



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 09:11 AM EST

PDB ID : 6W6V
EMDB ID : EMD-21564
Title : Structure of yeast RNase MRP holoenzyme
Authors : Perederina, A.; Li, D.; Lee, H.; Bator, C.; Berezin, I.; Hafenstein, S.L.; Krasilnikov, A.S.
Deposited on : 2020-03-17
Resolution : 3.00 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 ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

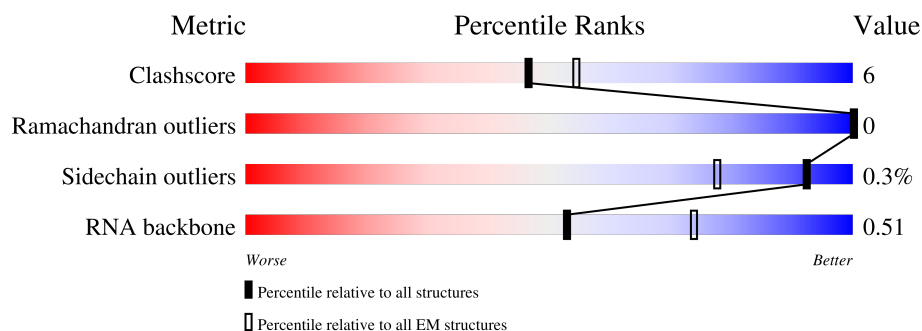
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	340	
2	B	875	
3	D	279	
4	E	173	
5	F	158	
6	G	140	
7	H	133	

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Mol	Chain	Length	Quality of chain
8	I	293	<div><div></div><div>68%15%17%</div></div>
8	J	293	<div><div></div><div>81%19%</div></div>
9	K	198	<div><div></div><div>32%8%60%</div></div>
10	L	201	<div><div></div><div>50%10%40%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24850 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 RNA chain called RNA component of RNase MRP NME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	294	Total	C	N	O	P	1	0
			6261	2805	1097	2064	295		

- Molecule 2 is a protein called Ribonucleases P/MRP protein subunit POP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	780	Total	C	N	O	S	0	0
			6345	4015	1154	1140	36		

- Molecule 3 is a protein called RNases MRP/P 32.9 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	212	Total	C	N	O	S	0	0
			1759	1131	300	320	8		

- Molecule 4 is a protein called Ribonuclease P/MRP protein subunit POP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	169	Total	C	N	O	S	0	0
			1335	837	237	253	8		

- Molecule 5 is a protein called Ribonucleases P/MRP protein subunit POP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	158	Total	C	N	O	S	0	0
			1280	809	223	243	5		

- Molecule 6 is a protein called Ribonucleases P/MRP protein subunit POP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	126	Total	C	N	O	S	0	0
			1006	635	177	192	2		

- Molecule 7 is a protein called Ribonucleases P/MRP protein subunit POP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	125	Total	C	N	O	S	0	0
			1033	655	169	207	2		

- Molecule 8 is a protein called Ribonuclease P/MRP protein subunit RPP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	243	Total	C	N	O	S	0	0
			1891	1194	342	346	9		
8	J	293	Total	C	N	O	S	0	0
			2260	1415	413	422	10		

- Molecule 9 is a protein called Ribonuclease MRP protein subunit SNM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	79	Total	C	N	O	S	0	0
			648	411	117	116	4		

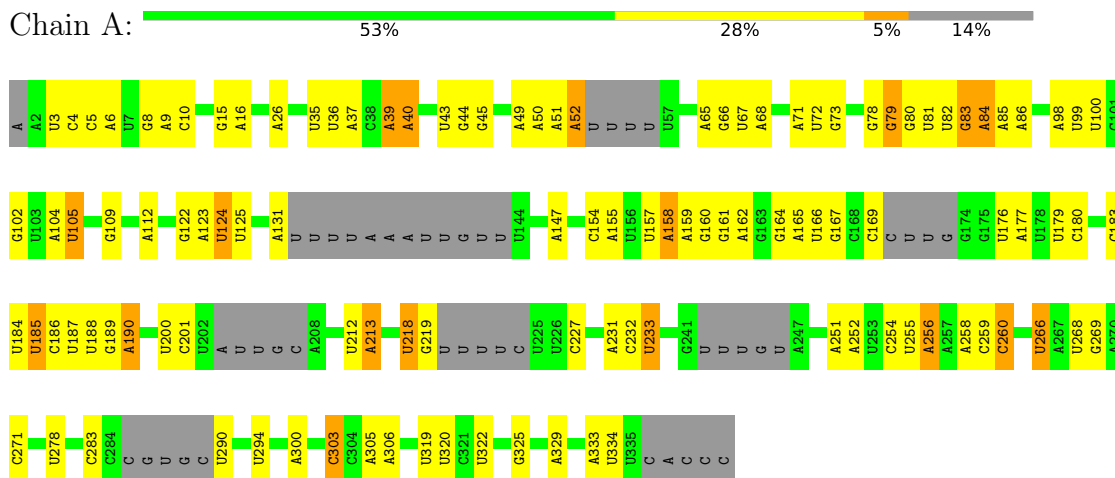
- Molecule 10 is a protein called Ribonuclease MRP protein subunit RMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	121	Total	C	N	O	S	0	0
			1032	665	189	172	6		

