



## Full wwPDB EM Validation Report ⓘ

Apr 13, 2026 – 04:19 PM JST

PDB ID : 9UH9 / pdb\_00009uh9  
EMDB ID : EMD-64159  
Title : human Ribonuclease MRP state 1  
Authors : Zhou, B.; Lan, P.; Wu, J.; Lei, M.  
Deposited on : 2025-04-14  
Resolution : 3.47 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](mailto: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>.

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

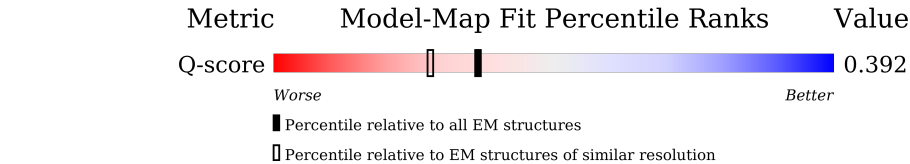
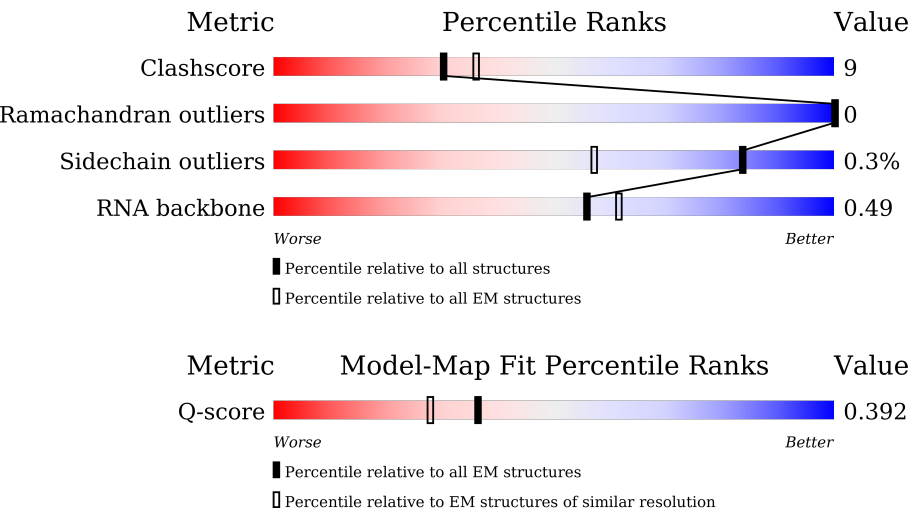
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.47 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.




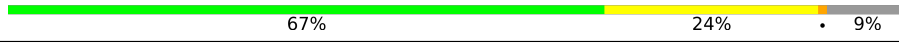
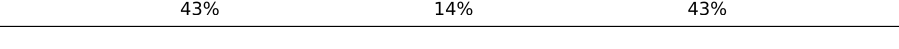



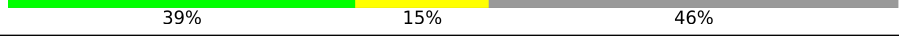
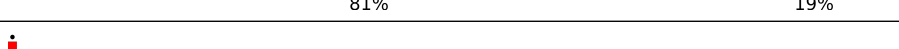


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13733 ( 2.97 - 3.97 )

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	270	<div><div>44%</div><div>45%</div><div>5%</div><div>6%</div></div>
2	B	1024	<div><div>58%</div><div>12%</div><div>30%</div></div>
3	C	283	<div><div>35%</div><div>14%</div><div>52%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	220	
5	E	163	
6	F	199	
7	G	140	
8	H	124	
9	I	268	
9	J	268	
10	K	220	
11	L	363	
12	M	567	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27111 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 (270-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	254	Total	C	N	O	P	0	0
			5391	2404	948	1785	254		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	718	Total	C	N	O	S	0	0
			5689	3628	1016	1006	39		

- Molecule 3 is a protein called Ribonuclease P protein subunit p38.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	137	Total	C	N	O	S	0	0
			1078	692	193	188	5		

- Molecule 4 is a protein called Ribonuclease P protein subunit p29.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	186	Total	C	N	O	S	0	0
			1502	960	268	269	5		

- Molecule 5 is a protein called Ribonuclease P/MRP protein subunit POP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	149	Total	C	N	O	S	0	0
			1215	773	222	212	8		

- Molecule 6 is a protein called Ribonuclease P protein subunit p25.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	114	Total	C	N	O	S	0	0
			869	547	166	151	5		

- Molecule 7 is a protein called Ribonuclease P protein subunit p20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	120	Total	C	N	O	S	0	0
			945	587	181	174	3		

- Molecule 8 is a protein called Ribonuclease P protein subunit p14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	122	Total	C	N	O	S	0	0
			946	614	153	174	5		

- Molecule 9 is a protein called Ribonuclease P protein subunit p30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	237	Total	C	N	O	S	0	0
			1829	1169	320	333	7		
9	J	248	Total	C	N	O	S	0	0
			1916	1227	336	346	7		

- Molecule 10 is a protein called UPF0711 protein C18orf21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	118	Total	C	N	O	S	0	0
			963	606	182	169	6		

- Molecule 11 is a protein called Ribonuclease P protein subunit p40.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	362	Total	C	N	O	S	0	0
			2939	1893	489	540	17		

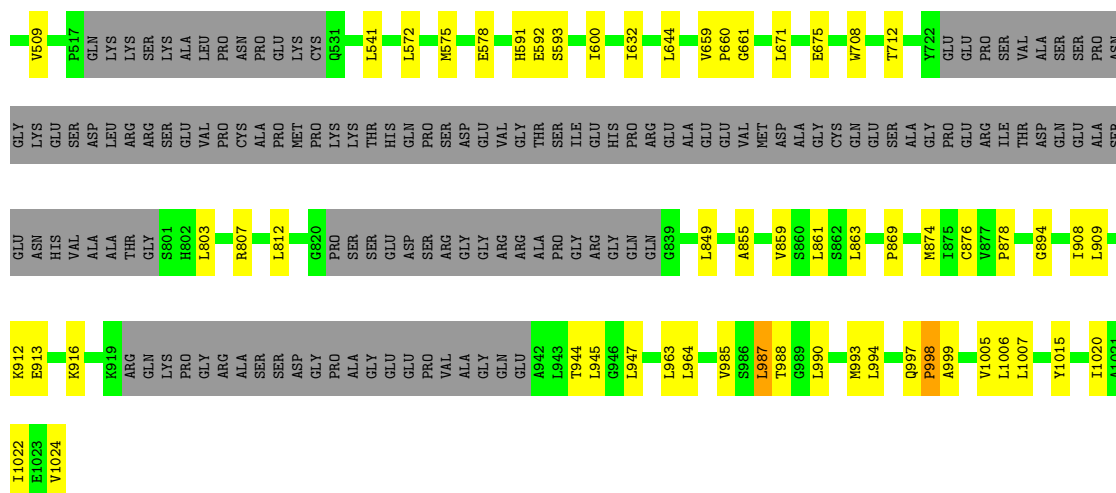
- Molecule 12 is a protein called Nucleolus and neural progenitor protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	230	Total	C	N	O	S	0	0
			1828	1190	309	315	14		

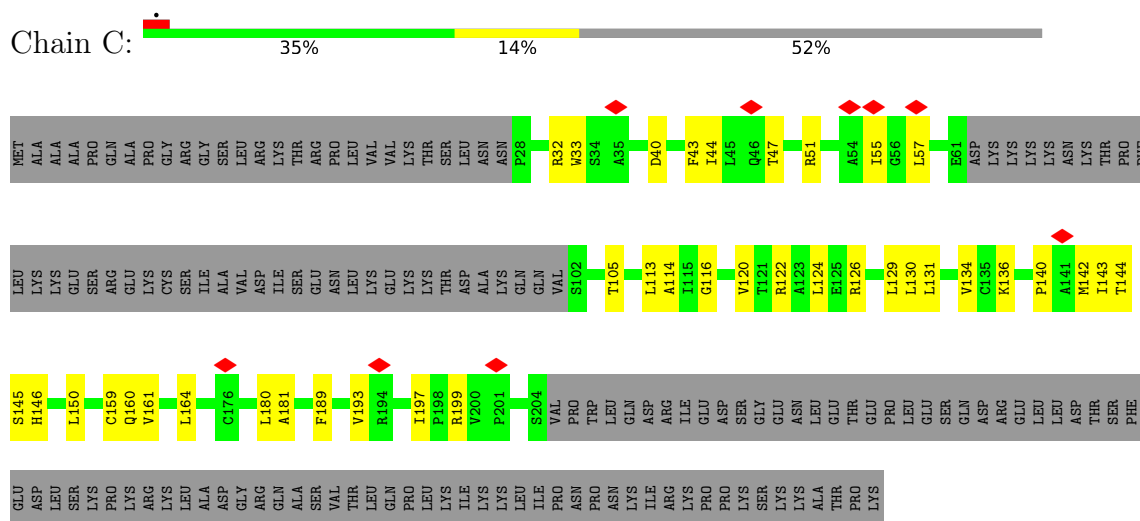
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	K	1	Total	Zn	0
			1	1	

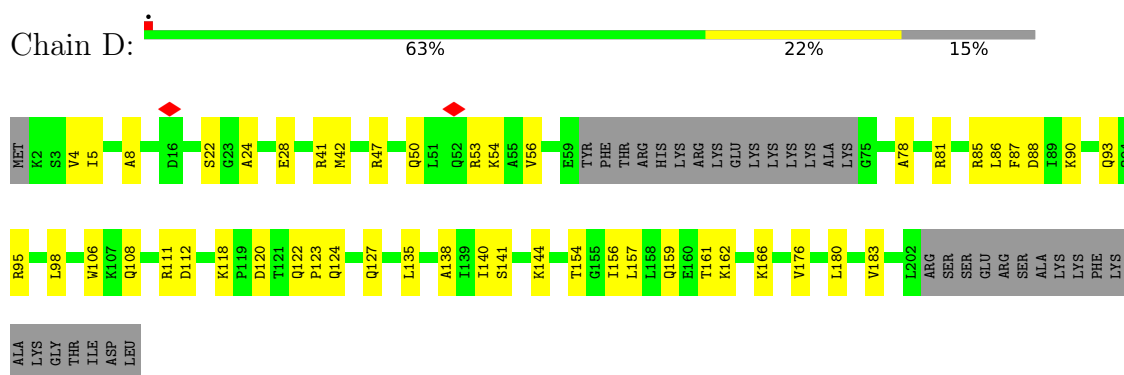




• Molecule 3: Ribonuclease P protein subunit p38

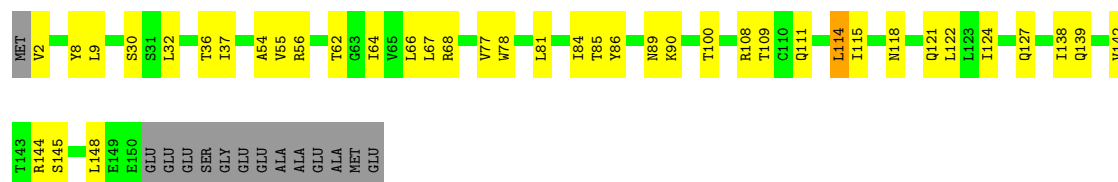


• Molecule 4: Ribonuclease P protein subunit p29



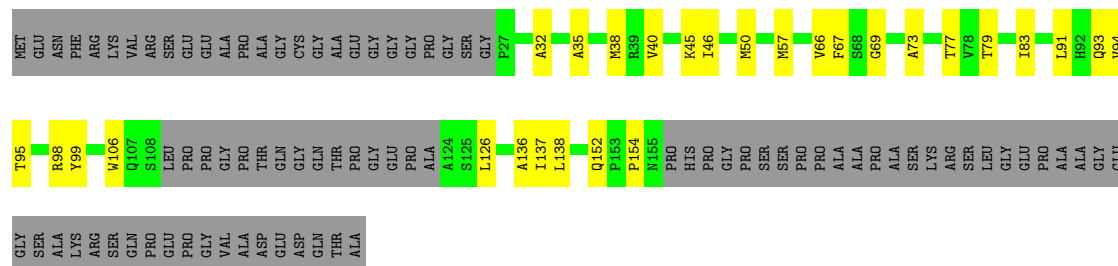
• Molecule 5: Ribonuclease P/MRP protein subunit POP5





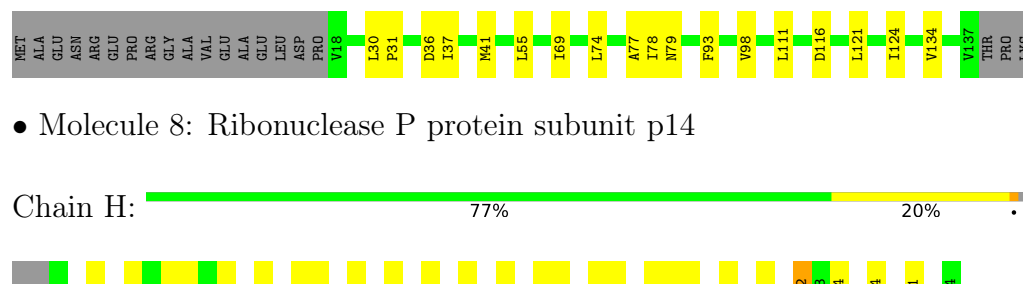
- Molecule 6: Ribonuclease P protein subunit p25

