Full wwPDB EM Validation Report (i)

Jun 10, 2025 – 02:24 PM JST

PDB ID	:	9JXS / pdb_00009jxs
EMDB ID	:	EMD-61880
Title	:	Cryo-EM structure of Cas5-HNH Cascade bound with dsDNA
Authors	:	Liu, Y.N.; Zhang, H.; Zhu, H.
Deposited on	:	2024-10-11
Resolution	:	2.93 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

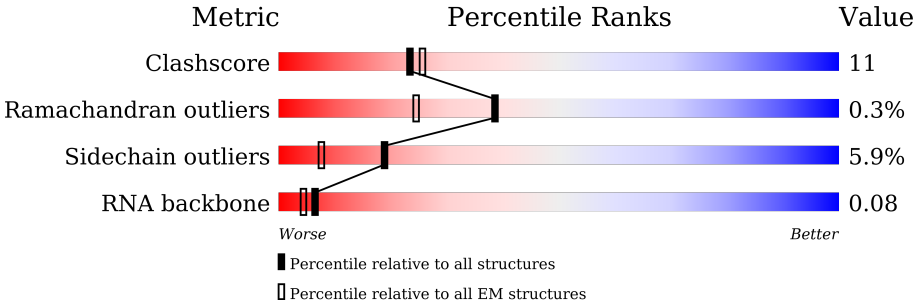
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	C	535	55% 24% • 18%
2	E	174	71% 23% • 5%
3	F	378	69% 26% • •
3	G	378	38% 25% • • 34%
3	H	378	75% 24% • •
3	I	378	75% 22% • •
3	J	378	73% 23% • •
3	K	378	71% 19% • 9%

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Mol	Chain	Length	Quality of chain
4	B	388	60% 27% • 11%
5	M	54	76% 15% 9%
6	D	272	68% 27% • •
7	A	61	15% 51% 31% •
8	N	54	13% 87%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 27905 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 CRISPR-associated protein Cse1 (CRISPR_cse1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	438	3460	2226	591	624	19	0	0

- Molecule 2 is a protein called CRISPR-associated protein Cse2 (CRISPR_cse2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	165	1352	875	238	233	6	0	0

- Molecule 3 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	368	2819	1782	489	536	12	0	0
3	H	375	2870	1808	503	547	12	0	0
3	I	370	2809	1769	493	535	12	0	0
3	J	371	2819	1779	491	537	12	0	0
3	K	345	2650	1672	466	501	11	0	0
3	G	249	1881	1191	327	356	7	0	0

- Molecule 4 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	346	2710	1709	500	484	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	333	ALA	HIS	conflict	UNP A0A1V6F8C5

- Molecule 5 is a DNA chain called DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	M	49	995	475	176	295	49	0	0

- Molecule 6 is a protein called CRISPR-associated endoribonuclease Cse3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	264	2134	1368	383	380	3	0	0

- Molecule 7 is a RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A	59	1258	562	225	413	58	0	0

- Molecule 8 is a DNA chain called non-target DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	N	7	146	69	27	43	7	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

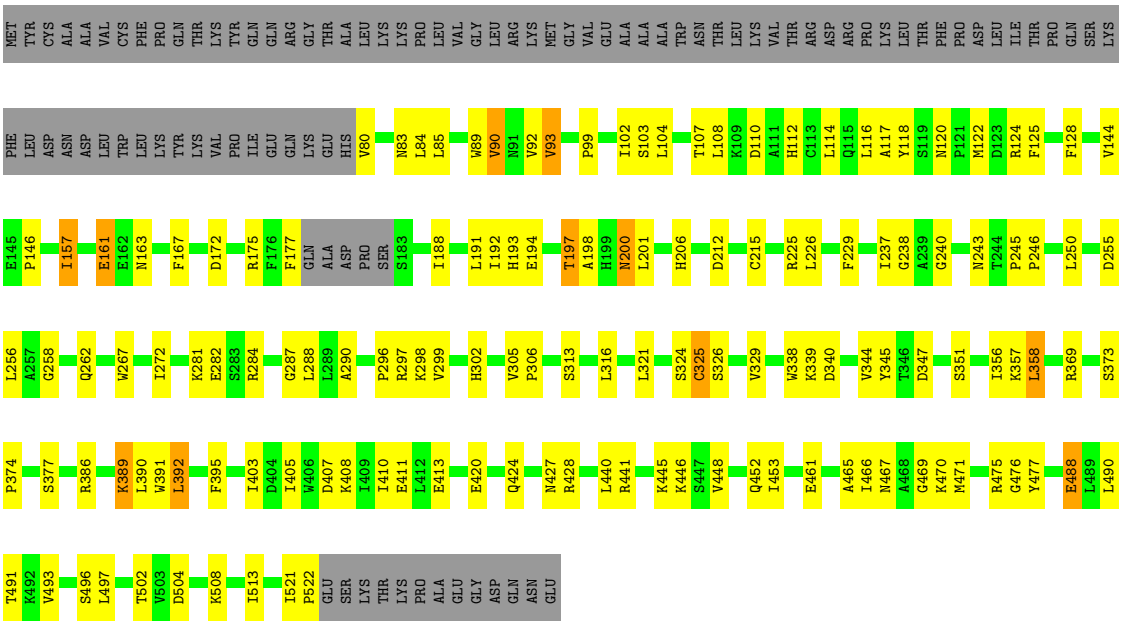
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	C	1	1	1	0
9	B	1	Total	Mg	0
			1	1	

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. 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. 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.

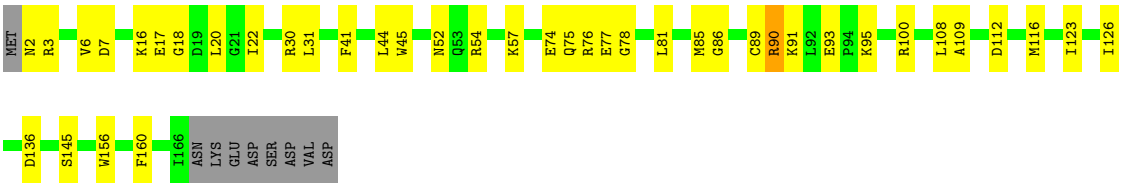
- Molecule 1: CRISPR-associated protein Cse1 (CRISPR_cse1)

Chain C: 55% 24% • 18%



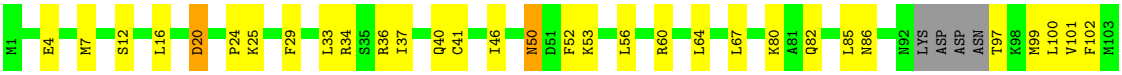
- Molecule 2: CRISPR-associated protein Cse2 (CRISPR_cse2)

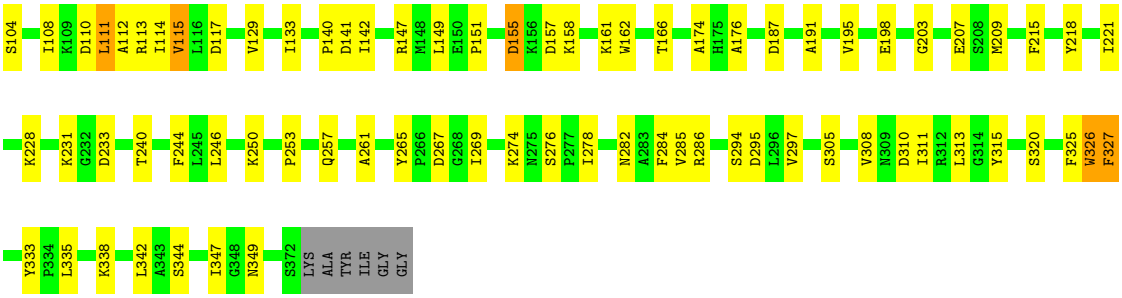
Chain E: 71% 23% • 5%



- Molecule 3: CRISPR system Cascade subunit CasC

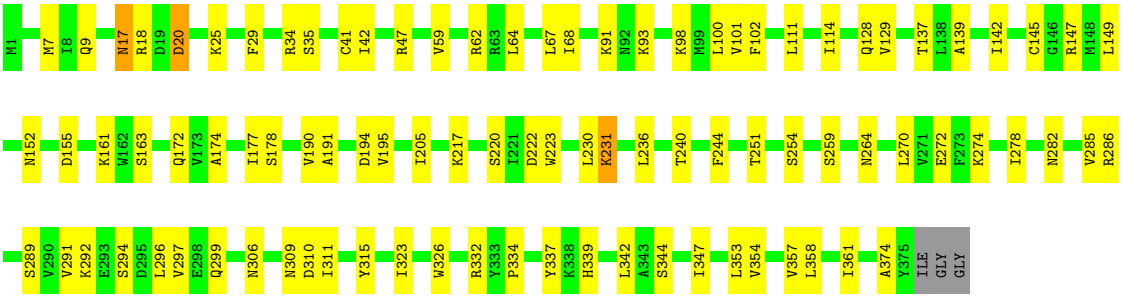
Chain F: 69% 26% • •





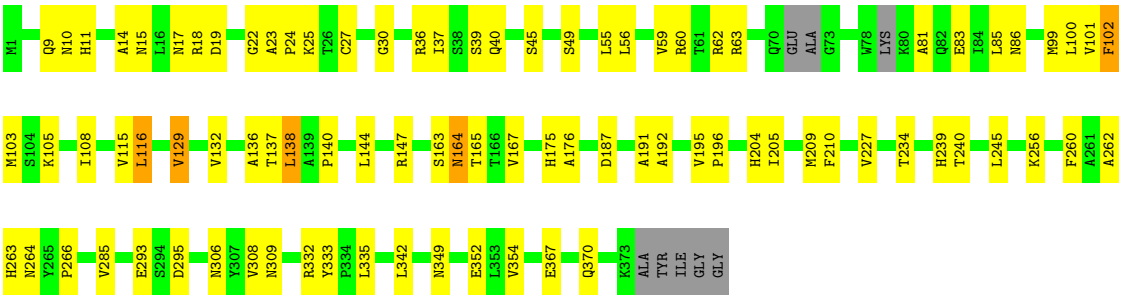
- Molecule 3: CRISPR system Cascade subunit CasC