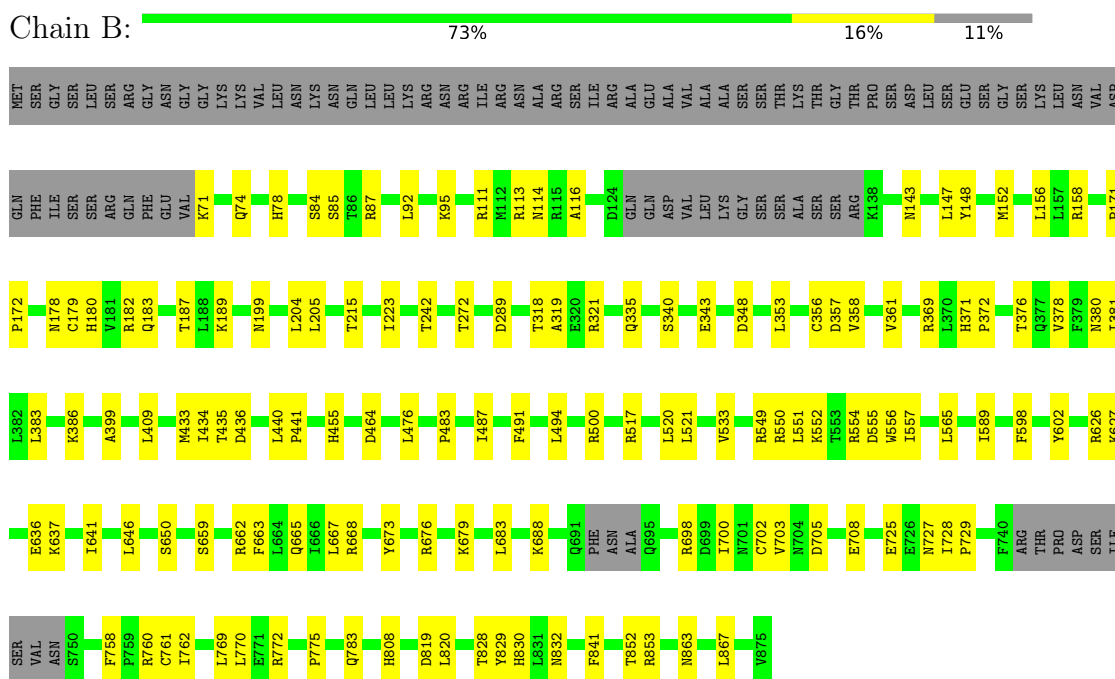
3 Residue-property plots

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.

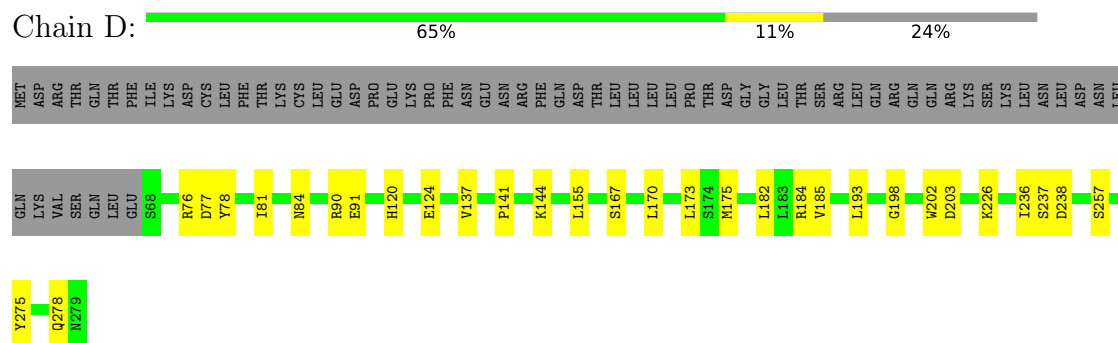
- Molecule 1: RNA component of RNase MRP NME1



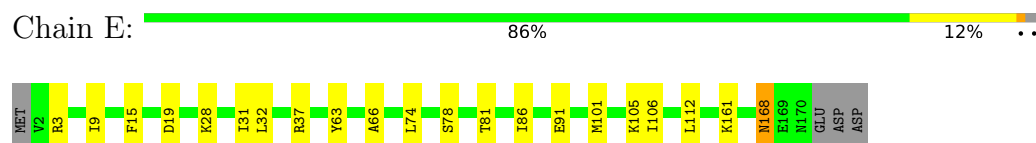
- Molecule 2: Ribonucleases P/MRP protein subunit POP1



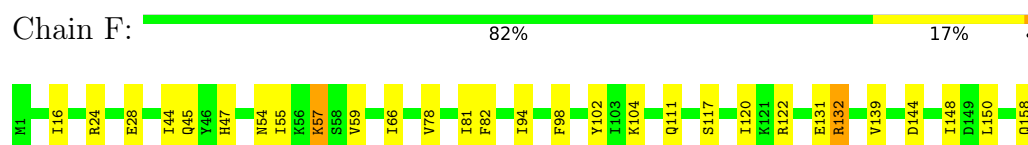
- Molecule 3: RNases MRP/P 32.9 kDa subunit



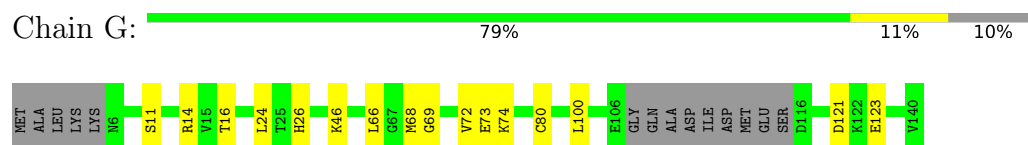
- Molecule 4: Ribonuclease P/MRP protein subunit POP5



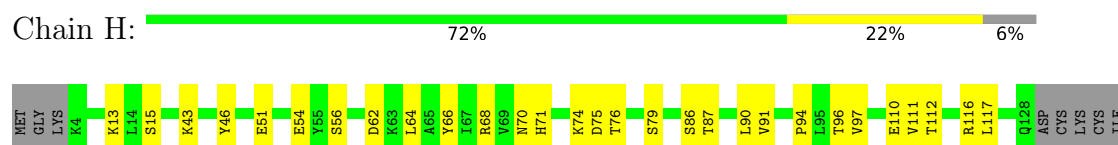
- Molecule 5: Ribonucleases P/MRP protein subunit POP6