Chain F: 43% 14% 43%



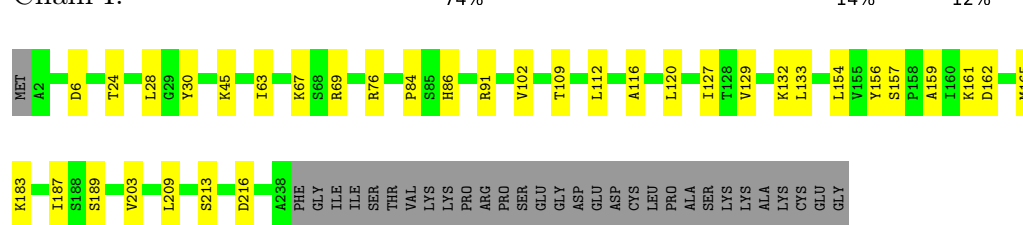
- Molecule 7: Ribonuclease P protein subunit p20

Chain G: 73% 13% 14%



- Molecule 8: Ribonuclease P protein subunit p14

Chain H: 77% 20% 3%



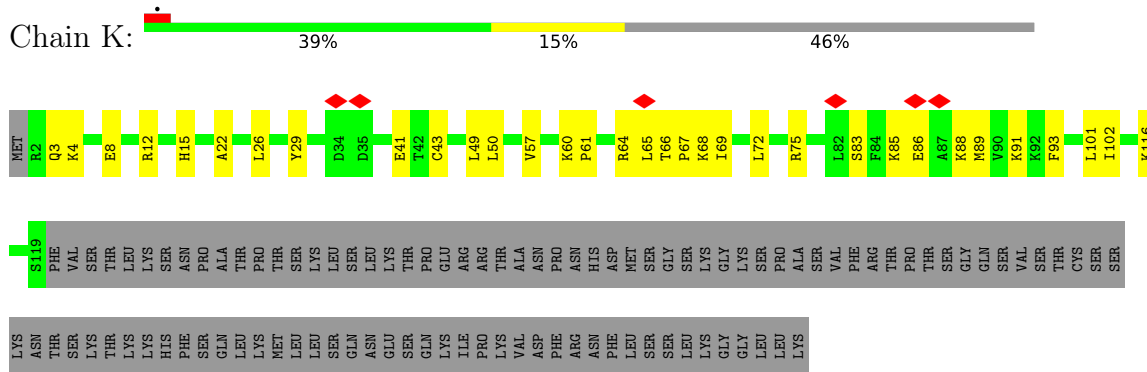
- Molecule 9: Ribonuclease P protein subunit p30

Chain I: 74% 14% 12%

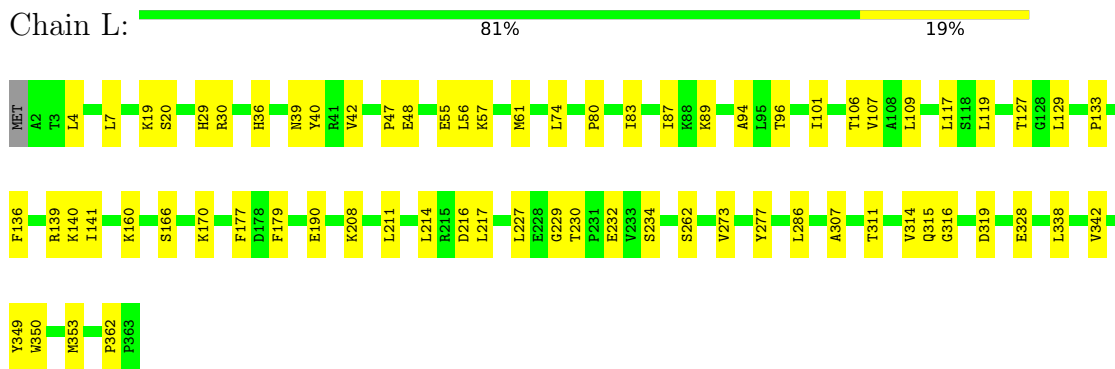




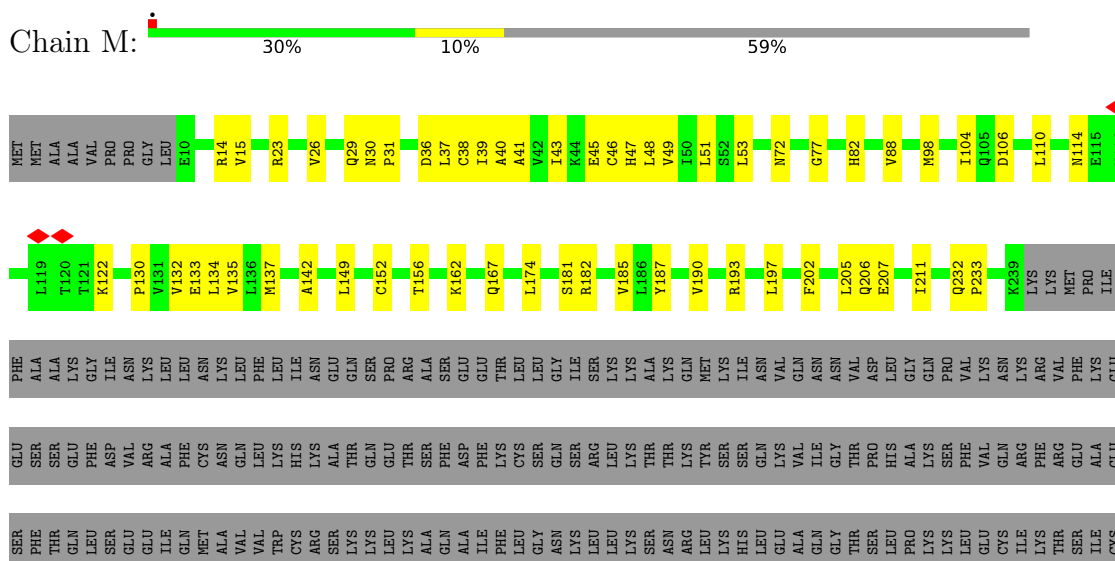
- Molecule 10: UPF0711 protein C18orf21



- Molecule 11: Ribonuclease P protein subunit p40



- Molecule 12: Nucleolus and neural progenitor protein



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432377	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size ( $\text{\AA}$ )	246.40001, 246.40001, 246.40001	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.08	0/6015	0.23	0/9368
2	B	0.12	0/5828	0.53	7/7885 (0.1%)
3	C	0.14	0/1095	0.34	0/1482
4	D	0.13	0/1529	0.31	0/2056
5	E	0.14	0/1238	0.38	0/1671
6	F	0.15	0/884	0.41	0/1194
7	G	0.13	0/957	0.37	0/1293
8	H	0.16	0/963	0.43	0/1303
9	I	0.11	0/1860	0.32	0/2522
9	J	0.14	0/1949	0.36	0/2641
10	K	0.13	0/982	0.37	0/1316
11	L	0.10	0/3021	0.33	2/4099 (0.0%)
12	M	0.14	0/1864	0.39	0/2526
All	All	0.12	0/28185	0.38	9/39356 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	999	ALA	N-CA-C	26.12	140.02	111.03
2	B	999	ALA	N-CA-CB	-15.19	87.95	109.98
2	B	998	PRO	N-CA-C	-14.83	81.93	112.47
2	B	299	LYS	CB-CA-C	-10.96	93.09	110.74
2	B	299	LYS	N-CA-C	8.86	123.53	108.02
2	B	300	TYR	N-CA-C	7.50	126.38	109.81
2	B	300	TYR	N-CA-CB	-6.88	98.13	110.37
11	L	229	GLY	CA-C-N	5.72	128.62	120.49
11	L	229	GLY	C-N-CA	5.72	128.62	120.49

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	5391	0	2746	90	0
2	B	5689	0	5775	97	0
3	C	1078	0	1156	26	0
4	D	1502	0	1561	38	0
5	E	1215	0	1232	31	0
6	F	869	0	912	18	0
7	G	945	0	971	17	0
8	H	946	0	977	24	0
9	I	1829	0	1914	25	0
9	J	1916	0	2015	35	0
10	K	963	0	990	20	0
11	L	2939	0	2884	41	0
12	M	1828	0	1926	44	0
13	K	1	0	0	0	0
All	All	27111	0	25059	468	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 9.