Chain H:



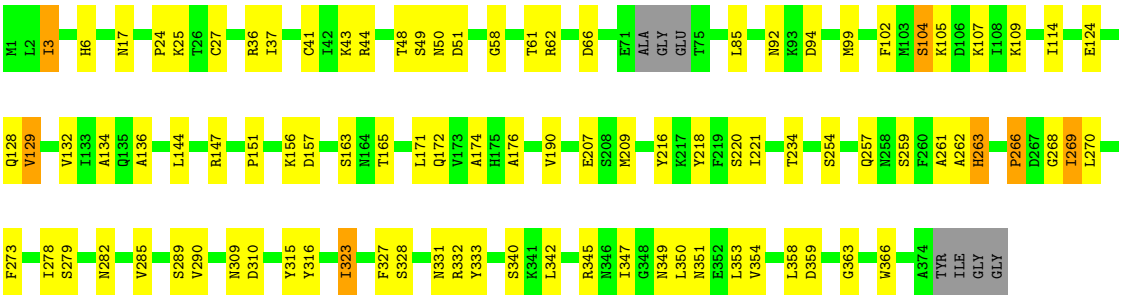
- Molecule 3: CRISPR system Cascade subunit CasC

Chain I:



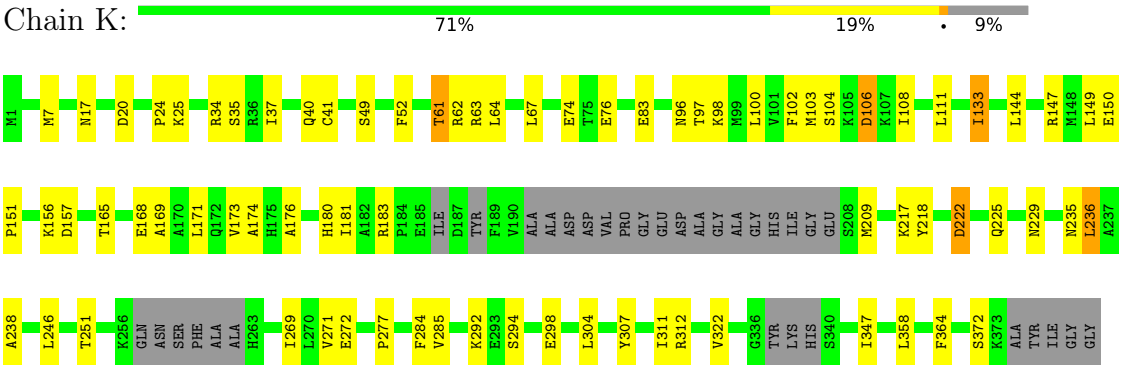
- Molecule 3: CRISPR system Cascade subunit CasC

Chain J:



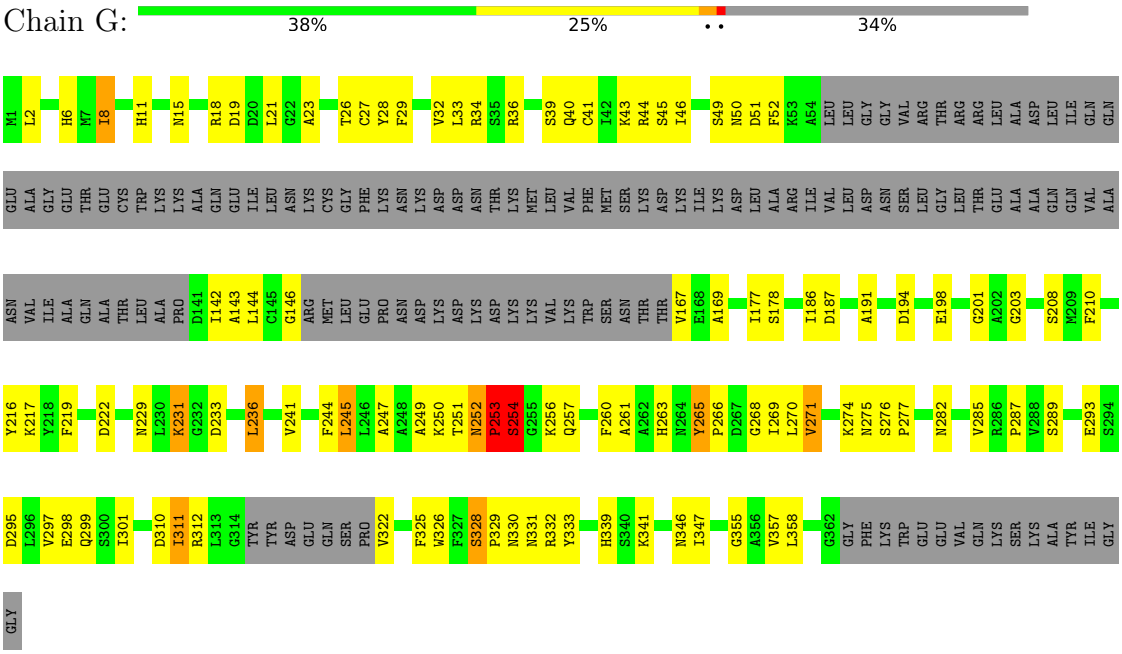
- Molecule 3: CRISPR system Cascade subunit CasC

Chain K:



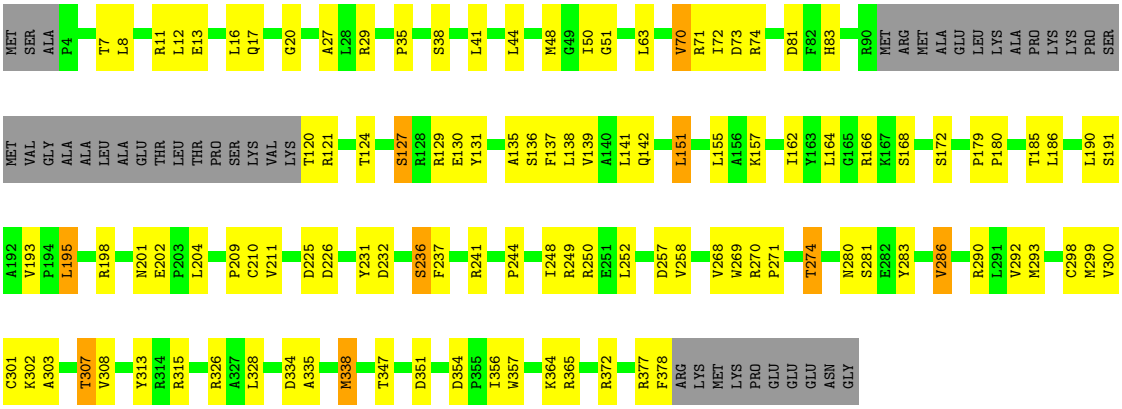
- Molecule 3: CRISPR system Cascade subunit CasC

Chain G:



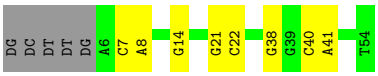
- Molecule 4: CRISPR system Cascade subunit CasD

Chain B:



- Molecule 5: DNA (54-MER)

Chain M: 76% 15% 9%



• Molecule 6: CRISPR-associated endoribonuclease Cse3

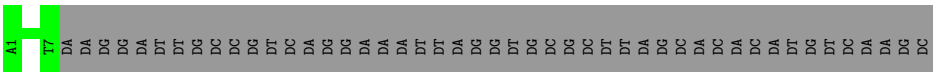
Chain D: 68% 27% • •

• Molecule 7: RNA (61-MER)

Chain A: 15% 51% 31% •

• Molecule 8: non-target DNA

Chain N: 13% 87%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73951	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.62	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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: MG

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	C	0.23	0/3559	0.60	3/4848 (0.1%)
2	E	0.23	0/1382	0.61	0/1862
3	F	0.23	0/2875	0.57	2/3900 (0.1%)
3	G	0.41	1/1920 (0.1%)	0.66	3/2606 (0.1%)
3	H	0.20	0/2926	0.48	1/3967 (0.0%)
3	I	0.20	0/2861	0.53	0/3878
3	J	0.38	2/2874 (0.1%)	0.60	2/3901 (0.1%)
3	K	0.18	0/2695	0.47	1/3644 (0.0%)
4	B	0.23	0/2779	0.64	3/3777 (0.1%)
5	M	0.27	0/1113	0.51	0/1713
6	D	0.23	0/2191	0.65	2/2968 (0.1%)
7	A	0.15	0/1405	0.40	0/2187
8	N	0.16	0/163	0.38	0/250
All	All	0.25	3/28743 (0.0%)	0.56	17/39501 (0.0%)

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
2	E	0	1
3	I	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	253	PRO	N-CD	10.29	1.62	1.47
3	J	262	ALA	CA-C	-5.80	1.46	1.53
3	J	263	HIS	CA-C	-5.48	1.47	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	266	PRO	N-CA-C	10.77	129.66	111.68
3	G	254	SER	N-CA-C	-7.58	99.77	108.49
6	D	117	LYS	CA-CB-CG	7.27	128.64	114.10
3	J	261	ALA	N-CA-C	6.74	120.96	111.52
1	C	146	PRO	CA-N-CD	-6.01	103.59	112.00
3	K	98	LYS	CA-CB-CG	5.97	126.03	114.10
1	C	389	LYS	CB-CG-CD	5.85	124.76	111.30
4	B	338	MET	CA-CB-CG	5.80	125.70	114.10
3	F	327	PHE	N-CA-C	-5.53	103.81	110.44
1	C	108	LEU	CA-CB-CG	5.50	135.56	116.30
3	H	292	LYS	CB-CG-CD	5.48	123.91	111.30
4	B	236	SER	CA-C-N	-5.28	112.96	122.46
4	B	236	SER	C-N-CA	-5.28	112.96	122.46
6	D	175	LEU	CA-CB-CG	5.23	134.61	116.30
3	F	231	LYS	CB-CG-CD	5.21	123.29	111.30
3	G	252	ASN	N-CA-C	-5.18	102.64	109.84
3	G	245	LEU	CA-CB-CG	5.14	134.29	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	90	ARG	Sidechain
3	I	102	PHE	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	C	3460	0	3373	92	0
2	E	1352	0	1387	23	0
3	F	2819	0	2745	75	0
3	G	1881	0	1802	75	0
3	H	2870	0	2797	56	0
3	I	2809	0	2716	65	0
3	J	2819	0	2714	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2650	0	2599	44	0
4	B	2710	0	2673	82	0
5	M	995	0	553	8	0
6	D	2134	0	2126	55	0
7	A	1258	0	638	37	0
8	N	146	0	80	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
All	All	27905	0	26203	583	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 11.