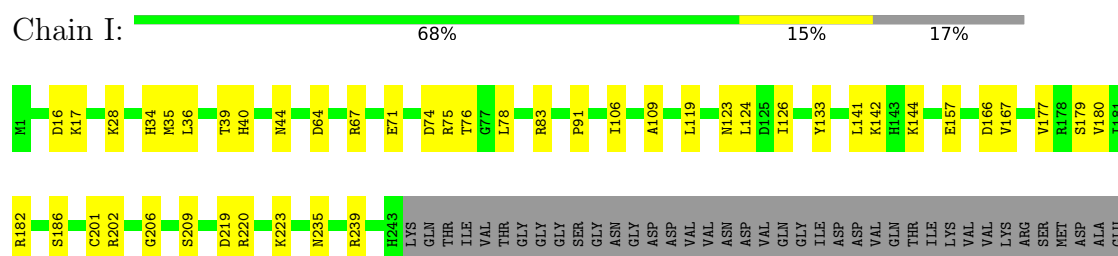
- Molecule 6: Ribonucleases P/MRP protein subunit POP7



- Molecule 7: Ribonucleases P/MRP protein subunit POP8

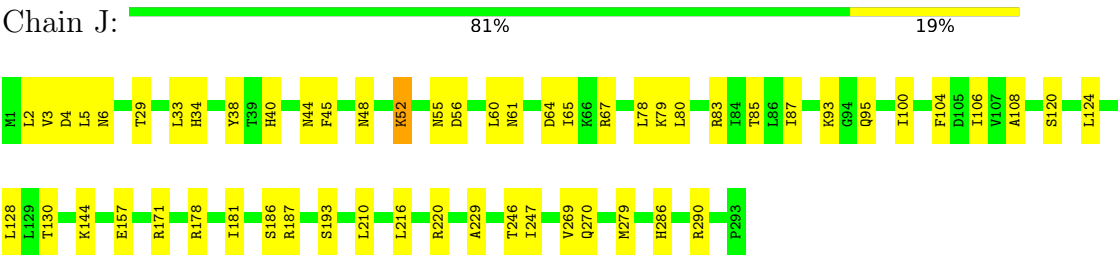


- Molecule 8: Ribonuclease P/MRP protein subunit RPP1

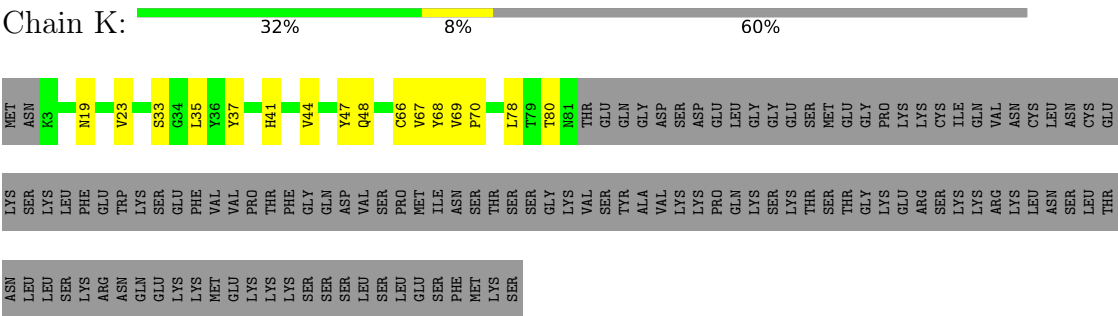


GLN
LEU
GLY
HIS
ALA
SER
LYS
ARG
HIS
LYS
PRO

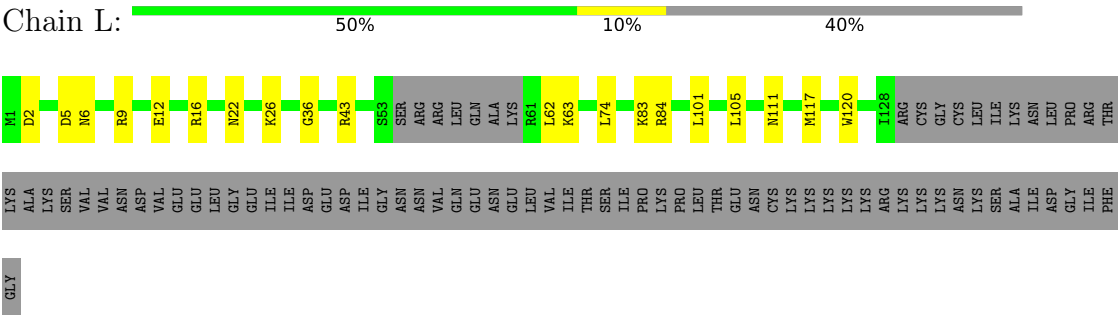
● Molecule 8: Ribonuclease P/MRP protein subunit RPP1



● Molecule 9: Ribonuclease MRP protein subunit SNM1



● Molecule 10: Ribonuclease MRP protein subunit RMP1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/6993	0.76	0/10870
2	B	0.29	0/6483	0.47	1/8734 (0.0%)
3	D	0.28	0/1790	0.47	0/2401
4	E	0.28	0/1351	0.45	0/1814
5	F	0.27	0/1298	0.48	0/1743
6	G	0.28	0/1019	0.55	1/1368 (0.1%)
7	H	0.28	0/1055	0.47	0/1428
8	I	0.27	0/1919	0.49	0/2592
8	J	0.26	0/2291	0.46	0/3092
9	K	0.27	0/662	0.53	0/891
10	L	0.28	0/1053	0.43	0/1418
All	All	0.30	0/25914	0.58	2/36351 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	66	LEU	CA-CB-CG	6.26	129.70	115.30
2	B	626	ARG	CA-CB-CG	5.15	124.73	113.40

There are no chirality outliers.

There are no planarity outliers.

