



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:31 PM UTC

PDB ID : 6YT9 / pdb_00006yt9
EMDB ID : EMD-10914
Title : Acinetobacter baumannii ribosome-tigecycline complex - 30S subunit body
Authors : Nicholson, D.; Edwards, T.A.; O'Neill, A.J.; Ranson, N.A.
Deposited on : 2020-04-24
Resolution : 2.70 Å (reported)
Based on initial models : 5MDZ, 5AFI

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:

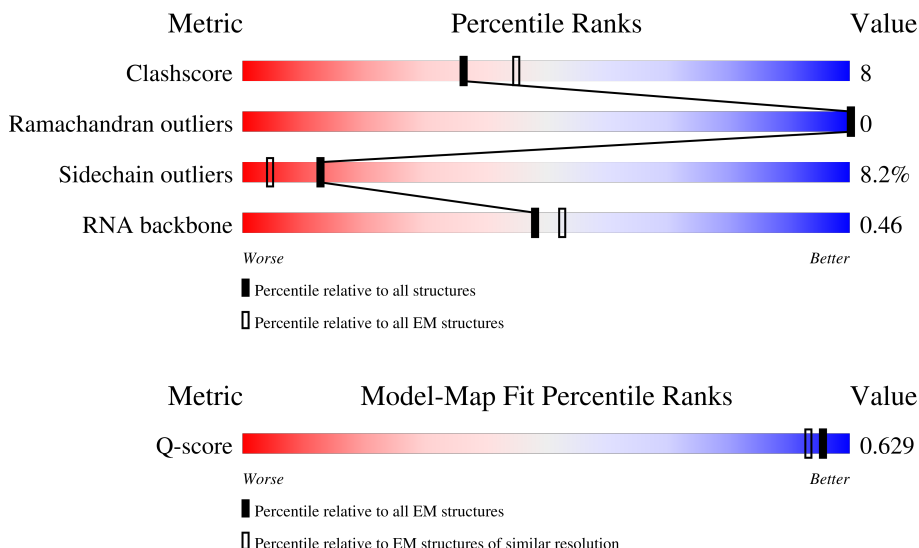
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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 $\leq 5\%$. 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	2	1544	
1	4	1544	
2	c	250	

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Mol	Chain	Length	Quality of chain
3	e	208	
4	f	165	
5	g	127	
6	i	131	
7	l	128	
8	m	124	
9	p	89	
10	q	83	
11	r	85	
12	s	75	
13	u	88	
14	v	71	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 33279 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	894	Total	C	N	O	P	0	0
			19228	8575	3556	6203	894		
1	4	146	Total	C	N	O	P	0	0
			3129	1395	572	1016	146		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	c	219	Total	C	N	O	0	0
			1079	641	219	219		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	207	Total	C	N	O	S	0	0
			1592	991	306	293	2		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	103	Total	C	N	O	S	0	0
			858	540	156	158	4		

- Molecule 6 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	130	Total	C	N	O	S	0	0
			984	615	177	186	6		

- Molecule 7 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	114	Total	C	N	O	S	0	0
			836	521	161	153	1		

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	p	88	Total	C	N	O	S	0	0
			704	434	144	125	1		

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	q	80	Total	C	N	O	S	0	0
			632	396	126	109	1		

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	r	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	s	53	Total	C	N	O	0	0
			434	277	76	81		

- Molecule 13 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	u	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

- Molecule 14 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	v	60	Total	C	N	O	0	0
			389	242	78	69		

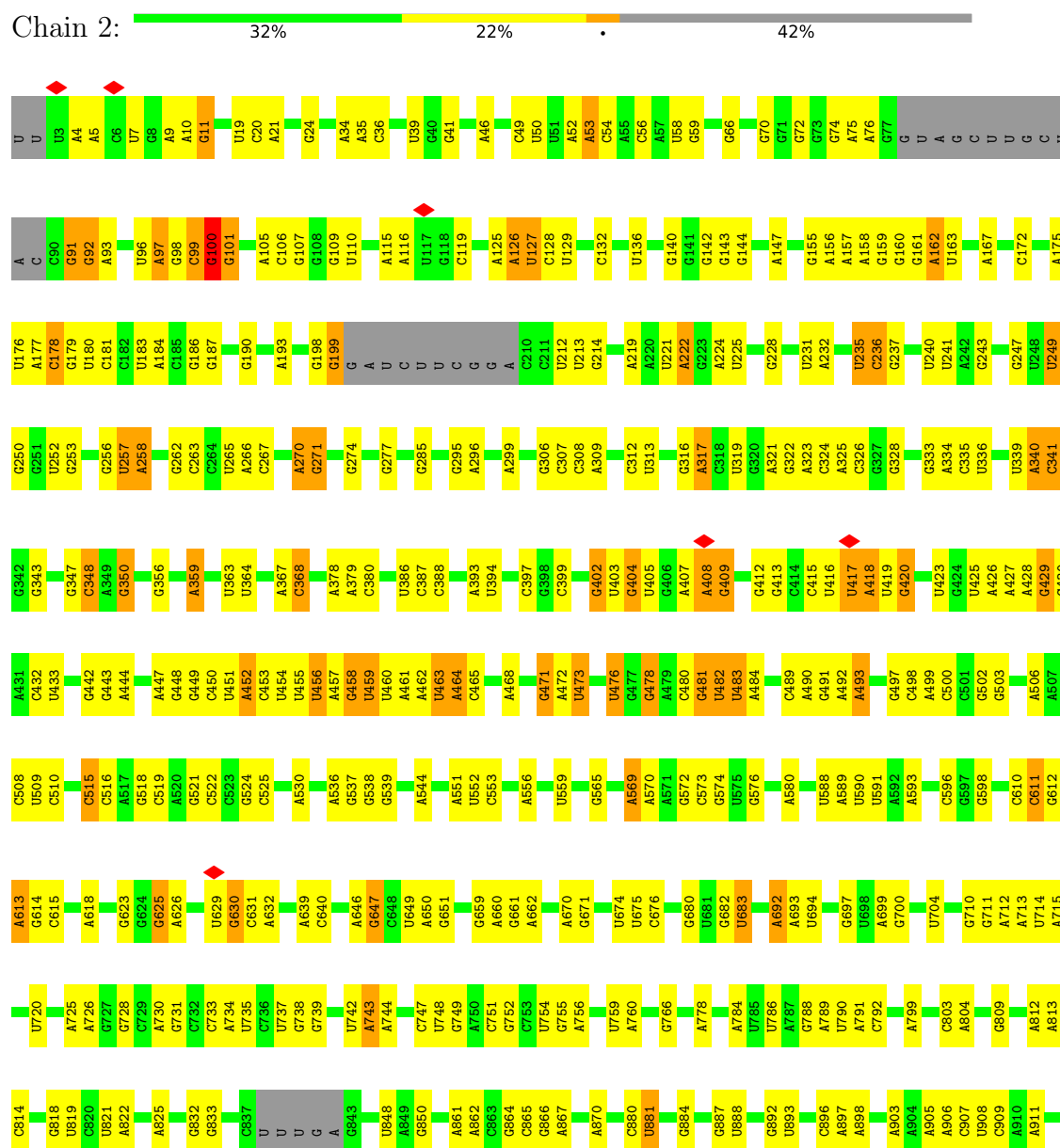
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