All (583) 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)
3:H:311:ILE:O	3:H:315:TYR:HB2	1.55	1.07
6:D:117:LYS:HD2	6:D:118:ALA:H	1.40	0.84
3:J:6:HIS:HB2	3:J:270:LEU:HB3	1.61	0.82
3:K:102:PHE:HB3	3:K:147:ARG:HD2	1.62	0.80
3:F:274:LYS:HG2	3:F:276:SER:H	1.46	0.78
3:I:103:MET:HE1	3:I:108:ILE:HG21	1.71	0.73
1:C:193:HIS:H	1:C:225:ARG:HH22	1.37	0.73
3:I:349:ASN:HB3	3:I:352:GLU:HG2	1.72	0.71
3:J:269:ILE:HB	3:J:327:PHE:HB3	1.70	0.71
1:C:157:ILE:O	1:C:161:GLU:HB3	1.89	0.71
4:B:298:CYS:SG	4:B:299:MET:N	2.64	0.70
3:G:29:PHE:HB3	3:G:34:ARG:HD2	1.74	0.70
4:B:334:ASP:OD2	4:B:372:ARG:NH2	2.25	0.69
3:F:29:PHE:HB3	3:F:34:ARG:HG3	1.75	0.69
7:A:-6:U:H1'	7:A:-4:A:H1'	1.75	0.68
3:G:275:ASN:HD21	4:B:157:LYS:HA	1.58	0.68
6:D:117:LYS:HE3	6:D:120:GLN:HE21	1.58	0.68
3:G:233:ASP:HB2	3:G:236:LEU:HB2	1.74	0.68
3:H:347:ILE:HG21	3:H:353:LEU:HB2	1.76	0.68
3:I:147:ARG:HB3	3:I:167:VAL:HB	1.76	0.68
6:D:129:ASN:HD21	6:D:255:ALA:HB2	1.58	0.67
3:G:328:SER:HB3	3:G:331:ASN:HA	1.76	0.67
2:E:81:LEU:O	2:E:85:MET:HB2	1.95	0.67
2:E:100:ARG:NH1	3:F:207:GLU:OE1	2.27	0.67
3:H:62:ARG:HG3	3:H:100:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:191:ALA:HB1	3:I:100:LEU:HD22	1.77	0.67
1:C:281:LYS:HE2	1:C:281:LYS:H	1.58	0.67
1:C:193:HIS:H	1:C:225:ARG:NH2	1.92	0.66
3:G:44:ARG:NH1	7:A:0:G:N3	2.43	0.66
3:I:10:ASN:ND2	3:J:282:ASN:OD1	2.27	0.66
4:B:301:CYS:SG	4:B:365:ARG:NH1	2.70	0.65
1:C:440:LEU:HD21	1:C:497:LEU:HD21	1.79	0.65
1:C:238:GLY:O	1:C:297:ARG:NH1	2.31	0.64
3:I:192:ALA:O	3:J:44:ARG:NH2	2.30	0.64
1:C:282:GLU:O	1:C:284:ARG:NH2	2.31	0.63
3:J:172:GLN:HB2	3:J:220:SER:HB2	1.80	0.63
6:D:201:LYS:O	6:D:223:ASN:ND2	2.31	0.63
3:F:20:ASP:OD1	3:F:20:ASP:N	2.29	0.63
4:B:195:LEU:HD21	4:B:204:LEU:HD21	1.81	0.63
3:G:40:GLN:HE22	4:B:83:HIS:HA	1.64	0.63
1:C:200:ASN:O	4:B:121:ARG:NH1	2.32	0.62
2:E:3:ARG:O	2:E:52:ASN:ND2	2.32	0.62
3:I:266:PRO:O	3:J:315:TYR:OH	2.17	0.62
4:B:130:GLU:O	4:B:166:ARG:NH2	2.32	0.62
3:I:309:ASN:HD22	3:I:342:LEU:HD13	1.64	0.62
3:I:27:CYS:HB3	3:I:36:ARG:HE	1.64	0.62
3:I:81:ALA:O	3:I:85:LEU:HB2	1.99	0.62
3:G:289:SER:O	3:G:299:GLN:NE2	2.33	0.62
3:J:6:HIS:HB2	3:J:270:LEU:CB	2.28	0.62
4:B:302:LYS:O	6:D:34:ARG:NH2	2.25	0.62
2:E:16:LYS:NZ	5:M:22:DC:OP2	2.33	0.62
1:C:110:ASP:O	1:C:112:HIS:ND1	2.31	0.61
2:E:108:LEU:HD22	2:E:116:MET:HE3	1.82	0.61
3:I:62:ARG:HH21	3:I:100:LEU:HB2	1.64	0.61
1:C:272:ILE:H	1:C:290:ALA:HB2	1.65	0.61
3:F:60:ARG:HG2	3:F:100:LEU:HD12	1.80	0.61
3:F:326:TRP:HE3	3:F:327:PHE:H	1.47	0.61
3:F:326:TRP:HE1	3:F:335:LEU:HB2	1.64	0.61
1:C:240:GLY:HA2	1:C:296:PRO:HB3	1.82	0.61
1:C:391:TRP:HE1	1:C:407:ASP:HB2	1.64	0.61
3:J:104:SER:OG	3:J:105:LYS:N	2.34	0.61
3:F:297:VAL:HG23	3:H:285:VAL:HG11	1.83	0.60
3:F:198:GLU:O	3:I:164:ASN:ND2	2.29	0.60
3:I:332:ARG:NH2	3:I:333:TYR:OH	2.34	0.60
4:B:338:MET:HG3	4:B:364:LYS:HB3	1.83	0.60
3:J:27:CYS:HB3	3:J:36:ARG:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:7:THR:HG23	4:B:141:LEU:H	1.65	0.60
1:C:471:MET:HA	1:C:477:TYR:HB3	1.84	0.60
2:E:85:MET:HE1	2:E:126:ILE:HD11	1.83	0.60
3:F:108:ILE:O	3:F:112:ALA:HB3	2.01	0.60
3:I:99:MET:HE3	3:I:101:VAL:HA	1.84	0.60
6:D:45:ARG:HH12	6:D:49:PRO:HA	1.66	0.60
4:B:300:VAL:O	6:D:98:ASN:ND2	2.34	0.60
6:D:123:ARG:HD3	6:D:236:LEU:HD12	1.84	0.60
3:K:67:LEU:HD13	3:K:108:ILE:HG12	1.85	0.59
4:B:120:THR:OG1	4:B:121:ARG:N	2.35	0.59
1:C:215:CYS:HA	1:C:321:LEU:HD22	1.84	0.59
1:C:120:ASN:ND2	1:C:194:GLU:OE1	2.35	0.59
3:G:254:SER:CA	3:G:257:GLN:HE22	2.14	0.59
3:I:264:ASN:ND2	3:J:279:SER:O	2.35	0.59
4:B:17:GLN:NE2	4:B:135:ALA:O	2.36	0.59
1:C:84:LEU:HB2	1:C:167:PHE:HB3	1.83	0.59
6:D:77:ASP:N	6:D:77:ASP:OD1	2.36	0.59
1:C:175:ARG:NH2	1:C:177:PHE:O	2.36	0.59
3:K:24:PRO:O	6:D:78:LYS:NZ	2.33	0.59
3:F:111:LEU:HA	3:F:114:ILE:HG13	1.84	0.58
3:J:62:ARG:HH22	5:M:21:DG:H5”	1.68	0.58
3:F:267:ASP:OD1	3:H:282:ASN:ND2	2.35	0.58
3:H:35:SER:HG	3:H:178:SER:HG	1.51	0.58
6:D:133:ARG:NH1	7:A:48:G:O6	2.36	0.58
4:B:71:ARG:HB2	4:B:190:LEU:HD21	1.84	0.58
3:G:15:ASN:HB2	3:G:210:PHE:HA	1.85	0.58
3:G:2:LEU:HB3	3:G:275:ASN:HA	1.86	0.58
6:D:129:ASN:OD1	6:D:129:ASN:N	2.36	0.58
3:G:26:THR:O	3:G:36:ARG:NH1	2.36	0.58
6:D:169:GLN:OE1	6:D:169:GLN:N	2.36	0.58
3:I:45:SER:O	3:I:49:SER:OG	2.22	0.58
3:G:254:SER:C	3:G:257:GLN:HE22	2.12	0.58
4:B:210:CYS:HB2	4:B:250:ARG:HB3	1.86	0.57
3:I:293:GLU:OE2	3:I:293:GLU:N	2.38	0.57
3:K:7:MET:HG2	3:K:269:ILE:HG12	1.85	0.57
3:J:43:LYS:NZ	7:A:23:G:OP1	2.37	0.57
3:F:101:VAL:HG13	3:F:149:LEU:HD21	1.86	0.57
3:F:102:PHE:HB3	3:F:147:ARG:HD2	1.85	0.57
1:C:237:ILE:HG13	1:C:329:VAL:HG21	1.86	0.57
3:F:218:TYR:OH	3:G:263:HIS:NE2	2.27	0.56
1:C:344:VAL:HG13	1:C:377:SER:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:77:GLU:OE2	2:E:78:GLY:N	2.37	0.56
3:G:18:ARG:NH2	7:A:3:U:OP2	2.38	0.56
3:G:36:ARG:NH2	4:B:81:ASP:OD1	2.38	0.56
3:G:301:ILE:HD11	3:G:326:TRP:CH2	2.41	0.56
4:B:307:THR:OG1	4:B:308:VAL:N	2.38	0.56
6:D:127:ARG:HE	6:D:231:LEU:HB2	1.70	0.56
3:H:297:VAL:HG23	3:I:285:VAL:HG11	1.87	0.56
1:C:358:LEU:HG	1:C:403:ILE:HD11	1.86	0.56
3:F:295:ASP:N	3:F:295:ASP:OD1	2.39	0.56
3:G:19:ASP:OD1	3:G:23:ALA:N	2.39	0.56
4:B:198:ARG:NH1	4:B:202:GLU:OE2	2.39	0.56
1:C:446:LYS:NZ	5:M:40:DC:OP1	2.34	0.56
3:F:187:ASP:OD1	3:H:25:LYS:NZ	2.39	0.56
3:I:18:ARG:HD3	3:I:22:GLY:HA2	1.88	0.56
3:I:60:ARG:HG3	3:I:102:PHE:HA	1.87	0.56
4:B:142:GLN:HE22	4:B:186:LEU:HA	1.71	0.56
3:F:4:GLU:OE1	3:F:274:LYS:NZ	2.39	0.55
1:C:197:THR:OG1	1:C:198:ALA:N	2.37	0.55
3:J:268:GLY:HA2	3:J:327:PHE:O	2.06	0.55
6:D:117:LYS:HA	6:D:241:PRO:HG3	1.88	0.55
1:C:92:VAL:HG12	1:C:116:LEU:HA	1.87	0.55
4:B:72:ILE:HG13	4:B:137:PHE:HE1	1.71	0.55
6:D:256:LYS:NZ	7:A:51:G:OP2	2.39	0.55
3:H:18:ARG:HH21	7:A:14:A:H8	1.54	0.55
3:J:345:ARG:HE	3:J:347:ILE:HD11	1.71	0.55
3:K:169:ALA:O	3:K:225:GLN:NE2	2.40	0.55
6:D:77:ASP:OD2	6:D:79:ARG:NH2	2.40	0.55
3:K:49:SER:HB2	3:K:251:THR:HG21	1.89	0.55
4:B:11:ARG:NH2	4:B:73:ASP:OD2	2.39	0.55
4:B:335:ALA:O	4:B:338:MET:HB2	2.07	0.55
2:E:3:ARG:O	2:E:3:ARG:NH1	2.40	0.55
3:I:37:ILE:HB	3:I:176:ALA:HB3	1.89	0.55
3:F:60:ARG:NH1	7:A:6:C:OP1	2.40	0.55
3:G:191:ALA:HB3	3:G:203:GLY:HA3	1.88	0.55
1:C:467:ASN:HB2	1:C:470:LYS:HB3	1.89	0.54
3:H:272:GLU:OE1	3:H:274:LYS:NZ	2.41	0.54
2:E:75:GLN:NE2	2:E:136:ASP:OD1	2.35	0.54
3:J:49:SER:OG	3:J:51:ASP:OD1	2.25	0.54
3:K:40:GLN:NE2	7:A:31:C:OP1	2.37	0.54
3:K:272:GLU:OE2	3:K:312:ARG:NH2	2.41	0.54
1:C:188:ILE:HG13	1:C:325:CYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:222:ASP:OD1	3:K:222:ASP:N	2.40	0.54
3:J:134:ALA:HA	3:J:165:THR:HG23	1.90	0.54
1:C:93:VAL:HG23	1:C:99:PRO:HG3	1.90	0.54
3:F:40:GLN:HB2	7:A:5:G:H3'	1.89	0.54
3:H:236:LEU:HD21	3:H:374:ALA:HB2	1.90	0.54
3:I:147:ARG:HD3	3:I:165:THR:HG22	1.89	0.54
6:D:168:ASP:OD1	6:D:168:ASP:N	2.38	0.54
3:G:256:LYS:HG3	3:G:260:PHE:HB2	1.89	0.54
6:D:117:LYS:HD2	6:D:118:ALA:N	2.17	0.54
3:F:310:ASP:OD1	3:F:310:ASP:N	2.41	0.54
1:C:411:GLU:HG3	1:C:469:GLY:HA3	1.90	0.54
3:F:320:SER:O	3:F:320:SER:OG	2.26	0.54
3:I:18:ARG:HH21	3:I:256:LYS:HD3	1.72	0.54
3:I:367:GLU:OE2	3:I:367:GLU:N	2.40	0.54
3:G:45:SER:HB2	3:G:253:PRO:HA	1.90	0.54
2:E:57:LYS:NZ	2:E:145:SER:O	2.39	0.53
3:F:246:LEU:O	3:F:250:LYS:HB2	2.08	0.53
3:F:305:SER:HB3	3:F:335:LEU:HG	1.90	0.53
3:F:282:ASN:HA	3:F:285:VAL:HG23	1.90	0.53
3:H:194:ASP:OD1	3:H:194:ASP:N	2.37	0.53
4:B:8:LEU:HD13	4:B:180:PRO:HG3	1.90	0.53
6:D:9:ILE:HD11	6:D:80:ALA:HB3	1.89	0.53
1:C:103:SER:OG	1:C:104:LEU:N	2.41	0.53
1:C:490:LEU:HD23	1:C:513:ILE:HA	1.90	0.53
3:F:99:MET:HE1	3:F:151:PRO:HA	1.90	0.53
3:I:191:ALA:N	3:I:204:HIS:O	2.39	0.53
6:D:206:ASN:HA	6:D:218:ARG:HB2	1.89	0.53
3:F:113:ARG:HH12	3:F:117:ASP:HB2	1.73	0.53
3:F:158:LYS:O	3:F:161:LYS:NZ	2.42	0.53
1:C:504:ASP:O	1:C:508:LYS:HG2	2.09	0.53
3:G:34:ARG:HD3	3:G:177:ILE:HG23	1.91	0.53
3:F:4:GLU:OE2	3:F:218:TYR:OH	2.21	0.53
3:G:27:CYS:HB2	3:G:36:ARG:HD3	1.91	0.53
3:H:102:PHE:HB3	3:H:147:ARG:HG3	1.90	0.53
1:C:243:ASN:OD1	1:C:351:SER:OG	2.27	0.53
1:C:470:LYS:NZ	1:C:470:LYS:O	2.42	0.53
3:H:296:LEU:HD22	3:I:30:GLY:HA2	1.90	0.53
3:H:334:PRO:HG2	3:H:337:TYR:HE1	1.73	0.53
3:G:51:ASP:N	3:G:51:ASP:OD1	2.41	0.53
7:A:32:A:O2'	7:A:33:G:N3	2.37	0.53
1:C:102:ILE:HD13	1:C:107:THR:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:168:GLU:OE2	3:K:168:GLU:N	2.35	0.52
1:C:85:LEU:HD13	1:C:104:LEU:HB3	1.91	0.52
3:F:313:LEU:HD23	3:G:330:ASN:HD21	1.74	0.52
4:B:50:ILE:HG22	4:B:51:GLY:H	1.75	0.52
3:F:7:MET:HG3	3:F:269:ILE:HD13	1.92	0.52
3:I:137:THR:OG1	3:I:147:ARG:NH1	2.43	0.52
3:J:254:SER:HA	3:J:257:GLN:HG3	1.92	0.52
1:C:428:ARG:NH2	1:C:461:GLU:OE2	2.40	0.52
3:G:229:ASN:O	3:G:231:LYS:N	2.41	0.52
4:B:16:LEU:HD22	4:B:131:TYR:HB3	1.92	0.52
3:F:253:PRO:O	3:F:257:GLN:NE2	2.43	0.52