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	6261	0	3165	59	0
2	B	6345	0	6427	94	0
3	D	1759	0	1817	21	0
4	E	1335	0	1380	21	0
5	F	1280	0	1317	17	0
6	G	1006	0	1048	14	0
7	H	1033	0	986	22	0
8	I	1891	0	1982	30	0
8	J	2260	0	2351	41	0
9	K	648	0	649	11	0
10	L	1032	0	1048	17	0
All	All	24850	0	22170	304	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 6.

All (304) 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)
1:A:167:G:H1	1:A:176:U:H3	1.28	0.80
5:F:47:HIS:HB3	5:F:81:ILE:HG22	1.65	0.79
1:A:79:G:H22	4:E:3:ARG:HH22	1.34	0.75
1:A:164:G:H1	1:A:179:U:H3	1.35	0.75
1:A:303:C:OP2	8:J:187:ARG:NH2	2.22	0.73
8:J:130:THR:HG22	8:J:157:GLU:HB3	1.71	0.73
2:B:521:LEU:HD13	10:L:74:LEU:HD21	1.71	0.71
3:D:90:ARG:NH1	3:D:91:GLU:OE2	2.23	0.70
4:E:91:GLU:OE2	8:J:178:ARG:NH1	2.24	0.70
2:B:494:LEU:O	2:B:500:ARG:NH1	2.24	0.69
2:B:242:THR:OG1	2:B:289:ASP:OD2	2.10	0.69
9:K:33:SER:OG	9:K:69:VAL:O	2.09	0.69
2:B:361:VAL:HG21	2:B:491:PHE:CE2	2.29	0.68
8:J:269:VAL:HG13	8:J:270:GLN:HG3	1.75	0.68
1:A:233:U:OP2	10:L:84:ARG:NH2	2.27	0.68
8:I:142:LYS:HE2	8:I:144:LYS:HD2	1.76	0.68
1:A:157:U:OP2	2:B:111:ARG:NH2	2.28	0.67
4:E:63:TYR:HB2	7:H:46:TYR:HE1	1.60	0.66
10:L:5:ASP:O	10:L:9:ARG:NH1	2.29	0.66
2:B:550:ARG:HD3	2:B:557:ILE:HD11	1.78	0.66
2:B:668:ARG:NH2	2:B:820:LEU:O	2.29	0.66
7:H:71:HIS:O	7:H:74:LYS:NZ	2.28	0.65
6:G:14:ARG:NH1	6:G:16:THR:OG1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:828:THR:HG22	2:B:829:TYR:H	1.61	0.65
2:B:550:ARG:NH2	2:B:555:ASP:OD2	2.29	0.64
5:F:122:ARG:NH2	5:F:131:GLU:OE2	2.31	0.64
4:E:168:ASN:O	4:E:168:ASN:ND2	2.28	0.64
1:A:290:U:O2	2:B:637:LYS:NZ	2.31	0.63
2:B:783:GLN:NE2	2:B:819:ASP:OD1	2.29	0.63
8:I:219:ASP:O	8:I:223:LYS:NZ	2.31	0.63
10:L:12:GLU:HG2	10:L:16:ARG:HH12	1.63	0.63
1:A:231:A:OP2	10:L:43:ARG:NH2	2.32	0.62
2:B:665:GLN:NE2	2:B:758:PHE:O	2.32	0.62
8:I:71:GLU:OE1	8:I:75:ARG:NH1	2.32	0.62
6:G:69:GLY:O	6:G:72:VAL:HG12	1.99	0.62
1:A:185:U:OP1	2:B:199:ASN:ND2	2.33	0.62
1:A:37:A:H2'	6:G:68:MET:HG2	1.82	0.61
8:J:44:ASN:OD1	8:J:45:PHE:N	2.33	0.61
10:L:2:ASP:OD1	10:L:6:ASN:ND2	2.33	0.61
2:B:673:TYR:OH	2:B:676:ARG:NH2	2.33	0.60
7:H:75:ASP:OD1	7:H:76:THR:N	2.33	0.60
2:B:357:ASP:HB2	2:B:369:ARG:HB2	1.84	0.60
2:B:71:LYS:N	10:L:111:ASN:HD21	2.00	0.60
3:D:184:ARG:NH1	8:J:279:MET:HG2	2.17	0.60
1:A:218:U:O4	2:B:179:CYS:N	2.35	0.59
8:J:181:ILE:HG23	8:J:186:SER:HB3	1.84	0.59
1:A:15:G:OP1	2:B:627:LYS:NZ	2.35	0.59
1:A:266:U:O2'	1:A:306:A:N6	2.35	0.58
8:J:120:SER:HA	8:J:124:LEU:HD12	1.84	0.58
1:A:40:A:H61	6:G:11:SER:HB3	1.68	0.58
8:I:91:PRO:HA	8:I:119:LEU:HD22	1.86	0.58
1:A:218:U:O4	2:B:180:HIS:N	2.35	0.58
2:B:215:THR:HG21	2:B:500:ARG:HH21	1.69	0.58
2:B:434:ILE:HG13	2:B:440:LEU:HD21	1.85	0.58
2:B:729:PRO:HG2	2:B:761:CYS:HA	1.86	0.58
2:B:178:ASN:O	2:B:182:ARG:NE	2.32	0.57
2:B:441:PRO:O	2:B:549:ARG:NH2	2.37	0.57
4:E:19:ASP:O	8:I:28:LYS:NZ	2.36	0.57
2:B:204:LEU:HG	2:B:205:LEU:H	1.68	0.57
2:B:434:ILE:HG22	2:B:436:ASP:H	1.70	0.57
9:K:41:HIS:HA	9:K:44:VAL:HG12	1.87	0.57
8:I:34:HIS:HB2	8:I:78:LEU:HD13	1.87	0.57
8:J:85:THR:HG22	8:J:108:ALA:HB3	1.87	0.56
2:B:319:ALA:O	2:B:321:ARG:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:206:GLY:O	8:I:209:SER:OG	2.19	0.56
1:A:212:U:H2'	1:A:213:A:H8	1.70	0.56
2:B:476:LEU:HD11	6:G:100:LEU:HD21	1.87	0.56
10:L:12:GLU:O	10:L:16:ARG:NH1	2.39	0.56
5:F:82:PHE:HB3	5:F:139:VAL:HG12	1.88	0.56
2:B:769:LEU:HD11	2:B:775:PRO:HD3	1.88	0.56
8:J:64:ASP:OD2	8:J:67:ARG:NH2	2.34	0.56
7:H:90:LEU:HD12	7:H:91:VAL:HG13	1.88	0.56
2:B:84:SER:OG	2:B:85:SER:N	2.39	0.55
8:I:201:CYS:O	8:I:202:ARG:NH1	2.30	0.55
8:J:286:HIS:O	8:J:290:ARG:NH1	2.39	0.55
2:B:455:HIS:O	2:B:517:ARG:NH2	2.39	0.55
