22	10:L:63:ARG:HD3	1.89	0.54
2:B:1033:LYS:HD3	2:B:1059:LEU:HD11	1.89	0.54
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.90	0.54
1:A:243:PRO:CB	1:A:244:PRO:HD2	2.37	0.54
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.88	0.54
1:A:975:HIS:H	6:H:136:LYS:NZ	2.05	0.54
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.08	0.54
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.90	0.54
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.90	0.54
2:B:751:VAL:HG13	2:B:812:LEU:HD13	1.90	0.54
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.89	0.54
2:B:950:ASP:OD2	2:B:969:ARG:NH1	2.31	0.54
6:H:36:CYS:HA	6:H:126:GLU:O	2.08	0.54
1:A:545:GLN:HG2	1:A:549:MET:CE	2.36	0.54
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.23	0.54
2:B:870:ILE:HG22	2:B:870:ILE:O	2.08	0.54
2:B:1053:GLU:OE1	2:B:1067:ARG:NH1	2.41	0.54
3:C:229:TYR:CD1	3:C:229:TYR:N	2.75	0.54
6:H:126:GLU:N	6:H:130:ARG:HH12	2.06	0.54
9:K:55:LYS:HB2	9:K:81:TYR:HE1	1.66	0.54
1:A:50:ILE:C	1:A:52:GLY:H	2.16	0.54
1:A:588:LEU:O	1:A:606:LEU:HA	2.08	0.54
1:A:903:ASN:ND2	1:A:905:ASP:H	2.04	0.54
2:B:315:LYS:HE2	7:I:13:MET:SD	2.48	0.54
7:I:8:ARG:HB3	7:I:34:TYR:CE1	2.42	0.54
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.90	0.53
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1084:GLN:HE22	3:C:192:TRP:H	0.81	0.53
3:C:178:PHE:C	3:C:178:PHE:CD2	2.86	0.53
1:A:740:LEU:HD21	3:C:193:TYR:CE2	2.43	0.53
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.90	0.53
2:B:69:LEU:HD12	2:B:90:ILE:HB	1.90	0.53
4:E:106:GLN:O	4:E:130:ALA:HA	2.08	0.53
1:A:47:ARG:O	1:A:48:ALA:HB2	2.08	0.53
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.55	0.53
1:A:1329:THR:CG2	1:A:1335:ILE:HG13	2.38	0.53
1:A:1438:THR:HG22	2:B:1142:GLY:O	2.08	0.53
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.39	0.53
2:B:1160:VAL:HG12	2:B:1161:HIS:H	1.72	0.53
2:B:1168:LEU:HB3	2:B:1170:THR:HG23	1.90	0.53
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.03	0.53
1:A:914:GLU:O	1:A:916:GLY:N	2.34	0.53
2:B:116:GLU:HG3	10:L:55:ILE:HD11	1.89	0.53
2:B:521:LEU:HD21	2:B:635:ARG:HD3	1.91	0.53
2:B:565:PRO:HG2	2:B:568:ASP:HB2	1.90	0.53
2:B:583:ASN:OD1	2:B:628:THR:N	2.41	0.53
3:C:114:TYR:HB3	3:C:140:ASN:O	2.08	0.53
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.39	0.53
1:A:84:ILE:HG22	1:A:241:VAL:HG23	1.90	0.53
2:B:40:GLU:OE1	2:B:680:THR:HG23	2.08	0.53
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.90	0.53
9:K:7:PHE:C	9:K:9:LEU:H	2.16	0.53
1:A:741:ASN:HD22	1:A:741:ASN:C	2.15	0.53
1:A:879:GLU:CD	1:A:962:ARG:HH22	2.17	0.53
2:B:705:MET:HE3	2:B:742:GLU:HG3	1.90	0.53
2:B:996:ARG:CZ	3:C:38:ILE:HG23	2.39	0.53
9:K:87:LEU:O	9:K:88:LYS:C	2.52	0.53
1:A:369:SER:OG	9:K:2:ASN:ND2	2.41	0.53
1:A:907:THR:HG22	1:A:908:LEU:N	2.24	0.53
2:B:541:LEU:HD11	2:B:808:ALA:HB1	1.91	0.53
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.64	0.53
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.90	0.53
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.89	0.53
4:E:88:VAL:HB	4:E:116:ILE:HG23	1.91	0.53
4:E:168:TYR:C	4:E:169:ARG:HG3	2.33	0.53
1:A:690:VAL:HG13	1:A:718:VAL:HG13	1.89	0.53
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.90	0.53
1:A:1341:ILE:HD11	1:A:1376:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1384:VAL:O	1:A:1386:ARG:N	2.42	0.53
3:C:31:ASN:O	3:C:35:ARG:HG3	2.08	0.53
1:A:401:GLY:O	1:A:435:HIS:ND1	2.42	0.53
1:A:1265:ASN:HD21	2:B:263:GLY:HA2	1.73	0.53
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.90	0.53
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.17	0.52
1:A:866:PHE:HZ	4:E:175:LEU:HD23	1.74	0.52
1:A:872:GLY:HA3	1:A:999:VAL:HG11	1.91	0.52
2:B:120:ARG:HG3	2:B:955:THR:CG2	2.39	0.52
2:B:121:ASN:HA	2:B:207:GLY:CA	2.39	0.52
2:B:185:THR:N	2:B:188:ASP:HB2	2.24	0.52
2:B:983:ARG:NH1	2:B:1091:TYR:CB	2.72	0.52
3:C:7:GLN:HG2	9:K:104:ASN:ND2	2.24	0.52
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.91	0.52
1:A:1164:PRO:C	1:A:1166:ASP:H	2.17	0.52
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.92	0.52
10:L:51:CYS:O	10:L:53:HIS:N	2.35	0.52
1:A:443:LEU:HG	1:A:455:MET:CE	2.40	0.52
1:A:598:LEU:O	1:A:599:SER:C	2.52	0.52
2:B:408:LEU:HD12	2:B:545:ILE:HD12	1.91	0.52
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.40	0.52
3:C:71:PRO:O	3:C:72:LEU:HD23	2.10	0.52
1:A:511:ILE:O	1:A:519:PRO:HA	2.09	0.52
1:A:1062:GLU:C	1:A:1064:VAL:N	2.67	0.52
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.90	0.52
2:B:1167:GLY:H	2:B:1217:TYR:HE2	1.57	0.52
3:C:167:HIS:CD2	3:C:169:LYS:H	2.21	0.52
4:E:15:ALA:O	4:E:19:VAL:HG23	2.09	0.52
1:A:49:LYS:CB	1:A:55:ASP:HB2	2.38	0.52
1:A:1333:ILE:HG12	1:A:1381:LEU:HD13	1.92	0.52
3:C:183:TRP:O	3:C:185:LYS:N	2.43	0.52
1:A:364:VAL:CG1	1:A:364:VAL:O	2.57	0.52
2:B:130:VAL:HG12	2:B:131:ASP:N	2.23	0.52
3:C:11:ARG:HE	3:C:209:TYR:HE2	1.55	0.52
10:L:31:CYS:HA	10:L:56:LEU:HA	1.92	0.52
1:A:90:VAL:HG13	1:A:297:GLN:NE2	2.25	0.52
1:A:1265:ASN:HD21	2:B:263:GLY:CA	2.23	0.52
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.39	0.52
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.92	0.52
2:B:361:LEU:HB3	2:B:364:ILE:HD12	1.92	0.52
4:E:6:GLU:OE2	4:E:43:LYS:NZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:31:THR:C	4:E:33:GLU:N	2.66	0.52
1:A:23:SER:CB	1:A:233:TRP:CE2	2.93	0.52
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.17	0.52
1:A:541:ILE:HG22	1:A:546:VAL:CG2	2.40	0.52
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.92	0.52
2:B:43:LEU:O	2:B:496:ARG:HD2	2.10	0.52
2:B:230:ALA:N	2:B:231:PRO:HD2	2.25	0.52
2:B:400:HIS:NE2	2:B:699:GLU:OE1	2.36	0.52
2:B:890:TYR:C	2:B:892:LYS:H	2.18	0.52
8:J:1:MET:N	8:J:1:MET:HE3	2.24	0.52
1:A:1341:ILE:HD12	1:A:1379:GLY:HA2	1.91	0.52
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.91	0.52
2:B:370:PHE:N	2:B:370:PHE:HD1	2.08	0.52
8:J:23:ASN:O	8:J:25:LEU:N	2.43	0.52
1:A:72:GLU:HB3	1:A:76:GLU:CB	2.37	0.52
1:A:362:ASP:OD2	1:A:362:ASP:N	2.41	0.52
1:A:1004:ASN:CG	4:E:167:ARG:HD2	2.35	0.52
1:A:1025:ARG:O	1:A:1035:TYR:HE1	1.93	0.52
1:A:399:HIS:O	1:A:435:HIS:ND1	2.43	0.51
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.45	0.51
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.92	0.51
8:J:23:ASN:C	8:J:25:LEU:N	2.63	0.51
1:A:19:PHE:O	1:A:1416:ALA:HA	2.11	0.51
1:A:534:LEU:O	1:A:534:LEU:HG	2.07	0.51
1:A:565:ILE:HG23	1:A:567:LYS:HE2	1.92	0.51
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.46	0.51
2:B:239:GLU:CG	2:B:255:GLN:HG2	2.40	0.51
2:B:287:ARG:NH1	2:B:324:ILE:O	2.43	0.51
2:B:550:ASP:OD1	2:B:552:MET:HG3	2.11	0.51
2:B:561:TRP:O	2:B:590:HIS:HE1	1.93	0.51
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.40	0.51
2:B:1162:ILE:HD13	2:B:1216:LEU:HB2	1.92	0.51
1:A:103:CYS:HB3	1:A:174:ILE:HD13	1.92	0.51
1:A:367:PRO:HB3	1:A:465:TYR:O	2.11	0.51
2:B:710:LEU:HD23	2:B:738:PHE:CD1	2.45	0.51
1:A:30:ILE:HB	2:B:1170:THR:HG21	1.92	0.51
1:A:437:MET:O	1:A:438:ASP:C	2.53	0.51
1:A:600:PRO:C	1:A:602:ASP:H	2.18	0.51
1:A:1222:ASN:C	1:A:1224:LEU:N	2.68	0.51
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.93	0.51
2:B:310:MET:O	2:B:313:MET:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.41	0.51
1:A:445:ASN:HD21	1:A:449:SER:HB3	1.75	0.51
1:A:47:ARG:O	1:A:48:ALA:CB	2.59	0.51
1:A:385:ILE:O	1:A:389:THR:HB	2.10	0.51
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.93	0.51
2:B:526:GLU:HG3	2:B:752:ALA:HB3	1.92	0.51
3:C:91:HIS:HB2	3:C:96:SER:OG	2.11	0.51
9:K:18:LYS:NZ	9:K:38:GLU:HG2	2.25	0.51
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.23	0.51
10:L:29:TYR:CE2	10:L:58:LYS:HG2	2.45	0.51
1:A:486:GLU:OE2	2:B:1102:LYS:HB3	2.11	0.51
1:A:567:LYS:HB3	6:H:95:TYR:HA	1.91	0.51
2:B:217:ARG:HD3	2:B:407:ASP:OD2	2.09	0.51
2:B:333:PHE:O	2:B:337:ARG:HG2	2.11	0.51
2:B:408:LEU:O	2:B:409:ALA:C	2.54	0.51
1:A:736:ASN:O	1:A:737:LEU:C	2.54	0.51
1:A:868:TYR:CZ	1:A:1064:VAL:HG22	2.46	0.51
2:B:18:PHE:N	2:B:18:PHE:CD2	2.77	0.51
2:B:845:SER:HB3	2:B:850:LEU:CD2	2.40	0.51
3:C:35:ARG:HD3	9:K:41:THR:HA	1.93	0.51
5:F:138:LEU:HB3	5:F:139:PRO:HD2	1.93	0.51
6:H:123:MET:HE1	6:H:142:LEU:HD11	1.92	0.51
1:A:600:PRO:HA	6:H:25:ARG:NH1	2.26	0.51
1:A:868:TYR:CE2	1:A:1366:ARG:HD3	2.46	0.51
1:A:1349:TYR:CD2	1:A:1349:TYR:O	2.64	0.51
2:B:62:ILE:HA	2:B:65:GLU:OE1	2.11	0.51
2:B:487:THR:HG22	2:B:490:SER:H	1.75	0.51
2:B:858:SER:HA	2:B:966:VAL:O	2.11	0.51
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.41	0.51
2:B:1138:MET:HE3	2:B:1143:ALA:HB3	1.93	0.51
3:C:180:TYR:HB3	3:C:228:PHE:HD2	1.76	0.51
9:K:47:ARG:HB3	9:K:47:ARG:NH1	2.26	0.51
9:K:58:PHE:HB3	9:K:76:GLN:CB	2.41	0.51
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.46	0.50
1:A:673:GLY:N	1:A:674:PRO:HD2	2.25	0.50
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.94	0.50
1:A:1206:ASP:CB	1:A:1274:ARG:HH12	2.24	0.50
1:A:1376:THR:O	4:E:212:ARG:NH2	2.43	0.50
2:B:680:THR:CG2	2:B:682:SER:HB2	2.41	0.50
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.46	0.50
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:7:ASP:O	6:H:8:ASP:HB2	2.11	0.50
1:A:145:LYS:HD2	1:A:149:GLU:OE1	2.12	0.50
1:A:185:TRP:O	1:A:197:PRO:HA	2.11	0.50
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.93	0.50
1:A:500:GLU:CD	1:A:1438:THR:HG21	2.35	0.50
1:A:817:ALA:HA	2:B:764:SER:OG	2.12	0.50
1:A:1015:VAL:CG1	1:A:1015:VAL:O	2.59	0.50
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.94	0.50
2:B:654:ARG:H	2:B:657:HIS:HD2	1.58	0.50
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.46	0.50
2:B:1004:GLU:OE2	2:B:1064:TYR:CE2	2.65	0.50
2:B:1027:ILE:HG12	2:B:1052:VAL:HG22	1.93	0.50
1:A:350:ARG:HA	1:A:487:MET:O	2.10	0.50
1:A:464:PRO:HB2	1:A:465:TYR:CD1	2.46	0.50
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.93	0.50
1:A:1072:ILE:HG23	1:A:1356:ILE:CD1	2.41	0.50
1:A:1139:GLU:HA	1:A:1279:ILE:HG22	1.93	0.50