All (468) 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:222:LEU:HD11	2:B:644:LEU:HD11	1.25	1.14
12:M:45:GLU:CB	12:M:197:LEU:HD13	1.88	1.04
4:D:161:THR:HG22	4:D:162:LYS:H	1.22	1.03
12:M:45:GLU:HB3	12:M:197:LEU:HD13	1.42	0.99
2:B:222:LEU:HD11	2:B:644:LEU:CD1	1.93	0.98
4:D:42:MET:HE2	4:D:47:ARG:HA	1.49	0.94
2:B:222:LEU:CD1	2:B:644:LEU:HD11	1.99	0.92
2:B:308:VAL:CG2	2:B:329:ILE:HG23	2.04	0.87
5:E:114:LEU:HD23	5:E:145:SER:HB2	1.55	0.87
4:D:161:THR:HG22	4:D:162:LYS:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:592:GLU:HG2	2:B:593:SER:H	1.40	0.85
2:B:659:VAL:HG23	2:B:661:GLY:H	1.46	0.81
12:M:45:GLU:HB2	12:M:197:LEU:HD13	1.62	0.79
4:D:159:GLN:HB2	4:D:166:LYS:HB2	1.66	0.78
2:B:222:LEU:CD1	2:B:644:LEU:CD1	2.61	0.77
4:D:161:THR:CG2	4:D:162:LYS:H	1.95	0.77
12:M:45:GLU:HB2	12:M:197:LEU:CD1	2.14	0.77
2:B:114:GLU:HG3	12:M:185:VAL:HG21	1.66	0.77
11:L:214:LEU:HB3	11:L:217:LEU:HD21	1.64	0.76
3:C:44:ILE:HD11	3:C:199:ARG:HH12	1.51	0.75
5:E:114:LEU:CD2	5:E:145:SER:HB2	2.17	0.75
2:B:280:ALA:HB3	2:B:283:CYS:HB2	1.68	0.75
2:B:997:GLN:C	2:B:998:PRO:O	2.18	0.74
3:C:57:LEU:HA	3:C:105:THR:O	1.88	0.73
11:L:311:THR:HG22	11:L:342:VAL:HG22	1.69	0.73
12:M:232:GLN:HG2	12:M:233:PRO:HD3	1.71	0.72
10:K:72:LEU:HD13	10:K:89:MET:HG2	1.72	0.72
1:A:62:C:H2'	9:I:67:LYS:HG2	1.70	0.72
5:E:9:LEU:HD11	5:E:67:LEU:HD12	1.72	0.72
6:F:95:THR:HB	6:F:137:ILE:HD13	1.70	0.72
9:J:84:PRO:HD3	9:J:112:LEU:HD11	1.71	0.71
2:B:144:MET:HE3	2:B:144:MET:HA	1.72	0.71
11:L:42:VAL:HG22	11:L:314:VAL:HG22	1.73	0.71
12:M:45:GLU:CB	12:M:197:LEU:CD1	2.67	0.70
3:C:136:LYS:HE2	3:C:160:GLN:HB3	1.72	0.69
2:B:308:VAL:HG21	2:B:329:ILE:HG23	1.74	0.69
10:K:57:VAL:HG22	10:K:102:ILE:HG12	1.74	0.69
1:A:157:C:H2'	1:A:158:G:H8	1.58	0.68
1:A:237:C:H5''	1:A:238:A:H5'	1.74	0.68
1:A:82:G:H2'	1:A:83:A:H8	1.60	0.66
2:B:108:ALA:HB2	12:M:174:LEU:HD21	1.76	0.66
5:E:78:TRP:HE1	5:E:100:THR:HG21	1.59	0.66
2:B:308:VAL:CG2	2:B:329:ILE:CG2	2.75	0.65
2:B:592:GLU:HG2	2:B:593:SER:N	2.11	0.65
1:A:121:C:H2'	1:A:122:A:H8	1.62	0.64
2:B:308:VAL:HG21	2:B:329:ILE:CG2	2.27	0.64
12:M:187:TYR:HA	12:M:190:VAL:HG12	1.78	0.64
5:E:138:ILE:O	5:E:142:VAL:HG23	1.98	0.63
1:A:232:C:H2'	1:A:233:G:H8	1.61	0.63
5:E:124:ILE:HD13	7:G:93:PHE:HE1	1.64	0.63
1:A:147:C:H2'	1:A:148:G:H8	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:C:H2'	1:A:112:G:C8	2.34	0.62
5:E:37:ILE:HD11	5:E:77:VAL:HA	1.81	0.62
1:A:122:A:C6	1:A:188:G:C2	2.88	0.62
2:B:863:LEU:HD11	2:B:869:PRO:HD3	1.81	0.62
3:C:114:ALA:HB3	3:C:181:ALA:HB3	1.82	0.62
11:L:96:THR:OG1	11:L:106:THR:HG23	2.00	0.61
1:A:8:U:H2'	1:A:9:G:H8	1.65	0.61
1:A:122:A:C6	1:A:188:G:N1	2.68	0.61
1:A:122:A:N6	1:A:188:G:N1	2.47	0.61
4:D:90:LYS:H	4:D:93:GLN:HE21	1.49	0.60
1:A:122:A:N1	1:A:188:G:C2	2.69	0.60
1:A:112:G:H2'	1:A:113:C:H6	1.67	0.60
9:I:116:ALA:HA	9:I:120:LEU:HD12	1.81	0.60
1:A:56:C:H2'	1:A:57:C:H6	1.66	0.60
5:E:54:ALA:HB3	5:E:68:ARG:HB3	1.84	0.60
9:J:26:ALA:HB2	9:J:71:ILE:HD13	1.82	0.60
5:E:111:GLN:O	5:E:115:ILE:HG12	2.02	0.60
1:A:222:U:H2'	1:A:223:G:H8	1.67	0.59
11:L:140:LYS:HD2	11:L:141:ILE:N	2.18	0.59
5:E:8:TYR:HB3	5:E:66:LEU:HD11	1.84	0.59
12:M:106:ASP:O	12:M:110:LEU:HD22	2.02	0.59
7:G:74:LEU:H	7:G:77:ALA:HB3	1.67	0.58
1:A:98:U:H2'	1:A:99:G:H8	1.67	0.58
2:B:1006:LEU:HD22	2:B:1015:TYR:HB3	1.86	0.58
3:C:193:VAL:O	3:C:197:ILE:HG12	2.03	0.58
2:B:89:ALA:HB1	2:B:92:GLU:HB2	1.86	0.58
5:E:62:THR:HG23	5:E:64:ILE:HG12	1.86	0.58
1:A:122:A:N6	1:A:188:G:C6	2.72	0.57
5:E:124:ILE:HD13	7:G:93:PHE:CE1	2.39	0.57
4:D:4:VAL:HG23	4:D:5:ILE:HD12	1.85	0.57
1:A:247:G:H2'	1:A:248:G:H8	1.69	0.57
1:A:8:U:H2'	1:A:9:G:C8	2.39	0.57
1:A:98:U:H2'	1:A:99:G:C8	2.39	0.57
10:K:83:SER:HB2	10:K:86:GLU:HB2	1.87	0.57
2:B:861:LEU:HG	2:B:1020:ILE:HG13	1.86	0.56
3:C:146:HIS:O	3:C:150:LEU:HG	2.05	0.56
7:G:41:MET:HE2	7:G:41:MET:H	1.70	0.56
2:B:203:GLU:HG2	2:B:204:THR:HG23	1.86	0.56
2:B:255:LEU:HB3	2:B:262:ILE:HD11	1.87	0.56
5:E:127:GLN:HE22	7:G:93:PHE:HB3	1.71	0.56
9:J:225:CYS:O	9:J:229:LEU:HD22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:G:O2'	10:K:67:PRO:HG2	2.06	0.56
2:B:913:GLU:HA	2:B:916:LYS:HZ2	1.70	0.56
11:L:89:LYS:HD2	11:L:190:GLU:OE2	2.05	0.56
2:B:878:PRO:HD3	2:B:1005:VAL:HA	1.88	0.56
3:C:134:VAL:HG11	3:C:144:THR:HB	1.87	0.55
9:J:143:ASN:O	9:J:146:ILE:HG22	2.07	0.55
10:K:65:LEU:HD21	10:K:93:PHE:CD2	2.42	0.55
11:L:353:MET:HE2	11:L:362:PRO:HB2	1.88	0.55
12:M:98:MET:HE1	12:M:142:ALA:HB2	1.89	0.55
1:A:8:U:H4'	4:D:180:LEU:HD23	1.87	0.55
9:J:57:LEU:HG	9:J:58:PHE:HD1	1.72	0.55
5:E:2:VAL:HG11	9:J:139:ARG:HH22	1.72	0.55
9:I:67:LYS:NZ	9:I:69:ARG:HB2	2.22	0.55
12:M:181:SER:O	12:M:185:VAL:HG23	2.07	0.55
7:G:111:LEU:HB2	7:G:121:LEU:HB2	1.88	0.55
9:J:229:LEU:O	9:J:233:GLU:HG3	2.07	0.55
9:J:246:LYS:HG3	9:J:248:PRO:HD3	1.87	0.55
12:M:137:MET:HE3	12:M:137:MET:HA	1.88	0.55
6:F:38:MET:HA	6:F:38:MET:HE2	1.87	0.54
12:M:49:VAL:O	12:M:53:LEU:HD12	2.07	0.54
3:C:193:VAL:HG23	3:C:197:ILE:HD11	1.88	0.54
4:D:95:ARG:HE	4:D:98:LEU:HD11	1.71	0.54
9:I:156:TYR:CZ	9:I:189:SER:HB3	2.43	0.54
10:K:66:THR:HG23	10:K:68:LYS:HG2	1.89	0.54
11:L:211:LEU:HD12	11:L:277:TYR:HE2	1.71	0.54
4:D:50:GLN:HE21	4:D:53:ARG:HH22	1.54	0.54
11:L:230:THR:HB	11:L:234:SER:H	1.72	0.54
2:B:308:VAL:HG22	2:B:329:ILE:HG23	1.86	0.54
2:B:855:ALA:HB3	2:B:987:LEU:HD22	1.90	0.54
9:I:84:PRO:HD3	9:I:112:LEU:HD21	1.88	0.54
5:E:118:ASN:OD1	5:E:142:VAL:HG13	2.08	0.54
1:A:91:C:H2'	1:A:92:A:H8	1.72	0.54
1:A:3:G:H22	1:A:267:U:H3	1.55	0.53
2:B:252:CYS:HA	2:B:329:ILE:O	2.08	0.53
1:A:40:A:H2'	1:A:41:G:H8	1.73	0.53
2:B:269:MET:HE1	2:B:342:GLU:HG3	1.89	0.53
1:A:263:C:H2'	1:A:264:G:H8	1.73	0.53
8:H:89:LEU:HD22	8:H:102:PHE:CE2	2.44	0.53
3:C:124:LEU:HG	3:C:129:LEU:HD12	1.89	0.53
5:E:114:LEU:HD23	5:E:145:SER:CB	2.32	0.53
5:E:139:GLN:HA	5:E:142:VAL:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:88:VAL:HG13	12:M:149:LEU:HD11	1.90	0.53
2:B:859:VAL:HG12	2:B:1022:ILE:HG12	1.91	0.53
9:J:130:THR:HA	9:J:165:MET:HE1	1.91	0.53
11:L:94:ALA:HB3	11:L:109:LEU:HB3	1.90	0.53
2:B:344:LYS:HB3	2:B:350:VAL:HG12	1.91	0.52
9:I:24:THR:O	9:I:28:LEU:HD12	2.09	0.52
8:H:90:THR:HG21	9:J:202:ASP:HB3	1.90	0.52
9:J:19:ARG:O	9:J:23:GLU:HG3	2.09	0.52
2:B:98:ILE:HG23	2:B:98:ILE:O	2.09	0.52
9:J:177:MET:HE3	9:J:177:MET:HA	1.91	0.52
5:E:85:THR:HG22	5:E:86:TYR:H	1.73	0.52
8:H:43:LEU:HD23	8:H:44:LEU:HD23	1.91	0.52
9:J:50:LYS:HD3	9:J:96:ARG:HH11	1.74	0.52
1:A:11:U:H2'	1:A:12:G:H8	1.75	0.52
11:L:166:SER:O	11:L:170:LYS:HB2	2.09	0.52
10:K:41:GLU:HB3	10:K:50:LEU:HG	1.92	0.52
6:F:45:LYS:HE3	6:F:45:LYS:HA	1.91	0.52
6:F:67:PHE:HB2	6:F:137:ILE:HG23	1.91	0.52
2:B:578:GLU:HG2	12:M:14:ARG:HH22	1.75	0.52
3:C:113:LEU:HD11	3:C:180:LEU:HG	1.92	0.51
11:L:19:LYS:HG2	11:L:227:LEU:HD22	1.92	0.51
2:B:252:CYS:SG	2:B:425:LEU:HB2	2.51	0.51
5:E:32:LEU:HD21	5:E:84:ILE:HG21	1.91	0.51
6:F:66:VAL:HG22	6:F:138:LEU:HB3	1.93	0.51
2:B:993:MET:HE2	2:B:994:LEU:HD12	1.93	0.51
2:B:259:GLU:HB3	2:B:325:ARG:HG3	1.93	0.51
9:J:17:ALA:O	9:J:21:LEU:HG	2.11	0.51
1:A:121:C:H2'	1:A:122:A:C8	2.44	0.51
1:A:6:C:H2'	1:A:7:G:C8	2.46	0.51
1:A:193:C:N4	2:B:146:HIS:CE1	2.79	0.51
7:G:37:ILE:HD11	7:G:55:LEU:HD22	1.93	0.51
1:A:82:G:H2'	1:A:83:A:C8	2.43	0.51
2:B:300:TYR:HB3	2:B:301:PRO:HD3	1.93	0.50
8:H:23:LYS:HG3	8:H:114:LEU:HD22	1.93	0.50
4:D:106:TRP:HE1	4:D:135:LEU:HA	1.76	0.50
11:L:216:ASP:HA	11:L:273:VAL:O	2.10	0.50
4:D:41:ARG:H	4:D:41:ARG:HD3	1.76	0.50
1:A:112:G:H2'	1:A:113:C:C6	2.47	0.50
2:B:242:CYS:HA	2:B:435:ILE:O	2.11	0.50
9:I:157:SER:O	9:I:161:LYS:HG2	2.11	0.50
9:J:22:VAL:HG12	9:J:62:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:C:C6	9:I:67:LYS:HE2	2.46	0.50
7:G:36:ASP:C	7:G:37:ILE:HD13	2.36	0.50
11:L:315:GLN:HG3	11:L:338:LEU:HB3	1.94	0.50
12:M:43:ILE:HA	12:M:46:CYS:SG	2.51	0.50
1:A:64:C:H2'	1:A:65:C:C6	2.46	0.50
1:A:184:G:H2'	1:A:185:G:H8	1.77	0.50
11:L:101:ILE:HD11	11:L:319:ASP:HA	1.92	0.49
4:D:140:ILE:HG12	4:D:157:LEU:HD22	1.95	0.49
7:G:41:MET:HE1	7:G:77:ALA:HB2	1.93	0.49
1:A:41:G:H2'	1:A:42:G:H8	1.78	0.49
2:B:859:VAL:HG21	2:B:1020:ILE:HD11	1.94	0.49
2:B:908:ILE:O	2:B:912:LYS:HG2	2.13	0.49
11:L:83:ILE:HA	11:L:87:ILE:HD13	1.93	0.49
8:H:44:LEU:O	8:H:48:VAL:HG23	2.12	0.49
10:K:8:GLU:HB3	10:K:12:ARG:NH2	2.27	0.49
2:B:452:VAL:HG12	2:B:453:HIS:N	2.27	0.49
10:K:22:ALA:O	10:K:26:LEU:HG	2.13	0.49
12:M:207:GLU:O	12:M:211:ILE:HG12	2.13	0.49
4:D:161:THR:CG2	4:D:162:LYS:N	2.59	0.49
2:B:812:LEU:HB3	2:B:1024:VAL:HG21	1.94	0.49
12:M:31:PRO:HD2	12:M:122:LYS:HB3	1.93	0.49
12:M:130:PRO:O	12:M:134:LEU:HD23	2.13	0.49
2:B:849:LEU:HD21	2:B:988:THR:HA	1.94	0.48
6:F:98:ARG:HH21	6:F:136:ALA:HB2	1.78	0.48
7:G:30:LEU:HG	7:G:31:PRO:HD2	1.94	0.48
7:G:41:MET:HE2	7:G:41:MET:N	2.27	0.48
10:K:66:THR:HG22	10:K:69:ILE:HG12	1.96	0.48
7:G:69:ILE:HG12	7:G:134:VAL:HB	1.95	0.48
9:I:162:ASP:HB3	9:I:165:MET:SD	2.54	0.48
5:E:56:ARG:NH2	5:E:144:ARG:HH22	2.11	0.48
12:M:77:GLY:HA2	12:M:82:HIS:CE1	2.48	0.48
1:A:22:A:H5'	1:A:23:U:OP2	2.14	0.48
1:A:224:C:H2'	1:A:225:G:C8	2.49	0.48
3:C:32:ARG:NE	3:C:32:ARG:HA	2.28	0.48
2:B:504:ILE:HG12	2:B:600:ILE:HG12	1.96	0.48
5:E:32:LEU:O	5:E:36:THR:HG22	2.14	0.48
9:I:183:LYS:HD3	9:I:183:LYS:N	2.28	0.48
1:A:56:C:H2'	1:A:57:C:C6	2.47	0.48
11:L:230:THR:HG22	11:L:232:GLU:H	1.79	0.48
5:E:30:SER:HB2	5:E:55:VAL:HG11	1.95	0.47
10:K:3:GLN:HG3	10:K:29:TYR:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:C:H2'	1:A:158:G:C8	2.45	0.47
3:C:130:LEU:HD11	3:C:193:VAL:HG11	1.96	0.47
1:A:202:C:H2'	1:A:202:C:O2	2.14	0.47
1:A:263:C:H2'	1:A:264:G:C8	2.49	0.47
9:I:127:ILE:O	9:I:129:VAL:HG23	2.14	0.47
10:K:15:HIS:CE1	10:K:49:LEU:HD13	2.49	0.47
12:M:40:ALA:O	12:M:43:ILE:HG12	2.14	0.47
5:E:86:TYR:CG	5:E:86:TYR:O	2.67	0.47
6:F:93:GLN:NE2	6:F:152:GLN:HG3	2.29	0.47
8:H:121:LEU:HD22	11:L:40:TYR:HE1	1.79	0.47
2:B:320:ASP:N	2:B:321:PRO:HD3	2.29	0.47
4:D:123:PRO:O	4:D:127:GLN:HG2	2.14	0.47
6:F:94:VAL:HB	6:F:138:LEU:HD11	1.94	0.47
11:L:48:GLU:HG2	11:L:273:VAL:HG13	1.96	0.47
2:B:659:VAL:HB	2:B:660:PRO:HD2	1.96	0.47
5:E:121:GLN:HA	5:E:124:ILE:HG22	1.95	0.47
11:L:106:THR:HG22	11:L:107:VAL:N	2.29	0.47
2:B:146:HIS:O	2:B:146:HIS:ND1	2.48	0.47
2:B:894:GLY:HA3	2:B:1015:TYR:O	2.15	0.47
4:D:122:GLN:HG2	4:D:124:GLN:H	1.79	0.47
9:I:63:ILE:HD12	9:I:63:ILE:HA	1.80	0.47
10:K:4:LYS:O	10:K:8:GLU:HG3	2.15	0.47
11:L:136:PHE:HE2	11:L:328:GLU:HG2	1.80	0.47
2:B:135:LEU:HD23	2:B:136:PRO:HD2	1.96	0.47
12:M:72:ASN:O	12:M:82:HIS:HE1	1.97	0.47
2:B:304:MET:HG3	2:B:807:ARG:NH1	2.30	0.47
2:B:671:LEU:HG	2:B:675:GLU:OE2	2.15	0.47
1:A:65:C:H2'	1:A:66:U:C6	2.51	0.46
2:B:280:ALA:HA	7:G:116:ASP:OD1	2.16	0.46
6:F:69:GLY:HA3	6:F:77:THR:HG21	1.97	0.46
6:F:106:TRP:HD1	6:F:126:LEU:HD23	1.80	0.46
8:H:77:ILE:HG21	8:H:85:LEU:HD22	1.95	0.46
1:A:222:U:H2'	1:A:223:G:C8	2.48	0.46
2:B:211:ARG:O	2:B:227:THR:HB	2.16	0.46
12:M:114:ASN:HD22	12:M:114:ASN:C	2.22	0.46