4:E:106:ILE:HD12	4:E:112:LEU:HD11	1.87	0.55
7:H:86:SER:OG	7:H:87:THR:N	2.38	0.55
1:A:218:U:C4	2:B:180:HIS:HB3	2.41	0.55
2:B:727:ASN:OD1	2:B:728:ILE:HG12	2.06	0.55
8:J:3:VAL:HG12	8:J:40:HIS:HB2	1.88	0.55
5:F:24:ARG:O	5:F:28:GLU:HG2	2.07	0.54
2:B:74:GLN:O	2:B:78:HIS:ND1	2.40	0.54
2:B:646:LEU:HD21	2:B:683:LEU:HD23	1.88	0.54
2:B:204:LEU:O	2:B:205:LEU:HG	2.08	0.53
4:E:105:LYS:HD2	4:E:105:LYS:O	2.07	0.53
9:K:78:LEU:HG	9:K:80:THR:H	1.73	0.53
2:B:182:ARG:O	2:B:183:GLN:HG3	2.07	0.53
1:A:158:A:H2'	1:A:159:A:H8	1.74	0.53
2:B:683:LEU:HA	2:B:703:VAL:HG12	1.91	0.53
7:H:62:ASP:OD1	7:H:62:ASP:N	2.42	0.53
2:B:113:ARG:NH2	2:B:114:ASN:OD1	2.42	0.53
1:A:161:G:H2'	1:A:162:A:H8	1.74	0.53
5:F:55:ILE:HG13	5:F:94:ILE:HG12	1.90	0.53
1:A:73:G:O6	6:G:46:LYS:NZ	2.35	0.53
8:I:64:ASP:OD1	8:I:67:ARG:HB3	2.09	0.53
10:L:117:MET:O	10:L:120:TRP:N	2.43	0.52
2:B:762:ILE:HD12	2:B:841:PHE:HB3	1.91	0.52
2:B:183:GLN:HA	2:B:187:THR:HB	1.92	0.52
1:A:158:A:H2'	1:A:159:A:C8	2.44	0.52
4:E:168:ASN:HD22	4:E:168:ASN:C	2.11	0.52
8:J:2:LEU:HB3	8:J:38:TYR:HD1	1.74	0.52
8:J:34:HIS:HB2	8:J:78:LEU:HD11	1.91	0.52
7:H:54:GLU:OE2	8:I:179:SER:OG	2.20	0.52
8:J:55:ASN:OD1	8:J:56:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:60:LEU:HD23	8:J:100:ILE:HD12	1.91	0.52
2:B:335:GLN:NE2	2:B:550:ARG:HD2	2.23	0.51
2:B:433:MET:SD	2:B:464:ASP:HB3	2.50	0.51
3:D:84:ASN:ND2	9:K:67:VAL:O	2.42	0.51
8:J:48:ASN:HA	8:J:87:ILE:HB	1.90	0.51
1:A:50:A:H2'	1:A:51:A:C8	2.45	0.51
8:J:6:ASN:OD1	8:J:83:ARG:NH1	2.43	0.51
2:B:399:ALA:HB1	2:B:565:LEU:HD22	1.92	0.51
1:A:256:A:H5''	2:B:87:ARG:HH12	1.76	0.51
1:A:176:U:H2'	1:A:177:A:C8	2.46	0.51
2:B:662:ARG:HH22	2:B:725:GLU:HB3	1.76	0.51
8:I:39:THR:OG1	8:I:40:HIS:ND1	2.38	0.51
7:H:15:SER:HB3	7:H:64:LEU:HA	1.93	0.51
1:A:15:G:H2'	1:A:83:G:N1	2.26	0.51
1:A:109:G:N2	1:A:112:A:OP2	2.42	0.51
7:H:56:SER:HB2	7:H:68:ARG:HG2	1.94	0.50
8:I:235:ASN:O	8:I:239:ARG:HG2	2.12	0.50
7:H:54:GLU:OE1	8:I:182:ARG:NE	2.40	0.50
2:B:828:THR:HG22	2:B:829:TYR:N	2.26	0.50
1:A:83:G:H1'	1:A:84:A:H4'	1.94	0.50
8:I:201:CYS:SG	8:I:202:ARG:N	2.85	0.50
2:B:641:ILE:HD13	2:B:863:ASN:HB3	1.95	0.49
4:E:32:LEU:HA	8:I:35:MET:HE1	1.93	0.49
2:B:378:VAL:O	2:B:381:ILE:HB	2.13	0.49
8:J:33:LEU:HD12	8:J:38:TYR:HD2	1.77	0.49
2:B:318:THR:HG23	2:B:319:ALA:O	2.11	0.49
4:E:31:ILE:HG22	8:I:35:MET:HE3	1.95	0.49
3:D:144:LYS:HE3	3:D:182:LEU:HB2	1.95	0.49
7:H:75:ASP:O	7:H:79:SER:OG	2.15	0.49
1:A:8:G:H2'	1:A:9:A:H8	1.78	0.49
8:J:40:HIS:CE1	8:J:79:LYS:HD2	2.48	0.49
1:A:154:C:H2'	1:A:155:A:H8	1.77	0.49
2:B:272:THR:HG22	2:B:589:ILE:HD11	1.96	0.48
5:F:117:SER:OG	6:G:80:CYS:SG	2.66	0.48
2:B:171:PRO:HB2	2:B:172:PRO:HD3	1.95	0.48
8:I:166:ASP:OD1	8:I:167:VAL:N	2.47	0.48
8:J:3:VAL:HG21	8:J:229:ALA:HB3	1.96	0.48
8:J:6:ASN:OD1	8:J:44:ASN:ND2	2.25	0.48
3:D:137:VAL:O	3:D:141:PRO:HD3	2.12	0.48
4:E:28:LYS:O	4:E:32:LEU:HD13	2.14	0.48
1:A:164:G:H2'	1:A:165:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:59:VAL:HG23	5:F:98:PHE:HB2	1.95	0.47
4:E:63:TYR:HB2	7:H:46:TYR:CE1	2.47	0.47
8:J:52:LYS:HA	8:J:95:GLN:NE2	2.28	0.47
9:K:47:TYR:O	9:K:48:GLN:HG2	2.15	0.47
1:A:232:C:N4	10:L:36:GLY:O	2.44	0.47
5:F:54:ASN:O	5:F:57:LYS:HG3	2.14	0.47
5:F:148:ILE:HG22	5:F:150:LEU:H	1.80	0.47
7:H:13:LYS:HG3	7:H:66:TYR:CE1	2.49	0.47
2:B:598:PHE:HA	2:B:602:TYR:CD1	2.50	0.47
10:L:83:LYS:HD2	10:L:83:LYS:HA	1.71	0.47
2:B:383:LEU:HD22	2:B:386:LYS:HD3	1.97	0.47
2:B:673:TYR:CD2	2:B:700:ILE:HG21	2.51	0.46
2:B:483:PRO:O	2:B:487:ILE:HG12	2.15	0.46
2:B:830:HIS:NE2	2:B:832:ASN:HB2	2.30	0.46
1:A:5:C:H2'	1:A:6:A:H8	1.80	0.46
8:I:44:ASN:HA	8:I:83:ARG:HG3	1.97	0.46
2:B:549:ARG:HB2	2:B:556:TRP:CZ3	2.50	0.46