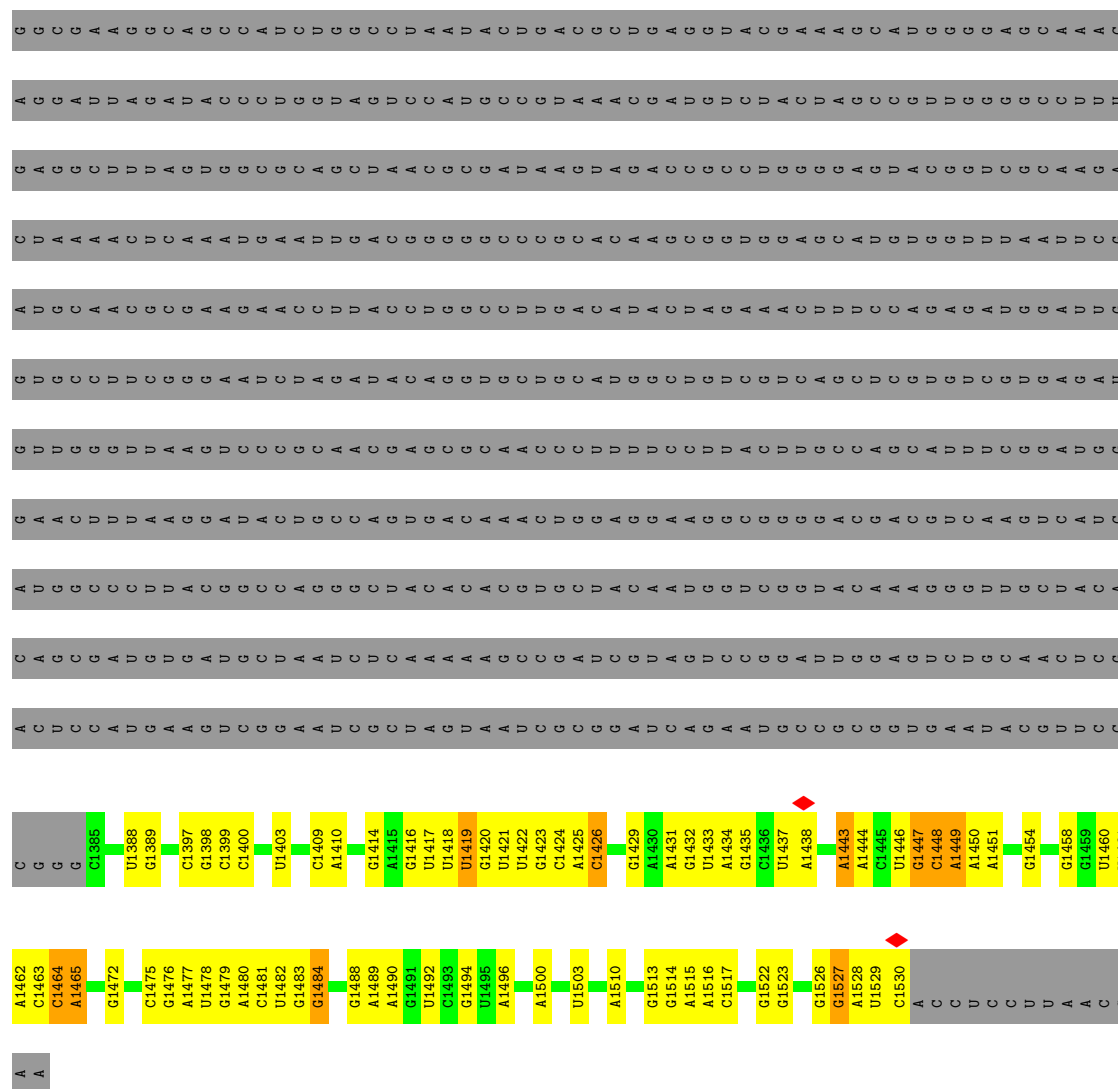
Mol	Chain	Residues	Atoms		AltConf
15	2	51	Total	Mg	0
			51	51	
15	4	5	Total	Mg	0
			5	5	

3 Residue-property plots

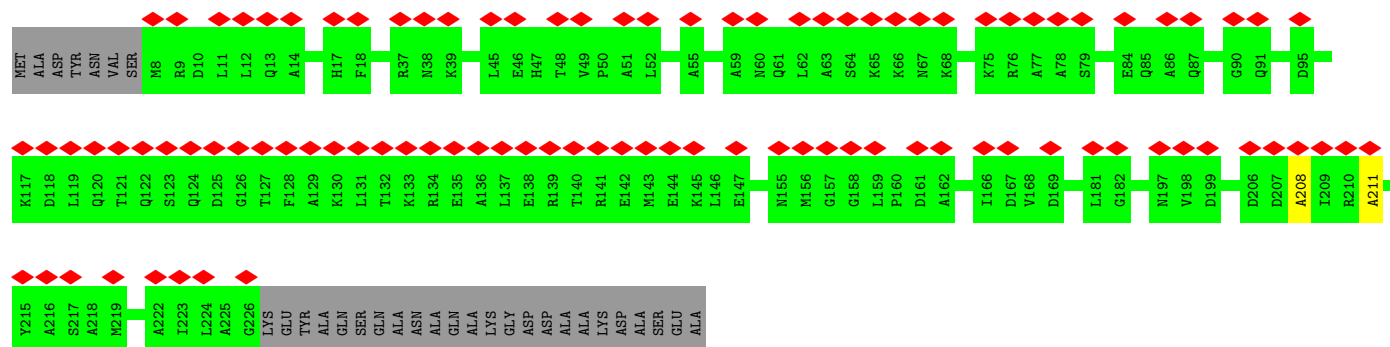
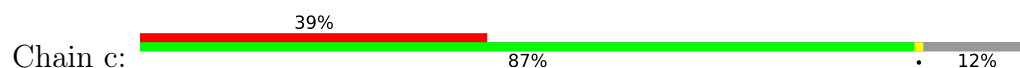
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 16S ribosomal RNA



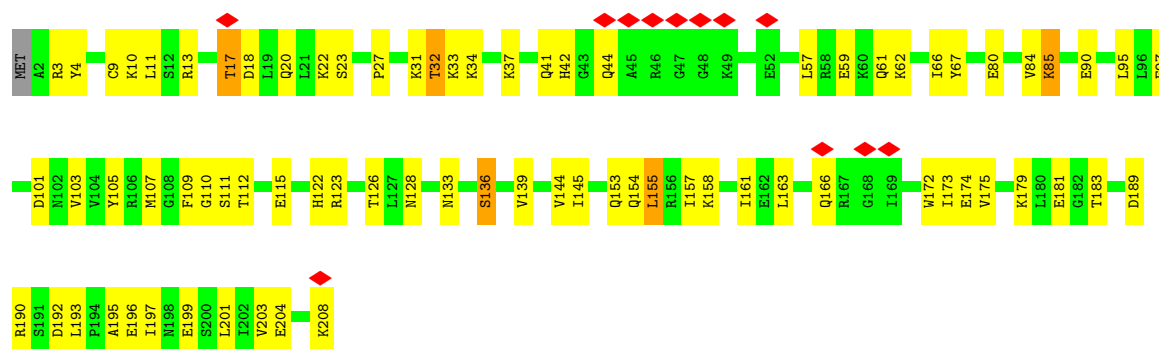


• Molecule 2: 30S ribosomal protein S2

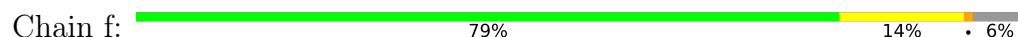


• Molecule 3: 30S ribosomal protein S4

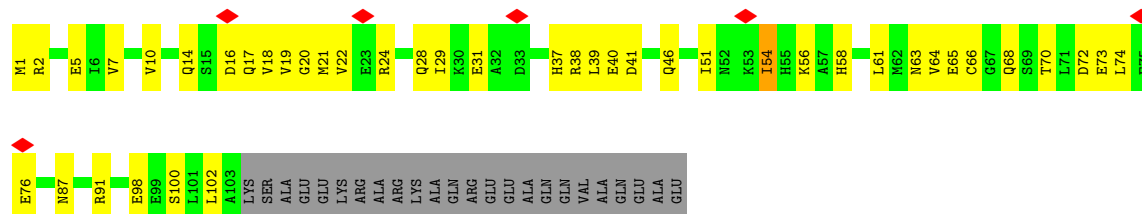




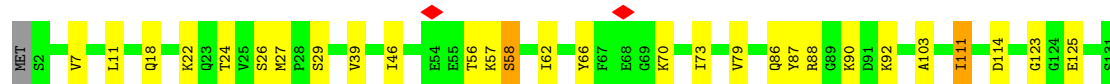
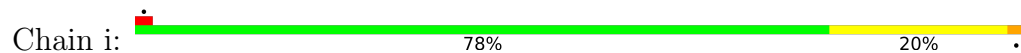
- Molecule 4: 30S ribosomal protein S5



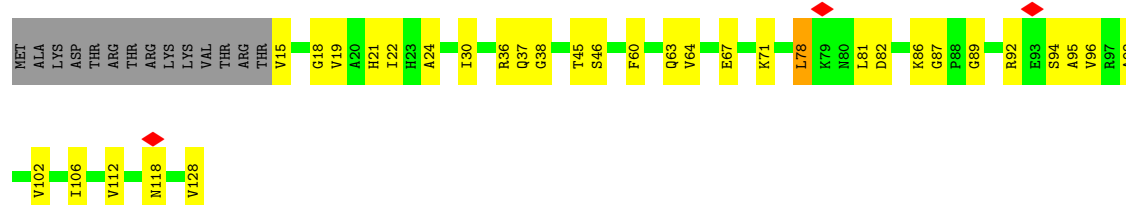
- Molecule 5: 30S ribosomal protein S6



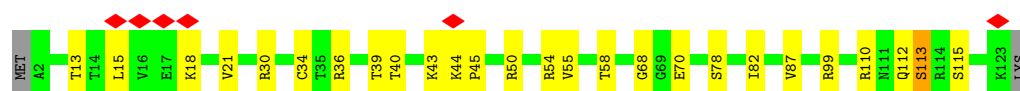
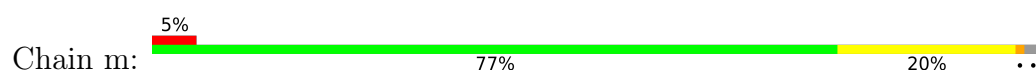
- Molecule 6: 30S ribosomal protein S8



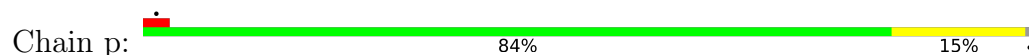
- Molecule 7: 30S ribosomal protein S11



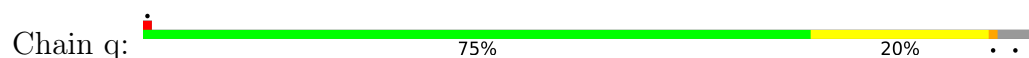
- Molecule 8: 30S ribosomal protein S12



- Molecule 9: 30S ribosomal protein S15



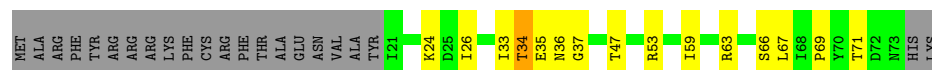
- Molecule 10: 30S ribosomal protein S16