4:D:86:LEU:HD23	4:D:87:PHE:H	1.80	0.46
8:H:26:LEU:HG	8:H:102:PHE:CE1	2.51	0.46
8:H:66:TYR:HD1	8:H:73:ALA:HB2	1.80	0.46
12:M:187:TYR:HA	12:M:190:VAL:CG1	2.43	0.46
1:A:40:A:H2'	1:A:41:G:C8	2.51	0.46
4:D:108:GLN:HA	4:D:111:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ILE:HG13	7:G:79:ASN:H	1.80	0.46
8:H:98:LYS:HD3	8:H:98:LYS:N	2.30	0.46
2:B:349:CYS:HB3	2:B:415:SER:HB2	1.96	0.46
4:D:8:ALA:HB3	12:M:182:ARG:HH22	1.81	0.46
4:D:138:ALA:H	4:D:157:LEU:HD23	1.80	0.46
8:H:24:VAL:HG11	8:H:102:PHE:CE2	2.50	0.46
2:B:102:ILE:HB	4:D:56:VAL:HB	1.97	0.46
6:F:40:VAL:HB	6:F:77:THR:HG22	1.98	0.46
1:A:6:C:H2'	1:A:7:G:H8	1.81	0.46
1:A:267:U:H5''	11:L:160:LYS:HE3	1.98	0.46
2:B:465:ARG:O	2:B:469:GLU:HG2	2.15	0.46
2:B:859:VAL:HG23	2:B:861:LEU:HD11	1.97	0.46
8:H:44:LEU:HD22	8:H:89:LEU:HD21	1.97	0.46
9:J:18:LEU:O	9:J:22:VAL:HG23	2.15	0.46
1:A:217:G:H2'	1:A:218:G:H8	1.80	0.46
4:D:118:LYS:HD2	4:D:120:ASP:HB2	1.96	0.46
12:M:47:HIS:O	12:M:51:LEU:HG	2.15	0.46
1:A:185:G:H2'	1:A:186:G:H8	1.80	0.46
12:M:29:GLN:HG2	12:M:30:ASN:OD1	2.16	0.46
1:A:223:G:H2'	1:A:224:C:C6	2.51	0.46
1:A:80:C:H2'	1:A:81:G:H8	1.79	0.45
2:B:944:THR:HG22	2:B:945:LEU:H	1.80	0.45
1:A:247:G:H2'	1:A:248:G:C8	2.49	0.45
8:H:62:ASP:HB2	11:L:262:SER:HA	1.98	0.45
12:M:202:PHE:O	12:M:206:GLN:HG3	2.17	0.45
1:A:250:C:H2'	1:A:251:U:C6	2.52	0.45
2:B:259:GLU:HA	2:B:262:ILE:HG22	1.99	0.45
9:J:216:ASP:HA	11:L:139:ARG:HH21	1.80	0.45
11:L:127:THR:HB	11:L:129:LEU:HD23	1.99	0.45
12:M:162:LYS:HE3	12:M:162:LYS:HB2	1.76	0.45
3:C:161:VAL:CG1	3:C:164:LEU:HB3	2.47	0.45
4:D:112:ASP:OD1	4:D:112:ASP:O	2.34	0.45
11:L:4:LEU:HA	11:L:7:LEU:HB2	1.98	0.45
11:L:47:PRO:HG2	11:L:307:ALA:HB1	1.99	0.45
1:A:81:G:H5'	2:B:210:LYS:HD3	1.99	0.45
1:A:99:G:H2'	1:A:100:C:C6	2.52	0.45
1:A:245:C:H2'	1:A:246:G:H8	1.81	0.45
2:B:222:LEU:C	2:B:222:LEU:HD12	2.42	0.45
9:J:133:LEU:HD12	9:J:133:LEU:H	1.82	0.45
11:L:117:LEU:HD12	11:L:119:LEU:HD21	1.99	0.45
2:B:235:TYR:O	2:B:239:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:81:VAL:HG22	9:J:112:LEU:HD23	1.97	0.45
2:B:105:SER:H	4:D:54:LYS:HZ1	1.65	0.44
2:B:249:TYR:O	2:B:333:PRO:HG3	2.17	0.44
3:C:33:TRP:CH2	3:C:159:CYS:HA	2.52	0.44
3:C:122:ARG:O	3:C:126:ARG:HD3	2.17	0.44
9:J:105:VAL:HG13	9:J:122:VAL:HG11	1.98	0.44
10:K:85:LYS:HA	10:K:88:LYS:HG2	1.99	0.44
2:B:964:LEU:HB3	2:B:985:VAL:HG13	1.99	0.44
3:C:43:PHE:O	3:C:47:THR:HG22	2.17	0.44
7:G:74:LEU:N	7:G:77:ALA:HB3	2.31	0.44
10:K:64:ARG:HG2	10:K:64:ARG:HH11	1.82	0.44
12:M:41:ALA:O	12:M:45:GLU:HG2	2.17	0.44
1:A:23:U:H4'	1:A:24:C:H3'	1.98	0.44
1:A:28:G:H2'	1:A:29:G:C8	2.52	0.44
2:B:442:ILE:HG13	2:B:443:LEU:N	2.31	0.44
9:I:187:ILE:HD13	9:I:203:VAL:HG13	2.00	0.44
1:A:128:C:H2'	1:A:129:G:C8	2.53	0.44
1:A:177:G:H4'	10:K:75:ARG:HD3	1.98	0.44
3:C:143:ILE:HD12	3:C:143:ILE:H	1.82	0.44
8:H:85:LEU:O	8:H:89:LEU:HD12	2.17	0.44
9:J:83:ASP:HB3	9:J:86:HIS:NE2	2.32	0.44
1:A:115:C:H2'	1:A:116:G:H8	1.82	0.44
2:B:876:CYS:HA	2:B:963:LEU:HA	1.98	0.44
4:D:93:GLN:HA	4:D:95:ARG:HH12	1.82	0.44
11:L:342:VAL:HB	11:L:350:TRP:HB2	2.00	0.44
12:M:132:VAL:HA	12:M:135:VAL:HG12	1.99	0.44
3:C:131:LEU:HD22	3:C:193:VAL:HG23	2.00	0.44
4:D:24:ALA:O	4:D:28:GLU:HG3	2.18	0.44
2:B:447:ILE:HG23	2:B:509:VAL:HG11	2.00	0.44
2:B:993:MET:O	2:B:997:GLN:HG2	2.18	0.44
12:M:205:LEU:HD12	12:M:205:LEU:HA	1.62	0.44
1:A:94:A:C8	2:B:209:ALA:HB1	2.52	0.44
2:B:541:LEU:HD21	7:G:124:ILE:HD13	1.99	0.44
9:J:31:SER:HA	9:J:71:ILE:HG22	1.99	0.44
11:L:39:ASN:HA	11:L:316:GLY:HA2	1.98	0.44
12:M:152:CYS:O	12:M:156:THR:HG22	2.18	0.44
1:A:12:G:H2'	1:A:13:A:C8	2.53	0.43
4:D:138:ALA:O	4:D:156:ILE:HA	2.18	0.43
6:F:91:LEU:H	6:F:154:PRO:HB3	1.82	0.43
9:I:178:GLN:NE2	9:I:179:ILE:HG12	2.33	0.43
9:J:117:CYS:HB2	9:J:145:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:177:PHE:HB2	11:L:179:PHE:CE1	2.53	0.43
9:I:6:ASP:HB2	9:I:30:TYR:CD1	2.53	0.43
1:A:11:U:H2'	1:A:12:G:C8	2.52	0.43
1:A:232:C:H2'	1:A:233:G:C8	2.48	0.43
2:B:472:LYS:HB2	2:B:472:LYS:HE2	1.80	0.43
2:B:591:HIS:O	2:B:592:GLU:HB3	2.19	0.43
2:B:874:MET:HE3	2:B:874:MET:HB2	1.89	0.43
9:I:109:THR:HB	9:I:112:LEU:HB2	1.99	0.43
4:D:159:GLN:HG3	4:D:166:LYS:NZ	2.34	0.43
5:E:108:ARG:HG3	5:E:109:THR:N	2.33	0.43
9:I:213:SER:HB3	9:I:216:ASP:OD2	2.18	0.43
1:A:115:C:H2'	1:A:116:G:C8	2.53	0.43
2:B:1006:LEU:O	2:B:1007:LEU:HD23	2.19	0.43
9:J:41:PHE:CE2	9:J:79:ILE:HD11	2.53	0.43
1:A:12:G:H2'	1:A:13:A:H8	1.84	0.43
5:E:111:GLN:HE22	5:E:148:LEU:HB2	1.83	0.43
2:B:987:LEU:HA	2:B:990:LEU:HB3	2.01	0.43
3:C:161:VAL:HB	3:C:164:LEU:HD23	2.01	0.43
6:F:73:ALA:O	6:F:77:THR:HG23	2.18	0.43
9:I:154:LEU:HD23	9:I:154:LEU:HA	1.81	0.43
9:J:8:ASP:HA	9:J:36:ASN:HB2	2.01	0.43
1:A:72:A:C8	1:A:253:A:N6	2.87	0.43
1:A:264:G:H4'	4:D:176:VAL:HB	2.00	0.43
3:C:51:ARG:HE	3:C:55:ILE:HD11	1.84	0.43
8:H:55:VAL:HG21	9:I:209:LEU:HD11	2.01	0.43
9:I:159:ALA:HB1	9:I:166:ARG:HG3	2.01	0.43
11:L:57:LYS:O	11:L:61:MET:SD	2.77	0.43
1:A:181:C:H2'	1:A:182:G:H8	1.83	0.43
2:B:148:VAL:HG21	2:B:151:LEU:HB3	2.01	0.43
2:B:222:LEU:HD13	2:B:644:LEU:HG	2.01	0.43
6:F:32:ALA:HB1	6:F:35:ALA:HB2	2.01	0.43
6:F:46:ILE:O	6:F:50:MET:SD	2.77	0.43
8:H:21:TYR:CE2	8:H:76:ARG:HD2	2.54	0.43
9:J:207:GLY:HA2	9:J:210:PHE:HD2	1.84	0.43
12:M:37:LEU:HD12	12:M:38:CYS:N	2.34	0.43
5:E:139:GLN:HA	5:E:142:VAL:HG23	2.01	0.42
3:C:140:PRO:HB2	3:C:142:MET:HG3	2.01	0.42
5:E:89:ASN:OD1	5:E:90:LYS:HG2	2.19	0.42
2:B:288:ARG:HB3	2:B:503:THR:H	1.85	0.42
4:D:144:LYS:HB3	4:D:183:VAL:HB	2.01	0.42
3:C:142:MET:HA	3:C:145:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:ASP:OD1	8:H:30:ASP:C	2.62	0.42
9:J:63:ILE:HD12	9:J:63:ILE:HA	1.86	0.42
1:A:253:A:H2'	1:A:254:U:C6	2.55	0.42
2:B:803:LEU:HD12	2:B:803:LEU:HA	1.84	0.42
8:H:9:GLU:N	8:H:9:GLU:OE1	2.53	0.42
11:L:29:HIS:NE2	11:L:30:ARG:HG3	2.34	0.42
2:B:572:LEU:HA	2:B:575:MET:HE1	2.02	0.42
11:L:80:PRO:HA	11:L:83:ILE:HD12	2.01	0.42
12:M:23:ARG:NH2	12:M:26:VAL:HA	2.34	0.42
1:A:5:U:H2'	1:A:6:C:C6	2.54	0.42
1:A:41:G:C2	1:A:42:G:N7	2.88	0.42
4:D:141:SER:HB3	4:D:154:THR:HG23	2.01	0.42
9:I:91:ARG:HG3	9:I:120:LEU:HD23	2.01	0.42
11:L:20:SER:HB3	11:L:349:TYR:CZ	2.53	0.42
1:A:194:C:N4	2:B:91:PRO:HA	2.35	0.42
4:D:140:ILE:HD13	4:D:140:ILE:HA	1.90	0.42
9:I:45:LYS:HA	9:I:45:LYS:HD2	1.81	0.42
11:L:74:LEU:HD23	11:L:74:LEU:HA	1.84	0.42
12:M:48:LEU:HB3	12:M:193:ARG:HH12	1.85	0.42
1:A:147:C:H2'	1:A:148:G:C8	2.49	0.42
2:B:148:VAL:HG21	2:B:151:LEU:HD23	2.01	0.42
9:I:133:LEU:HD12	9:I:133:LEU:HA	1.88	0.42
11:L:55:GLU:HG2	11:L:56:LEU:N	2.34	0.42
12:M:133:GLU:OE1	12:M:205:LEU:HD11	2.20	0.42
2:B:113:ALA:HB2	4:D:22:SER:HB3	2.01	0.41
2:B:632:ILE:HD13	2:B:632:ILE:HA	1.89	0.41
4:D:41:ARG:HH22	12:M:167:GLN:HB2	1.84	0.41
6:F:79:THR:O	6:F:83:ILE:HG12	2.20	0.41
7:G:98:VAL:HG12	7:G:134:VAL:HG22	2.01	0.41
9:J:124:LEU:HD23	9:J:124:LEU:HA	1.90	0.41
11:L:133:PRO:HB3	11:L:141:ILE:HG21	2.01	0.41
12:M:77:GLY:HA2	12:M:82:HIS:ND1	2.35	0.41
1:A:51:C:H2'	1:A:52:C:C6	2.55	0.41
1:A:52:C:H2'	1:A:53:U:C6	2.55	0.41
1:A:127:C:H2'	1:A:128:C:C6	2.55	0.41
1:A:164:C:H5''	10:K:101:LEU:HD13	2.03	0.41
2:B:252:CYS:HG	2:B:425:LEU:HB2	1.86	0.41
8:H:43:LEU:HD12	8:H:95:TYR:CG	2.55	0.41
8:H:91:LEU:HD13	9:J:160:ILE:HD13	2.01	0.41
11:L:208:LYS:HB2	11:L:208:LYS:HE2	1.89	0.41
1:A:152:A:H2	10:K:116:LYS:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ARG:CG	2:B:303:GLU:HG3	2.51	0.41
2:B:909:LEU:H	2:B:909:LEU:HD12	1.84	0.41
10:K:60:LYS:HA	10:K:61:PRO:HD3	1.93	0.41
10:K:91:LYS:HB3	10:K:91:LYS:HE3	1.75	0.41
12:M:49:VAL:HG21	12:M:197:LEU:HD22	2.03	0.41
1:A:163:C:H2'	1:A:164:C:O4'	2.21	0.41
2:B:105:SER:H	4:D:54:LYS:NZ	2.19	0.41
3:C:40:ASP:HB3	3:C:199:ARG:HD2	2.02	0.41
4:D:85:ARG:HG3	4:D:88:ASP:HB2	2.03	0.41
4:D:78:ALA:HA	4:D:81:ARG:HD3	2.03	0.41
4:D:166:LYS:HB3	4:D:166:LYS:HE2	1.97	0.41
5:E:81:LEU:HD23	5:E:81:LEU:HA	1.88	0.41
8:H:86:TRP:CZ2	8:H:104:VAL:HG21	2.56	0.41
9:J:2:ALA:HA	9:J:226:ARG:HH21	1.86	0.41
1:A:267:U:H2'	1:A:268:G:C8	2.56	0.41
3:C:189:PHE:O	3:C:193:VAL:HG12	2.21	0.41
6:F:57:MET:HA	6:F:57:MET:HE2	2.03	0.41
2:B:198:LYS:HD2	2:B:198:LYS:HA	1.86	0.41
2:B:214:MET:HA	2:B:214:MET:HE3	2.03	0.41
2:B:452:VAL:CG1	2:B:453:HIS:N	2.83	0.41
2:B:944:THR:HB	2:B:947:LEU:HB2	2.03	0.41
9:J:77:LEU:O	9:J:103:VAL:HA	2.21	0.41
9:J:122:VAL:HG23	9:J:150:LEU:HD23	2.03	0.41
12:M:104:ILE:HD12	12:M:104:ILE:HA	1.86	0.41
1:A:86:U:O2'	2:B:157:GLU:HG3	2.20	0.41
3:C:51:ARG:NE	3:C:55:ILE:HD11	2.36	0.41
5:E:55:VAL:O	5:E:56:ARG:HD2	2.21	0.41
1:A:193:C:N4	2:B:146:HIS:HE1	2.19	0.40
1:A:229:C:H3'	1:A:230:C:H6	1.85	0.40
8:H:77:ILE:HD13	8:H:85:LEU:HD23	2.02	0.40
9:J:76:ARG:HG3	9:J:102:VAL:HB	2.02	0.40
1:A:199:G:N3	1:A:199:G:H2'	2.35	0.40
1:A:245:C:H2'	1:A:246:G:C8	2.56	0.40
2:B:708:TRP:O	2:B:712:THR:HG23	2.20	0.40
8:H:121:LEU:HD22	11:L:40:TYR:CE1	2.56	0.40
9:J:88:ASN:HA	9:J:91:ARG:HB2	2.02	0.40
9:J:156:TYR:CZ	9:J:189:SER:HB3	2.56	0.40
1:A:159:U:H3'	1:A:160:A:C5'	2.51	0.40
6:F:138:LEU:HD12	6:F:138:LEU:O	2.21	0.40
1:A:266:C:H2'	1:A:267:U:C6	2.56	0.40
2:B:578:GLU:O	12:M:15:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:GLY:O	3:C:120:VAL:HG22	2.22	0.40
8:H:21:TYR:HE2	8:H:76:ARG:HD2	1.87	0.40
11:L:286:LEU:HD23	11:L:286:LEU:HA	1.89	0.40
12:M:36:ASP:O	12:M:39:ILE:HG13	2.21	0.40
5:E:122:LEU:HD11	5:E:142:VAL:HG21	2.03	0.40
9:I:76:ARG:HG2	9:I:102:VAL:HB	2.03	0.40
9:I:132:LYS:HE3	9:I:132:LYS:HB2	1.82	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	
2	B	704/1024 (69%)	665 (94%)	39 (6%)	0	100	100
3	C	133/283 (47%)	131 (98%)	2 (2%)	0	100	100
4	D	182/220 (83%)	171 (94%)	11 (6%)	0	100	100
5	E	147/163 (90%)	140 (95%)	7 (5%)	0	100	100
6	F	110/199 (55%)	109 (99%)	1 (1%)	0	100	100
7	G	118/140 (84%)	114 (97%)	4 (3%)	0	100	100
8	H	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
9	I	235/268 (88%)	226 (96%)	9 (4%)	0	100	100
9	J	246/268 (92%)	238 (97%)	8 (3%)	0	100	100
10	K	116/220 (53%)	109 (94%)	7 (6%)	0	100	100
11	L	360/363 (99%)	351 (98%)	9 (2%)	0	100	100
12	M	228/567 (40%)	225 (99%)	3 (1%)	0	100	100
All	All	2699/3839 (70%)	2593 (96%)	106 (4%)	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	624/883 (71%)	622 (100%)	2 (0%)	86	83
3	C	122/255 (48%)	122 (100%)	0	100	100
4	D	166/196 (85%)	166 (100%)	0	100	100
5	E	133/143 (93%)	132 (99%)	1 (1%)	73	76
6	F	92/150 (61%)	91 (99%)	1 (1%)	65	74
7	G	102/118 (86%)	102 (100%)	0	100	100
8	H	104/106 (98%)	103 (99%)	1 (1%)	68	75
9	I	202/228 (89%)	201 (100%)	1 (0%)	81	80
9	J	212/228 (93%)	212 (100%)	0	100	100
10	K	107/201 (53%)	106 (99%)	1 (1%)	70	75
11	L	331/332 (100%)	330 (100%)	1 (0%)	86	83
12	M	208/513 (40%)	208 (100%)	0	100	100
All	All	2403/3353 (72%)	2395 (100%)	8 (0%)	84	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	201	TRP
2	B	987	LEU
5	E	114	LEU
6	F	99	TYR
8	H	102	PHE
9	I	86	HIS
10	K	43	CYS
11	L	36	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	208	HIS