8:I:16:ASP:OD1	8:I:17:LYS:N	2.48	0.46
9:K:66:CYS:HB2	9:K:68:TYR:CZ	2.51	0.46
9:K:68:TYR:HD1	9:K:70:PRO:HD3	1.80	0.46
1:A:160:G:H2'	1:A:161:G:C8	2.49	0.46
3:D:184:ARG:HH12	8:J:279:MET:HG2	1.80	0.46
4:E:78:SER:OG	4:E:81:THR:O	2.31	0.46
3:D:182:LEU:HD12	3:D:198:GLY:O	2.15	0.46
4:E:66:ALA:HB2	8:J:171:ARG:HG2	1.97	0.46
8:I:123:ASN:O	8:I:124:LEU:HD22	2.15	0.46
1:A:8:G:H2'	1:A:9:A:C8	2.51	0.46
2:B:371:HIS:CG	2:B:372:PRO:HD2	2.51	0.46
2:B:659:SER:O	2:B:659:SER:OG	2.34	0.45
8:I:177:VAL:HA	8:I:180:VAL:HG12	1.97	0.45
3:D:155:LEU:HD11	3:D:173:LEU:HD21	1.97	0.45
6:G:123:GLU:OE2	6:G:123:GLU:N	2.48	0.45
7:H:110:GLU:HG2	7:H:116:ARG:HG3	1.99	0.45
3:D:185:VAL:HG11	3:D:193:LEU:HD23	1.98	0.45
5:F:111:GLN:NE2	5:F:158:GLN:OE1	2.49	0.45
8:I:133:TYR:OH	8:I:157:GLU:O	2.21	0.45
8:J:246:THR:HG23	8:J:247:ILE:HG12	1.99	0.45
2:B:772:ARG:HE	2:B:808:HIS:CE1	2.34	0.45
7:H:96:THR:HG22	7:H:97:VAL:N	2.31	0.45
2:B:204:LEU:HG	2:B:205:LEU:N	2.32	0.45
8:J:4:ASP:OD1	8:J:193:SER:OG	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:33:LEU:HD12	8:J:38:TYR:CD2	2.51	0.45
2:B:116:ALA:HB2	2:B:156:LEU:HD12	1.98	0.45
8:J:29:THR:O	8:J:33:LEU:HD23	2.17	0.45
1:A:160:G:N2	1:A:184:U:O2	2.49	0.45
4:E:9:ILE:HB	4:E:86:ILE:HG22	1.99	0.45
1:A:105:U:H3	2:B:156:LEU:HD21	1.82	0.45
1:A:190:A:OP2	2:B:158:ARG:NH1	2.50	0.45
5:F:44:ILE:HA	5:F:78:VAL:O	2.17	0.45
2:B:435:THR:HG21	6:G:24:LEU:HB2	1.99	0.45
2:B:700:ILE:O	2:B:700:ILE:HG22	2.17	0.45
2:B:550:ARG:HB2	2:B:555:ASP:OD1	2.16	0.44
3:D:167:SER:HA	3:D:170:LEU:HD12	1.99	0.44
8:I:202:ARG:HD3	8:I:202:ARG:HA	1.80	0.44
2:B:698:ARG:HH22	2:B:708:GLU:CD	2.21	0.44
3:D:77:ASP:OD1	3:D:78:TYR:N	2.50	0.44
5:F:102:TYR:OH	5:F:144:ASP:OD1	2.29	0.44
1:A:123:A:H5''	1:A:124:U:OP1	2.17	0.44
1:A:268:U:H5''	1:A:269:G:H5'	1.99	0.44
2:B:520:LEU:HD11	2:B:533:VAL:HA	1.99	0.44
2:B:673:TYR:HD2	2:B:700:ILE:HG21	1.82	0.44
3:D:120:HIS:CE1	3:D:124:GLU:HG3	2.52	0.44
8:J:5:LEU:O	8:J:83:ARG:NH1	2.51	0.44
8:J:210:LEU:HD12	8:J:210:LEU:H	1.82	0.44
10:L:26:LYS:HE2	10:L:26:LYS:HA	1.99	0.44
2:B:760:ARG:HA	2:B:760:ARG:HD3	1.88	0.44
5:F:66:ILE:HD11	5:F:144:ASP:HB2	2.00	0.44
6:G:73:GLU:HG2	6:G:74:LYS:N	2.33	0.44
1:A:79:G:N2	4:E:3:ARG:HH22	2.08	0.43
3:D:81:ILE:HD13	9:K:37:TYR:CE1	2.52	0.43
4:E:101:MET:HE3	8:I:206:GLY:HA3	2.00	0.43
8:J:2:LEU:HB3	8:J:38:TYR:CD1	2.52	0.43
4:E:161:LYS:HA	4:E:161:LYS:HD2	1.80	0.43
8:I:83:ARG:HB3	8:I:106:ILE:HB	2.01	0.43
2:B:551:LEU:O	2:B:554:ARG:HG2	2.19	0.43
3:D:184:ARG:CZ	8:J:279:MET:HG2	2.49	0.43
8:I:186:SER:O	8:I:220:ARG:NH2	2.51	0.43
2:B:335:GLN:OE1	2:B:552:LYS:HB3	2.19	0.43
2:B:343:GLU:HA	2:B:348:ASP:CG	2.38	0.43
7:H:46:TYR:CD2	7:H:76:THR:HG23	2.53	0.43
1:A:161:G:N2	1:A:183:C:N3	2.66	0.43
7:H:54:GLU:HG3	7:H:70:ASN:HD21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:216:LEU:HD11	8:J:220:ARG:HD2	2.00	0.43
5:F:45:GLN:N	5:F:45:GLN:OE1	2.52	0.43
7:H:86:SER:O	7:H:94:PRO:HB3	2.19	0.43
2:B:409:LEU:HD23	2:B:409:LEU:HA	1.79	0.43
3:D:175:MET:HG2	3:D:257:SER:O	2.19	0.43
8:J:83:ARG:HG2	8:J:106:ILE:HB	2.01	0.43
1:A:251:A:H2'	1:A:252:A:C8	2.53	0.43
3:D:202:TRP:CE2	9:K:35:LEU:HD12	2.54	0.43
10:L:22:ASN:O	10:L:26:LYS:HE3	2.19	0.43
1:A:212:U:H2'	1:A:213:A:C8	2.50	0.42
8:I:109:ALA:HB2	8:I:126:ILE:HG21	2.01	0.42
9:K:66:CYS:HB2	9:K:68:TYR:CE1	2.53	0.42
10:L:12:GLU:HG2	10:L:16:ARG:NH1	2.29	0.42
1:A:4:C:H2'	1:A:5:C:C6	2.54	0.42
6:G:26:HIS:O	6:G:26:HIS:ND1	2.52	0.42
1:A:251:A:H2'	1:A:252:A:H8	1.84	0.42
1:A:278:U:O2'	1:A:322:U:OP1	2.33	0.42
2:B:705:ASP:O	2:B:708:GLU:HG3	2.20	0.42
4:E:15:PHE:HB3	4:E:37:ARG:CZ	2.49	0.42
1:A:164:G:H2'	1:A:165:A:H8	1.84	0.42
2:B:683:LEU:O	2:B:702:CYS:HB3	2.20	0.42
2:B:688:LYS:HD2	2:B:688:LYS:HA	1.63	0.42