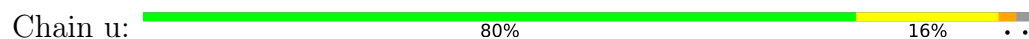
- Molecule 11: 30S ribosomal protein S17



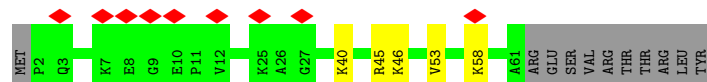
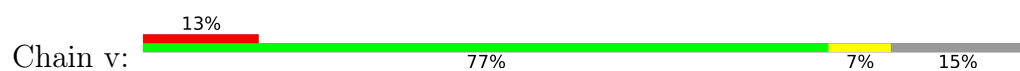
- Molecule 12: 30S ribosomal protein S18



- Molecule 13: 30S ribosomal protein S20



- Molecule 14: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	231159	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 ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.545	Depositor
Minimum map value	-0.279	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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	2	0.56	0/21541	0.42	1/33605 (0.0%)
1	4	0.49	0/3501	0.38	0/5459
2	c	0.16	0/1078	0.36	0/1498
3	e	0.35	0/1612	0.52	0/2162
4	f	0.39	0/1141	0.50	0/1537
5	g	0.34	0/873	0.45	0/1178
6	i	0.42	0/992	0.44	0/1331
7	l	0.32	0/852	0.44	0/1155
8	m	0.42	0/958	0.51	0/1284
9	p	0.40	0/714	0.45	0/958
10	q	0.45	0/643	0.48	0/862
11	r	0.35	0/628	0.46	0/847
12	s	0.40	0/440	0.45	0/594
13	u	0.41	0/669	0.44	0/892
14	v	0.27	0/392	0.47	0/528
All	All	0.50	0/36034	0.43	1/53890 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	100	G	N9-C1'-C2'	-5.57	103.64	112.00

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	2	19228	0	9654	219	0
1	4	3129	0	1579	50	0
2	c	1079	0	518	1	0
3	e	1592	0	1611	49	0
4	f	1129	0	1174	11	0
5	g	858	0	855	22	0
6	i	984	0	1047	16	0
7	l	836	0	850	16	0
8	m	945	0	998	12	0
9	p	704	0	712	9	0
10	q	632	0	646	13	0
11	r	621	0	665	13	0
12	s	434	0	453	8	0
13	u	663	0	715	12	0
14	v	389	0	318	3	0
15	2	51	0	0	0	0
15	4	5	0	0	0	0
All	All	33279	0	21795	407	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 8.