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Mol	Chain	Res	Type
2	B	289	GLN
2	B	658	ASN
3	C	42	HIS
3	C	149	GLN
4	D	124	GLN
4	D	127	GLN
5	E	102	HIS
5	E	116	GLN
7	G	97	GLN
7	G	126	ASN
8	H	29	GLN
8	H	39	GLN
9	I	114	HIS
9	I	224	ASN
9	J	184	ASN
10	K	15	HIS
11	L	34	GLN
11	L	205	HIS
11	L	255	ASN
11	L	345	ASN
12	M	82	HIS
12	M	129	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	252/270 (93%)	54 (21%)	2 (0%)

All (54) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	G
1	A	22	A
1	A	23	U
1	A	34	A
1	A	35	C
1	A	36	A
1	A	37	C
1	A	38	U
1	A	39	G
1	A	50	U

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Mol	Chain	Res	Type
1	A	55	C
1	A	56	C
1	A	62	C
1	A	69	G
1	A	70	G
1	A	72	A
1	A	74	A
1	A	76	U
1	A	82	G
1	A	89	G
1	A	109	U
1	A	110	A
1	A	111	C
1	A	112	G
1	A	118	A
1	A	119	G
1	A	120	A
1	A	153	G
1	A	160	A
1	A	161	U
1	A	169	A
1	A	170	G
1	A	175	G
1	A	180	G
1	A	191	A
1	A	192	U
1	A	193	C
1	A	194	C
1	A	195	G
1	A	199	G
1	A	203	C
1	A	205	U
1	A	206	C
1	A	207	U
1	A	208	A
1	A	209	G
1	A	212	A
1	A	227	G
1	A	228	U
1	A	233	G
1	A	243	C
1	A	244	A

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Mol	Chain	Res	Type
1	A	245	C
1	A	269	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	117	U
1	A	174	C

## 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 1 ligands modelled in this entry, 1 is 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.

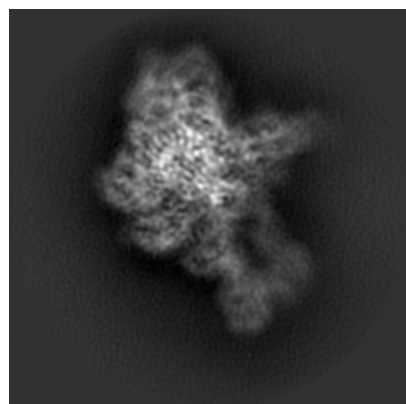
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64159. These allow visual inspection of the internal detail of the map and identification of artifacts.