3:J:114:ILE:HD13	3:J:128:GLN:HE22	1.75	0.52
3:J:282:ASN:HA	3:J:285:VAL:HG23	1.91	0.52
3:H:29:PHE:HB3	3:H:34:ARG:HG3	1.92	0.52
3:J:309:ASN:HB2	3:J:342:LEU:HD21	1.92	0.52
1:C:117:ALA:HB1	4:B:244:PRO:HG3	1.92	0.52
3:I:11:HIS:HD2	3:I:264:ASN:HB2	1.75	0.52
3:K:34:ARG:NH2	3:K:285:VAL:O	2.43	0.52
2:E:17:GLU:OE2	2:E:17:GLU:N	2.37	0.51
3:J:6:HIS:HB3	3:J:216:TYR:HE1	1.75	0.51
3:G:6:HIS:HB2	3:G:270:LEU:HB2	1.92	0.51
1:C:470:LYS:HZ1	1:C:476:GLY:H	1.55	0.51
3:F:112:ALA:HA	3:F:115:VAL:HG12	1.92	0.51
3:H:190:VAL:HG12	3:H:205:ILE:HG22	1.91	0.51
3:K:62:ARG:O	3:K:97:THR:N	2.35	0.51
4:B:300:VAL:HG12	4:B:328:LEU:HD21	1.93	0.51
3:I:19:ASP:N	3:I:23:ALA:O	2.43	0.51
1:C:267:TRP:HE3	1:C:288:LEU:HD11	1.75	0.51
3:G:217:LYS:HG3	3:G:219:PHE:HE1	1.76	0.51
3:G:355:GLY:HA2	3:G:358:LEU:HD12	1.90	0.51
3:F:16:LEU:HD13	3:F:253:PRO:HG2	1.93	0.51
3:J:358:LEU:HD11	3:J:366:TRP:HE3	1.75	0.51
6:D:126:LEU:HB2	6:D:263:LEU:HD23	1.93	0.51
3:I:14:ALA:HA	3:I:260:PHE:HB3	1.93	0.51
3:K:149:LEU:O	3:K:165:THR:OG1	2.29	0.51
3:G:326:TRP:HD1	3:G:346:ASN:HA	1.76	0.51
4:B:17:GLN:HB3	4:B:164:LEU:HD13	1.93	0.50
3:F:295:ASP:HB2	3:H:285:VAL:HG12	1.92	0.50
1:C:340:ASP:H	1:C:345:TYR:HE2	1.60	0.50
3:H:358:LEU:HD23	3:H:361:ILE:HD11	1.94	0.50
3:G:52:PHE:HZ	3:G:251:THR:HB	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:PHE:HB2	1:C:405:ILE:HD13	1.94	0.50
4:B:29:ARG:HH11	4:B:129:ARG:HH12	1.60	0.50
6:D:125:ARG:HA	6:D:233:GLU:HA	1.94	0.50
3:F:311:ILE:HA	3:F:315:TYR:HB2	1.93	0.50
3:I:15:ASN:ND2	3:I:209:MET:O	2.44	0.50
3:G:34:ARG:HB2	3:G:178:SER:HB3	1.94	0.50
1:C:125:PHE:HE1	1:C:250:LEU:HD13	1.77	0.50
1:C:188:ILE:HB	1:C:324:SER:HA	1.94	0.50
3:H:139:ALA:H	3:H:142:ILE:HD11	1.77	0.50
3:I:187:ASP:HB2	3:I:210:PHE:HE1	1.76	0.50
3:J:92:ASN:ND2	3:J:94:ASP:O	2.38	0.50
3:K:156:LYS:NZ	3:K:157:ASP:O	2.45	0.50
3:G:32:VAL:HG11	3:G:287:PRO:HG3	1.94	0.50
3:K:37:ILE:HG12	3:K:176:ALA:HB3	1.94	0.50
6:D:158:SER:OG	7:A:37:U:OP1	2.28	0.50
6:D:254:LYS:NZ	7:A:50:G:OP2	2.45	0.50
3:F:64:LEU:HB3	3:F:85:LEU:HD11	1.92	0.49
6:D:44:ARG:H	6:D:44:ARG:HD3	1.77	0.49
3:K:74:GLU:OE1	3:K:76:GLU:N	2.45	0.49
4:B:292:VAL:HB	6:D:218:ARG:NH2	2.26	0.49
3:H:270:LEU:HD23	3:H:326:TRP:HE3	1.78	0.49
4:B:290:ARG:HA	4:B:293:MET:HB3	1.94	0.49
3:F:37:ILE:HB	3:F:176:ALA:HB3	1.94	0.49
3:G:143:ALA:O	3:G:229:ASN:ND2	2.45	0.49
1:C:347:ASP:OD1	1:C:347:ASP:N	2.46	0.49
3:G:241:VAL:O	3:G:245:LEU:HD22	2.12	0.49
3:G:245:LEU:HD21	3:G:357:VAL:HG11	1.93	0.49
1:C:281:LYS:HE2	1:C:281:LYS:N	2.27	0.49
3:I:10:ASN:HB3	3:J:282:ASN:HD21	1.78	0.49
3:J:58:GLY:HA2	3:J:104:SER:HB2	1.94	0.49
3:K:34:ARG:NH1	3:K:284:PHE:O	2.44	0.49
3:K:358:LEU:HG	3:K:364:PHE:HB2	1.95	0.49
4:B:44:LEU:HD11	4:B:151:LEU:HD21	1.93	0.49
3:G:301:ILE:HD13	3:G:333:TYR:HB3	1.95	0.49
6:D:255:ALA:O	6:D:257:SER:N	2.46	0.49
1:C:90:VAL:HG22	1:C:92:VAL:HG13	1.95	0.49
1:C:262:GLN:OE1	1:C:386:ARG:NH2	2.46	0.49
3:I:23:ALA:HB2	3:I:209:MET:HE2	1.94	0.49
3:I:308:VAL:HG12	3:I:342:LEU:HD21	1.93	0.49
1:C:496:SER:HB2	3:G:33:LEU:HB3	1.95	0.49
3:H:101:VAL:HA	3:H:149:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:309:ASN:HB2	3:H:342:LEU:HD22	1.94	0.49
3:J:6:HIS:O	3:J:270:LEU:N	2.31	0.49
3:J:207:GLU:OE2	6:D:19:ARG:NH2	2.45	0.49
6:D:60:PHE:O	6:D:62:LYS:NZ	2.46	0.49
3:F:294:SER:H	3:H:286:ARG:HH21	1.60	0.49
1:C:255:ASP:HB3	1:C:258:GLY:H	1.78	0.48
3:G:252:ASN:HB3	3:G:253:PRO:HD2	1.94	0.48
3:I:39:SER:H	3:I:175:HIS:CE1	2.31	0.48
3:K:236:LEU:HG	3:K:372:SER:HB3	1.96	0.48
3:I:25:LYS:HE2	3:I:36:ARG:HH22	1.78	0.48
2:E:74:GLU:OE2	2:E:76:ARG:NH2	2.45	0.48
3:J:157:ASP:OD1	3:J:157:ASP:N	2.41	0.48
3:G:274:LYS:HB2	3:G:322:VAL:HG21	1.95	0.48
6:D:126:LEU:HD23	6:D:263:LEU:HG	1.94	0.48
1:C:427:ASN:OD1	1:C:427:ASN:N	2.47	0.48
3:F:265:TYR:CE1	3:H:278:ILE:HD12	2.48	0.48
3:J:44:ARG:O	3:J:48:THR:OG1	2.30	0.48
3:I:9:GLN:HG2	3:I:266:PRO:HB3	1.96	0.48
4:B:302:LYS:HB3	4:B:302:LYS:HE2	1.68	0.48
3:J:107:LYS:HZ3	3:J:107:LYS:HB2	1.78	0.48
3:G:187:ASP:N	3:G:208:SER:O	2.40	0.48
6:D:126:LEU:HD21	6:D:252:ILE:HB	1.96	0.48
3:J:41:CYS:SG	7:A:24:C:O2'	2.71	0.48
3:F:141:ASP:OD1	3:F:141:ASP:N	2.45	0.47
6:D:70:ASP:OD2	6:D:125:ARG:NH1	2.47	0.47
6:D:167:PRO:HA	6:D:170:ALA:HB3	1.96	0.47
6:D:186:LEU:HG	6:D:236:LEU:HD22	1.97	0.47
1:C:192:ILE:HG22	1:C:194:GLU:HG2	1.96	0.47
1:C:452:GLN:HE21	1:C:497:LEU:HD22	1.79	0.47
5:M:7:DC:H2'	5:M:8:DA:H4'	1.95	0.47
3:J:109:LYS:HE3	3:J:109:LYS:HB3	1.71	0.47
3:G:52:PHE:CZ	3:G:251:THR:HB	2.50	0.47
4:B:377:ARG:HE	4:B:378:PHE:N	2.12	0.47
3:J:174:ALA:HB3	3:J:218:TYR:HB3	1.96	0.47
3:K:41:CYS:SG	7:A:30:G:O2'	2.66	0.47
3:G:285:VAL:HG11	4:B:198:ARG:HB3	1.97	0.47
3:K:103:MET:HG2	3:K:133:ILE:HG23	1.97	0.47
4:B:226:ASP:OD1	4:B:226:ASP:N	2.48	0.47
1:C:408:LYS:NZ	1:C:465:ALA:O	2.44	0.47
4:B:354:ASP:OD1	4:B:354:ASP:N	2.38	0.47
1:C:356:ILE:HD11	1:C:369:ARG:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:112:ASP:O	2:E:116:MET:HG3	2.14	0.47
3:H:111:LEU:HD11	3:H:129:VAL:HG13	1.97	0.47
3:K:292:LYS:HE2	3:K:292:LYS:H	1.78	0.47
3:G:27:CYS:SG	3:G:28:TYR:N	2.88	0.47
3:G:247:ALA:HA	3:G:250:LYS:HB2	1.97	0.47
5:M:40:DC:H6	5:M:40:DC:H2'	1.62	0.47
1:C:114:LEU:HD11	1:C:256:LEU:HD22	1.96	0.47
1:C:357:LYS:HA	1:C:357:LYS:HD3	1.74	0.47
3:F:50:ASN:N	3:F:50:ASN:OD1	2.48	0.47
3:H:20:ASP:OD1	3:H:20:ASP:N	2.45	0.47
3:I:309:ASN:HB2	3:I:342:LEU:HD22	1.97	0.47
3:K:17:ASN:HB3	3:K:25:LYS:HG3	1.96	0.47
4:B:27:ALA:HB1	4:B:127:SER:HA	1.96	0.47
6:D:134:ARG:HB3	6:D:137:PRO:HG3	1.97	0.47
6:D:156:ARG:NH1	7:A:51:G:O6	2.48	0.47
3:I:144:LEU:HD21	3:I:240:THR:HG21	1.96	0.46
1:C:200:ASN:OD1	1:C:200:ASN:N	2.47	0.46
2:E:85:MET:HB3	2:E:160:PHE:HE2	1.79	0.46
3:F:285:VAL:HG11	3:G:297:VAL:HG22	1.97	0.46
3:K:174:ALA:HB3	3:K:218:TYR:HB3	1.98	0.46
4:B:313:TYR:O	4:B:347:THR:OG1	2.33	0.46
5:M:14:DG:H1	7:A:31:C:H41	1.63	0.46
3:F:155:ASP:OD1	3:F:155:ASP:N	2.48	0.46
3:J:263:HIS:CG	3:K:277:PRO:HB2	2.50	0.46
3:G:271:VAL:HG13	3:G:325:PHE:HB3	1.97	0.46
4:B:71:ARG:HH12	4:B:258:VAL:HG21	1.81	0.46
1:C:344:VAL:HG21	1:C:374:PRO:HB2	1.96	0.46
1:C:466:ILE:HD12	1:C:467:ASN:N	2.30	0.46
3:H:137:THR:O	3:H:231:LYS:NZ	2.48	0.46
3:H:230:LEU:C	3:H:231:LYS:HD2	2.40	0.46
3:G:198:GLU:OE2	3:G:198:GLU:N	2.36	0.46
3:G:310:ASP:O	3:G:312:ARG:N	2.40	0.46
7:A:-2:C:O2'	7:A:-1:C:O4'	2.33	0.46
1:C:287:GLY:O	1:C:338:TRP:NE1	2.40	0.46
3:I:18:ARG:HA	3:I:24:PRO:HA	1.98	0.46
7:A:41:C:H3'	7:A:42:A:H8	1.80	0.46
3:H:9:GLN:NE2	3:H:264:ASN:O	2.40	0.46
3:I:295:ASP:HB2	3:J:285:VAL:HG12	1.97	0.46
3:J:3:ILE:HD12	3:J:221:ILE:HB	1.98	0.46
4:B:72:ILE:HD13	4:B:209:PRO:HB2	1.98	0.46
1:C:488:GLU:O	1:C:491:THR:OG1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:191:ALA:O	3:F:203:GLY:N	2.38	0.46
4:B:191:SER:HB2	4:B:257:ASP:HB3	1.98	0.46
1:C:212:ASP:HB2	1:C:313:SER:HB2	1.97	0.46
2:E:85:MET:HE2	2:E:123:ILE:HD12	1.97	0.46
2:E:86:GLY:HA2	2:E:89:CYS:HB2	1.97	0.46
3:F:174:ALA:HB2	3:G:261:ALA:HB3	1.96	0.46
3:F:113:ARG:NH2	3:F:117:ASP:OD2	2.39	0.46
3:J:273:PHE:HB2	3:J:323:ILE:HD11	1.98	0.46
4:B:72:ILE:HB	4:B:209:PRO:HD2	1.98	0.46
6:D:167:PRO:HG2	6:D:191:LEU:HD21	1.98	0.46
3:F:295:ASP:OD2	3:F:333:TYR:OH	2.34	0.46
3:K:168:GLU:O	3:K:229:ASN:ND2	2.48	0.46
1:C:316:LEU:HG	4:B:241:ARG:HG2	1.97	0.45
3:H:114:ILE:HD13	3:H:128:GLN:HB3	1.97	0.45
3:G:49:SER:OG	3:G:51:ASP:OD1	2.25	0.45
6:D:127:ARG:HD2	6:D:260:PHE:HD1	1.81	0.45
1:C:172:ASP:OD1	1:C:172:ASP:N	2.39	0.45
1:C:389:LYS:HE3	1:C:389:LYS:HA	1.98	0.45
1:C:521:ILE:HD12	1:C:522:PRO:HD3	1.98	0.45
3:H:91:LYS:HG2	3:H:152:ASN:ND2	2.30	0.45
3:G:8:ILE:HG22	3:G:268:GLY:H	1.81	0.45
3:G:201:GLY:HA3	5:M:38:DG:H8	1.80	0.45
3:G:249:ALA:HB1	3:G:266:PRO:HG2	1.97	0.45
7:A:4:U:H2'	7:A:5:G:C4	2.51	0.45
3:H:47:ARG:NH1	3:H:145:CYS:SG	2.87	0.45
4:B:41:LEU:HD21	4:B:63:LEU:HD11	1.99	0.45
3:I:136:ALA:O	3:I:138:LEU:HD22	2.17	0.45
3:J:17:ASN:HB3	3:J:25:LYS:HD2	1.98	0.45
3:K:61:THR:OG1	3:K:62:ARG:N	2.50	0.45
3:K:171:LEU:HG	3:K:173:VAL:HG23	1.99	0.45
6:D:28:ILE:HA	6:D:31:VAL:HB	1.99	0.45
3:K:209:MET:HB2	6:D:188:ARG:HH21	1.80	0.45
1:C:206:HIS:NE2	7:A:-2:C:N3	2.64	0.45
3:H:354:VAL:HA	3:H:357:VAL:HG12	1.98	0.45
3:J:349:ASN:OD1	3:J:351:ASN:ND2	2.36	0.45
3:J:359:ASP:HA	3:J:363:GLY:HA2	1.98	0.45
3:K:104:SER:OG	3:K:106:ASP:OD1	2.35	0.45
3:K:307:TYR:CE1	3:K:311:ILE:HG13	2.51	0.45
4:B:236:SER:OG	4:B:237:PHE:N	2.49	0.45
3:G:39:SER:O	3:G:43:LYS:HB2	2.17	0.45
3:H:64:LEU:O	3:H:68:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:11:HIS:HB3	3:I:262:ALA:HB1	1.97	0.45
3:K:235:ASN:OD1	3:K:372:SER:OG	2.32	0.45
6:D:40:PRO:HG3	6:D:94:TYR:CD2	2.52	0.45
1:C:420:GLU:O	1:C:424:GLN:HG2	2.17	0.45
3:I:18:ARG:NH2	7:A:21:G:OP2	2.48	0.45
3:K:63:ARG:HH21	3:K:96:ASN:HB3	1.82	0.45
2:E:41:PHE:O	2:E:45:TRP:HB3	2.17	0.44