All (407) 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)
1:2:75:A:N6	1:2:92:G:H1	1.22	1.38
1:2:74:G:H1	1:2:93:A:N6	1.26	1.31
1:2:76:A:N6	1:2:91:G:H1	1.31	1.25
1:2:74:G:N2	1:2:93:A:N1	2.12	0.98
1:2:198:G:HO2'	1:2:464:A:H8	1.04	0.96
1:2:76:A:N1	1:2:91:G:N2	2.17	0.92
1:2:651:G:H1	1:2:751:C:H5	1.18	0.89
1:2:75:A:N1	1:2:92:G:N2	2.21	0.87
1:2:142:G:H1	1:2:172:C:H5	1.20	0.86
1:4:1447:G:H21	1:4:1450:A:H2	1.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:423:U:OP1	3:e:13:ARG:NH2	2.12	0.82
1:2:99:C:HO2'	1:2:100:G:H8	1.32	0.76
5:g:68:GLN:NE2	5:g:72:ASP:OD1	2.19	0.75
1:2:161:G:H2'	1:2:162:A:H8	1.51	0.75
1:2:612:G:HO2'	1:2:613:A:H8	1.35	0.74
5:g:40:GLU:OE1	5:g:100:SER:OG	2.06	0.72
1:2:179:G:N2	1:2:219:A:O2'	2.23	0.72
1:4:1527:G:O6	14:v:46:LYS:NZ	2.22	0.72
1:2:661:G:H22	1:2:738:G:H1	1.36	0.71
7:l:24:ALA:HB1	7:l:89:GLY:HA3	1.72	0.71
5:g:28:GLN:NE2	5:g:73:GLU:OE2	2.23	0.71
1:2:674:U:H3	1:2:710:G:H22	1.36	0.70
1:2:832:G:OP1	12:s:53:ARG:NH2	2.24	0.70
10:q:4:ILE:HG12	10:q:21:VAL:HG22	1.72	0.70
1:2:481:G:H4'	1:2:482:U:H5'	1.72	0.70
1:4:1429:G:O2'	1:4:1465:A:N6	2.24	0.70
5:g:5:GLU:OE2	12:s:24:LYS:NZ	2.25	0.69
9:p:4:THR:HG23	9:p:6:ALA:H	1.57	0.69
1:2:125:A:O2'	1:2:126:A:H2'	1.93	0.69
5:g:10:VAL:HG22	5:g:58:HIS:HB3	1.75	0.69
1:2:179:G:H1	1:2:190:G:H22	1.39	0.68
1:2:178:C:H3'	1:2:179:G:H8	1.59	0.68
1:2:456:U:H2'	1:2:457:A:H8	1.58	0.68
1:2:747:C:O2'	9:p:21:ASP:O	2.08	0.67
7:l:30:ILE:HG23	7:l:45:THR:HG22	1.77	0.67
7:l:87:GLY:O	7:l:92:ARG:NH1	2.27	0.67
1:2:907:C:OP2	8:m:18:LYS:NZ	2.28	0.67
1:2:670:A:H2'	1:2:671:G:C8	2.30	0.67
1:2:733:C:H2'	1:2:734:A:C8	2.30	0.67
10:q:14:ARG:HH22	10:q:44:GLN:HE21	1.43	0.66
1:2:714:U:H4'	7:l:118:ASN:HD22	1.58	0.66
1:2:161:G:H2'	1:2:162:A:C8	2.31	0.66
1:4:1522:G:OP2	14:v:40:LYS:NZ	2.28	0.65
1:2:408:A:H62	1:2:427:A:H61	1.45	0.65
1:2:125:A:H1'	1:2:126:A:C8	2.31	0.65
11:r:59:VAL:HB	11:r:81:GLU:HB2	1.77	0.65
11:r:29:ARG:HG2	11:r:38:SER:HB2	1.76	0.65
1:2:99:C:OP1	13:u:12:ARG:NH2	2.30	0.65
1:2:447:A:H61	1:2:478:G:H5'	1.61	0.65
1:2:680:G:N2	7:l:38:GLY:O	2.29	0.65
1:4:1513:G:N2	1:4:1516:A:OP2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:33:THR:HG22	4:f:51:LYS:HG2	1.79	0.64
1:4:1419:U:O4	1:4:1475:C:N3	2.31	0.64
1:2:784:A:N1	1:2:792:C:N4	2.45	0.63
1:2:399:C:OP1	3:e:136:SER:OG	2.16	0.63
1:2:632:A:O2'	11:r:7:ARG:NH2	2.32	0.63
1:4:1388:U:H2'	1:4:1389:G:C8	2.34	0.63
1:2:462:A:O2'	1:2:463:U:O2	2.16	0.62
3:e:27:PRO:HA	3:e:31:LYS:HB3	1.81	0.61
1:2:10:A:N6	3:e:204:GLU:O	2.33	0.61
7:l:67:GLU:OE1	7:l:71:LYS:NZ	2.34	0.61
4:f:114:LEU:HD13	4:f:122:VAL:HG11	1.81	0.61
1:2:409:G:N7	3:e:33:LYS:NZ	2.48	0.60
1:4:1410:A:H2	1:4:1484:G:H22	1.49	0.60
8:m:34:CYS:SG	8:m:78:SER:HB2	2.41	0.60
1:2:75:A:N6	1:2:92:G:C6	2.59	0.60
1:2:99:C:O2'	1:2:100:G:H8	1.84	0.60
1:4:1454:G:H5'	13:u:30:THR:HG21	1.84	0.60
1:2:456:U:H2'	1:2:457:A:C8	2.36	0.60
1:4:1488:G:H2'	1:4:1489:A:C8	2.37	0.59
3:e:107:MET:HG2	3:e:173:ILE:HG21	1.84	0.59
6:i:79:VAL:HG12	6:i:86:GLN:HG3	1.84	0.59
11:r:48:HIS:HB2	11:r:72:LYS:HD3	1.84	0.58
1:2:629:U:H5''	1:2:630:G:C8	2.39	0.58
3:e:174:GLU:N	3:e:174:GLU:OE2	2.35	0.58
1:2:198:G:O2'	1:2:464:A:H8	1.79	0.57
1:2:403:U:H2'	1:2:404:G:H5''	1.86	0.57
1:2:710:G:H2'	1:2:711:G:C8	2.39	0.57
11:r:51:ASN:HB2	11:r:53:VAL:HG23	1.86	0.57
1:2:109:G:H1'	1:2:350:G:H5'	1.86	0.57
4:f:102:THR:O	4:f:121:ASN:ND2	2.24	0.57
1:2:482:U:O2'	1:2:483:U:OP1	2.22	0.57
1:2:610:C:H2'	1:2:611:C:C6	2.40	0.57
1:2:199:G:O2'	1:2:461:A:N6	2.38	0.56
1:2:177:A:O2'	1:2:179:G:O6	2.19	0.56
1:2:265:U:H2'	1:2:266:A:C8	2.40	0.56
4:f:110:MET:HE2	4:f:126:CYS:SG	2.45	0.56
8:m:44:LYS:HB3	8:m:45:PRO:HD3	1.86	0.56
1:2:623:G:O2'	10:q:51:ARG:NH2	2.38	0.56
1:2:125:A:H62	1:2:228:G:H1	1.54	0.56
1:2:612:G:O2'	1:2:613:A:H8	1.89	0.56
6:i:22:LYS:O	6:i:66:TYR:OH	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:596:C:H4'	6:i:123:GLY:O	2.06	0.55
7:l:36:ARG:HB2	7:l:37:GLN:HE21	1.71	0.55
1:2:423:U:OP2	3:e:34:LYS:NZ	2.39	0.55
12:s:34:THR:OG1	12:s:36:ASN:OD1	2.25	0.55
1:4:1460:U:H2'	1:4:1461:U:C6	2.41	0.55
7:l:86:LYS:HB2	7:l:112:VAL:HG23	1.88	0.55
1:2:813:A:OP1	1:4:1523:G:O2'	2.24	0.55
3:e:174:GLU:HG2	3:e:183:THR:HG23	1.88	0.55
9:p:47:LYS:O	9:p:53:ARG:NH2	2.40	0.55
1:2:449:G:O6	1:2:476:U:O4	2.24	0.54
1:2:887:G:N2	1:2:888:U:O4	2.25	0.54
1:2:733:C:H2'	1:2:734:A:H8	1.72	0.54
3:e:37:LYS:HG3	3:e:44:GLN:HA	1.88	0.54
1:2:316:G:H2'	1:2:317:A:O4'	2.08	0.53
1:4:1432:G:H2'	1:4:1433:U:C6	2.43	0.53
3:e:20:GLN:OE1	3:e:105:TYR:OH	2.27	0.53
3:e:123:ARG:HG3	3:e:133:ASN:HB3	1.90	0.53
4:f:55:VAL:O	4:f:59:ILE:HG13	2.08	0.53
11:r:55:LYS:N	11:r:58:ASP:OD1	2.33	0.53
1:2:588:U:H2'	1:2:589:A:C8	2.44	0.53
3:e:67:TYR:OH	3:e:97:GLU:OE2	2.13	0.53
1:2:905:A:H2'	1:2:906:A:C8	2.44	0.53
10:q:48:GLU:OE1	10:q:51:ARG:NH1	2.42	0.53
1:2:92:G:H2'	1:2:93:A:H8	1.73	0.53
1:2:75:A:N6	1:2:92:G:N1	2.00	0.53
1:2:143:G:H2'	1:2:144:G:C8	2.43	0.53
1:2:598:G:OP1	6:i:90:LYS:NZ	2.42	0.53
1:2:821:U:H2'	1:2:822:A:C8	2.45	0.52
1:2:443:G:N1	1:2:483:U:OP2	2.39	0.52
5:g:29:ILE:HD11	5:g:74:LEU:HD11	1.92	0.52
3:e:111:SER:OG	3:e:115:GLU:OE1	2.27	0.52
1:2:19:U:H2'	1:2:20:C:C6	2.45	0.52
1:2:521:G:H2'	1:2:522:C:C6	2.45	0.52
1:2:52:A:O2'	1:2:356:G:N2	2.43	0.52
1:2:715:A:H5'	7:l:118:ASN:HB2	1.91	0.52
5:g:21:MET:HG2	5:g:24:ARG:HH21	1.75	0.52
3:e:157:ILE:O	3:e:161:ILE:HG12	2.10	0.51
3:e:154:GLN:HG3	3:e:157:ILE:HD12	1.92	0.51
1:2:127:U:H2'	1:2:128:C:C6	2.45	0.51
1:4:1478:U:H2'	1:4:1479:G:C8	2.45	0.51
3:e:23:SER:H	3:e:112:THR:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:114:ASP:OD2	6:i:114:ASP:N	2.37	0.51
1:2:651:G:N1	1:2:751:C:H5	1.99	0.51
1:4:1434:A:OP1	13:u:29:ARG:NH2	2.43	0.51
6:i:29:SER:HB3	6:i:58:SER:HB3	1.92	0.51
1:2:100:G:OP1	13:u:16:LYS:NZ	2.38	0.51
1:2:693:A:H2'	1:2:694:U:H6	1.76	0.50
1:2:892:G:H2'	1:2:893:U:C6	2.46	0.50
3:e:179:LYS:HE2	3:e:181:GLU:OE1	2.11	0.50
5:g:20:GLY:O	5:g:24:ARG:HG3	2.11	0.50
1:2:386:U:H2'	1:2:387:C:C6	2.46	0.50
1:2:754:U:OP1	1:2:819:U:O2'	2.25	0.50
10:q:59:HIS:O	10:q:63:GLN:HG2	2.12	0.50
1:4:1478:U:H2'	1:4:1479:G:H8	1.77	0.50
1:2:132:C:O2'	10:q:66:GLN:NE2	2.45	0.50
1:2:183:U:OP1	13:u:77:SER:OG	2.29	0.50
1:2:661:G:OP1	12:s:53:ARG:NH1	2.44	0.49
1:4:1523:G:OP1	14:v:45:ARG:NH2	2.44	0.49
4:f:74:ASP:OD2	4:f:74:ASP:N	2.34	0.49
1:2:675:U:H2'	1:2:676:C:C6	2.46	0.49
1:2:142:G:N1	1:2:172:C:H5	2.01	0.49
1:2:367:A:H2'	1:2:368:C:O4'	2.12	0.49
1:2:519:C:H41	8:m:50:ARG:NH2	2.10	0.49
1:2:743:A:H2'	1:2:744:A:C8	2.48	0.49
1:2:458:G:H3'	1:2:459:U:H6	1.78	0.49
1:2:552:U:H2'	1:2:553:C:C6	2.48	0.49
3:e:172:TRP:CZ3	3:e:192:ASP:HB3	2.48	0.49
1:2:426:A:OP2	3:e:22:LYS:NZ	2.46	0.49
3:e:57:LEU:O	3:e:61:GLN:HG2	2.12	0.49
1:2:231:U:H2'	1:2:232:A:C8	2.48	0.49
1:4:1409:C:H2'	1:4:1410:A:C8	2.47	0.49
3:e:189:ASP:N	3:e:189:ASP:OD1	2.45	0.49
1:2:96:U:O2'	1:2:97:A:N7	2.41	0.49
8:m:36:ARG:HB3	8:m:54:ARG:HB3	1.95	0.49
1:2:306:G:H5''	10:q:31:ARG:HB2	1.95	0.48
1:2:737:U:OP1	9:p:2:ALA:N	2.46	0.48
1:2:766:G:H4'	1:4:1510:A:H4'	1.95	0.48
1:2:198:G:O2'	1:2:464:A:H2'	2.12	0.48
11:r:50:GLU:OE1	11:r:50:GLU:N	2.45	0.48
1:2:402:G:O3'	3:e:3:ARG:NH2	2.46	0.48
1:2:449:G:O6	1:2:476:U:C4	2.67	0.48
1:2:471:G:O2'	1:2:472:A:H5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:551:A:H2'	1:2:552:U:C6	2.48	0.48
1:4:1437:U:O2	1:4:1458:G:O6	2.32	0.48
8:m:68:GLY:O	8:m:99:ARG:NH1	2.44	0.48
1:2:429:G:H2'	1:2:430:C:C6	2.48	0.48
3:e:32:THR:C	3:e:34:LYS:H	2.21	0.48
1:4:1462:A:H2'	1:4:1463:C:C6	2.48	0.48
1:2:489:C:H2'	1:2:490:A:C8	2.49	0.48
5:g:10:VAL:HG21	5:g:18:VAL:HG11	1.94	0.48
5:g:16:ASP:HB2	5:g:17:GLN:HE21	1.79	0.48
1:2:4:A:N1	1:2:5:A:N6	2.62	0.47
3:e:155:LEU:HB3	3:e:158:LYS:HZ1	1.78	0.47
1:4:1431:A:H2'	1:4:1432:G:O4'	2.14	0.47
1:4:1443:A:O2'	1:4:1444:A:H5'	2.13	0.47
3:e:110:GLY:HA2	3:e:115:GLU:OE2	2.14	0.47
6:i:46:ILE:HD12	6:i:62:ILE:HG23	1.96	0.47
8:m:110:ARG:NH1	8:m:112:GLN:O	2.48	0.47
9:p:4:THR:HG23	9:p:6:ALA:N	2.28	0.47
1:2:92:G:H2'	1:2:93:A:C8	2.49	0.47
3:e:17:THR:HG22	3:e:18:ASP:H	1.78	0.47
12:s:26:ILE:HD11	12:s:67:LEU:HD13	1.95	0.47
1:2:759:U:H2'	1:2:760:A:C8	2.50	0.47
1:4:1420:G:H2'	1:4:1421:U:C6	2.50	0.47
7:l:63:GLN:HG2	7:l:98:ALA:HB2	1.96	0.47
1:2:158:A:H2'	1:2:159:G:O4'	2.15	0.47
1:2:404:G:OP1	3:e:112:THR:OG1	2.31	0.47
3:e:128:ASN:HD21	3:e:144:VAL:H	1.62	0.47
5:g:73:GLU:HA	5:g:76:GLU:HG3	1.97	0.47
1:2:419:U:H2'	1:2:420:G:O4'	2.15	0.46
6:i:39:VAL:HG21	6:i:111:ILE:HG22	1.98	0.46
1:2:250:G:OP1	11:r:69:SER:OG	2.28	0.46
3:e:101:ASP:OD2	3:e:101:ASP:N	2.45	0.46
13:u:86:LEU:HA	13:u:86:LEU:HD23	1.79	0.46
1:2:497:G:H2'	1:2:498:C:C6	2.49	0.46
1:2:590:U:H2'	1:2:591:U:C6	2.50	0.46
7:l:64:VAL:O	7:l:67:GLU:HG3	2.15	0.46
9:p:21:ASP:O	9:p:23:GLY:N	2.48	0.46
1:2:308:C:H2'	1:2:309:A:C8	2.51	0.46
12:s:37:GLY:O	12:s:63:ARG:NH2	2.42	0.46
1:2:478:G:O2'	1:2:480:C:N4	2.48	0.46
1:2:235:U:H5''	1:2:235:U:H6	1.81	0.46
6:i:87:TYR:CE1	6:i:125:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:39:U:O2'	1:2:497:G:H4'	2.16	0.46
1:2:340:A:H5''	1:2:341:C:H5	1.81	0.46
1:2:572:G:O2'	1:2:818:G:H5'	2.16	0.46
1:2:588:U:H2'	1:2:589:A:H8	1.81	0.46