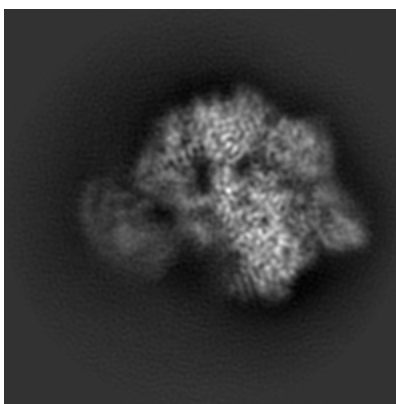
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

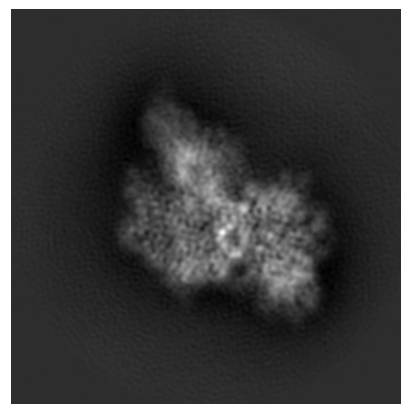
#### 6.1.1 Primary map



X

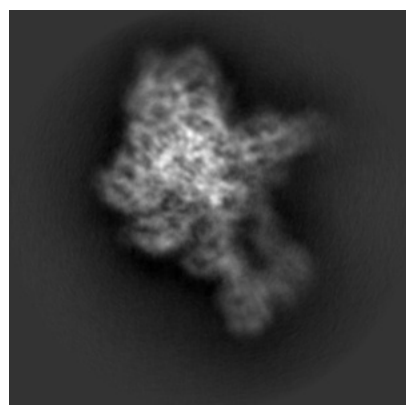


Y

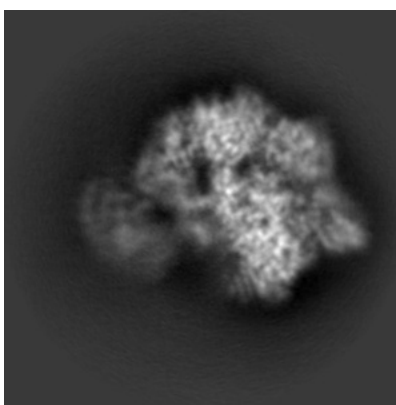


Z

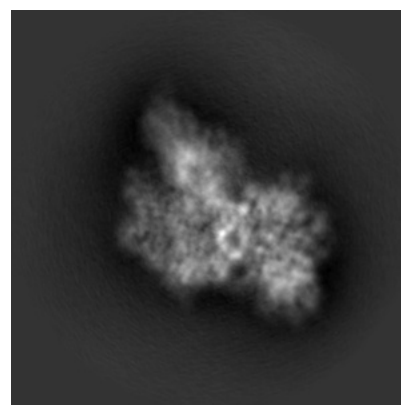
#### 6.1.2 Raw map



X



Y

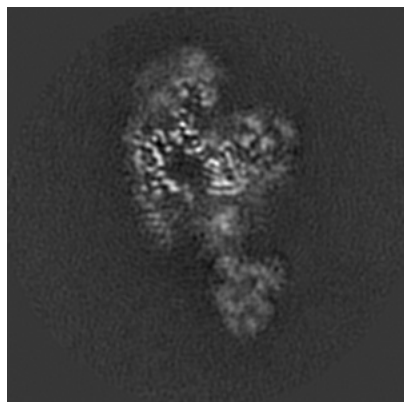


Z

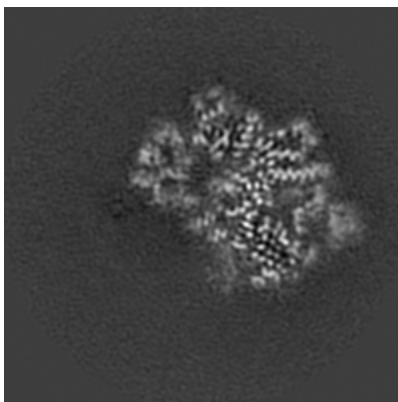
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

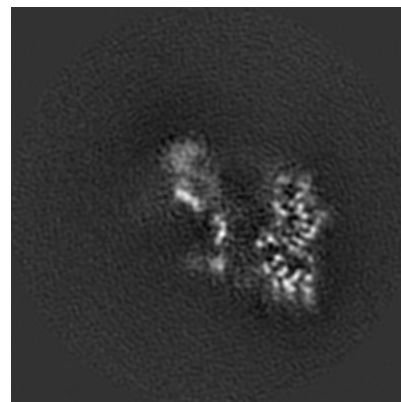
### 6.2.1 Primary map



X Index: 112

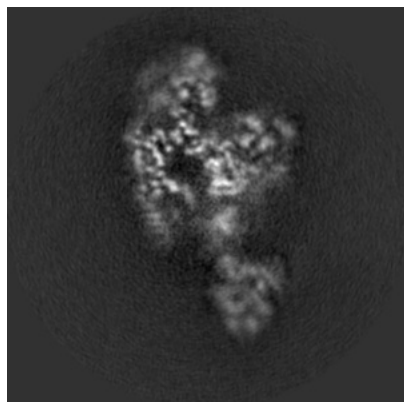


Y Index: 112

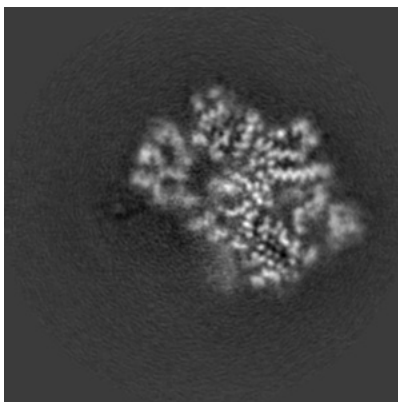


Z Index: 112

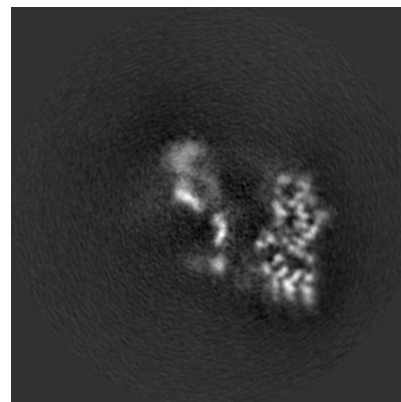
### 6.2.2 Raw map



X Index: 112



Y Index: 112

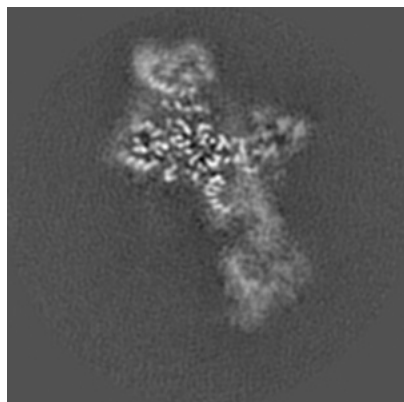


Z Index: 112

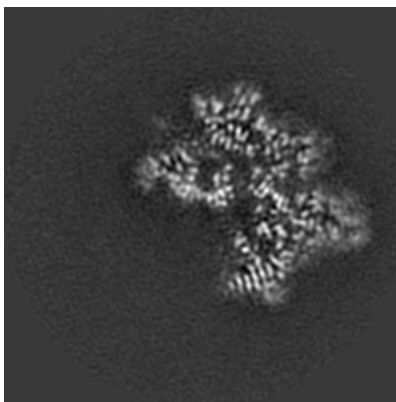
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

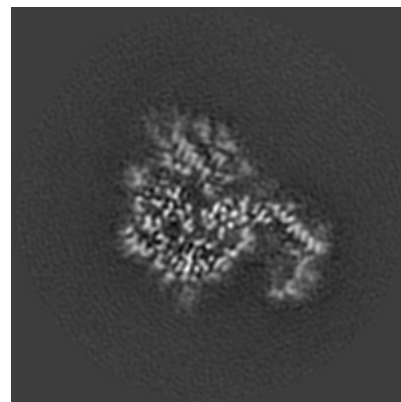
### 6.3.1 Primary map



X Index: 97

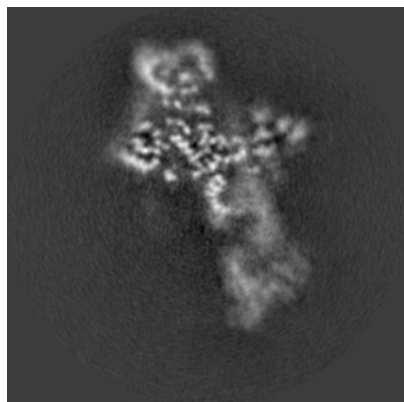


Y Index: 100

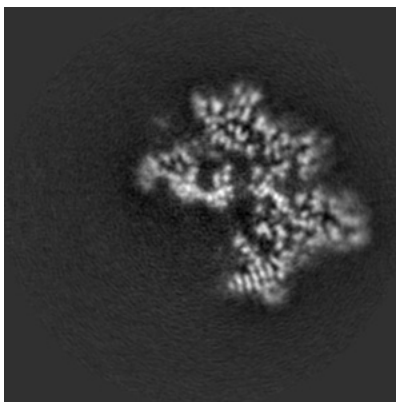


Z Index: 143

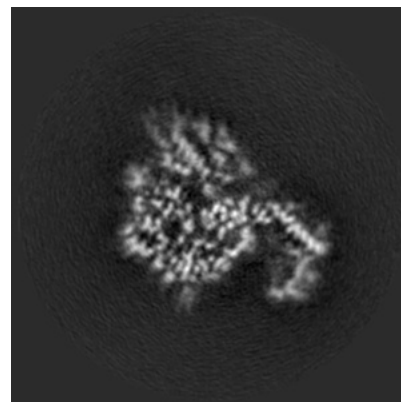
### 6.3.2 Raw map



X Index: 98



Y Index: 100



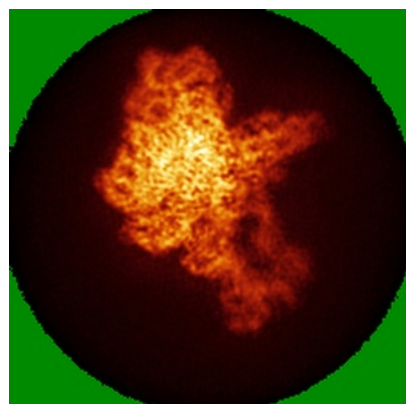
Z Index: 143

The images above show the largest variance slices of the map in three orthogonal directions.

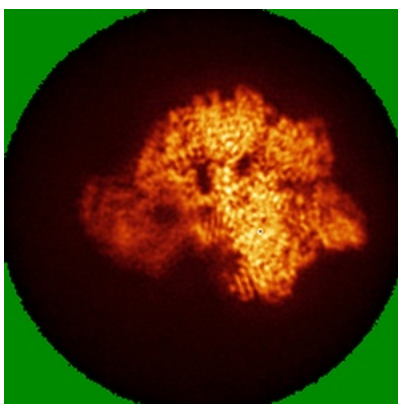


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

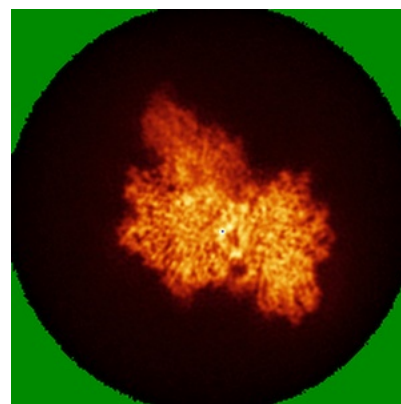
### 6.4.1 Primary map



X

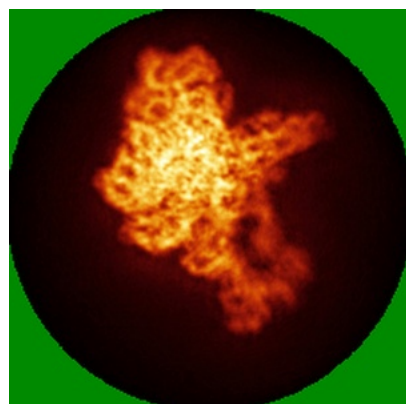


Y

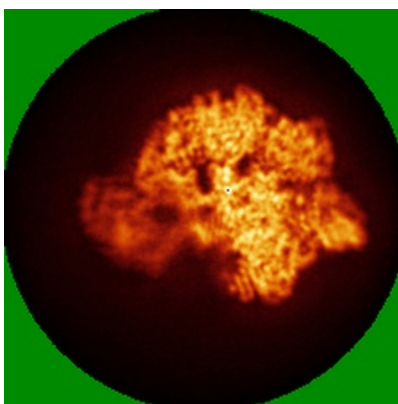


Z

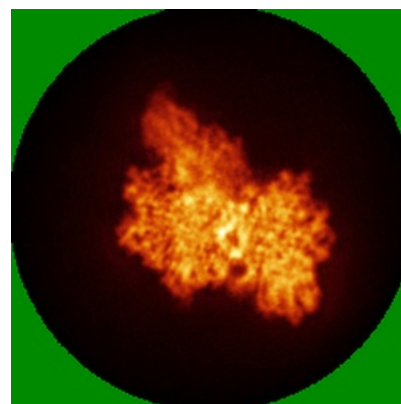
### 6.4.2 Raw map



X



Y

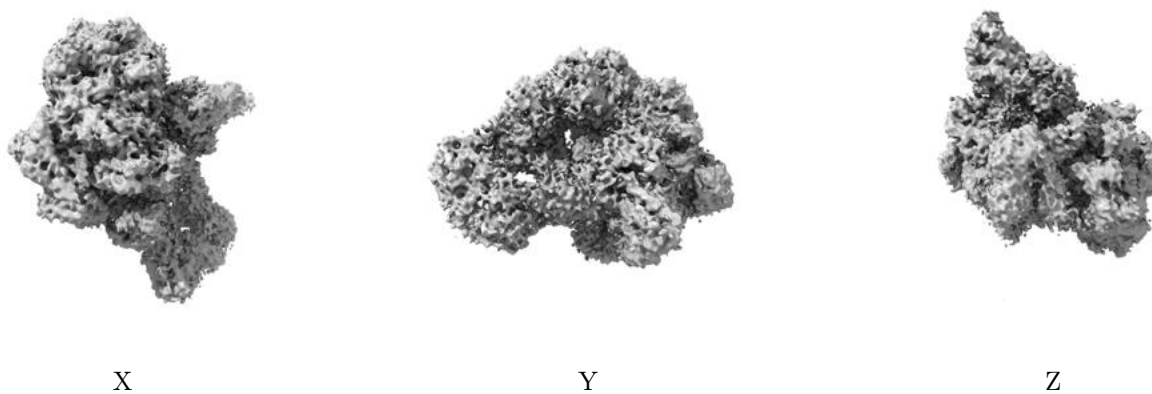


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

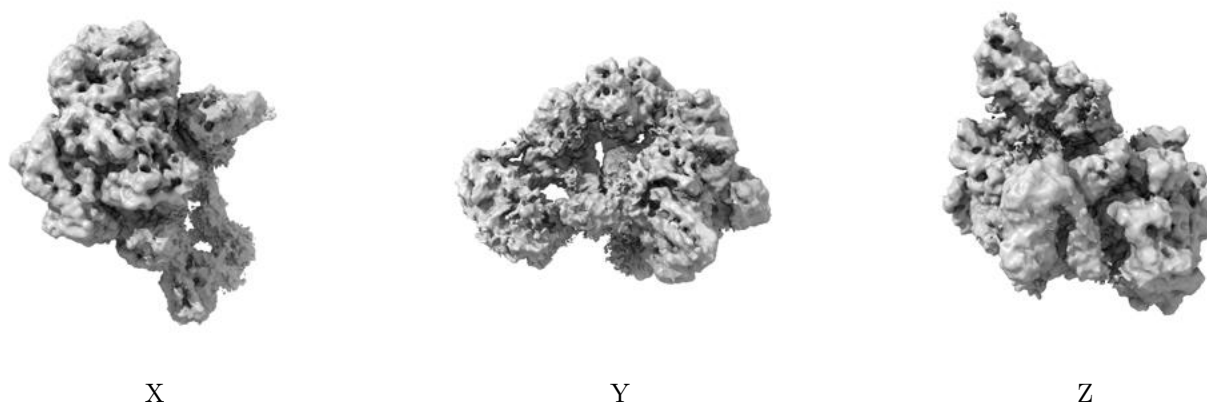
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