6:G:72:VAL:HG13	6:G:73:GLU:H	1.84	0.42
7:H:111:VAL:HG22	7:H:112:THR:HG23	2.01	0.42
2:B:356:CYS:SG	2:B:358:VAL:HG23	2.60	0.42
2:B:698:ARG:NH1	2:B:708:GLU:OE2	2.52	0.42
8:I:141:LEU:H	8:I:141:LEU:HD23	1.84	0.42
6:G:121:ASP:OD1	6:G:121:ASP:N	2.53	0.42
1:A:10:C:OP1	3:D:226:LYS:NZ	2.53	0.42
8:I:36:LEU:HD12	8:I:201:CYS:SG	2.60	0.42
8:I:74:ASP:C	8:I:76:THR:H	2.23	0.42
8:J:93:LYS:HA	8:J:93:LYS:HD3	1.87	0.42
1:A:3:U:H2'	1:A:4:C:C6	2.55	0.42
1:A:5:C:H2'	1:A:6:A:C8	2.55	0.42
1:A:51:A:H2'	1:A:52:A:C8	2.55	0.42
3:D:237:SER:OG	3:D:238:ASP:N	2.51	0.42
3:D:275:TYR:HA	3:D:278:GLN:HB2	2.02	0.42
1:A:50:A:H2'	1:A:51:A:H8	1.85	0.41
2:B:335:GLN:HE22	2:B:550:ARG:HD2	1.85	0.41
7:H:43:LYS:HB2	7:H:51:GLU:OE2	2.19	0.41
2:B:679:LYS:HD3	2:B:679:LYS:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:203:ASP:OD1	3:D:203:ASP:N	2.42	0.41
2:B:770:LEU:HD12	2:B:867:LEU:HD23	2.02	0.41
2:B:663:PHE:CZ	2:B:667:LEU:HD22	2.56	0.41
7:H:46:TYR:CE2	7:H:76:THR:HG23	2.56	0.41
9:K:19:ASN:O	9:K:23:VAL:HG23	2.21	0.41
1:A:254:C:H2'	1:A:255:U:C6	2.56	0.41
3:D:236:ILE:HG23	3:D:237:SER:N	2.36	0.41
8:J:61:ASN:HB3	8:J:104:PHE:CE1	2.56	0.41
2:B:852:THR:OG1	2:B:853:ARG:N	2.53	0.41
4:E:19:ASP:OD1	4:E:19:ASP:N	2.53	0.41
4:E:74:LEU:HD12	4:E:74:LEU:HA	1.89	0.41
5:F:104:LYS:HA	5:F:104:LYS:HD3	1.86	0.41
1:A:39:A:C6	1:A:65:A:C5	3.08	0.41
2:B:340:SER:HB3	2:B:353:LEU:HD11	2.02	0.41
5:F:120:ILE:O	5:F:132:ARG:HA	2.20	0.41
10:L:62:LEU:HD11	10:L:63:LYS:HE3	2.02	0.41
2:B:143:ASN:HB3	2:B:147:LEU:HG	2.03	0.41
8:J:128:LEU:HD23	8:J:128:LEU:HA	1.97	0.41
1:A:9:A:H2'	1:A:10:C:C6	2.55	0.40
2:B:376:THR:O	2:B:380:ASN:ND2	2.47	0.40
2:B:636:GLU:O	2:B:650:SER:OG	2.31	0.40
5:F:16:ILE:HG13	5:F:120:ILE:HD11	2.03	0.40
1:A:260:C:O2'	2:B:95:LYS:HE2	2.22	0.40
8:J:65:ILE:HD13	8:J:80:LEU:HB3	2.04	0.40
10:L:101:LEU:O	10:L:105:LEU:HD13	2.21	0.40
1:A:49:A:H2'	1:A:50:A:C8	2.57	0.40
1:A:258:A:N6	2:B:92:LEU:HD23	2.37	0.40
2:B:223:ILE:H	2:B:223:ILE:HD12	1.86	0.40
6:G:14:ARG:HH11	6:G:14:ARG:HG2	1.86	0.40
1:A:78:G:O2'	1:A:268:U:O2	2.33	0.40
7:H:117:LEU:HD23	7:H:117:LEU:HA	1.93	0.40
8:J:40:HIS:ND1	8:J:79:LYS:HD2	2.36	0.40
8:J:78:LEU:HD23	8:J:78:LEU:HA	1.91	0.40
2:B:148:TYR:CZ	2:B:152:MET:HG3	2.57	0.40
10:L:22:ASN:O	10:L:26:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	
2	B	772/875 (88%)	690 (89%)	82 (11%)	0	100	100
3	D	210/279 (75%)	189 (90%)	21 (10%)	0	100	100
4	E	167/173 (96%)	146 (87%)	21 (13%)	0	100	100
5	F	156/158 (99%)	142 (91%)	14 (9%)	0	100	100
6	G	122/140 (87%)	113 (93%)	9 (7%)	0	100	100
7	H	123/133 (92%)	105 (85%)	18 (15%)	0	100	100
8	I	241/293 (82%)	211 (88%)	30 (12%)	0	100	100
8	J	291/293 (99%)	259 (89%)	32 (11%)	0	100	100
9	K	77/198 (39%)	64 (83%)	13 (17%)	0	100	100
10	L	117/201 (58%)	108 (92%)	9 (8%)	0	100	100
All	All	2276/2743 (83%)	2027 (89%)	249 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	
2	B	704/785 (90%)	703 (100%)	1 (0%)	93	98
3	D	196/261 (75%)	195 (100%)	1 (0%)	88	96
4	E	156/160 (98%)	155 (99%)	1 (1%)	86	95
5	F	149/149 (100%)	147 (99%)	2 (1%)	69	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	116/127 (91%)	116 (100%)	0	100	100
7	H	116/123 (94%)	116 (100%)	0	100	100
8	I	217/258 (84%)	217 (100%)	0	100	100
8	J	258/258 (100%)	256 (99%)	2 (1%)	81	93
9	K	73/184 (40%)	73 (100%)	0	100	100
10	L	110/182 (60%)	110 (100%)	0	100	100
All	All	2095/2487 (84%)	2088 (100%)	7 (0%)	92	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	189	LYS
3	D	76	ARG
4	E	168	ASN
5	F	57	LYS
5	F	132	ARG
8	J	52	LYS
8	J	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	111	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	285/340 (83%)	67 (23%)	0