3:F:286:ARG:NE	3:G:295:ASP:OD1	2.50	0.44
3:H:17:ASN:HD22	3:H:17:ASN:HA	1.60	0.44
3:I:56:LEU:HG	3:I:105:LYS:HZ3	1.82	0.44
3:I:295:ASP:OD1	3:I:295:ASP:N	2.50	0.44
3:J:102:PHE:O	3:J:147:ARG:NH1	2.50	0.44
1:C:89:TRP:CD1	1:C:90:VAL:HG12	2.52	0.44
3:F:176:ALA:HB1	3:F:215:PHE:HB3	1.99	0.44
3:G:274:LYS:HA	3:G:322:VAL:HG11	1.99	0.44
4:B:35:PRO:HD2	4:B:70:VAL:HG11	1.99	0.44
3:F:174:ALA:HB3	3:F:218:TYR:HB3	1.98	0.44
3:K:64:LEU:HD12	3:K:111:LEU:HD12	1.99	0.44
3:K:180:HIS:CE1	3:K:183:ARG:HE	2.35	0.44
3:H:7:MET:HE2	3:H:217:LYS:HD3	1.99	0.44
3:J:269:ILE:HG21	3:J:353:LEU:HD21	1.99	0.44
3:G:144:LEU:HD11	3:G:244:PHE:HE2	1.83	0.44
3:G:310:ASP:O	3:G:311:ILE:HG13	2.18	0.44
3:F:52:PHE:O	3:F:56:LEU:N	2.50	0.44
3:F:149:LEU:HD12	3:F:149:LEU:HA	1.87	0.44
3:F:151:PRO:HG3	3:F:162:TRP:CE2	2.53	0.44
3:H:93:LYS:HD3	3:H:93:LYS:HA	1.83	0.44
4:B:280:ASN:OD1	4:B:281:SER:N	2.45	0.44
5:M:40:DC:H2"	5:M:41:DA:O4'	2.17	0.44
1:C:122:MET:HB2	1:C:229:PHE:CE2	2.53	0.44
3:H:161:LYS:HD3	3:H:161:LYS:HA	1.73	0.44
3:K:165:THR:OG1	3:K:165:THR:O	2.35	0.44
4:B:20:GLY:HA3	7:A:-5:G:H3'	1.99	0.44
4:B:48:MET:HE3	4:B:48:MET:HA	1.99	0.44
4:B:372:ARG:HB3	6:D:18:PRO:HD3	2.00	0.44
1:C:83:ASN:ND2	1:C:167:PHE:O	2.50	0.44
3:J:129:VAL:HA	3:J:132:VAL:HG12	2.00	0.44
4:B:298:CYS:N	4:B:303:ALA:O	2.51	0.44
1:C:466:ILE:HD12	1:C:467:ASN:H	1.83	0.44
3:F:221:ILE:HD11	3:F:244:PHE:CD2	2.53	0.44
3:J:124:GLU:OE2	3:J:124:GLU:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:HIS:CE1	3:G:216:TYR:HH	2.36	0.44
6:D:143:ASP:OD1	6:D:143:ASP:N	2.45	0.44
6:D:166:THR:OG1	6:D:168:ASP:OD1	2.23	0.44
1:C:374:PRO:HG2	1:C:392:LEU:HD11	1.99	0.44
1:C:390:LEU:HB3	1:C:410:ILE:HG22	1.99	0.44
3:F:24:PRO:HD3	3:F:209:MET:HB2	2.00	0.44
3:I:55:LEU:HD21	3:I:140:PRO:HB2	2.00	0.44
1:C:413:GLU:OE2	1:C:475:ARG:NH1	2.51	0.43
6:D:9:ILE:HG21	6:D:24:TRP:HZ3	1.83	0.43
3:I:367:GLU:H	3:I:367:GLU:CD	2.25	0.43
4:B:191:SER:HB3	4:B:252:LEU:HD11	2.00	0.43
7:A:28:U:H2'	7:A:29:A:C8	2.53	0.43
3:H:332:ARG:NH1	3:I:306:ASN:OD1	2.51	0.43
3:K:7:MET:HE2	3:K:217:LYS:HD2	2.00	0.43
1:C:175:ARG:NH2	1:C:299:VAL:O	2.52	0.43
3:H:222:ASP:OD1	3:H:223:TRP:N	2.51	0.43
1:C:118:TYR:HB2	1:C:124:ARG:HG3	2.00	0.43
3:J:37:ILE:HB	3:J:176:ALA:HB3	2.01	0.43
7:A:41:C:H3'	7:A:42:A:C8	2.53	0.43
2:E:31:LEU:HD23	2:E:31:LEU:H	1.84	0.43
4:B:13:GLU:OE1	4:B:74:ARG:NH1	2.50	0.43
1:C:448:VAL:HB	3:G:21:LEU:HB3	2.00	0.43
3:G:266:PRO:HB2	3:G:269:ILE:HD11	1.99	0.43
4:B:248:ILE:HG21	4:B:250:ARG:HH21	1.82	0.43
3:K:238:ALA:HB1	3:K:358:LEU:HD11	2.01	0.43
4:B:274:THR:OG1	4:B:315:ARG:NH1	2.52	0.43
3:F:110:ASP:OD1	3:F:111:LEU:N	2.52	0.43
3:H:102:PHE:O	3:H:147:ARG:NH1	2.52	0.43
3:I:332:ARG:HD3	3:J:310:ASP:OD2	2.19	0.43
3:G:282:ASN:HA	3:G:285:VAL:HG23	2.00	0.43
4:B:201:ASN:OD1	4:B:201:ASN:N	2.51	0.43
1:C:441:ARG:NH1	3:F:20:ASP:OD2	2.51	0.43
3:F:278:ILE:HD11	3:G:265:TYR:CD2	2.54	0.43
3:I:59:VAL:HG23	3:I:105:LYS:HE3	2.00	0.43
3:I:263:HIS:NE2	3:J:172:GLN:OE1	2.42	0.43
6:D:108:GLU:OE1	6:D:108:GLU:N	2.52	0.43
3:H:236:LEU:HD12	3:H:236:LEU:HA	1.88	0.42
3:H:357:VAL:O	3:H:361:ILE:HG12	2.19	0.42
3:J:24:PRO:HD3	3:J:209:MET:HB2	2.01	0.42
3:G:254:SER:C	3:G:257:GLN:NE2	2.76	0.42
1:C:238:GLY:H	1:C:329:VAL:HG11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:THR:HA	1:C:513:ILE:HD11	2.00	0.42
3:G:295:ASP:OD1	3:G:295:ASP:N	2.51	0.42
4:B:298:CYS:HB3	4:B:302:LYS:HA	2.01	0.42
3:I:103:MET:HB2	3:I:103:MET:HE2	1.54	0.42
4:B:157:LYS:HA	4:B:157:LYS:HD2	1.81	0.42
1:C:502:THR:HG22	2:E:109:ALA:HB3	2.00	0.42
3:F:286:ARG:NH2	3:G:293:GLU:O	2.46	0.42
3:H:139:ALA:HB3	3:H:142:ILE:HG12	2.02	0.42
3:G:341:LYS:HB2	3:G:341:LYS:HE2	1.85	0.42
4:B:138:LEU:HD11	4:B:193:VAL:HG11	2.00	0.42
4:B:268:VAL:HG13	4:B:270:ARG:HG2	2.00	0.42
6:D:106:PRO:HA	6:D:107:PRO:HD3	1.90	0.42
1:C:128:PHE:CD2	1:C:250:LEU:HD21	2.54	0.42
3:I:83:GLU:O	3:I:86:ASN:ND2	2.42	0.42
3:F:40:GLN:NE2	7:A:7:C:OP1	2.39	0.42
3:K:181:ILE:HA	3:K:181:ILE:HD13	1.84	0.42
4:B:38:SER:O	4:B:38:SER:OG	2.32	0.42
2:E:2:ASN:HD21	2:E:54:ARG:HB3	1.85	0.42
3:I:370:GLN:H	3:I:370:GLN:HG2	1.61	0.42
6:D:134:ARG:HG3	6:D:136:ILE:H	1.84	0.42
6:D:155:LYS:NZ	7:A:38:C:OP2	2.51	0.42
3:F:261:ALA:HB3	3:H:174:ALA:HB2	2.01	0.42
3:J:144:LEU:HB3	3:J:171:LEU:HD13	2.02	0.42
3:G:50:ASN:OD1	3:G:50:ASN:N	2.52	0.42
3:G:301:ILE:HD11	3:G:326:TRP:HH2	1.83	0.42
4:B:249:ARG:HA	4:B:249:ARG:HD3	1.83	0.42
6:D:125:ARG:HG2	6:D:233:GLU:HB3	2.02	0.42
3:H:172:GLN:HB2	3:H:220:SER:HB3	2.02	0.42
3:J:136:ALA:HB3	3:J:147:ARG:HH22	1.84	0.42
1:C:201:LEU:HD23	4:B:121:ARG:HH12	1.85	0.42
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.92	0.42
3:F:33:LEU:HD12	3:F:33:LEU:HA	1.93	0.42
3:F:140:PRO:HB2	3:F:240:THR:HG21	2.01	0.42
3:H:240:THR:O	3:H:244:PHE:HB3	2.20	0.42
6:D:254:LYS:HZ1	7:A:49:U:H5"	1.85	0.42
1:C:245:PRO:HA	1:C:246:PRO:HD3	1.91	0.41
3:F:53:LYS:H	3:F:53:LYS:HG2	1.68	0.41
3:H:306:ASN:O	3:H:310:ASP:HB2	2.20	0.41
3:F:315:TYR:HE2	3:G:265:TYR:HB3	1.85	0.41
3:I:335:LEU:HD23	3:I:335:LEU:HA	1.84	0.41
3:K:20:ASP:OD1	3:K:20:ASP:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:283:TYR:HA	4:B:286:VAL:HG12	2.01	0.41
7:A:43:C:H1'	7:A:48:G:C6	2.55	0.41
1:C:452:GLN:HE22	1:C:497:LEU:HD13	1.86	0.41
3:F:41:CYS:SG	7:A:6:C:O2'	2.76	0.41
3:I:18:ARG:HH22	7:A:21:G:P	2.43	0.41
4:B:155:LEU:HD23	4:B:155:LEU:HA	1.89	0.41
4:B:326:ARG:NH2	4:B:351:ASP:OD1	2.46	0.41
2:E:18:GLY:O	2:E:22:ILE:HG23	2.20	0.41
3:F:129:VAL:O	3:F:133:ILE:HG13	2.21	0.41
1:C:157:ILE:HD12	1:C:157:ILE:HA	1.87	0.41
1:C:339:LYS:HE2	1:C:339:LYS:HB2	1.94	0.41
3:H:195:VAL:O	3:I:63:ARG:NH2	2.53	0.41
3:I:115:VAL:HG23	3:I:116:LEU:HD23	2.03	0.41
3:J:190:VAL:O	7:A:29:A:O2'	2.33	0.41
4:B:211:VAL:HG22	4:B:249:ARG:HH11	1.86	0.41
1:C:493:VAL:HG22	3:G:33:LEU:HD22	2.03	0.41
3:F:25:LYS:HB3	3:F:36:ARG:NH2	2.35	0.41
3:K:246:LEU:HD12	3:K:246:LEU:HA	1.85	0.41
4:B:12:LEU:HB2	4:B:137:PHE:HB2	2.02	0.41
4:B:179:PRO:HA	4:B:180:PRO:HD3	1.94	0.41
6:D:254:LYS:NZ	7:A:49:U:H5"	2.36	0.41
3:F:347:ILE:HD12	3:F:349:ASN:H	1.86	0.41
4:B:250:ARG:HD3	4:B:250:ARG:HA	1.67	0.41
1:C:212:ASP:OD1	1:C:212:ASP:N	2.51	0.41
1:C:445:LYS:H	1:C:445:LYS:HG3	1.64	0.41
2:E:30:ARG:H	2:E:30:ARG:HG3	1.68	0.41
3:F:34:ARG:NH1	3:F:284:PHE:O	2.54	0.41
3:F:102:PHE:CE2	3:F:142:ILE:HG12	2.56	0.41
3:H:20:ASP:HA	7:A:13:G:N7	2.36	0.41
3:H:111:LEU:HD12	3:H:111:LEU:HA	1.91	0.41
3:H:294:SER:OG	3:H:299:GLN:OE1	2.31	0.41
3:I:116:LEU:HD21	3:I:129:VAL:HG23	2.03	0.41
3:I:195:VAL:HA	3:I:196:PRO:HD3	1.90	0.41
3:I:349:ASN:HD21	3:J:316:TYR:HB3	1.86	0.41
3:K:150:GLU:HA	3:K:151:PRO:HD3	1.84	0.41
4:B:44:LEU:HD12	4:B:44:LEU:HA	1.74	0.41
4:B:72:ILE:HG13	4:B:137:PHE:CE1	2.53	0.41
7:A:22:U:H2'	7:A:23:G:C8	2.55	0.41
3:I:55:LEU:HD12	3:I:239:HIS:CD2	2.56	0.41
3:G:276:SER:HA	3:G:277:PRO:HD3	1.96	0.41
7:A:43:C:N3	7:A:47:U:O4	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:46:ILE:HD13	3:F:244:PHE:CE1	2.56	0.40
4:B:13:GLU:O	4:B:172:SER:N	2.49	0.40
6:D:132:VAL:HB	7:A:47:U:H5'	2.03	0.40
3:H:98:LYS:HE3	3:H:98:LYS:HB3	1.85	0.40
3:K:103:MET:HE3	3:K:133:ILE:HG12	2.02	0.40
4:B:44:LEU:HD11	4:B:151:LEU:CD2	2.51	0.40
3:F:308:VAL:HG12	3:F:342:LEU:HD21	2.03	0.40
3:I:245:LEU:HD23	3:I:354:VAL:HG22	2.03	0.40
3:J:332:ARG:NH1	3:J:333:TYR:OH	2.54	0.40
3:G:146:GLY:H	3:G:169:ALA:HB2	1.86	0.40
4:B:269:TRP:CH2	4:B:271:PRO:HG3	2.56	0.40
6:D:162:ASP:OD2	6:D:165:SER:N	2.55	0.40
2:E:90:ARG:HH12	2:E:91:LYS:NZ	2.20	0.40
3:K:62:ARG:HG3	3:K:100:LEU:HD13	2.03	0.40
3:G:298:GLU:O	3:G:301:ILE:HG22	2.21	0.40
3:G:329:PRO:O	3:G:332:ARG:HD3	2.22	0.40
4:B:168:SER:O	4:B:168:SER:OG	2.36	0.40
4:B:225:ASP:N	4:B:225:ASP:OD1	2.54	0.40
4:B:268:VAL:HG13	4:B:270:ARG:HH11	1.86	0.40
4:B:356:ILE:HD12	4:B:357:TRP:N	2.36	0.40
1:C:316:LEU:HA	1:C:316:LEU:HD23	1.87	0.40
3:F:295:ASP:HB3	3:H:286:ARG:HB2	2.03	0.40
3:J:85:LEU:HD23	3:J:85:LEU:HA	1.93	0.40
3:J:350:LEU:O	3:J:354:VAL:HG23	2.22	0.40
4:B:231:TYR:HA	4:B:244:PRO:HA	2.02	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	434/535 (81%)	389 (90%)	44 (10%)	1 (0%)	44 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	163/174 (94%)	154 (94%)	9 (6%)	0	100	100
3	F	364/378 (96%)	339 (93%)	25 (7%)	0	100	100
3	G	241/378 (64%)	209 (87%)	29 (12%)	3 (1%)	11	28
3	H	373/378 (99%)	348 (93%)	25 (7%)	0	100	100
3	I	364/378 (96%)	328 (90%)	36 (10%)	0	100	100
3	J	367/378 (97%)	336 (92%)	29 (8%)	2 (0%)	25	50
3	K	334/378 (88%)	309 (92%)	25 (8%)	0	100	100
4	B	342/388 (88%)	284 (83%)	58 (17%)	0	100	100
6	D	262/272 (96%)	227 (87%)	32 (12%)	3 (1%)	12	30
All	All	3244/3637 (89%)	2923 (90%)	312 (10%)	9 (0%)	38	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	306	PRO
3	J	151	PRO
3	G	253	PRO
3	G	311	ILE
6	D	117	LYS
6	D	256	LYS
3	J	104	SER
3	G	231	LYS
6	D	140	VAL