1:2:91:G:H2'	1:2:92:G:C8	2.51	0.46
4:f:80:LEU:HD11	4:f:95:MET:HB3	1.97	0.46
1:2:905:A:H2'	1:2:906:A:H8	1.81	0.46
1:4:1464:C:H2'	1:4:1465:A:C8	2.51	0.46
7:l:18:GLY:HA3	7:l:78:LEU:HD11	1.98	0.46
13:u:79:LEU:O	13:u:83:VAL:HG13	2.15	0.46
1:2:659:G:H2'	1:2:660:A:C8	2.50	0.45
1:4:1423:G:H2'	1:4:1424:C:C6	2.51	0.45
1:4:1460:U:H2'	1:4:1461:U:H6	1.81	0.45
7:l:60:PHE:O	7:l:64:VAL:HG23	2.15	0.45
1:2:100:G:O2'	1:2:101:G:P	2.74	0.45
1:2:518:G:H4'	8:m:70:GLU:HG2	1.99	0.45
1:2:335:C:H2'	1:2:336:U:H6	1.81	0.45
1:2:335:C:H2'	1:2:336:U:C6	2.51	0.45
1:2:447:A:N6	1:2:478:G:H5'	2.30	0.45
1:2:725:A:H2'	1:2:726:A:C8	2.52	0.45
1:2:295:G:H2'	1:2:296:A:C8	2.52	0.45
2:c:208:ALA:HB3	2:c:211:ALA:HB3	1.97	0.45
1:4:1447:G:H5'	1:4:1448:C:OP2	2.16	0.45
1:2:464:A:H3'	1:2:465:C:H6	1.80	0.45
1:2:451:U:H2'	1:2:452:A:C8	2.52	0.45
3:e:128:ASN:ND2	3:e:144:VAL:H	2.15	0.45
5:g:46:GLN:HB2	5:g:56:LYS:HZ3	1.80	0.45
1:4:1414:G:O2'	1:4:1480:A:N6	2.46	0.45
1:2:339:U:O3'	1:2:340:A:H8	2.00	0.45
3:e:204:GLU:OE1	4:f:111:ARG:NH2	2.45	0.45
10:q:56:ARG:HA	10:q:56:ARG:HD2	1.62	0.45
1:2:611:C:H2'	1:2:612:G:H5'	1.98	0.44
3:e:107:MET:HG2	3:e:173:ILE:HD13	1.99	0.44
4:f:79:THR:OG1	4:f:121:ASN:O	2.28	0.44
5:g:1:MET:HG3	5:g:66:CYS:C	2.42	0.44
5:g:18:VAL:O	5:g:22:VAL:HG23	2.17	0.44
1:2:98:G:C2'	1:2:99:C:H5'	2.47	0.44
1:2:610:C:H2'	1:2:611:C:H6	1.80	0.44
1:2:611:C:C2'	1:2:612:G:H5'	2.47	0.44
1:2:908:U:H2'	1:2:909:C:C6	2.51	0.44
3:e:80:GLU:HG3	3:e:95:LEU:HD11	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:r:41:ARG:HD2	11:r:41:ARG:HA	1.73	0.44
1:2:803:C:H2'	1:2:804:A:H8	1.83	0.44
1:2:897:A:H2'	1:2:898:A:C8	2.52	0.44
1:4:1419:U:H2'	1:4:1420:G:O4'	2.17	0.44
1:4:1489:A:H2'	1:4:1490:A:O4'	2.16	0.44
1:2:538:G:H2'	1:2:539:G:O4'	2.17	0.44
10:q:55:ASP:OD2	10:q:56:ARG:N	2.50	0.44
3:e:59:GLU:HG2	3:e:201:LEU:HB2	1.99	0.44
3:e:196:GLU:HG2	3:e:197:ILE:HD12	2.00	0.44
1:2:76:A:N6	1:2:91:G:N1	2.14	0.44
1:2:155:G:O2'	1:2:157:A:N7	2.47	0.44
1:2:397:C:O2'	1:2:618:A:N3	2.48	0.44
1:2:509:U:H2'	1:2:510:C:C6	2.51	0.44
3:e:103:VAL:O	3:e:107:MET:HG3	2.18	0.44
1:2:249:U:O2'	11:r:18:MET:SD	2.76	0.44
1:2:693:A:H2'	1:2:694:U:C6	2.52	0.44
1:4:1529:U:H2'	1:4:1530:C:O4'	2.18	0.44
3:e:4:TYR:CE1	3:e:11:LEU:HD11	2.52	0.44
3:e:90:GLU:H	3:e:90:GLU:HG2	1.65	0.44
1:2:156:A:H2'	1:2:157:A:O4'	2.18	0.43
1:2:471:G:C6	1:2:472:A:N6	2.86	0.43
5:g:2:ARG:HG2	5:g:91:ARG:HH21	1.83	0.43
8:m:113:SER:O	8:m:113:SER:OG	2.26	0.43
1:2:491:G:O2'	1:2:493:A:H1'	2.18	0.43
1:4:1476:G:H2'	1:4:1477:A:C8	2.52	0.43
3:e:31:LYS:HB2	3:e:31:LYS:HE3	1.76	0.43
13:u:52:LYS:HA	13:u:52:LYS:HD2	1.70	0.43
1:2:861:A:H2'	1:2:862:A:C8	2.53	0.43
3:e:172:TRP:HZ3	3:e:192:ASP:HB3	1.81	0.43
6:i:27:MET:HE2	6:i:27:MET:HB3	1.84	0.43
1:4:1425:A:H2'	1:4:1426:C:O4'	2.18	0.43
1:2:53:A:N7	1:2:110:U:O2'	2.51	0.43
1:2:91:G:O2'	1:2:92:G:OP1	2.27	0.43
1:2:483:U:H2'	1:2:484:A:C8	2.53	0.43
1:4:1417:U:H2'	1:4:1418:U:O4'	2.18	0.43
1:2:456:U:C2	1:2:457:A:C8	3.07	0.43
5:g:22:VAL:HG11	5:g:39:LEU:HD21	2.00	0.43
7:l:22:ILE:HD13	7:l:95:ALA:HB3	2.00	0.43
1:2:35:A:H2'	1:2:36:C:C6	2.53	0.43
1:2:580:A:N6	1:2:755:G:O2'	2.50	0.43
1:4:1462:A:H2'	1:4:1463:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:1476:G:H2'	1:4:1477:A:H8	1.83	0.43
1:4:1424:C:H2'	1:4:1425:A:C8	2.54	0.43
1:4:1435:G:OP1	13:u:33:LYS:NZ	2.45	0.43
13:u:53:LYS:HB3	13:u:53:LYS:HE2	1.78	0.43
1:2:190:G:H4'	13:u:59:ASP:HB3	2.01	0.43
1:2:221:U:C2'	1:2:222:A:H5'	2.48	0.43
1:2:417:U:H3'	1:2:418:A:H8	1.83	0.43
1:4:1483:G:H2'	1:4:1484:G:O4'	2.18	0.43
10:q:42:THR:OG1	10:q:43:ALA:N	2.51	0.43
1:2:433:U:O2'	3:e:122:HIS:ND1	2.35	0.42
1:2:502:G:H2'	1:2:503:G:H8	1.83	0.42
1:4:1448:C:O2'	1:4:1449:A:H3'	2.19	0.42
5:g:38:ARG:HB3	5:g:63:ASN:HB2	2.01	0.42
1:2:179:G:C5	1:2:180:U:C5	3.07	0.42
1:2:359:A:OP1	8:m:58:THR:OG1	2.22	0.42
10:q:25:ARG:HE	10:q:25:ARG:HB2	1.71	0.42
1:2:178:C:H3'	1:2:179:G:C8	2.46	0.42
1:2:270:A:O2'	1:2:271:G:O4'	2.37	0.42
1:2:919:G:H2'	1:2:920:A:C8	2.55	0.42
3:e:190:ARG:NH1	3:e:195:ALA:HA	2.34	0.42
1:2:412:G:H2'	1:2:413:G:H8	1.85	0.42
1:2:660:A:H2'	1:2:661:G:O4'	2.20	0.42
1:2:748:U:H2'	1:2:749:G:O4'	2.19	0.42
1:4:1398:G:H2'	1:4:1399:C:O4'	2.20	0.42
3:e:103:VAL:HG11	3:e:145:ILE:HD13	2.00	0.42
6:i:70:LYS:HB3	6:i:70:LYS:HE3	1.68	0.42
13:u:44:TYR:HB2	13:u:87:ALA:HB3	2.02	0.42
1:2:646:A:H2'	1:2:647:G:O4'	2.20	0.42
1:2:692:A:H2'	1:2:693:A:C8	2.55	0.42
1:2:786:U:O2'	1:2:788:G:N7	2.49	0.42
1:2:58:U:H2'	1:2:59:G:C8	2.54	0.42
1:2:502:G:H2'	1:2:503:G:C8	2.54	0.42
1:2:734:A:H2'	1:2:735:U:C6	2.54	0.42
1:2:864:G:O2'	1:2:870:A:N1	2.46	0.42
1:2:499:A:OP1	8:m:115:SER:HB2	2.19	0.42
1:2:675:U:H2'	1:2:676:C:H6	1.85	0.42
5:g:41:ASP:CG	5:g:58:HIS:HE2	2.26	0.42
6:i:88:ARG:HA	6:i:88:ARG:HD3	1.78	0.42
1:2:266:A:H2'	1:2:267:C:C6	2.55	0.42
1:2:499:A:H2'	1:2:500:C:O4'	2.19	0.42
1:2:742:U:OP1	1:2:848:U:O2'	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:7:VAL:O	6:i:11:LEU:HG	2.20	0.42
11:r:8:THR:HG23	11:r:61:THR:HG23	2.02	0.42
12:s:69:PRO:HB2	12:s:71:THR:O	2.20	0.42
1:2:472:A:O2'	1:2:473:U:H6	2.02	0.42
1:2:649:U:O4	1:2:749:G:O2'	2.31	0.42
1:2:682:G:O2'	1:2:683:U:H5'	2.20	0.42
1:4:1424:C:H2'	1:4:1425:A:H8	1.84	0.42
1:4:1513:G:H2'	1:4:1515:A:OP2	2.19	0.42
5:g:7:VAL:O	5:g:87:ASN:HA	2.20	0.42
10:q:73:SER:O	10:q:77:GLN:HG2	2.19	0.42
3:e:199:GLU:O	3:e:203:VAL:HG23	2.20	0.41
9:p:53:ARG:O	9:p:57:ILE:HG12	2.20	0.41
1:2:144:G:O2'	1:4:1443:A:N3	2.48	0.41
1:2:180:U:H2'	1:2:181:C:H6	1.83	0.41
1:2:221:U:O2'	1:2:222:A:H5'	2.20	0.41
6:i:103:ALA:HB3	6:i:114:ASP:HB3	2.01	0.41
1:2:712:A:H2'	1:2:713:A:C8	2.54	0.41
4:f:43:GLY:O	4:f:73:VAL:N	2.42	0.41
5:g:51:ILE:O	5:g:54:ILE:HB	2.20	0.41
1:2:428:A:H3'	1:2:429:G:H8	1.86	0.41
1:2:162:A:H2'	1:2:163:U:H6	1.85	0.41
1:2:235:U:H5'	1:2:236:C:OP1	2.19	0.41
1:2:240:U:O4	1:2:903:A:H1'	2.20	0.41
1:2:625:G:H2'	1:2:626:A:C8	2.56	0.41
11:r:69:SER:OG	11:r:70:LYS:N	2.53	0.41
1:2:175:A:H2'	1:2:176:U:C6	2.56	0.41
1:2:257:U:H5'	1:2:258:A:OP2	2.20	0.41
1:2:515:C:H5''	1:2:516:C:C6	2.56	0.41
9:p:31:LEU:O	9:p:35:GLN:HG2	2.19	0.41
1:2:75:A:H2'	1:2:76:A:O4'	2.21	0.41
1:2:483:U:H2'	1:2:484:A:H8	1.85	0.41
1:2:536:A:H2'	1:2:537:G:C8	2.56	0.41
6:i:18:GLN:HE21	6:i:73:ILE:HB	1.85	0.41
1:2:880:C:O2'	1:2:881:U:H5'	2.21	0.41
1:4:1416:G:N2	1:4:1478:U:O2	2.47	0.41
5:g:29:ILE:HG21	5:g:64:VAL:HG13	2.03	0.41
1:2:307:C:OP1	10:q:31:ARG:NH1	2.51	0.41
1:4:1421:U:H2'	1:4:1422:U:H6	1.86	0.41
3:e:62:LYS:HE2	3:e:62:LYS:HB3	1.76	0.41
1:2:162:A:H2'	1:2:163:U:C6	2.56	0.41
1:4:1414:G:H2'	1:4:1479:G:N2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:1481:C:H2'	1:4:1482:U:O4'	2.20	0.41
3:e:9:CYS:O	3:e:13:ARG:HG3	2.20	0.41
5:g:37:HIS:NE2	5:g:65:GLU:HB2	2.36	0.41
1:2:252:U:H2'	1:2:253:G:H8	1.86	0.40
1:2:462:A:H2'	1:2:464:A:C2	2.56	0.40
1:2:865:C:H2'	1:2:866:G:O4'	2.21	0.40
3:e:85:LYS:HB3	3:e:85:LYS:HE2	1.73	0.40
8:m:43:LYS:HB3	8:m:44:LYS:H	1.78	0.40
11:r:31:GLN:HA	11:r:38:SER:HA	2.03	0.40
12:s:33:ILE:HD11	12:s:59:ILE:HG12	2.03	0.40
1:2:11:G:H5'	4:f:107:GLY:HA3	2.02	0.40
1:2:348:C:H4'	1:2:350:G:OP1	2.21	0.40
1:2:408:A:H62	1:2:427:A:N6	2.16	0.40
1:2:415:C:H2'	1:2:416:U:O4'	2.22	0.40
1:2:711:G:H2'	1:2:712:A:C8	2.56	0.40
7:l:98:ALA:O	7:l:102:VAL:HG13	2.20	0.40
9:p:47:LYS:HB2	9:p:47:LYS:HE2	1.78	0.40
1:2:308:C:H2'	1:2:309:A:H8	1.86	0.40
1:2:378:A:H2'	1:2:379:A:C8	2.56	0.40
1:2:639:A:H2'	1:2:640:C:H6	1.85	0.40
1:2:704:U:H4'	7:l:21:HIS:CD2	2.56	0.40
1:2:106:C:H2'	1:2:107:G:O4'	2.21	0.40
1:2:896:C:H2'	1:2:897:A:C8	2.57	0.40
1:4:1399:C:H2'	1:4:1400:C:O4'	2.20	0.40
6:i:57:LYS:HE2	6:i:57:LYS:HB3	1.92	0.40
1:2:21:A:O2'	1:2:569:A:N1	2.48	0.40
1:2:738:G:H2'	1:2:739:G:O4'	2.21	0.40
3:e:139:VAL:HG11	3:e:145:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	c	217/250 (87%)	200 (92%)	17 (8%)	0	100	100
3	e	205/208 (99%)	169 (82%)	36 (18%)	0	100	100
4	f	153/165 (93%)	146 (95%)	7 (5%)	0	100	100
5	g	101/127 (80%)	94 (93%)	7 (7%)	0	100	100
6	i	128/131 (98%)	121 (94%)	7 (6%)	0	100	100
7	l	112/128 (88%)	103 (92%)	9 (8%)	0	100	100
8	m	120/124 (97%)	111 (92%)	9 (8%)	0	100	100
9	p	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
10	q	78/83 (94%)	71 (91%)	7 (9%)	0	100	100
11	r	77/85 (91%)	71 (92%)	6 (8%)	0	100	100
12	s	51/75 (68%)	50 (98%)	1 (2%)	0	100	100
13	u	84/88 (96%)	84 (100%)	0	0	100	100
14	v	58/71 (82%)	52 (90%)	6 (10%)	0	100	100
All	All	1470/1624 (90%)	1351 (92%)	119 (8%)	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	
3	e	158/171 (92%)	140 (89%)	18 (11%)	5	14
4	f	113/120 (94%)	104 (92%)	9 (8%)	11	28
5	g	93/111 (84%)	85 (91%)	8 (9%)	10	25
6	i	108/109 (99%)	102 (94%)	6 (6%)	19	44
7	l	85/98 (87%)	75 (88%)	10 (12%)	5	13
8	m	104/106 (98%)	94 (90%)	10 (10%)	8	20
9	p	71/72 (99%)	68 (96%)	3 (4%)	26	55
10	q	62/63 (98%)	60 (97%)	2 (3%)	34	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	r	71/76 (93%)	65 (92%)	6 (8%)	10	25
12	s	47/66 (71%)	43 (92%)	4 (8%)	10	25
13	u	65/67 (97%)	61 (94%)	4 (6%)	16	39
14	v	21/62 (34%)	19 (90%)	2 (10%)	8	20
All	All	998/1121 (89%)	916 (92%)	82 (8%)	13	27