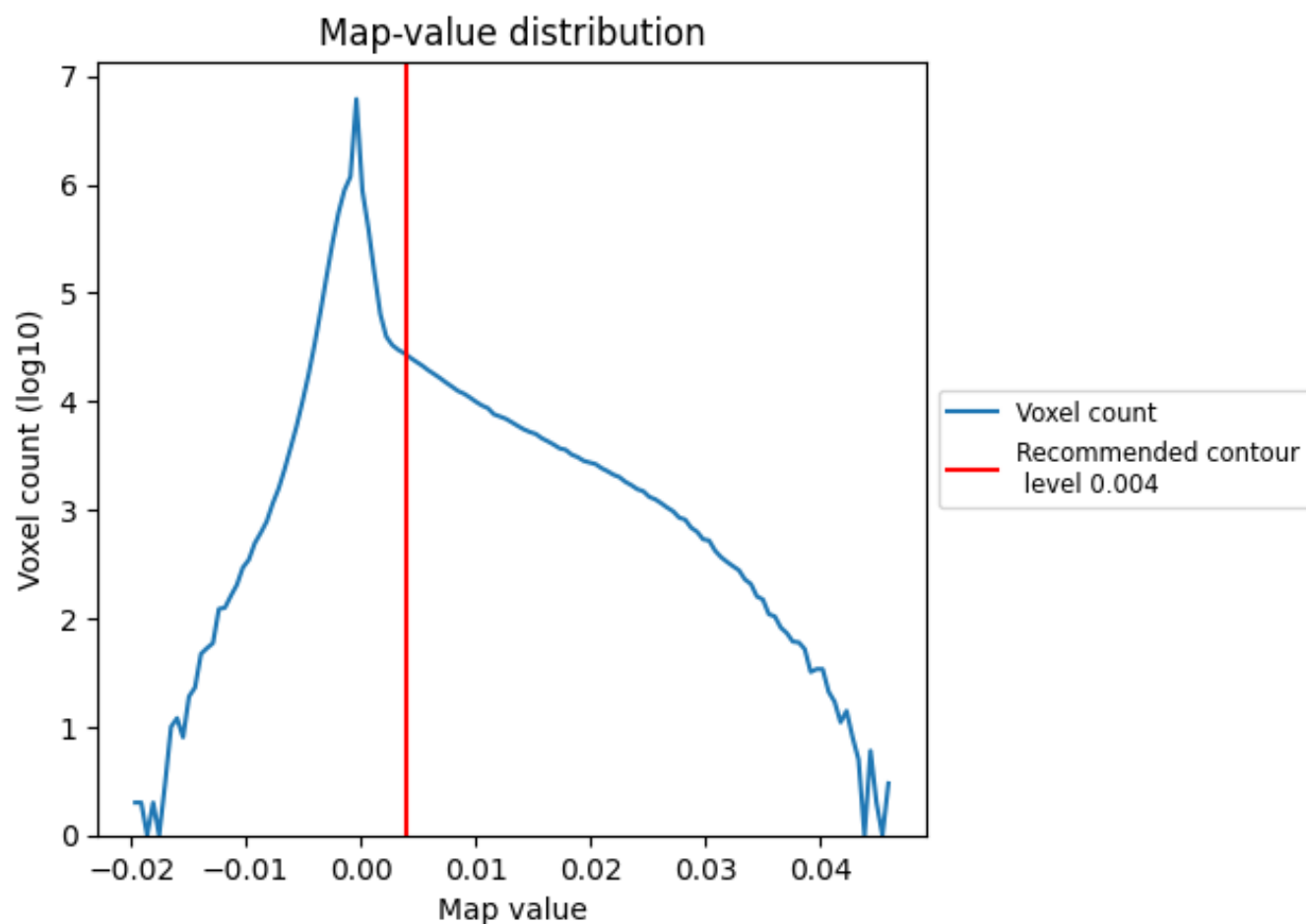
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

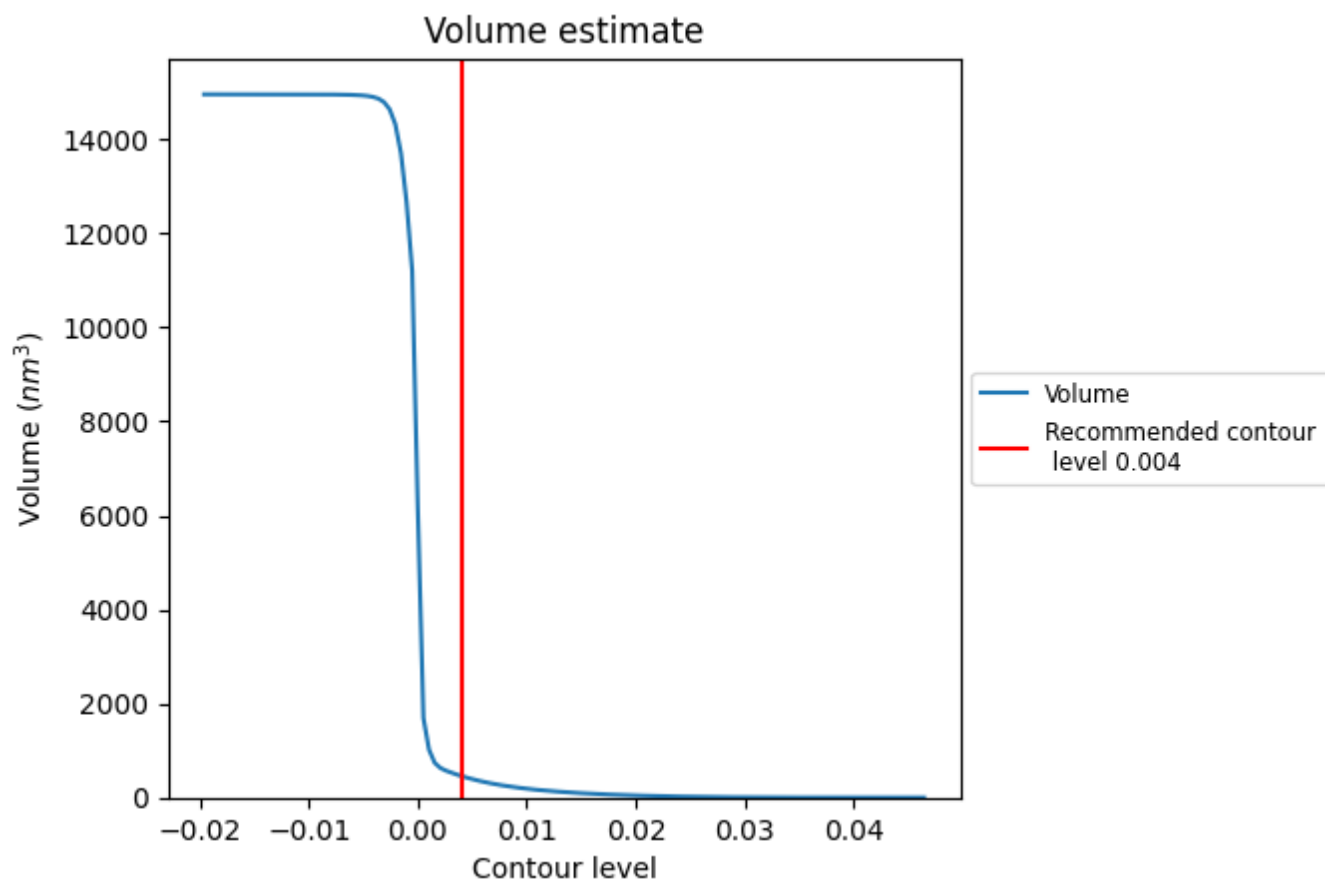
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

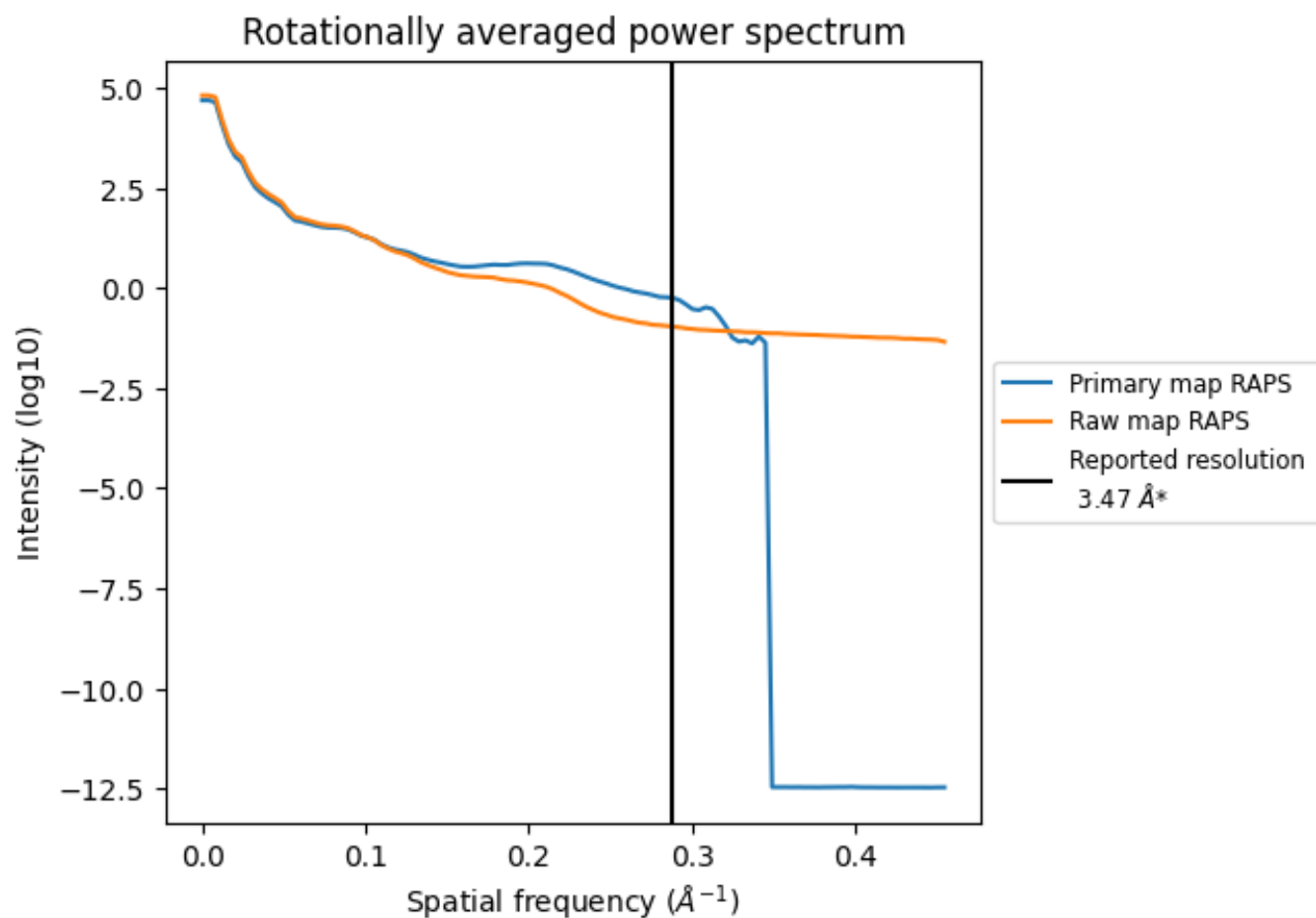
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 458  $\text{nm}^3$ ; this corresponds to an approximate mass of 413 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