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.11	0.50
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.47	0.50
5:F:109:VAL:CG1	5:F:110:ASP:H	2.24	0.50
1:A:682:THR:HG23	1:A:728:LYS:HG3	1.92	0.50
1:A:1392:SER:O	1:A:1393:ASN:HB2	2.12	0.50
2:B:241:ARG:HH21	2:B:251:ILE:HD11	1.77	0.50
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.94	0.50
9:K:78:THR:CG2	9:K:79:GLU:N	2.74	0.50
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.93	0.50
1:A:1142:THR:O	1:A:1145:SER:OG	2.29	0.50
2:B:744:HIS:HD2	2:B:746:SER:OG	1.94	0.50
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.44	0.50
1:A:112:LYS:HD2	1:A:165:GLY:HA3	1.94	0.50
2:B:89:GLU:N	2:B:137:TYR:HB2	2.27	0.50
2:B:120:ARG:HH21	2:B:956:THR:HB	1.76	0.50
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.93	0.50
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.94	0.50
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.50
1:A:1359:ASP:O	1:A:1361:SER:N	2.44	0.50
2:B:408:LEU:CD1	2:B:545:ILE:HD12	2.41	0.50
2:B:515:HIS:O	2:B:516:ASN:C	2.55	0.50
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.26	0.50
1:A:987:VAL:HG23	1:A:1028:THR:OG1	2.11	0.50
2:B:125:SER:HA	2:B:171:PRO:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.12	0.50
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.92	0.50
3:C:89:GLU:O	3:C:90:ASP:HB2	2.12	0.50
6:H:97:MET:HE3	6:H:142:LEU:HD23	1.94	0.50
7:I:69:PRO:HG2	7:I:85:PHE:O	2.12	0.50
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.47	0.49
1:A:465:TYR:CD1	1:A:465:TYR:N	2.77	0.49
1:A:562:THR:HG23	6:H:79:TRP:CD1	2.46	0.49
1:A:1198:ASP:O	1:A:1202:MET:HB2	2.12	0.49
1:A:1434:ALA:C	1:A:1436:ILE:H	2.19	0.49
2:B:604:ARG:NH2	2:B:697:GLU:OE1	2.39	0.49
2:B:1037:LEU:HD13	2:B:1062:HIS:HB3	1.94	0.49
3:C:43:THR:HG22	3:C:44:LEU:N	2.25	0.49
4:E:158:SER:O	4:E:162:ARG:HG3	2.12	0.49
9:K:39:ASP:OD1	9:K:40:HIS:N	2.45	0.49
1:A:55:ASP:H	1:A:56:PRO:CD	2.16	0.49
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.92	0.49
1:A:381:THR:HG23	1:A:383:TYR:CD1	2.47	0.49
1:A:441:PRO:HG2	1:A:498:ARG:HG2	1.93	0.49
1:A:527:THR:HG21	1:A:650:GLN:HA	1.93	0.49
1:A:557:ASP:HA	9:K:26:LYS:HD2	1.94	0.49
2:B:604:ARG:CZ	2:B:615:MET:HE2	2.43	0.49
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.92	0.49
3:C:62:PHE:O	3:C:66:ARG:HG3	2.12	0.49
5:F:128:LYS:NZ	5:F:151:LEU:O	2.39	0.49
7:I:103:CYS:HB3	7:I:108:HIS:H	1.77	0.49
1:A:460:VAL:CG1	1:A:461:LYS:N	2.75	0.49
1:A:939:ASP:OD2	1:A:1023:ARG:HD2	2.13	0.49
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.94	0.49
2:B:63:ILE:HG23	2:B:63:ILE:O	2.12	0.49
2:B:103:ASN:HB2	2:B:169:ARG:HH12	1.77	0.49
2:B:684:LEU:HD23	2:B:689:LEU:HD13	1.93	0.49
2:B:704:ALA:HB3	2:B:741:CYS:HB2	1.94	0.49
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.94	0.49
1:A:858:ASN:C	1:A:858:ASN:ND2	2.68	0.49
1:A:864:ILE:HD13	1:A:1374:VAL:HG22	1.95	0.49
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.47	0.49
2:B:235:SER:HB3	2:B:261:ARG:HA	1.93	0.49
2:B:770:GLN:HG2	2:B:983:ARG:O	2.12	0.49
2:B:806:THR:HG22	2:B:808:ALA:N	2.27	0.49
1:A:493:GLN:NE2	1:A:493:GLN:CA	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ARG:NH2	2:B:701:ILE:O	2.40	0.49
2:B:25:ILE:HD12	2:B:653:VAL:CB	2.38	0.49
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.45	0.49
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.94	0.49
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	1.94	0.49
1:A:1151:GLU:HG2	7:I:42:LEU:HD11	1.95	0.49
2:B:120:ARG:CZ	10:L:54:ARG:HH11	2.26	0.49
2:B:542:MET:HE2	2:B:747:MET:HG3	1.95	0.49
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.94	0.49
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.42	0.49
1:A:1293:SER:HB3	1:A:1299:VAL:CG2	2.42	0.49
2:B:1152:MET:HA	2:B:1152:MET:HE3	1.94	0.49
4:E:23:VAL:CG1	4:E:30:ILE:HD11	2.43	0.49
8:J:48:ARG:NE	8:J:49:MET:HE1	2.28	0.49
1:A:532:ARG:HH12	1:A:745:GLN:NE2	2.10	0.49
1:A:572:TRP:N	1:A:572:TRP:CE3	2.80	0.49
1:A:781:ASP:OD2	7:I:91:ARG:NH2	2.46	0.49
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.37	0.49
2:B:251:ILE:O	2:B:251:ILE:HG22	2.11	0.49
2:B:1152:MET:HA	2:B:1152:MET:HE2	1.95	0.49
5:F:111:LEU:HD12	5:F:111:LEU:H	1.77	0.49
6:H:47:PHE:O	6:H:47:PHE:HD2	1.96	0.49
1:A:709:THR:CG2	7:I:94:ASP:HA	2.43	0.49
1:A:1111:MET:CE	1:A:1331:SER:HB2	2.43	0.49
2:B:167:ILE:HG22	2:B:167:ILE:O	2.12	0.49
2:B:229:ALA:C	2:B:231:PRO:HD2	2.38	0.49
2:B:604:ARG:HH21	2:B:614:SER:HA	1.76	0.49
3:C:43:THR:CG2	3:C:44:LEU:N	2.75	0.49
3:C:52:GLU:HA	10:L:64:LEU:HD21	1.93	0.49
5:F:134:ILE:HD12	5:F:151:LEU:HD12	1.93	0.49
1:A:530:GLY:HA2	1:A:657:LEU:HD13	1.93	0.49
1:A:534:LEU:O	1:A:574:GLY:HA3	2.13	0.49
2:B:283:VAL:HG21	2:B:318:VAL:HA	1.95	0.49
2:B:648:HIS:CD2	2:B:648:HIS:N	2.80	0.49
2:B:1031:LEU:O	2:B:1032:SER:C	2.56	0.49
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.81	0.49
4:E:12:LEU:HD22	4:E:55:ARG:CZ	2.43	0.49
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.94	0.48
2:B:879:ARG:HB3	2:B:883:LEU:HD22	1.94	0.48
2:B:890:TYR:HD2	2:B:893:LEU:HD11	1.77	0.48
2:B:1159:ARG:CD	2:B:1193:GLN:HG3	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:62:ALA:HB3	4:E:78:LEU:HB2	1.93	0.48
5:F:81:THR:HG21	5:F:136:ARG:HD2	1.92	0.48
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.78	0.48
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.95	0.48
4:E:5:ASN:HD21	4:E:53:PRO:HD3	1.77	0.48
9:K:40:HIS:O	9:K:41:THR:C	2.56	0.48
1:A:914:GLU:C	1:A:916:GLY:N	2.70	0.48
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.13	0.48
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.95	0.48
2:B:918:ILE:HD12	2:B:935:ARG:HH11	1.78	0.48
4:E:113:GLN:HG2	4:E:137:GLU:OE1	2.13	0.48
1:A:103:CYS:SG	1:A:207:ILE:HG23	2.53	0.48
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.94	0.48
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.53	0.48
7:I:84:VAL:O	7:I:84:VAL:CG1	2.61	0.48
8:J:23:ASN:C	8:J:25:LEU:H	2.22	0.48
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.96	0.48
2:B:986:GLN:HA	2:B:986:GLN:NE2	2.27	0.48
3:C:65:HIS:CE1	3:C:69:LEU:HD11	2.48	0.48
6:H:89:LEU:C	6:H:91:ASP:H	2.22	0.48
1:A:497:THR:HG21	2:B:1149:GLU:CD	2.38	0.48
2:B:893:LEU:HD21	2:B:910:VAL:HG12	1.93	0.48
6:H:95:TYR:CE2	6:H:97:MET:HE2	2.48	0.48
1:A:917:SER:C	1:A:919:ILE:H	2.21	0.48
1:A:1128:GLN:OE1	1:A:1284:MET:HE1	2.12	0.48
1:A:1154:TYR:OH	7:I:18:GLU:HG3	2.13	0.48
2:B:227:LYS:HD3	2:B:236:HIS:CE1	2.49	0.48
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.49	0.48
3:C:47:ASP:HA	3:C:169:LYS:HZ1	1.79	0.48
3:C:99:LEU:HD23	3:C:118:LEU:HB3	1.95	0.48
1:A:1044:TRP:CE2	1:A:1048:ASN:ND2	2.82	0.48
1:A:1077:THR:O	1:A:1078:GLN:NE2	2.46	0.48
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.14	0.48
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.48
4:E:23:VAL:HG11	4:E:30:ILE:HD11	1.96	0.48
1:A:67:CYS:O	1:A:68:GLN:HB2	2.14	0.48
1:A:562:THR:HB	6:H:98:TYR:CE2	2.48	0.48
1:A:838:GLN:HE22	1:A:1070:GLN:HG2	1.79	0.48
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.62	0.48
2:B:564:GLU:N	2:B:589:VAL:O	2.45	0.48
2:B:680:THR:HG22	2:B:682:SER:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1096:ARG:HG2	2:B:1096:ARG:HH11	1.79	0.48
4:E:109:ILE:HG23	4:E:135:PHE:HD1	1.79	0.48
6:H:47:PHE:O	6:H:47:PHE:CD2	2.67	0.48
9:K:7:PHE:HB2	9:K:11:LEU:CD2	2.44	0.48
1:A:360:GLU:OE2	1:A:651:LYS:NZ	2.46	0.48
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.49	0.48
4:E:145:THR:HA	4:E:150:VAL:HG11	1.96	0.48
6:H:103:LYS:HZ2	6:H:114:VAL:CB	2.26	0.48
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.94	0.47
1:A:741:ASN:C	1:A:741:ASN:ND2	2.72	0.47
2:B:597:MET:HE1	2:B:615:MET:HB2	1.96	0.47
2:B:801:LYS:O	8:J:52:THR:CG2	2.55	0.47
3:C:82:TYR:O	3:C:83:SER:C	2.54	0.47
7:I:62:ILE:O	7:I:68:LEU:HD12	2.13	0.47
9:K:7:PHE:O	9:K:9:LEU:N	2.47	0.47
1:A:339:ASN:HD21	1:A:344:ARG:CZ	2.27	0.47
1:A:672:ASP:O	1:A:673:GLY:C	2.57	0.47
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.44	0.47
1:A:1371:LEU:O	1:A:1375:MET:HG3	2.13	0.47
2:B:1004:GLU:OE2	2:B:1064:TYR:HE2	1.97	0.47
3:C:50:GLU:OE1	3:C:156:THR:HB	2.14	0.47
1:A:836:TYR:CE2	1:A:1385:THR:HG22	2.49	0.47
1:A:967:ALA:HB1	1:A:1041:ALA:HB1	1.96	0.47
1:A:1059:HIS:CE1	5:F:87:LYS:H	2.32	0.47
2:B:755:ILE:HA	2:B:809:MET:HE3	1.96	0.47
3:C:97:VAL:CG2	3:C:129:ILE:CG2	2.92	0.47
4:E:31:THR:C	4:E:33:GLU:H	2.22	0.47
1:A:186:LYS:HE2	1:A:197:PRO:HD3	1.96	0.47
1:A:333:GLU:HG3	1:A:337:ARG:HH21	1.80	0.47
1:A:473:SER:C	1:A:475:THR:H	2.23	0.47
1:A:682:THR:CG2	1:A:728:LYS:HG3	2.45	0.47
1:A:825:ILE:HG22	1:A:826:ASP:N	2.29	0.47
1:A:868:TYR:CZ	1:A:1064:VAL:CG2	2.97	0.47
1:A:874:ASP:HB2	1:A:1058:VAL:HA	1.96	0.47
2:B:523:CYS:HB2	2:B:750:GLY:N	2.29	0.47
9:K:58:PHE:O	9:K:75:ILE:HA	2.15	0.47
1:A:55:ASP:N	1:A:56:PRO:HD2	2.15	0.47
1:A:91:PHE:CD1	1:A:99:ILE:HD13	2.49	0.47
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.79	0.47
1:A:752:LYS:HD2	2:B:1015:HIS:O	2.15	0.47
1:A:1264:GLU:HA	1:A:1267:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.45	0.47
2:B:406:LEU:CD1	2:B:498:THR:OG1	2.62	0.47
2:B:416:LEU:HD11	2:B:466:TRP:CE2	2.50	0.47
5:F:90:ARG:HG3	5:F:125:LEU:HD21	1.96	0.47
5:F:128:LYS:NZ	5:F:148:VAL:O	2.48	0.47
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.97	0.47
1:A:619:LYS:O	1:A:620:LYS:C	2.58	0.47
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.47	0.47
3:C:115:SER:O	3:C:118:LEU:HB2	2.14	0.47
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.97	0.47
1:A:92:HIS:HD2	1:A:94:GLY:N	2.12	0.47
1:A:672:ASP:CB	1:A:736:ASN:ND2	2.41	0.47
1:A:848:ILE:CD1	1:A:1374:VAL:HG21	2.42	0.47
1:A:857:ARG:CZ	5:F:139:PRO:HG3	2.45	0.47
1:A:1199:ARG:CA	1:A:1202:MET:HB2	2.45	0.47
1:A:1438:THR:CG2	2:B:1144:ALA:H	2.26	0.47
2:B:546:SER:CB	2:B:612:GLU:HG3	2.44	0.47
2:B:569:TYR:CD1	2:B:589:VAL:HG21	2.50	0.47
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.50	0.47
3:C:146:LYS:O	8:J:61:LEU:HD21	2.14	0.47