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	366/459 (80%)	346 (94%)	20 (6%)	18	39
2	E	143/153 (94%)	136 (95%)	7 (5%)	21	43
3	F	295/313 (94%)	274 (93%)	21 (7%)	12	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	194/313 (62%)	178 (92%)	16 (8%)	9	23
3	H	300/313 (96%)	282 (94%)	18 (6%)	16	35
3	I	291/313 (93%)	280 (96%)	11 (4%)	28	52
3	J	290/313 (93%)	271 (93%)	19 (7%)	14	31
3	K	280/313 (90%)	265 (95%)	15 (5%)	18	40
4	B	281/321 (88%)	268 (95%)	13 (5%)	23	46
6	D	228/238 (96%)	211 (92%)	17 (8%)	11	26
All	All	2668/3049 (88%)	2511 (94%)	157 (6%)	19	36

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	80	VAL
1	C	90	VAL
1	C	93	VAL
1	C	144	VAL
1	C	157	ILE
1	C	161	GLU
1	C	163	ASN
1	C	191	LEU
1	C	197	THR
1	C	200	ASN
1	C	298	LYS
1	C	302	HIS
1	C	305	VAL
1	C	325	CYS
1	C	326	SER
1	C	358	LEU
1	C	373	SER
1	C	392	LEU
1	C	453	ILE
1	C	488	GLU
2	E	6	VAL
2	E	7	ASP
2	E	20	LEU
2	E	44	LEU
2	E	93	GLU
2	E	95	LYS
2	E	156	TRP
3	F	12	SER