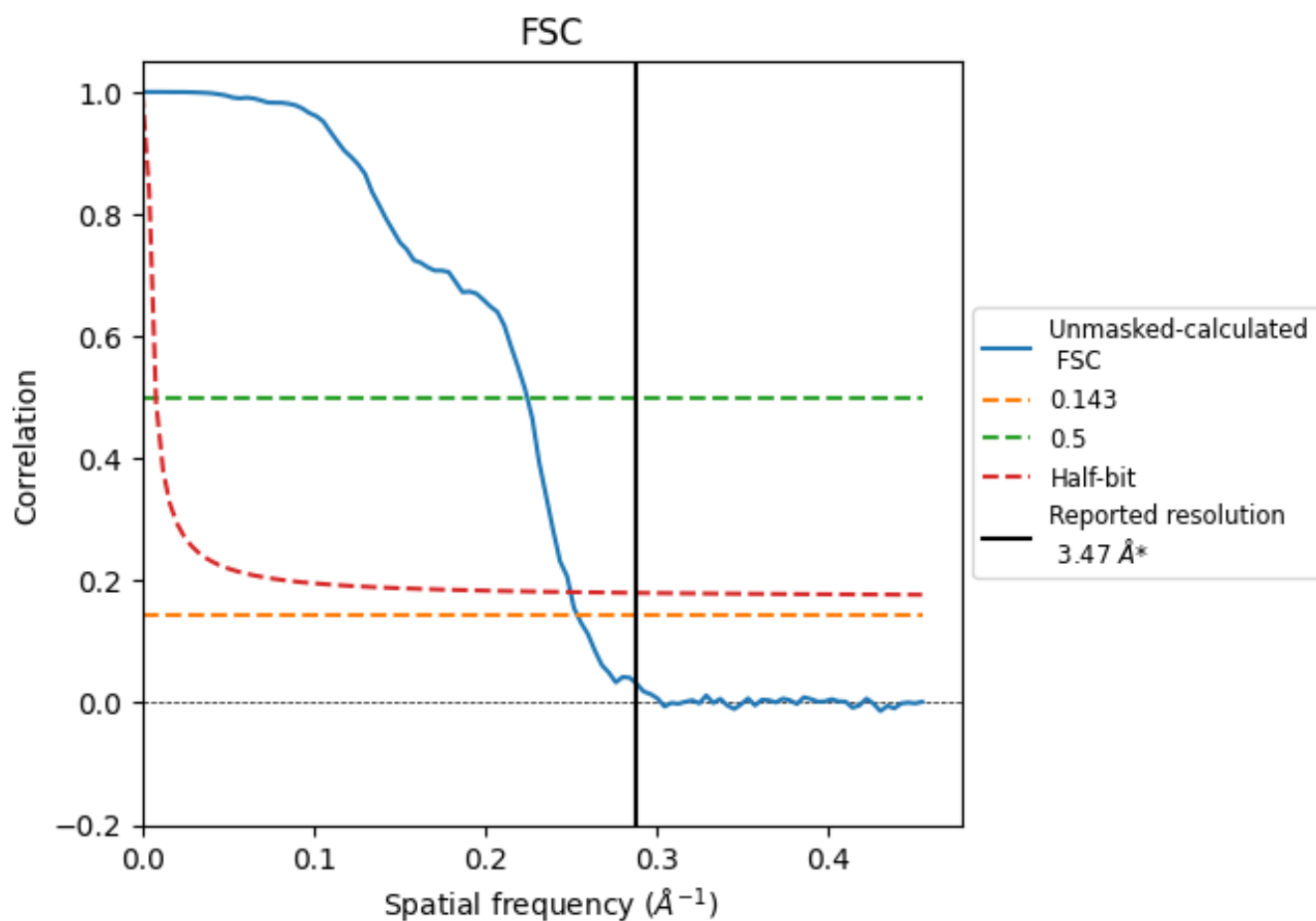


\*Reported resolution corresponds to spatial frequency of 0.288 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.288  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

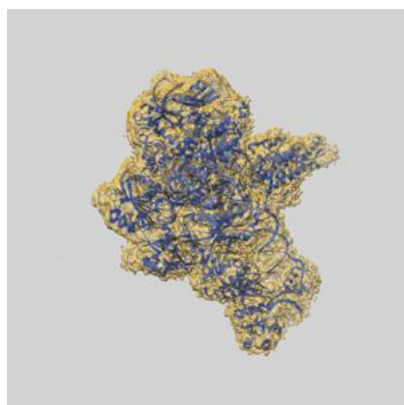
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	4.46	4.01

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.47 by more than 10 %

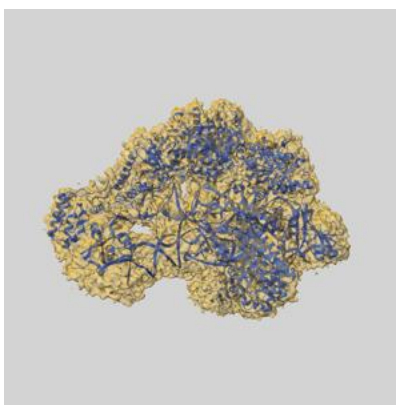
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64159 and PDB model 9UH9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

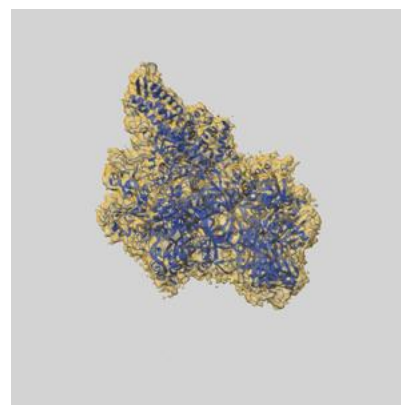
### 9.1 Map-model overlay [i](#)



X



Y

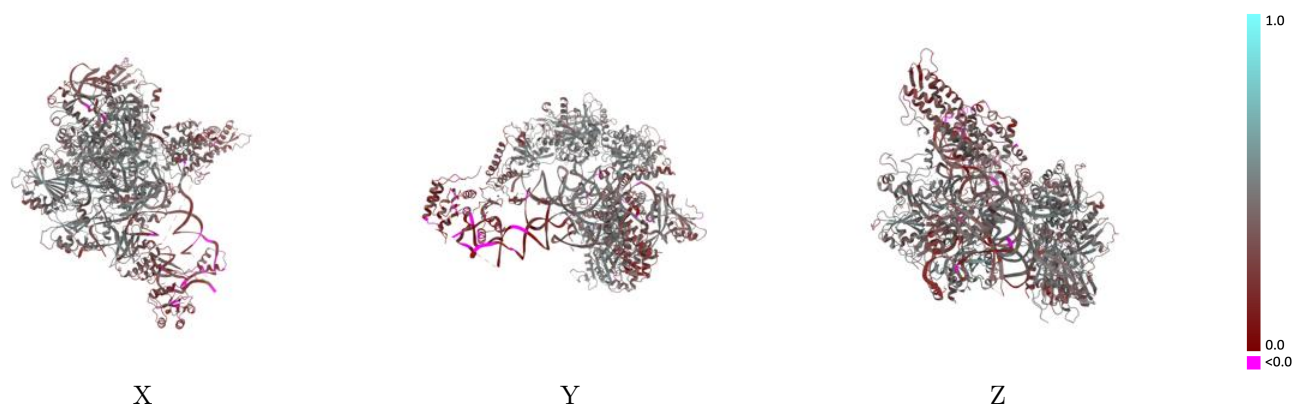


Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

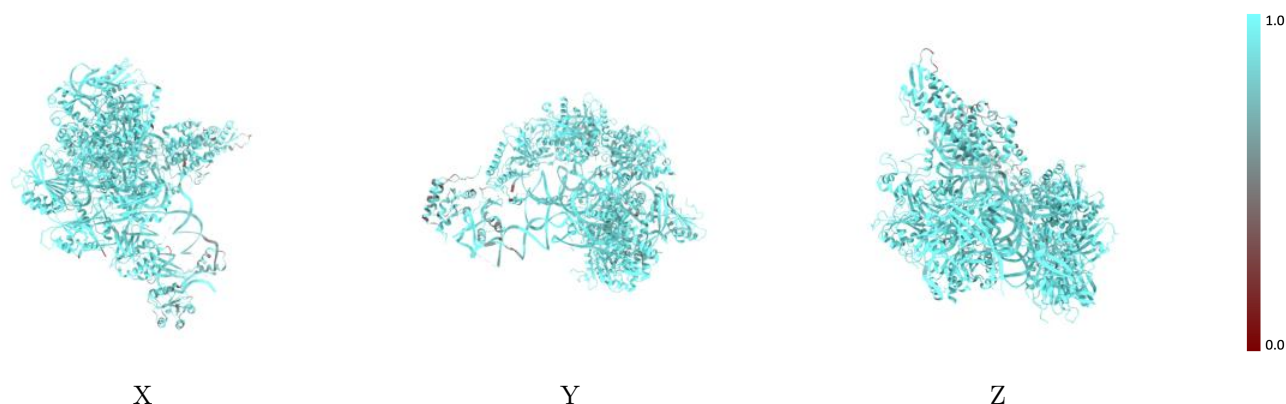


## 9.2 Q-score mapped to coordinate model [i](#)



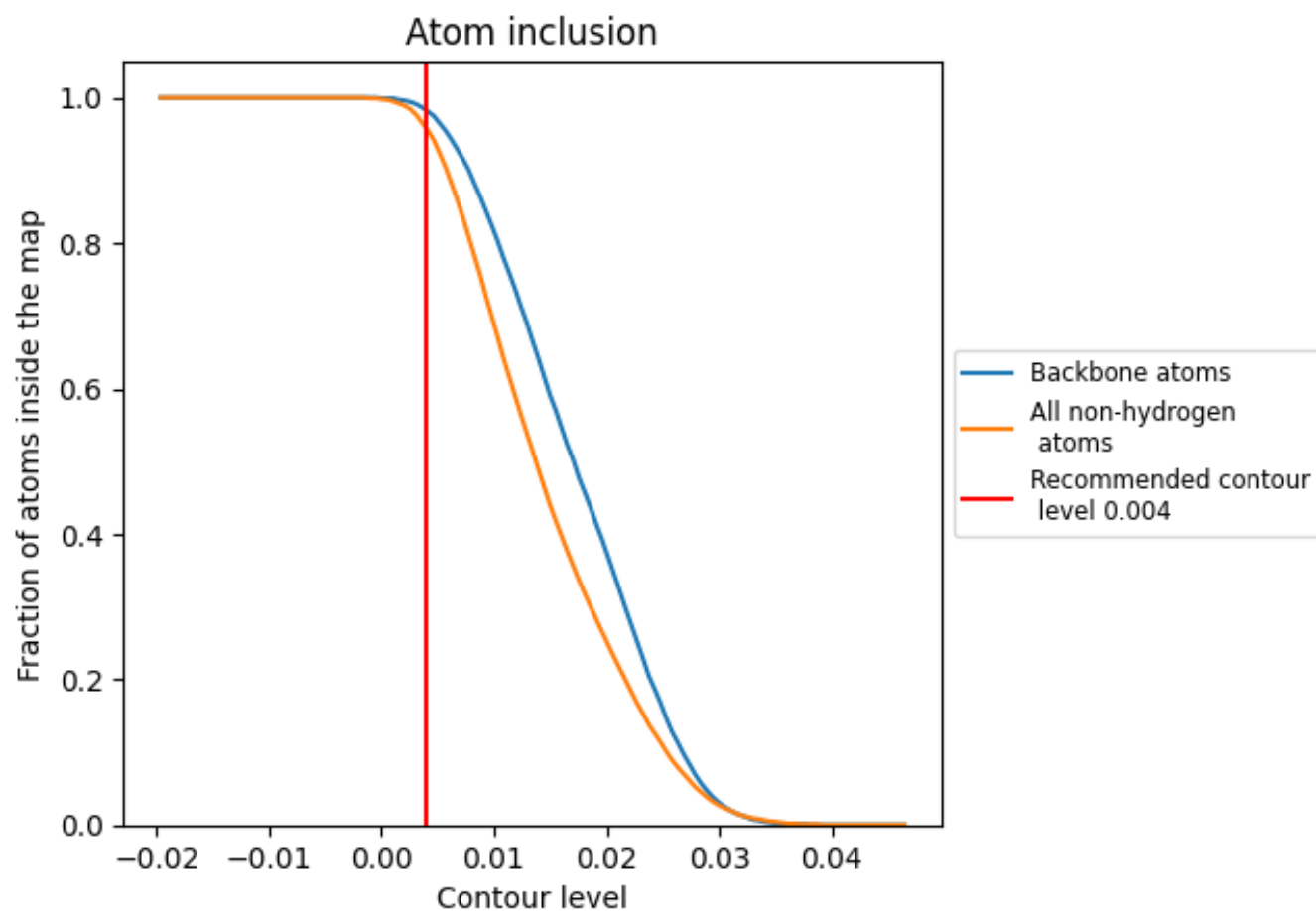
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.3920
A	 0.9530	 0.3210
B	 0.9770	 0.4570
C	 0.8180	 0.1940
D	 0.9300	 0.3650
E	 0.9690	 0.4530
F	 0.9910	 0.3200
G	 0.9760	 0.4410
H	 0.9850	 0.4690
I	 0.9820	 0.4040
J	 0.9850	 0.4510
K	 0.8560	 0.2650
L	 0.9850	 0.4580
M	 0.9340	 0.3510