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	e	10	LYS
3	e	17	THR
3	e	32	THR
3	e	41	GLN
3	e	42	HIS
3	e	66	ILE
3	e	84	VAL
3	e	85	LYS
3	e	109	PHE
3	e	126	THR
3	e	136	SER
3	e	153	GLN
3	e	155	LEU
3	e	163	LEU
3	e	166	GLN
3	e	175	VAL
3	e	193	LEU
3	e	208	LYS
4	f	18	ASP
4	f	38	VAL
4	f	68	ARG
4	f	74	ASP
4	f	102	THR
4	f	130	THR
4	f	147	THR
4	f	160	VAL
4	f	161	GLU
5	g	14	GLN
5	g	19	VAL
5	g	31	GLU
5	g	54	ILE
5	g	61	LEU

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Mol	Chain	Res	Type
5	g	70	THR
5	g	98	GLU
5	g	102	LEU
6	i	24	THR
6	i	26	SER
6	i	56	THR
6	i	58	SER
6	i	92	LYS
6	i	111	ILE
7	l	15	VAL
7	l	19	VAL
7	l	46	SER
7	l	78	LEU
7	l	81	LEU
7	l	82	ASP
7	l	94	SER
7	l	96	VAL
7	l	106	ILE
7	l	128	VAL
8	m	13	THR
8	m	15	LEU
8	m	21	VAL
8	m	30	ARG
8	m	39	THR
8	m	40	THR
8	m	55	VAL
8	m	82	ILE
8	m	87	VAL
8	m	113	SER
9	p	20	ASN
9	p	22	THR
9	p	54	ARG
10	q	42	THR
10	q	52	LEU
11	r	5	THR
11	r	8	THR
11	r	14	VAL
11	r	15	SER
11	r	61	THR
11	r	80	VAL
12	s	34	THR
12	s	35	GLU