4:E:114:ASN:OD1	4:E:115:ASN:N	2.48	0.47
5:F:97:ARG:HE	5:F:124:GLU:CD	2.22	0.47
6:H:125:LEU:C	6:H:130:ARG:HH12	2.23	0.47
8:J:48:ARG:O	8:J:52:THR:HB	2.14	0.47
1:A:629:LEU:O	1:A:633:VAL:HG23	2.15	0.47
1:A:751:SER:O	1:A:752:LYS:C	2.58	0.47
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.50	0.47
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.14	0.47
2:B:572:HIS:C	2:B:572:HIS:CD2	2.93	0.47
2:B:787:VAL:O	2:B:787:VAL:HG12	2.15	0.47
2:B:973:ILE:O	2:B:974:PRO:C	2.57	0.47
3:C:40:GLU:HG2	3:C:163:ILE:HG21	1.97	0.47
1:A:32:VAL:HG23	1:A:58:LEU:HD23	1.96	0.47
1:A:313:GLN:HE21	1:A:322:VAL:HG12	1.80	0.47
1:A:364:VAL:O	1:A:364:VAL:HG13	2.15	0.47
1:A:706:HIS:NE2	1:A:1139:GLU:OE1	2.48	0.47
1:A:779:PHE:CZ	2:B:517:THR:HA	2.50	0.47
1:A:1199:ARG:O	1:A:1200:ALA:C	2.58	0.47
2:B:211:VAL:O	2:B:480:SER:HA	2.14	0.47
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.96	0.47
2:B:836:GLU:O	2:B:837:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:839:MET:HG2	2:B:1012:ILE:HG22	1.97	0.47
2:B:1128:LEU:O	2:B:1128:LEU:HG	2.15	0.47
1:A:329:LEU:HD12	1:A:1406:VAL:HG22	1.96	0.47
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.15	0.47
2:B:130:VAL:HB	2:B:167:ILE:HD12	1.96	0.47
2:B:800:GLN:CB	8:J:52:THR:CG2	2.60	0.47
2:B:842:ASN:O	2:B:846:ILE:HG13	2.15	0.47
1:A:345:VAL:HG11	2:B:1129:ARG:HA	1.97	0.46
1:A:445:ASN:ND2	1:A:449:SER:HB3	2.31	0.46
1:A:579:SER:OG	1:A:612:ILE:HG23	2.15	0.46
1:A:855:THR:HG21	1:A:857:ARG:CZ	2.44	0.46
2:B:343:ILE:HG22	2:B:348:ARG:HG3	1.97	0.46
2:B:571:PRO:C	2:B:573:GLN:N	2.72	0.46
4:E:84:ASP:O	4:E:113:GLN:NE2	2.48	0.46
7:I:2:THR:HG22	7:I:2:THR:O	2.15	0.46
9:K:103:THR:O	9:K:104:ASN:C	2.58	0.46
1:A:22:PHE:HB3	1:A:27:VAL:HG22	1.97	0.46
1:A:620:LYS:O	1:A:625:SER:OG	2.34	0.46
1:A:1276:VAL:CG1	1:A:1279:ILE:HD13	2.45	0.46
2:B:314:LEU:O	2:B:315:LYS:C	2.59	0.46
2:B:422:LYS:HD2	2:B:422:LYS:HA	1.74	0.46
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.45	0.46
3:C:70:ILE:HG21	3:C:115:SER:HB3	1.97	0.46
3:C:142:VAL:CG1	8:J:5:VAL:HG22	2.45	0.46
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.47	0.46
1:A:32:VAL:HG22	1:A:81:PHE:O	2.16	0.46
1:A:778:GLY:HA3	2:B:516:ASN:ND2	2.30	0.46
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.80	0.46
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.96	0.46
3:C:246:ARG:HA	3:C:249:ASP:CB	2.46	0.46
1:A:122:MET:HE1	1:A:138:ILE:HG23	1.97	0.46
1:A:1191:TRP:CZ3	7:I:43:VAL:HG21	2.51	0.46
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.80	0.46
2:B:552:MET:N	2:B:553:PRO:HD2	2.30	0.46
2:B:851:PHE:CD2	2:B:1094:ARG:HB2	2.50	0.46
3:C:10:ILE:HG21	9:K:112:GLN:HG3	1.96	0.46
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.97	0.46
6:H:99:GLY:HA3	6:H:118:PHE:CD2	2.50	0.46
1:A:767:GLN:HA	1:A:799:PHE:HA	1.96	0.46
2:B:65:GLU:O	2:B:65:GLU:HG2	2.15	0.46
2:B:906:SER:O	2:B:907:GLY:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:VAL:O	3:C:243:VAL:N	2.48	0.46
1:A:868:TYR:CD1	1:A:1064:VAL:HG11	2.50	0.46
1:A:1215:ARG:HA	1:A:1218:GLN:HE21	1.80	0.46
2:B:47:GLN:NE2	2:B:408:LEU:HD21	2.31	0.46
2:B:770:GLN:HB2	2:B:985:GLY:H	1.80	0.46
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.50	0.46
6:H:87:ARG:O	6:H:89:LEU:N	2.44	0.46
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.16	0.46
9:K:45:LEU:HG	9:K:94:ILE:CD1	2.45	0.46
2:B:173:MET:HE1	2:B:409:ALA:HB2	1.98	0.46
2:B:557:PHE:CD2	2:B:557:PHE:C	2.94	0.46
2:B:841:MET:HB2	2:B:990:ILE:HG12	1.98	0.46
3:C:44:LEU:CD2	3:C:130:GLY:HA2	2.46	0.46
3:C:164:ALA:HB2	3:C:171:GLY:HA2	1.98	0.46
3:C:167:HIS:CD2	3:C:169:LYS:HB3	2.51	0.46
6:H:103:LYS:CD	6:H:114:VAL:HB	2.46	0.46
1:A:87:ALA:HB2	1:A:277:GLU:HG3	1.97	0.46
1:A:590:ARG:HG2	1:A:605:MET:HB3	1.97	0.46
1:A:1164:PRO:O	1:A:1166:ASP:N	2.49	0.46
2:B:515:HIS:CD2	2:B:517:THR:H	2.33	0.46
3:C:243:VAL:O	3:C:244:VAL:C	2.59	0.46
8:J:2:ILE:HG12	8:J:57:ILE:HG21	1.97	0.46
1:A:456:MET:HB3	1:A:507:VAL:HG22	1.98	0.46
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.41	0.46
1:A:1116:LEU:HD23	1:A:1316:VAL:HG11	1.96	0.46
2:B:25:ILE:HD12	2:B:653:VAL:CG2	2.46	0.46
2:B:823:ALA:O	2:B:1089:PRO:HA	2.15	0.46
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.45	0.46
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.97	0.46
3:C:262:LEU:HD21	9:K:87:LEU:HD23	1.98	0.46
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.98	0.46
1:A:567:LYS:CB	6:H:95:TYR:HA	2.46	0.46
1:A:873:MET:HE3	1:A:957:PRO:HG3	1.98	0.46
2:B:306:ASN:O	2:B:308:TRP:N	2.43	0.46
2:B:322:PHE:CE1	7:I:30:ARG:HG3	2.51	0.46
2:B:657:HIS:O	2:B:660:LYS:HB2	2.15	0.46
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.15	0.46
8:J:1:MET:O	8:J:57:ILE:HG22	2.16	0.46
1:A:361:LEU:O	1:A:361:LEU:HG	2.11	0.45
1:A:663:SER:O	1:A:742:ASN:HB3	2.16	0.45
1:A:909:ASP:C	1:A:911:SER:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:GLN:CG	1:A:1188:GLN:H	2.28	0.45
2:B:291:ILE:HD12	2:B:300:HIS:CE1	2.51	0.45
2:B:416:LEU:O	2:B:420:LEU:N	2.50	0.45
2:B:816:GLU:OE1	2:B:816:GLU:N	2.49	0.45
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.16	0.45
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.36	0.45
3:C:175:ALA:HB2	8:J:43:ARG:CZ	2.46	0.45
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.77	0.45
5:F:93:ILE:O	5:F:94:LEU:C	2.58	0.45
8:J:31:ASP:OD1	8:J:34:THR:OG1	2.32	0.45
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.98	0.45
1:A:456:MET:HE1	1:A:474:VAL:HG22	1.98	0.45
1:A:497:THR:HG21	2:B:1149:GLU:OE2	2.17	0.45
1:A:848:ILE:HD13	1:A:1370:LEU:HD11	1.98	0.45
2:B:899:ILE:CG2	2:B:903:VAL:HB	2.47	0.45
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.98	0.45
1:A:1220:PHE:CE1	1:A:1271:ILE:HD11	2.51	0.45
1:A:1341:ILE:HD13	4:E:212:ARG:NH2	2.32	0.45
2:B:515:HIS:O	2:B:518:HIS:HB2	2.16	0.45
1:A:470:LEU:CD1	1:A:487:MET:CE	2.75	0.45
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.29	0.45
1:A:842:VAL:O	1:A:843:LYS:C	2.58	0.45
1:A:843:LYS:HZ3	1:A:1386:ARG:HB3	1.79	0.45
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.16	0.45
1:A:1433:MET:HE2	1:A:1439:GLY:CA	2.47	0.45
2:B:20:ASP:C	2:B:22:SER:H	2.24	0.45
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.98	0.45
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.97	0.45
2:B:1065:GLN:NE2	2:B:1069:PHE:H	2.05	0.45
1:A:27:VAL:HB	1:A:238:CYS:SG	2.56	0.45
1:A:329:LEU:HD21	2:B:1203:LEU:HD13	1.98	0.45
1:A:1076:ALA:C	1:A:1078:GLN:H	2.25	0.45
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.98	0.45
2:B:89:GLU:HB2	2:B:137:TYR:CD1	2.52	0.45
2:B:519:TRP:CD1	2:B:519:TRP:C	2.95	0.45
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.45
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.79	0.45
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.98	0.45
2:B:1002:THR:O	2:B:1003:ALA:C	2.60	0.45
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.47	0.45
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:147:HIS:HD2	4:E:149:LEU:N	2.09	0.45
7:I:34:TYR:HE2	7:I:36:GLU:HG2	1.81	0.45
1:A:391:LEU:HD12	1:A:434:ARG:HB3	1.99	0.45
1:A:405:VAL:HB	1:A:413:ILE:HD12	1.99	0.45
1:A:553:VAL:CG2	1:A:652:VAL:HG21	2.43	0.45
1:A:556:TRP:HD1	1:A:580:VAL:HG11	1.81	0.45
1:A:848:ILE:HD11	1:A:1374:VAL:CG2	2.44	0.45
1:A:880:LYS:HG3	1:A:955:PRO:HD3	1.98	0.45
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.98	0.45
4:E:71:LYS:O	4:E:73:PRO:HD3	2.17	0.45
1:A:17:VAL:HA	2:B:1215:ARG:O	2.17	0.45
1:A:445:ASN:HB2	1:A:455:MET:HE3	1.98	0.45
1:A:565:ILE:CG2	1:A:567:LYS:HE2	2.46	0.45
1:A:838:GLN:NE2	1:A:1070:GLN:HG2	2.31	0.45
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.21	0.45
2:B:808:ALA:O	2:B:812:LEU:HG	2.15	0.45
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.17	0.45
3:C:259:LEU:HD21	9:K:88:LYS:HA	1.99	0.45
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.51	0.45
1:A:325:ILE:HA	1:A:328:ARG:HB2	1.99	0.45
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.77	0.45
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.42	0.45
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.48	0.45
2:B:890:TYR:HD2	2:B:893:LEU:CD1	2.30	0.45
2:B:1098:MET:O	2:B:1099:VAL:C	2.60	0.45
1:A:11:LEU:HD11	2:B:1195:HIS:NE2	2.32	0.45
1:A:699:ALA:O	1:A:700:ASN:CB	2.65	0.45
2:B:801:LYS:HG2	8:J:52:THR:O	2.17	0.45
2:B:859:TYR:OH	2:B:942:ARG:HG3	2.16	0.45
1:A:243:PRO:C	1:A:245:PRO:HD2	2.41	0.45
1:A:809:THR:HG22	2:B:730:ARG:HG2	1.99	0.45
1:A:1276:VAL:HG12	1:A:1279:ILE:HD13	1.97	0.45
2:B:535:LEU:HD23	2:B:535:LEU:HA	1.77	0.45
2:B:783:THR:HG23	2:B:817:LEU:HD21	1.99	0.45
3:C:26:ASP:O	3:C:27:LEU:C	2.60	0.45
3:C:263:THR:C	3:C:265:MET:N	2.75	0.45
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.17	0.45
1:A:780:VAL:HG23	2:B:699:GLU:OE2	2.17	0.44
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	1.99	0.44
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.98	0.44
2:B:406:LEU:HD13	2:B:498:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG23	3:C:58:LEU:H	1.82	0.44
6:H:18:GLY:C	6:H:20:TYR:H	2.25	0.44
1:A:95:PHE:O	1:A:96:ILE:C	2.61	0.44
1:A:911:SER:O	1:A:978:PRO:CB	2.63	0.44
2:B:40:GLU:OE1	2:B:680:THR:CG2	2.66	0.44
2:B:234:ILE:HG22	2:B:236:HIS:O	2.18	0.44
2:B:405:ARG:NE	2:B:632:ARG:HG3	2.33	0.44
2:B:623:GLU:OE1	2:B:625:LYS:HE3	2.17	0.44
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.82	0.44
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.99	0.44
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.99	0.44
3:C:145:CYS:SG	3:C:146:LYS:N	2.90	0.44
8:J:23:ASN:O	8:J:24:LEU:C	2.59	0.44
1:A:937:VAL:O	1:A:938:LYS:C	2.61	0.44
2:B:99:LYS:HB3	2:B:180:TYR:CE2	2.53	0.44
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.99	0.44
2:B:350:GLN:O	2:B:354:ASP:OD2	2.35	0.44
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.98	0.44
2:B:882:THR:HG21	2:B:935:ARG:HG3	2.00	0.44
1:A:523:ILE:HG23	1:A:527:THR:HB	2.00	0.44
1:A:560:ILE:HD11	9:K:58:PHE:HD1	1.81	0.44