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Mol	Chain	Res	Type
3	F	20	ASP
3	F	50	ASN
3	F	67	LEU
3	F	80	LYS
3	F	82	GLN
3	F	86	ASN
3	F	97	THR
3	F	104	SER
3	F	111	LEU
3	F	115	VAL
3	F	155	ASP
3	F	157	ASP
3	F	166	THR
3	F	195	VAL
3	F	228	LYS
3	F	233	ASP
3	F	325	PHE
3	F	326	TRP
3	F	338	LYS
3	F	344	SER
3	H	17	ASN
3	H	20	ASP
3	H	41	CYS
3	H	42	ILE
3	H	59	VAL
3	H	67	LEU
3	H	155	ASP
3	H	163	SER
3	H	177	ILE
3	H	231	LYS
3	H	251	THR
3	H	254	SER
3	H	259	SER
3	H	289	SER
3	H	291	VAL
3	H	323	ILE
3	H	339	HIS
3	H	344	SER
3	I	17	ASN
3	I	40	GLN
3	I	116	LEU
3	I	129	VAL

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Mol	Chain	Res	Type
3	I	132	VAL
3	I	138	LEU
3	I	163	SER
3	I	164	ASN
3	I	205	ILE
3	I	227	VAL
3	I	234	THR
3	J	3	ILE
3	J	50	ASN
3	J	61	THR
3	J	66	ASP
3	J	99	MET
3	J	129	VAL
3	J	156	LYS
3	J	163	SER
3	J	234	THR
3	J	259	SER
3	J	266	PRO
3	J	269	ILE
3	J	278	ILE
3	J	289	SER
3	J	290	VAL
3	J	323	ILE
3	J	328	SER
3	J	331	ASN
3	J	340	SER
3	K	35	SER
3	K	52	PHE
3	K	61	THR
3	K	83	GLU
3	K	106	ASP
3	K	133	ILE
3	K	144	LEU
3	K	222	ASP
3	K	236	LEU
3	K	271	VAL
3	K	294	SER
3	K	298	GLU
3	K	304	LEU
3	K	322	VAL
3	K	347	ILE
3	G	8	ILE