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Mol	Chain	Res	Type
12	s	47	THR
12	s	66	SER
13	u	25	ARG
13	u	27	MET
13	u	30	THR
13	u	77	SER
14	v	53	VAL
14	v	58	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	e	128	ASN
3	e	148	HIS
4	f	42	ASN
4	f	69	ASN
4	f	120	HIS
4	f	137	ASN
5	g	17	GLN
5	g	63	ASN
6	i	18	GLN
6	i	41	GLN
7	l	21	HIS
7	l	23	HIS
7	l	37	GLN
7	l	39	ASN
7	l	107	ASN
7	l	117	HIS
7	l	118	ASN
8	m	111	ASN
9	p	46	HIS
10	q	44	GLN
10	q	46	GLN
10	q	59	HIS
10	q	63	GLN
10	q	66	GLN
12	s	52	GLN
13	u	6	GLN
14	v	57	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	890/1544 (57%)	180 (20%)	4 (0%)
1	4	145/1544 (9%)	25 (17%)	0
All	All	1035/3088 (33%)	205 (19%)	4 (0%)

All (205) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	7	U
1	2	9	A
1	2	11	G
1	2	24	G
1	2	34	A
1	2	41	G
1	2	46	A
1	2	49	C
1	2	50	U
1	2	53	A
1	2	54	C
1	2	56	C
1	2	66	G
1	2	70	G
1	2	72	G
1	2	91	G
1	2	92	G
1	2	97	A
1	2	99	C
1	2	100	G
1	2	101	G
1	2	105	A
1	2	115	A
1	2	116	A
1	2	119	C
1	2	126	A
1	2	127	U
1	2	129	U
1	2	136	U
1	2	140	G
1	2	147	A
1	2	160	G
1	2	162	A
1	2	167	A
1	2	178	C
1	2	184	A

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Mol	Chain	Res	Type
1	2	186	G
1	2	187	G
1	2	193	A
1	2	199	G
1	2	212	U
1	2	213	U
1	2	214	G
1	2	222	A
1	2	224	A
1	2	225	U
1	2	235	U
1	2	236	C
1	2	237	G
1	2	241	U
1	2	243	G
1	2	247	G
1	2	249	U
1	2	256	G
1	2	257	U
1	2	258	A
1	2	262	G
1	2	263	C
1	2	271	G
1	2	274	G
1	2	277	G
1	2	285	G
1	2	299	A
1	2	312	C
1	2	313	U
1	2	317	A
1	2	319	U
1	2	321	A
1	2	322	G
1	2	323	A
1	2	324	C
1	2	325	A
1	2	326	C
1	2	328	G
1	2	333	G
1	2	334	A
1	2	340	A
1	2	341	C

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Mol	Chain	Res	Type
1	2	343	G
1	2	347	G
1	2	348	C
1	2	350	G
1	2	359	A
1	2	363	U
1	2	364	U
1	2	368	C
1	2	380	C
1	2	388	C
1	2	393	A
1	2	394	U
1	2	402	G
1	2	404	G
1	2	405	U
1	2	407	A
1	2	408	A
1	2	409	G
1	2	417	U
1	2	418	A
1	2	420	G
1	2	425	U
1	2	429	G
1	2	432	C
1	2	442	G
1	2	444	A
1	2	448	G
1	2	450	C
1	2	452	A
1	2	453	C
1	2	454	U
1	2	455	U
1	2	456	U
1	2	458	G
1	2	459	U
1	2	460	U
1	2	463	U
1	2	464	A
1	2	468	A
1	2	471	G
1	2	473	U
1	2	476	U

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Mol	Chain	Res	Type
1	2	478	G
1	2	481	G
1	2	482	U
1	2	483	U
1	2	492	A
1	2	493	A
1	2	506	A
1	2	508	C
1	2	515	C
1	2	524	G
1	2	525	C
1	2	530	A
1	2	544	A
1	2	556	A
1	2	559	U
1	2	565	G
1	2	569	A
1	2	570	A
1	2	573	C
1	2	574	G
1	2	576	G
1	2	593	A
1	2	611	C
1	2	613	A
1	2	614	G
1	2	615	C
1	2	625	G
1	2	630	G
1	2	631	C
1	2	647	G
1	2	650	A
1	2	662	A
1	2	683	U
1	2	692	A
1	2	697	G
1	2	699	A
1	2	700	G
1	2	720	U
1	2	728	G
1	2	730	A
1	2	731	G
1	2	743	A

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Mol	Chain	Res	Type
1	2	752	G
1	2	756	A
1	2	778	A
1	2	789	A
1	2	790	U
1	2	791	A
1	2	799	A
1	2	809	G
1	2	812	A
1	2	814	C
1	2	825	A
1	2	833	G
1	2	850	G
1	2	867	A
1	2	881	U
1	2	884	G
1	2	911	A
1	2	923	G
1	4	1397	C
1	4	1403	U
1	4	1419	U
1	4	1426	C
1	4	1438	A
1	4	1443	A
1	4	1446	U
1	4	1447	G
1	4	1448	C
1	4	1449	A
1	4	1451	A
1	4	1464	C
1	4	1465	A
1	4	1472	G
1	4	1484	G
1	4	1492	U
1	4	1494	G
1	4	1496	A
1	4	1500	A
1	4	1503	U
1	4	1514	G
1	4	1517	C
1	4	1526	G
1	4	1527	G

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Mol	Chain	Res	Type
1	4	1528	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	91	G
1	2	100	G
1	2	186	G
1	2	270	A

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 56 ligands modelled in this entry, 56 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.

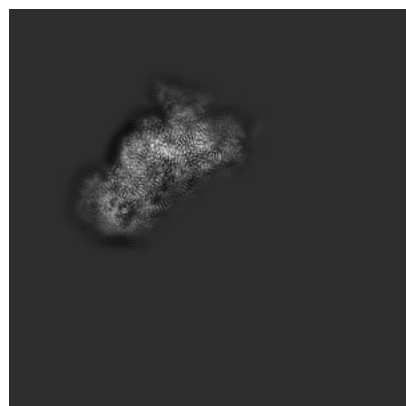
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10914. These allow visual inspection of the internal detail of the map and identification of artifacts.