1:A:600:PRO:O	1:A:602:ASP:N	2.50	0.44
1:A:777:PHE:CE1	1:A:792:TYR:CZ	3.04	0.44
1:A:1153:TYR:CZ	7:I:42:LEU:HD13	2.53	0.44
1:A:1397:LEU:HB3	1:A:1429:ILE:HD12	2.00	0.44
2:B:322:PHE:HE1	7:I:30:ARG:HG3	1.82	0.44
3:C:6:PRO:HG2	9:K:97:LYS:O	2.18	0.44
3:C:240:VAL:O	3:C:241:ASP:C	2.60	0.44
6:H:15:VAL:HG13	6:H:24:CYS:HB3	1.99	0.44
6:H:135:LEU:HD13	6:H:137:GLN:HB2	1.99	0.44
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.33	0.44
1:A:596:THR:HG22	1:A:597:LEU:H	1.83	0.44
2:B:53:GLN:NE2	2:B:57:TYR:HB2	2.33	0.44
2:B:235:SER:HB3	2:B:260:GLY:O	2.18	0.44
2:B:235:SER:C	2:B:236:HIS:CD2	2.96	0.44
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.99	0.44
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.82	0.44
2:B:1001:PHE:CZ	2:B:1073:TYR:CB	2.99	0.44
2:B:1002:THR:HG22	2:B:1006:ILE:HB	2.00	0.44
1:A:605:MET:HE3	1:A:607:ILE:CG1	2.48	0.44
1:A:617:VAL:CG1	1:A:622:VAL:HB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:TRP:HA	1:A:955:PRO:HD2	1.64	0.44
1:A:1215:ARG:HD2	1:A:1218:GLN:HE21	1.82	0.44
2:B:680:THR:HG21	2:B:682:SER:HB2	1.99	0.44
3:C:18:VAL:O	3:C:20:PHE:N	2.50	0.44
3:C:22:LEU:HD12	3:C:230:MET:HE3	2.00	0.44
1:A:913:LEU:HD12	1:A:914:GLU:H	1.83	0.44
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.51	0.44
2:B:170:LEU:HD13	2:B:457:LEU:HD13	2.00	0.44
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.44
2:B:334:ILE:O	2:B:335:GLY:C	2.61	0.44
2:B:863:GLU:CD	2:B:962:LYS:HB2	2.43	0.44
2:B:1002:THR:HG22	2:B:1006:ILE:O	2.17	0.44
3:C:80:LEU:HD12	3:C:94:LYS:O	2.18	0.44
3:C:205:LYS:HB3	3:C:206:ASN:OD1	2.18	0.44
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.42	0.44
1:A:523:ILE:HB	1:A:622:VAL:HG13	2.00	0.44
1:A:903:ASN:C	1:A:905:ASP:N	2.75	0.44
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.99	0.44
2:B:360:PHE:CE2	2:B:374:LYS:HB3	2.52	0.44
2:B:651:LEU:CD2	2:B:741:CYS:HB3	2.47	0.44
2:B:826:ALA:HB2	2:B:1087:PHE:HE1	1.81	0.44
2:B:976:ILE:O	2:B:1099:VAL:HG21	2.18	0.44
4:E:178:ILE:HG23	4:E:214:CYS:HA	2.00	0.44
5:F:119:ARG:HA	5:F:122:MET:HE2	2.00	0.44
5:F:151:LEU:HD23	5:F:151:LEU:HA	1.78	0.44
9:K:107:THR:HG22	9:K:108:GLU:N	2.33	0.44
10:L:27:LEU:HD22	10:L:37:LYS:HD3	1.99	0.44
1:A:687:LYS:NZ	1:A:795:GLU:HG3	2.33	0.44
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.18	0.44
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.58	0.44
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.18	0.44
2:B:1163:CYS:SG	2:B:1187:ASN:ND2	2.91	0.44
4:E:20:LYS:HE3	4:E:34:GLU:HG2	2.00	0.44
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.25	0.44
1:A:329:LEU:O	1:A:333:GLU:N	2.39	0.43
1:A:474:VAL:O	1:A:474:VAL:HG13	2.17	0.43
1:A:704:ALA:HB1	1:A:708:MET:O	2.18	0.43
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.50	0.43
1:A:1006:ILE:HB	4:E:167:ARG:HG3	1.98	0.43
1:A:1017:LEU:HB2	4:E:206:GLY:N	2.33	0.43
1:A:1064:VAL:HG13	1:A:1370:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.32	0.43
2:B:99:LYS:HB3	2:B:180:TYR:CZ	2.53	0.43
2:B:287:ARG:NH1	2:B:321:GLY:O	2.50	0.43
4:E:17:ARG:O	4:E:20:LYS:HB2	2.18	0.43
6:H:26:ILE:CD1	6:H:42:ILE:HB	2.48	0.43
9:K:105:PHE:O	9:K:106:GLU:C	2.61	0.43
1:A:566:ILE:HD11	6:H:98:TYR:HB2	2.00	0.43
1:A:909:ASP:O	1:A:911:SER:N	2.51	0.43
2:B:195:CYS:SG	2:B:782:LEU:HD22	2.58	0.43
2:B:199:MET:HE3	2:B:488:TYR:CZ	2.52	0.43
2:B:601:ARG:HA	2:B:615:MET:HE1	2.00	0.43
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.00	0.43
3:C:226:ASP:O	3:C:227:THR:HB	2.17	0.43
3:C:234:SER:HB2	3:C:240:VAL:HG13	2.00	0.43
10:L:62:LYS:C	10:L:64:LEU:H	2.26	0.43
1:A:41:MET:HG2	1:A:48:ALA:O	2.17	0.43
1:A:367:PRO:HB3	1:A:466:SER:HA	2.00	0.43
1:A:528:LEU:HD23	1:A:751:SER:N	2.33	0.43
1:A:549:MET:SD	1:A:577:ILE:CD1	3.06	0.43
1:A:630:ILE:O	1:A:631:HIS:C	2.60	0.43
1:A:724:GLU:O	1:A:728:LYS:HG2	2.18	0.43
1:A:1134:ILE:HG22	1:A:1306:LEU:CD1	2.48	0.43
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	2.00	0.43
1:A:1422:ARG:HA	1:A:1435:PRO:CG	2.49	0.43
2:B:120:ARG:NH2	10:L:54:ARG:HD2	2.33	0.43
2:B:212:LEU:HD21	2:B:461:LEU:HG	1.99	0.43
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.99	0.43
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.83	0.43
4:E:198:ILE:CD1	4:E:212:ARG:HG3	2.48	0.43
5:F:93:ILE:CG2	5:F:130:ILE:HD13	2.48	0.43
6:H:18:GLY:O	6:H:20:TYR:N	2.50	0.43
6:H:31:THR:O	6:H:32:THR:CB	2.65	0.43
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.19	0.43
1:A:605:MET:HE2	1:A:607:ILE:HD11	2.00	0.43
1:A:830:LYS:HG2	1:A:1079:MET:O	2.17	0.43
1:A:1066:VAL:O	1:A:1067:LEU:C	2.60	0.43
2:B:384:ARG:HE	2:B:384:ARG:HB3	1.60	0.43
2:B:593:PRO:O	2:B:596:LEU:HB3	2.18	0.43
2:B:597:MET:HG3	2:B:601:ARG:NH1	2.33	0.43
2:B:904:ARG:NH2	2:B:948:ILE:HD11	2.33	0.43
3:C:41:ILE:HG22	3:C:172:PRO:HG3	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:12:VAL:HG22	6:H:28:ALA:HB2	2.00	0.43
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.34	0.43
9:K:7:PHE:C	9:K:9:LEU:N	2.76	0.43
1:A:187:LYS:O	1:A:188:ASP:HB2	2.18	0.43
1:A:239:LEU:HD23	1:A:240:PRO:O	2.19	0.43
1:A:277:GLU:C	1:A:279:LEU:H	2.27	0.43
1:A:337:ARG:HH22	1:A:1403:GLU:HA	1.82	0.43
1:A:664:THR:HA	1:A:668:ASP:OD2	2.19	0.43
1:A:849:MET:HE2	1:A:1063:MET:SD	2.59	0.43
2:B:620:ARG:NH2	7:I:86:PHE:CB	2.81	0.43
2:B:847:ASP:O	3:C:65:HIS:HE1	2.01	0.43
3:C:108:GLU:HG2	3:C:149:LYS:CD	2.49	0.43
3:C:121:VAL:O	3:C:121:VAL:CG1	2.65	0.43
6:H:91:ASP:C	6:H:93:TYR:N	2.75	0.43
7:I:50:THR:HB	7:I:92:ARG:NH2	2.34	0.43
1:A:48:ALA:O	1:A:49:LYS:HG3	2.19	0.43
1:A:219:PHE:C	1:A:219:PHE:HD1	2.25	0.43
1:A:266:LEU:HA	1:A:269:ILE:HD12	2.00	0.43
1:A:655:PHE:CD2	1:A:655:PHE:C	2.96	0.43
1:A:845:LEU:HB3	1:A:848:ILE:HD12	2.01	0.43
1:A:1438:THR:HA	5:F:88:TYR:HB3	2.00	0.43
2:B:1169:MET:HE2	2:B:1204:PHE:HB2	2.00	0.43
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.44	0.43
3:C:263:THR:O	3:C:265:MET:N	2.52	0.43
9:K:113:THR:O	9:K:114:LEU:CB	2.67	0.43
1:A:399:HIS:C	1:A:401:GLY:N	2.75	0.43
1:A:541:ILE:HD12	1:A:541:ILE:N	2.33	0.43
1:A:785:PRO:HG3	2:B:698:GLU:HG2	1.99	0.43
1:A:974:ASP:HA	6:H:136:LYS:HE2	2.01	0.43
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.18	0.43
2:B:31:TRP:CZ2	2:B:744:HIS:CD2	3.06	0.43
2:B:785:TYR:CD1	2:B:785:TYR:C	2.96	0.43
2:B:955:THR:HG22	2:B:956:THR:H	1.83	0.43
2:B:1152:MET:HE3	2:B:1152:MET:CA	2.48	0.43
4:E:144:ILE:HG13	4:E:145:THR:N	2.32	0.43
4:E:167:ARG:HA	4:E:167:ARG:HD3	1.75	0.43
8:J:14:VAL:HG13	8:J:50:ILE:CD1	2.44	0.43
1:A:387:ARG:O	1:A:391:LEU:HG	2.19	0.43
1:A:483:ASP:HB3	2:B:837:ASP:HB3	2.00	0.43
2:B:120:ARG:HH11	2:B:122:LEU:HD11	1.83	0.43
2:B:336:ARG:HG2	2:B:348:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.34	0.43
2:B:1080:LYS:HG3	3:C:180:TYR:CZ	2.54	0.43
9:K:18:LYS:O	9:K:35:PHE:HA	2.19	0.43
9:K:49:GLU:HG3	9:K:94:ILE:HG13	2.00	0.43
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.59	0.43
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.87	0.43
1:A:596:THR:HB	1:A:598:LEU:H	1.83	0.43
1:A:1398:MET:O	1:A:1399:ARG:C	2.61	0.43
3:C:115:SER:HB2	3:C:132:PRO:HB3	2.00	0.43
4:E:19:VAL:HG11	4:E:80:VAL:CG1	2.41	0.43
5:F:134:ILE:HD12	5:F:151:LEU:CD1	2.48	0.43
8:J:30:LEU:HD22	8:J:34:THR:HB	2.00	0.43
9:K:23:PRO:O	9:K:24:ASP:C	2.61	0.43
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.44	0.43
1:A:663:SER:OG	1:A:664:THR:N	2.52	0.43
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.53	0.43
2:B:29:ASP:CB	2:B:658:ILE:HD12	2.41	0.43
2:B:280:ILE:HA	2:B:281:PRO:HD2	1.87	0.43
2:B:1103:ILE:O	2:B:1104:HIS:C	2.61	0.43
4:E:111:VAL:HA	4:E:135:PHE:O	2.19	0.43
5:F:77:ASP:O	5:F:78:GLN:HB2	2.19	0.43
5:F:147:SER:O	5:F:150:GLU:N	2.50	0.43
6:H:110:ASP:O	6:H:128:ASN:ND2	2.52	0.43
8:J:21:TYR:HB2	8:J:39:LEU:CD1	2.47	0.43
9:K:31:VAL:O	9:K:74:ARG:HA	2.19	0.43
1:A:49:LYS:HB3	1:A:55:ASP:CB	2.48	0.42
1:A:493:GLN:HA	1:A:493:GLN:HE21	1.80	0.42
1:A:619:LYS:HD2	1:A:750:GLY:HA3	2.00	0.42
1:A:781:ASP:O	1:A:782:ARG:HB3	2.19	0.42
1:A:849:MET:CE	1:A:1063:MET:SD	3.07	0.42
1:A:1293:SER:HB3	1:A:1299:VAL:HG21	2.00	0.42
2:B:515:HIS:N	2:B:518:HIS:HD2	2.07	0.42
2:B:1010:LEU:HA	2:B:1010:LEU:HD12	1.82	0.42
3:C:175:ALA:HB2	8:J:43:ARG:NE	2.33	0.42
9:K:57:LEU:N	9:K:76:GLN:O	2.52	0.42
10:L:51:CYS:C	10:L:53:HIS:N	2.74	0.42
1:A:1104:ILE:HG22	1:A:1105:LEU:N	2.33	0.42
1:A:1201:ALA:HB1	1:A:1205:LYS:NZ	2.34	0.42
2:B:234:ILE:HG21	2:B:257:LYS:HB3	2.00	0.42
2:B:578:THR:HA	2:B:622:LYS:O	2.18	0.42
2:B:651:LEU:CD1	2:B:707:PRO:HB3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:VAL:HG13	2:B:689:LEU:HB3	2.00	0.42
2:B:890:TYR:O	2:B:892:LYS:N	2.52	0.42
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.33	0.42
1:A:123:ARG:HH22	1:A:155:GLU:HG2	1.83	0.42
1:A:407:ARG:O	1:A:408:ASP:C	2.62	0.42
1:A:445:ASN:ND2	1:A:455:MET:HG2	2.34	0.42
1:A:741:ASN:HD22	1:A:743:VAL:N	2.17	0.42
1:A:1137:ALA:HB2	1:A:1274:ARG:HH21	1.84	0.42
2:B:377:PHE:CE2	2:B:381:MET:HE2	2.54	0.42
3:C:56:THR:HG21	3:C:63:ILE:HD11	2.01	0.42
8:J:24:LEU:HD23	8:J:24:LEU:HA	1.83	0.42
10:L:53:HIS:C	10:L:55:ILE:H	2.26	0.42
1:A:350:ARG:HD2	2:B:1128:LEU:HB2	2.02	0.42
1:A:567:LYS:NZ	6:H:95:TYR:CZ	2.69	0.42
1:A:837:ILE:HD12	1:A:1098:VAL:HG13	2.01	0.42
1:A:903:ASN:C	1:A:903:ASN:ND2	2.76	0.42
1:A:925:LEU:O	1:A:928:LEU:N	2.52	0.42
1:A:928:LEU:HD11	1:A:984:LYS:HG2	2.00	0.42
2:B:728:ARG:HD2	2:B:730:ARG:HH21	1.84	0.42
2:B:1182:CYS:HB3	2:B:1187:ASN:HB2	2.01	0.42
3:C:178:PHE:C	3:C:178:PHE:HD2	2.27	0.42
6:H:80:ARG:HG2	9:K:57:LEU:HD22	2.02	0.42
8:J:48:ARG:O	8:J:52:THR:CB	2.68	0.42
1:A:463:ILE:HD13	1:A:469:ARG:HD2	2.01	0.42
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.54	0.42
1:A:738:LYS:NZ	3:C:194:GLU:C	2.78	0.42
2:B:104:GLU:HG3	10:L:54:ARG:CZ	2.50	0.42
2:B:287:ARG:HG2	2:B:292:ILE:HA	2.01	0.42
2:B:615:MET:HB2	2:B:615:MET:HE3	1.92	0.42
2:B:666:TYR:C	2:B:668:ASP:H	2.28	0.42
2:B:776:GLN:HA	2:B:1096:ARG:NH1	2.34	0.42
2:B:882:THR:C	2:B:884:ARG:H	2.28	0.42
3:C:91:HIS:HB2	3:C:96:SER:CB	2.49	0.42