All (67) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	A
1	A	26	A
1	A	35	U
1	A	36	U
1	A	39	A

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Mol	Chain	Res	Type
1	A	40	A
1	A	43	U
1	A	44	G
1	A	45	G
1	A	52	A
1	A	66	G
1	A	67	U
1	A	68	A
1	A	71	A
1	A	72	U
1	A	79	G
1	A	80	G
1	A	81	U
1	A	82	U
1	A	83	G
1	A	84	A
1	A	85	A
1	A	86	A
1	A	98	A
1	A	99	U
1	A	100	U
1	A	102	G
1	A	104	A
1	A	105	U
1	A	122	G
1	A	124	U
1	A	125	U
1	A	131	A
1	A	147	A
1	A	158	A
1	A	166	U
1	A	169	C
1	A	180	C
1	A	185	U
1	A	186	C
1	A	187	U
1	A	188	U
1	A	189	G
1	A	190	A
1	A	200	U
1	A	201	C
1	A	213	A

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Mol	Chain	Res	Type
1	A	218	U
1	A	219	G
1	A	227	C
1	A	233	U
1	A	256	A
1	A	259	C
1	A	260	C
1	A	266	U
1	A	271	C
1	A	283	C
1	A	294	U
1	A	300	A
1	A	303	C
1	A	305	A
1	A	319	U
1	A	320	U
1	A	325	G
1	A	329	A
1	A	333	A
1	A	334	U

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.