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Mol	Chain	Res	Type
3	G	11	HIS
3	G	41	CYS
3	G	46	ILE
3	G	142	ILE
3	G	167	VAL
3	G	186	ILE
3	G	194	ASP
3	G	222	ASP
3	G	236	LEU
3	G	254	SER
3	G	265	TYR
3	G	271	VAL
3	G	328	SER
3	G	339	HIS
3	G	347	ILE
4	B	70	VAL
4	B	124	THR
4	B	127	SER
4	B	136	SER
4	B	139	VAL
4	B	151	LEU
4	B	162	ILE
4	B	185	THR
4	B	195	LEU
4	B	232	ASP
4	B	274	THR
4	B	286	VAL
4	B	307	THR
6	D	37	MET
6	D	41	SER
6	D	69	VAL
6	D	84	VAL
6	D	129	ASN
6	D	136	ILE
6	D	147	ILE
6	D	151	LYS
6	D	153	LEU
6	D	164	SER
6	D	165	SER
6	D	179	SER
6	D	189	CYS
6	D	200	SER

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Mol	Chain	Res	Type
6	D	220	HIS
6	D	235	VAL
6	D	257	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	280	GLN
1	C	452	GLN
1	C	501	GLN
2	E	132	GLN
3	F	92	ASN
3	F	225	GLN
3	F	257	GLN
3	F	275	ASN
3	H	17	ASN
3	H	128	GLN
3	H	152	ASN
3	H	264	ASN
3	H	346	ASN
3	I	15	ASN
3	I	17	ASN
3	I	69	GLN
3	I	92	ASN
3	I	225	GLN
3	I	229	ASN
3	I	239	HIS
3	J	70	GLN
3	J	135	GLN
3	J	309	ASN
3	K	70	GLN
3	K	118	ASN
3	K	131	ASN
3	K	331	ASN
3	G	258	ASN
3	G	330	ASN
4	B	142	GLN
4	B	196	GLN
4	B	279	ASN
4	B	376	GLN
6	D	71	ASN
6	D	120	GLN

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Mol	Chain	Res	Type
6	D	145	GLN
6	D	206	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	57/61 (93%)	36 (63%)	0

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	-6	U
7	A	-1	C
7	A	1	G
7	A	5	G
7	A	6	C
7	A	7	C
7	A	8	G
7	A	9	U
7	A	10	C
7	A	11	A
7	A	12	G
7	A	13	G
7	A	14	A
7	A	19	A
7	A	21	G
7	A	23	G
7	A	24	C
7	A	25	G
7	A	26	C
7	A	27	U
7	A	29	A
7	A	31	C
7	A	32	A
7	A	33	G
7	A	34	U
7	A	36	U
7	A	39	C
7	A	40	C
7	A	42	A
7	A	43	C

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Mol	Chain	Res	Type
7	A	44	G
7	A	45	C
7	A	48	G
7	A	50	G
7	A	51	G
7	A	52	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.