4:E:85:GLU:HA	4:E:86:PRO:HD3	1.85	0.42
7:I:50:THR:HG22	7:I:51:ASN:N	2.35	0.42
1:A:535:THR:HG21	1:A:616:VAL:CA	2.49	0.42
1:A:566:ILE:O	1:A:567:LYS:O	2.38	0.42
1:A:715:GLU:OE1	1:A:774:ARG:NH1	2.53	0.42
1:A:782:ARG:NH2	2:B:699:GLU:O	2.52	0.42
1:A:1067:LEU:HD23	1:A:1367:HIS:HE1	1.85	0.42
1:A:1124:HIS:HB2	1:A:1130:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:ARG:HB3	1:A:1301:GLU:O	2.19	0.42
2:B:46:GLN:NE2	2:B:496:ARG:HA	2.32	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.42
2:B:515:HIS:HB3	2:B:518:HIS:CD2	2.55	0.42
3:C:61:GLU:HB3	10:L:67:PHE:CE2	2.55	0.42
3:C:71:PRO:C	3:C:72:LEU:HD23	2.45	0.42
3:C:180:TYR:HD1	3:C:181:ASP:HB2	1.84	0.42
4:E:4:GLU:O	4:E:5:ASN:C	2.63	0.42
1:A:298:PHE:HE2	1:A:312:PRO:HG3	1.85	0.42
1:A:562:THR:HG23	6:H:79:TRP:HD1	1.85	0.42
1:A:567:LYS:HB3	6:H:95:TYR:CA	2.50	0.42
1:A:1215:ARG:HH11	1:A:1218:GLN:NE2	2.17	0.42
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.01	0.42
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.99	0.42
4:E:96:PHE:CE2	4:E:100:ILE:HD11	2.53	0.42
1:A:365:GLY:O	1:A:468:PHE:HA	2.20	0.42
1:A:451:HIS:O	1:A:452:LYS:C	2.63	0.42
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.89	0.42
1:A:1165:GLU:H	1:A:1165:GLU:HG3	1.60	0.42
2:B:36:ALA:CB	2:B:661:LEU:HD22	2.50	0.42
2:B:204:ILE:O	2:B:205:ILE:HG12	2.19	0.42
2:B:953:LEU:O	2:B:964:VAL:HA	2.20	0.42
3:C:99:LEU:HD12	3:C:99:LEU:N	2.35	0.42
8:J:16:ASP:OD1	8:J:17:LYS:CG	2.67	0.42
1:A:151:ASP:HB3	1:A:161:LEU:HB3	2.02	0.42
1:A:329:LEU:O	1:A:333:GLU:CG	2.68	0.42
1:A:704:ALA:HB2	1:A:710:LEU:CD1	2.44	0.42
1:A:733:ALA:O	1:A:737:LEU:HG	2.20	0.42
1:A:825:ILE:HD11	2:B:512:ARG:C	2.45	0.42
1:A:848:ILE:HB	1:A:1065:GLY:HA3	2.02	0.42
1:A:993:LEU:O	1:A:996:ASN:HB2	2.20	0.42
1:A:1080:THR:O	1:A:1081:LEU:HD23	2.20	0.42
1:A:1166:ASP:HA	1:A:1169:ILE:CG2	2.43	0.42
2:B:194:GLU:O	2:B:195:CYS:C	2.62	0.42
2:B:899:ILE:HD12	2:B:911:ILE:HA	2.02	0.42
3:C:5:GLY:C	3:C:24:ASN:HD22	2.27	0.42
3:C:167:HIS:C	3:C:169:LYS:H	2.28	0.42
7:I:101:PHE:CD1	7:I:101:PHE:N	2.88	0.42
1:A:286:HIS:C	1:A:288:ALA:N	2.77	0.42
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.55	0.42
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:HB2	2:B:985:GLY:N	2.35	0.42
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.20	0.42
2:B:890:TYR:CZ	2:B:910:VAL:HG21	2.54	0.42
2:B:1084:GLN:HE21	3:C:201:TRP:HZ2	1.65	0.42
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.34	0.42
9:K:1:MET:HE3	9:K:1:MET:HB2	1.94	0.42
1:A:1436:ILE:HG13	2:B:1144:ALA:HB2	2.00	0.41
2:B:789:MET:HE3	2:B:789:MET:HB3	1.91	0.41
7:I:97:MET:HE3	7:I:97:MET:HB2	1.89	0.41
1:A:741:ASN:ND2	1:A:743:VAL:H	2.18	0.41
1:A:994:GLN:HE22	1:A:1023:ARG:HH21	1.68	0.41
1:A:1220:PHE:O	1:A:1221:LYS:C	2.63	0.41
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.33	0.41
1:A:1359:ASP:C	1:A:1361:SER:N	2.77	0.41
2:B:185:THR:H	2:B:188:ASP:HB2	1.84	0.41
2:B:792:MET:HE2	2:B:857:ARG:HH22	1.85	0.41
2:B:1162:ILE:HD11	2:B:1216:LEU:HD12	2.01	0.41
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.55	0.41
5:F:114:GLU:OE2	5:F:119:ARG:HG2	2.20	0.41
8:J:2:ILE:HG22	8:J:3:VAL:H	1.85	0.41
8:J:48:ARG:HE	8:J:49:MET:HE1	1.84	0.41
9:K:65:HIS:HB3	9:K:68:PHE:CD1	2.55	0.41
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.35	0.41
1:A:974:ASP:C	1:A:976:THR:H	2.29	0.41
1:A:1106:ASN:O	1:A:1107:VAL:C	2.62	0.41
2:B:224:GLN:HB3	2:B:226:PHE:CZ	2.56	0.41
2:B:1072:MET:SD	2:B:1085:ILE:HD12	2.60	0.41
9:K:35:PHE:CE1	9:K:73:LEU:HD12	2.55	0.41
1:A:146:MET:HE3	1:A:146:MET:HB2	1.78	0.41
1:A:216:VAL:O	1:A:220:THR:HB	2.20	0.41
2:B:63:ILE:HB	2:B:95:ILE:HD11	2.01	0.41
2:B:335:GLY:O	2:B:339:THR:HB	2.21	0.41
2:B:1167:GLY:N	2:B:1217:TYR:HE2	2.17	0.41
3:C:56:THR:CG2	3:C:63:ILE:HD11	2.49	0.41
10:L:49:LYS:O	10:L:50:ASP:HB2	2.19	0.41
1:A:95:PHE:HB3	1:A:234:MET:SD	2.60	0.41
2:B:809:MET:CG	2:B:814:PHE:HB3	2.51	0.41
2:B:1002:THR:HG23	2:B:1004:GLU:HB2	2.01	0.41
2:B:1038:SER:C	2:B:1040:ASN:H	2.28	0.41
7:I:61:ASP:O	7:I:64:SER:N	2.49	0.41
8:J:5:VAL:O	8:J:14:VAL:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:5:ASP:HB3	9:K:7:PHE:CE2	2.56	0.41
1:A:21:LEU:HD21	1:A:95:PHE:CZ	2.55	0.41
1:A:32:VAL:CG2	1:A:58:LEU:HD23	2.51	0.41
1:A:91:PHE:HB3	1:A:96:ILE:HG12	2.02	0.41
1:A:805:LEU:O	1:A:805:LEU:HG	2.18	0.41
1:A:834:THR:HG21	1:A:1077:THR:HA	2.02	0.41
2:B:420:LEU:HD13	2:B:453:ILE:HA	2.02	0.41
2:B:842:ASN:HB3	2:B:1009:ASP:HA	2.02	0.41
3:C:66:ARG:O	3:C:67:LEU:C	2.64	0.41
8:J:5:VAL:HG12	8:J:6:ARG:HG3	2.02	0.41
1:A:455:MET:HB3	1:A:455:MET:HE2	1.75	0.41
1:A:550:LEU:HD11	1:A:561:PRO:HD2	2.02	0.41
1:A:584:ASN:O	1:A:637:LYS:HE3	2.20	0.41
1:A:1025:ARG:HD3	1:A:1025:ARG:HA	1.89	0.41
1:A:1276:VAL:HG11	1:A:1312:ASN:HB3	2.01	0.41
2:B:654:ARG:H	2:B:657:HIS:CD2	2.38	0.41
2:B:680:THR:HG22	2:B:682:SER:HB2	2.03	0.41
3:C:21:ILE:HD11	3:C:209:TYR:HD2	1.85	0.41
4:E:112:TYR:HE1	4:E:115:ASN:HA	1.82	0.41
4:E:138:ALA:HA	4:E:141:VAL:HG23	2.03	0.41
5:F:124:GLU:HB3	5:F:130:ILE:HG13	2.03	0.41
1:A:345:VAL:HA	2:B:1150:ARG:HH12	1.86	0.41
1:A:452:LYS:HB2	1:A:452:LYS:HE2	1.86	0.41
1:A:1104:ILE:HD11	1:A:1351:GLU:HB3	2.03	0.41
1:A:1122:PRO:HD3	1:A:1323:ASP:OD2	2.21	0.41
2:B:986:GLN:HE21	2:B:986:GLN:C	2.28	0.41
2:B:1171:VAL:HG22	2:B:1182:CYS:HB2	2.03	0.41
6:H:40:LEU:HD11	6:H:97:MET:HE1	2.03	0.41
9:K:19:LEU:HD21	9:K:35:PHE:CE2	2.56	0.41
1:A:548:ASN:O	1:A:549:MET:C	2.64	0.41
1:A:852:TYR:HA	1:A:1060:PRO:CG	2.51	0.41
1:A:1111:MET:HE2	1:A:1331:SER:HB2	2.03	0.41
2:B:203:PHE:O	2:B:209:GLU:HA	2.20	0.41
2:B:393:LYS:HD3	2:B:393:LYS:HA	1.71	0.41
2:B:546:SER:HA	2:B:634:TYR:HE2	1.85	0.41
2:B:600:LEU:HD23	2:B:600:LEU:HA	1.88	0.41
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.54	0.41
2:B:779:GLY:O	2:B:795:ILE:HA	2.21	0.41
2:B:786:ASN:O	2:B:967:ARG:NH2	2.54	0.41
2:B:825:VAL:HA	2:B:1010:LEU:O	2.21	0.41
2:B:950:ASP:O	2:B:951:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:5:ASN:HD21	4:E:52:ARG:HA	1.86	0.41
4:E:52:ARG:HA	4:E:53:PRO:HD3	1.88	0.41
4:E:136:ASN:O	4:E:137:GLU:C	2.63	0.41
6:H:15:VAL:HG22	6:H:26:ILE:HG13	2.02	0.41
7:I:75:CYS:C	7:I:77:LYS:H	2.29	0.41
8:J:28:ASP:OD1	8:J:28:ASP:N	2.54	0.41
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.36	0.41
10:L:30:ILE:HG22	10:L:31:CYS:H	1.83	0.41
1:A:55:ASP:N	1:A:56:PRO:CD	2.82	0.41
1:A:313:GLN:O	1:A:320:ARG:HA	2.21	0.41
1:A:817:ALA:HB1	2:B:524:PRO:HB2	2.02	0.41
1:A:871:ASP:OD1	1:A:873:MET:HB2	2.21	0.41
1:A:922:ASP:O	1:A:923:LEU:C	2.62	0.41
1:A:1163:ILE:HA	1:A:1164:PRO:HD2	1.84	0.41
2:B:176:SER:O	2:B:177:LYS:C	2.63	0.41
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.51	0.41
2:B:539:LEU:HD22	2:B:543:SER:HB2	2.03	0.41
2:B:786:ASN:OD1	2:B:967:ARG:NH2	2.54	0.41
2:B:983:ARG:CD	2:B:1091:TYR:HD2	2.34	0.41
3:C:22:LEU:HD23	3:C:22:LEU:HA	1.91	0.41
3:C:240:VAL:C	3:C:242:GLN:N	2.78	0.41
4:E:58:MET:O	4:E:59:SER:C	2.64	0.41
6:H:103:LYS:HZ2	6:H:114:VAL:C	2.28	0.41
8:J:6:ARG:HB3	8:J:11:GLY:HA2	2.03	0.41
1:A:249:SER:HB2	1:A:258:GLY:O	2.21	0.40
1:A:367:PRO:HA	1:A:463:ILE:O	2.21	0.40
1:A:582:ILE:HG21	1:A:610:GLY:HA2	2.03	0.40
1:A:715:GLU:CD	1:A:774:ARG:HH12	2.28	0.40
1:A:840:ARG:HA	1:A:840:ARG:HD3	1.93	0.40
1:A:902:LEU:HD23	1:A:921:GLY:HA2	2.02	0.40
2:B:374:LYS:O	2:B:375:ALA:C	2.64	0.40
2:B:806:THR:CG2	2:B:807:ARG:N	2.84	0.40
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	2.03	0.40
2:B:1194:ILE:O	2:B:1194:ILE:HG13	2.21	0.40
5:F:98:ALA:HB2	5:F:118:LEU:HA	2.03	0.40
9:K:42:LEU:O	9:K:43:GLY:C	2.63	0.40
1:A:35:ILE:HD13	1:A:241:VAL:HG11	2.03	0.40
1:A:289:ILE:O	1:A:293:GLU:N	2.48	0.40
1:A:414:ASP:C	1:A:416:ARG:N	2.79	0.40
1:A:415:LEU:HD21	1:A:424:ILE:HD12	2.03	0.40
1:A:437:MET:HE3	1:A:437:MET:HB2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:VAL:HG12	1:A:461:LYS:N	2.37	0.40
1:A:531:ILE:CD1	1:A:578:LEU:HD21	2.47	0.40
1:A:858:ASN:HD22	1:A:861:GLY:H	1.68	0.40
1:A:1335:ILE:O	1:A:1336:MET:C	2.64	0.40
2:B:299:GLU:OE2	2:B:572:HIS:ND1	2.42	0.40
2:B:408:LEU:CD2	2:B:409:ALA:H	2.30	0.40
2:B:547:VAL:H	2:B:612:GLU:CD	2.29	0.40
3:C:250:THR:O	3:C:254:LYS:HG3	2.21	0.40
1:A:269:ILE:HD11	1:A:303:TYR:CB	2.51	0.40
1:A:767:GLN:HG3	1:A:768:GLN:O	2.21	0.40
1:A:846:GLU:OE1	2:B:1135:ARG:NH2	2.52	0.40
1:A:879:GLU:O	1:A:955:PRO:HA	2.22	0.40
1:A:1327:ILE:O	4:E:147:HIS:HE1	2.04	0.40
2:B:120:ARG:HB3	2:B:122:LEU:HG	2.01	0.40
2:B:654:ARG:C	2:B:656:GLY:N	2.78	0.40
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.56	0.40
2:B:901:PRO:HD2	10:L:59:ALA:O	2.21	0.40
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.99	0.40
6:H:12:VAL:CG1	6:H:26:ILE:HG23	2.48	0.40
8:J:57:ILE:O	8:J:60:PHE:N	2.52	0.40
1:A:170:THR:HG21	1:A:186:LYS:O	2.21	0.40
1:A:359:LEU:HB3	1:A:363:GLN:HB2	2.03	0.40
1:A:567:LYS:HB3	6:H:95:TYR:C	2.46	0.40
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.56	0.40
1:A:1424:VAL:HG21	2:B:1139:ILE:HG12	2.02	0.40
2:B:839:MET:HE1	2:B:980:PHE:HB2	2.04	0.40
2:B:839:MET:HE2	2:B:839:MET:HB2	1.85	0.40
2:B:892:LYS:HD2	2:B:909:ASP:OD2	2.22	0.40
6:H:104:PHE:O	6:H:106:GLU:N	2.54	0.40
1:A:505:CYS:O	1:A:506:ALA:C	2.65	0.40
1:A:858:ASN:ND2	1:A:861:GLY:H	2.19	0.40
2:B:1070:GLU:OE2	8:J:44:TYR:OH	2.32	0.40
2:B:1103:ILE:O	2:B:1103:ILE:HG22	2.21	0.40
2:B:1210:MET:O	2:B:1212:ILE:HG13	2.21	0.40
3:C:8:VAL:HG23	9:K:101:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	1411/1733 (81%)	1182 (84%)	174 (12%)	55 (4%)	2 15
2	B	1074/1224 (88%)	924 (86%)	122 (11%)	28 (3%)	4 22
3	C	264/318 (83%)	221 (84%)	34 (13%)	9 (3%)	3 17
4	E	213/215 (99%)	179 (84%)	30 (14%)	4 (2%)	6 26
5	F	82/155 (53%)	68 (83%)	11 (13%)	3 (4%)	2 16
6	H	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	0 3
7	I	120/122 (98%)	96 (80%)	21 (18%)	3 (2%)	4 22
8	J	63/70 (90%)	53 (84%)	8 (13%)	2 (3%)	3 18
9	K	112/120 (93%)	92 (82%)	14 (12%)	6 (5%)	1 10
10	L	44/70 (63%)	25 (57%)	12 (27%)	7 (16%)	0 0
All	All	3512/4173 (84%)	2935 (84%)	448 (13%)	129 (4%)	2 16

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	415	LEU
1	A	464	PRO
1	A	567	LYS
1	A	752	LYS
1	A	1223	ASP
1	A	1386	ARG
1	A	1393	ASN
3	C	90	ASP
3	C	231	ASN
6	H	18	GLY
6	H	32	THR

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Mol	Chain	Res	Type
10	L	39	SER
10	L	59	ALA
10	L	64	LEU
1	A	188	ASP
1	A	226	GLU
1	A	601	LYS
1	A	628	GLY
1	A	736	ASN
1	A	915	SER
1	A	958	VAL
1	A	1063	MET
1	A	1127	ASP
1	A	1165	GLU
1	A	1200	ALA
1	A	1360	GLY
1	A	1385	THR
1	A	1391	ARG
1	A	1392	SER
1	A	1399	ARG
1	A	1400	CYS
2	B	165	VAL
2	B	266	ALA
2	B	864	LYS
2	B	884	ARG
2	B	891	ASP
2	B	1099	VAL
3	C	4	GLU
3	C	19	ASP
3	C	88	CYS
4	E	3	GLN
4	E	59	SER
4	E	137	GLU
5	F	112	GLU
6	H	19	ARG
6	H	81	PRO
6	H	88	SER
6	H	103	LYS
6	H	105	GLU
6	H	128	ASN
8	J	29	GLU
9	K	8	GLU
1	A	45	GLN

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Mol	Chain	Res	Type
1	A	67	CYS
1	A	408	ASP
1	A	409	SER
1	A	517	ASN
1	A	737	LEU
1	A	926	GLN
2	B	304	ASP
6	H	82	PRO
6	H	138	GLU
9	K	103	THR
9	K	104	ASN
10	L	56	LEU
1	A	56	PRO
1	A	196	GLU
1	A	451	HIS
1	A	466	SER
1	A	467	THR
1	A	777	PHE
1	A	904	THR
2	B	249	ARG
2	B	383	ASN
2	B	907	GLY
2	B	1222	ARG
3	C	168	ALA
3	C	241	ASP
4	E	5	ASN
6	H	61	SER
8	J	41	LEU
9	K	107	THR
10	L	38	LEU
1	A	35	ILE
1	A	79	GLY
1	A	154	SER
1	A	673	GLY
1	A	700	ASN
1	A	986	ILE
2	B	90	ILE
2	B	303	TYR
2	B	307	ASP
2	B	367	LEU
2	B	369	GLY
2	B	541	LEU

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Mol	Chain	Res	Type
2	B	648	HIS
2	B	708	GLU
2	B	879	ARG
2	B	883	LEU
2	B	1104	HIS
2	B	1167	GLY
3	C	264	GLN
5	F	73	ALA
6	H	139	ASN
7	I	9	ASP
7	I	76	PRO
10	L	54	ARG
1	A	253	ASN
1	A	599	SER
2	B	711	GLU
3	C	240	VAL
7	I	39	GLY
9	K	93	SER
10	L	52	GLY
1	A	955	PRO
2	B	743	ILE
1	A	51	GLY
1	A	308	ILE
2	B	901	PRO
5	F	93	ILE
9	K	43	GLY
1	A	178	GLY
1	A	399	HIS
1	A	910	PRO
2	B	1214	PRO
2	B	571	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1239/1520 (82%)	1077 (87%)	162 (13%)	3 13
2	B	950/1061 (90%)	840 (88%)	110 (12%)	4 17
3	C	234/274 (85%)	202 (86%)	32 (14%)	3 11
4	E	197/197 (100%)	180 (91%)	17 (9%)	8 29
5	F	74/137 (54%)	68 (92%)	6 (8%)	9 31
6	H	117/128 (91%)	115 (98%)	2 (2%)	56 74
7	I	116/116 (100%)	105 (90%)	11 (10%)	7 25
8	J	60/65 (92%)	47 (78%)	13 (22%)	1 2
9	K	99/102 (97%)	84 (85%)	15 (15%)	2 9
10	L	40/57 (70%)	34 (85%)	6 (15%)	2 9
All	All	3126/3657 (86%)	2752 (88%)	374 (12%)	4 16

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	13	THR
1	A	30	ILE
1	A	44	THR
1	A	61	ILE
1	A	69	THR
1	A	71	GLN
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	106	VAL
1	A	112	LYS
1	A	117	GLU
1	A	140	THR
1	A	146	MET
1	A	157	ASP
1	A	159	THR
1	A	162	VAL
1	A	200	ARG
1	A	204	THR
1	A	208	LEU
1	A	219	PHE

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Mol	Chain	Res	Type
1	A	220	THR
1	A	232	GLU
1	A	247	ARG
1	A	250	ILE
1	A	266	LEU
1	A	268	ASP
1	A	291	GLU
1	A	308	ILE
1	A	316	GLN
1	A	345	VAL
1	A	351	THR
1	A	368	LYS
1	A	372	LYS
1	A	373	THR
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	437	MET
1	A	445	ASN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	455	MET
1	A	461	LYS
1	A	463	ILE
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	479	ASN
1	A	493	GLN
1	A	496	GLU
1	A	497	THR
1	A	501	LEU
1	A	503	GLN
1	A	504	LEU
1	A	513	SER
1	A	515	GLN
1	A	523	ILE

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Mol	Chain	Res	Type
1	A	524	VAL
1	A	527	THR
1	A	535	THR
1	A	543	LEU
1	A	544	ASP
1	A	567	LYS
1	A	571	LEU
1	A	577	ILE
1	A	580	VAL
1	A	588	LEU
1	A	596	THR
1	A	597	LEU
1	A	612	ILE
1	A	613	ILE
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	641	VAL
1	A	666	ILE
1	A	677	ARG
1	A	702	LEU
1	A	709	THR
1	A	740	LEU
1	A	741	ASN
1	A	756	ILE
1	A	774	ARG
1	A	780	VAL
1	A	821	ARG
1	A	822	GLU
1	A	824	LEU
1	A	825	ILE
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	845	LEU
1	A	855	THR
1	A	858	ASN
1	A	867	ILE
1	A	885	THR
1	A	903	ASN
1	A	913	LEU
1	A	919	ILE

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Mol	Chain	Res	Type
1	A	920	LEU
1	A	926	GLN
1	A	969	GLN
1	A	973	ILE
1	A	988	LEU
1	A	991	LYS
1	A	1006	ILE
1	A	1015	VAL
1	A	1030	ARG
1	A	1048	ASN
1	A	1064	VAL
1	A	1095	THR
1	A	1118	VAL
1	A	1133	LEU
1	A	1134	ILE
1	A	1138	ILE
1	A	1141	THR
1	A	1143	LEU
1	A	1146	VAL
1	A	1161	THR
1	A	1162	VAL
1	A	1169	ILE
1	A	1192	LEU
1	A	1204	ASP
1	A	1214	GLU
1	A	1227	ILE
1	A	1237	ILE
1	A	1238	ILE
1	A	1240	CYS
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1264	GLU
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1325	THR
1	A	1335	ILE
1	A	1338	VAL
1	A	1359	ASP
1	A	1361	SER

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Mol	Chain	Res	Type
1	A	1372	VAL
1	A	1374	VAL
1	A	1376	THR
1	A	1377	THR
1	A	1382	THR
1	A	1383	SER
1	A	1385	THR
1	A	1387	HIS
1	A	1399	ARG
1	A	1417	GLU
1	A	1419	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1449	SER
2	B	18	PHE
2	B	19	GLU
2	B	20	ASP
2	B	22	SER
2	B	40	GLU
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	65	GLU
2	B	68	THR
2	B	69	LEU
2	B	97	VAL
2	B	98	THR
2	B	102	VAL
2	B	128	LEU
2	B	136	THR
2	B	170	LEU
2	B	174	LEU
2	B	178	ASN
2	B	183	GLU
2	B	194	GLU
2	B	205	ILE
2	B	217	ARG
2	B	221	ASN
2	B	225	VAL
2	B	234	ILE
2	B	252	SER
2	B	253	THR

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	276	ILE
2	B	277	LYS
2	B	291	ILE
2	B	305	VAL
2	B	313	MET
2	B	323	VAL
2	B	337	ARG
2	B	339	THR
2	B	365	THR
2	B	367	LEU
2	B	370	PHE
2	B	408	LEU
2	B	424	LEU
2	B	451	LYS
2	B	455	SER
2	B	485	ARG
2	B	487	THR
2	B	496	ARG
2	B	498	THR
2	B	513	GLN
2	B	540	SER
2	B	543	SER
2	B	544	CYS
2	B	547	VAL
2	B	556	THR
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	572	HIS
2	B	579	ARG
2	B	589	VAL
2	B	592	ASN
2	B	597	MET
2	B	599	THR
2	B	604	ARG
2	B	612	GLU
2	B	615	MET
2	B	619	ILE
2	B	628	THR
2	B	646	LEU
2	B	648	HIS

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Mol	Chain	Res	Type
2	B	653	VAL
2	B	680	THR
2	B	706	GLN
2	B	708	GLU
2	B	737	THR
2	B	743	ILE
2	B	755	ILE
2	B	783	THR
2	B	790	ASP
2	B	796	LEU
2	B	801	LYS
2	B	806	THR
2	B	825	VAL
2	B	831	SER
2	B	857	ARG
2	B	860	MET
2	B	864	LYS
2	B	873	THR
2	B	889	THR
2	B	915	THR
2	B	946	ASN
2	B	955	THR
2	B	971	THR
2	B	983	ARG
2	B	996	ARG
2	B	999	MET
2	B	1019	SER
2	B	1045	SER
2	B	1049	ASP
2	B	1060	ARG
2	B	1099	VAL
2	B	1101	ASP
2	B	1152	MET
2	B	1153	GLU
2	B	1159	ARG
2	B	1169	MET
2	B	1196	ILE
2	B	1216	LEU
2	B	1218	THR
2	B	1219	ASP
3	C	3	GLU
3	C	9	LYS

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Mol	Chain	Res	Type
3	C	11	ARG
3	C	25	VAL
3	C	26	ASP
3	C	50	GLU
3	C	52	GLU
3	C	55	THR
3	C	57	VAL
3	C	69	LEU
3	C	77	ILE
3	C	83	SER
3	C	89	GLU
3	C	116	LYS
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	136	ASP
3	C	154	LYS
3	C	156	THR
3	C	178	PHE
3	C	186	LEU
3	C	189	THR
3	C	203	GLN
3	C	209	TYR
3	C	215	GLU
3	C	240	VAL
3	C	258	ILE
3	C	260	LEU
3	C	264	GLN
3	C	265	MET
3	C	266	ASP
4	E	8	ASN
4	E	18	THR
4	E	19	VAL
4	E	37	LEU
4	E	47	CYS
4	E	69	ILE
4	E	81	GLU
4	E	87	SER
4	E	92	THR
4	E	98	ILE
4	E	116	ILE
4	E	123	LEU

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Mol	Chain	Res	Type
4	E	149	LEU
4	E	154	ILE
4	E	169	ARG
4	E	196	VAL
4	E	204	THR
5	F	79	ARG
5	F	82	THR
5	F	111	LEU
5	F	133	VAL
5	F	140	ASP
5	F	149	GLU
6	H	42	ILE
6	H	62	SER
7	I	7	CYS
7	I	17	ARG
7	I	24	ARG
7	I	35	VAL
7	I	50	THR
7	I	51	ASN
7	I	52	ILE
7	I	55	THR
7	I	84	VAL
7	I	98	VAL
7	I	109	ILE
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	12	LYS
8	J	14	VAL
8	J	19	GLU
8	J	20	SER
8	J	22	LEU
8	J	28	ASP
8	J	34	THR
8	J	48	ARG
8	J	57	ILE
9	K	1	MET
9	K	6	ARG
9	K	11	LEU
9	K	14	GLU
9	K	25	THR

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Mol	Chain	Res	Type
9	K	29	ASN
9	K	31	VAL
9	K	33	ILE
9	K	47	ARG
9	K	63	VAL
9	K	66	PRO
9	K	73	LEU
9	K	75	ILE
9	K	101	LEU
9	K	113	THR
10	L	27	LEU
10	L	42	ARG
10	L	56	LEU
10	L	64	LEU
10	L	65	VAL
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS
1	A	160	GLN
1	A	256	GLN
1	A	281	HIS
1	A	299	HIS
1	A	313	GLN
1	A	445	ASN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	548	ASN
1	A	587	HIS
1	A	631	HIS
1	A	648	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	838	GLN

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Mol	Chain	Res	Type
1	A	858	ASN
1	A	862	ASN
1	A	903	ASN
1	A	926	GLN
1	A	966	ASN
1	A	994	GLN
1	A	1048	ASN
1	A	1052	GLN
1	A	1078	GLN
1	A	1140	HIS
1	A	1173	HIS
1	A	1218	GLN
1	A	1265	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	53	GLN
2	B	121	ASN
2	B	236	HIS
2	B	300	HIS
2	B	325	GLN
2	B	383	ASN
2	B	433	GLN
2	B	449	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	648	HIS
2	B	734	HIS
2	B	744	HIS
2	B	881	ASN
2	B	958	GLN
2	B	986	GLN
2	B	1065	GLN
2	B	1084	GLN
2	B	1193	GLN
2	B	1211	ASN
3	C	17	ASN
3	C	24	ASN
3	C	31	ASN
3	C	65	HIS

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Mol	Chain	Res	Type
3	C	73	GLN
3	C	79	GLN
3	C	102	GLN
3	C	112	ASN
3	C	131	HIS
3	C	167	HIS
3	C	242	GLN
3	C	267	GLN
4	E	5	ASN
4	E	147	HIS
6	H	3	ASN
6	H	11	GLN
6	H	21	ASN
7	I	12	ASN
7	I	114	GLN
7	I	116	ASN
8	J	26	GLN
8	J	53	HIS
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN
9	K	92	ASN
10	L	53	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1419/1733 (81%)	-0.28	13 (0%) 81 73	41, 79, 162, 188	0
2	B	1094/1224 (89%)	-0.28	13 (1%) 76 68	47, 80, 140, 167	0
3	C	266/318 (83%)	-0.34	0 100 100	58, 78, 111, 133	0
4	E	215/215 (100%)	-0.30	0 100 100	51, 98, 130, 145	0
5	F	84/155 (54%)	-0.45	0 100 100	52, 71, 92, 98	0
6	H	133/146 (91%)	0.30	10 (7%) 22 21	103, 119, 147, 149	0
7	I	122/122 (100%)	-0.13	1 (0%) 82 75	75, 107, 129, 150	0
8	J	65/70 (92%)	-0.63	0 100 100	58, 70, 91, 94	0
9	K	114/120 (95%)	-0.42	0 100 100	58, 85, 107, 126	0
10	L	46/70 (65%)	0.24	0 100 100	87, 137, 144, 145	0
All	All	3558/4173 (85%)	-0.27	37 (1%) 79 71	41, 82, 146, 188	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	4.8
7	I	55	THR	3.7
6	H	140	ALA	3.3
1	A	250	ILE	3.3
2	B	247	GLY	3.2
1	A	329	LEU	3.2
1	A	1176	LEU	2.9
2	B	1098	MET	2.8
1	A	1446	ASP	2.8
6	H	104	PHE	2.8
2	B	883	LEU	2.8
1	A	342	GLY	2.8
2	B	1102	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1396	ALA	2.6
1	A	1400	CYS	2.6
2	B	90	ILE	2.5
6	H	59	ILE	2.5
2	B	729	ILE	2.4
6	H	127	GLY	2.4
6	H	136	LYS	2.4
2	B	248	SER	2.4
2	B	726	ALA	2.3
2	B	728	ARG	2.3
1	A	61	ILE	2.3
1	A	308	ILE	2.2
2	B	1103	ILE	2.2
1	A	1069	ALA	2.2
6	H	90	ALA	2.2
6	H	134	ASN	2.2
1	A	1390	ASN	2.1
2	B	1224	PHE	2.1
6	H	63	LEU	2.1
2	B	640	VAL	2.1
1	A	171	GLN	2.0
6	H	60	ALA	2.0
2	B	731	VAL	2.0
6	H	79	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	MN	A	3010	1/1	0.79	0.13	50,50,50,50	0
11	ZN	I	3004	1/1	0.98	0.04	117,117,117,117	0
11	ZN	L	3005	1/1	0.98	0.04	128,128,128,128	0
11	ZN	A	3008	1/1	0.98	0.05	143,143,143,143	0
11	ZN	B	3007	1/1	0.99	0.02	87,87,87,87	0
12	MN	A	3009	1/1	0.99	0.03	49,49,49,49	0
11	ZN	A	3006	1/1	0.99	0.02	95,95,95,95	0
11	ZN	I	3003	1/1	1.00	0.02	97,97,97,97	0
11	ZN	C	3002	1/1	1.00	0.02	79,79,79,79	0
11	ZN	J	3001	1/1	1.00	0.01	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.