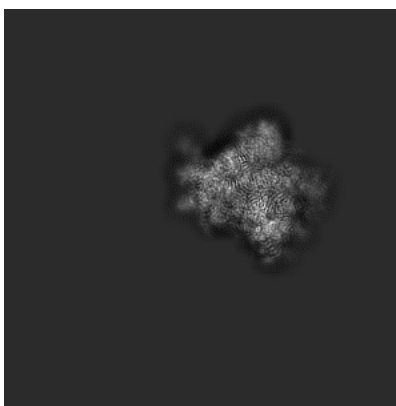
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

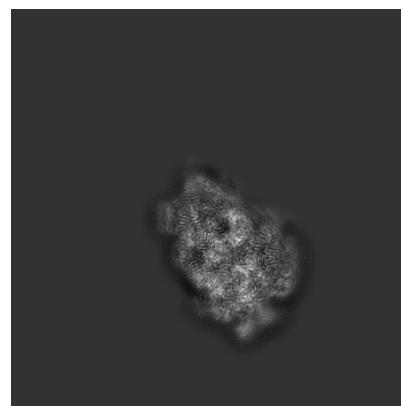
6.1.1 Primary map



X

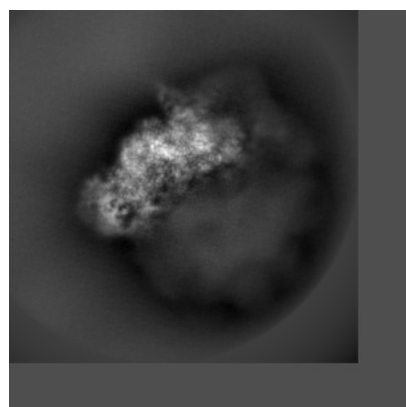


Y

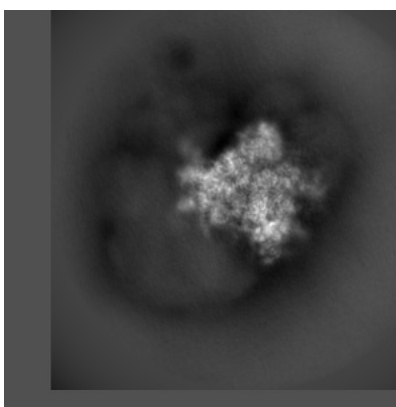


Z

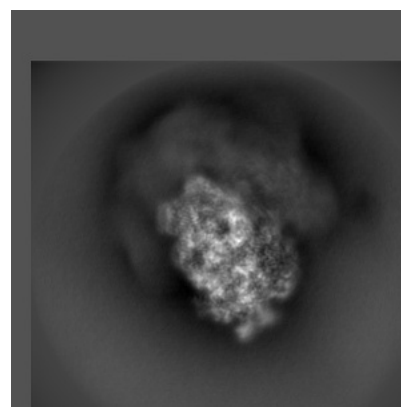
6.1.2 Raw map



X



Y

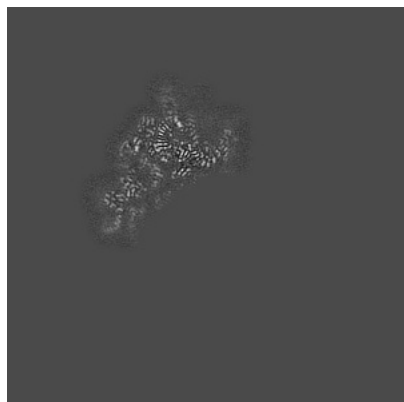


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

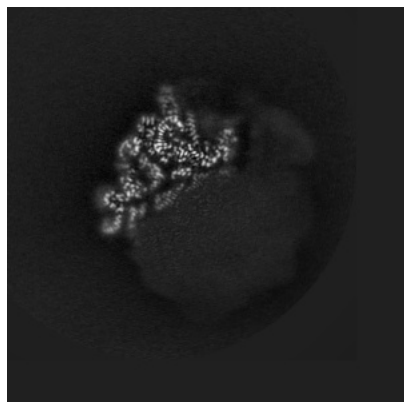


Y Index: 200

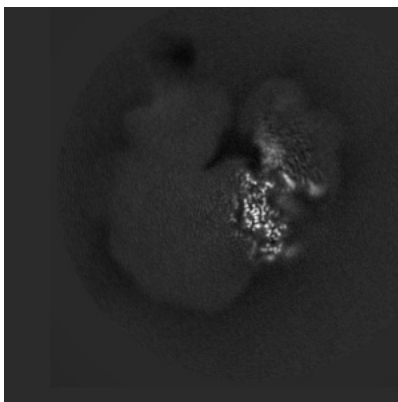


Z Index: 200

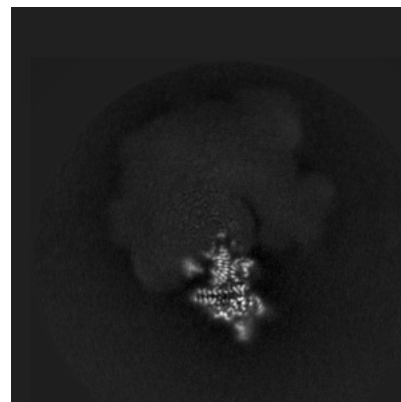
6.2.2 Raw map



X Index: 200



Y Index: 200

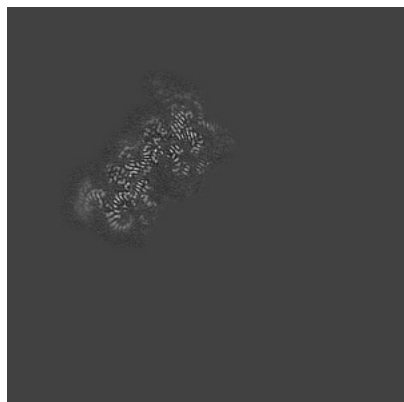


Z Index: 200

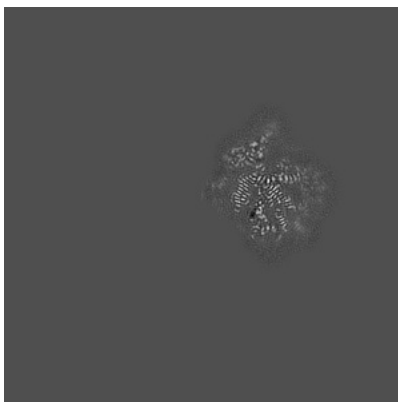
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

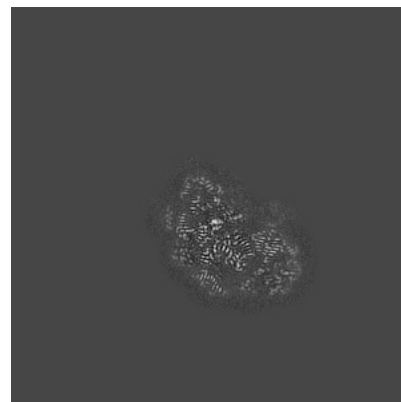
6.3.1 Primary map



X Index: 230

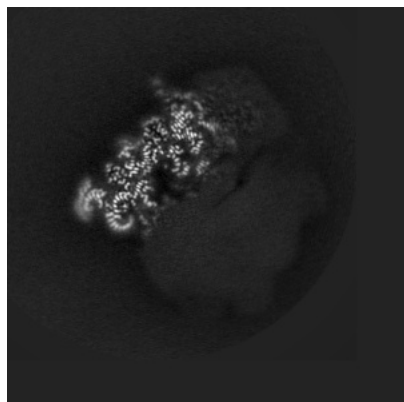


Y Index: 168

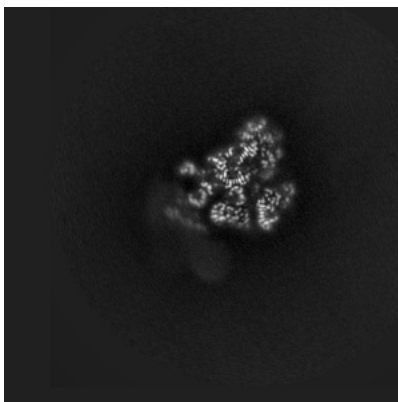


Z Index: 257

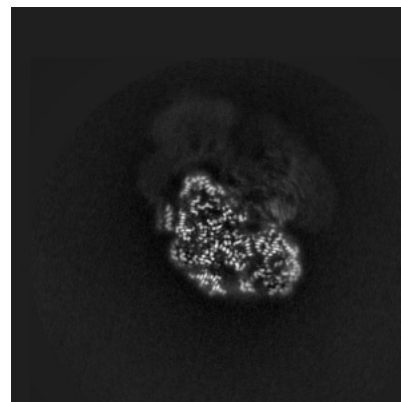
6.3.2 Raw map



X Index: 230



Y Index: 130

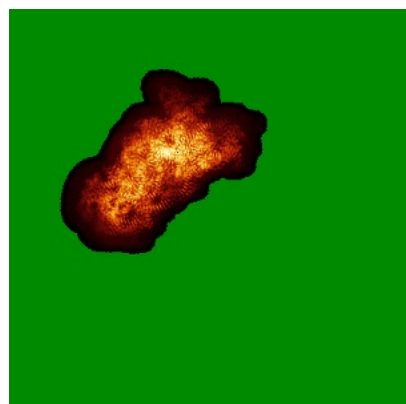


Z Index: 258

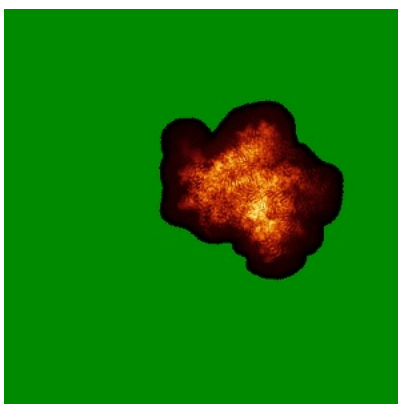
The images above show the largest variance slices of the map in three orthogonal directions.

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

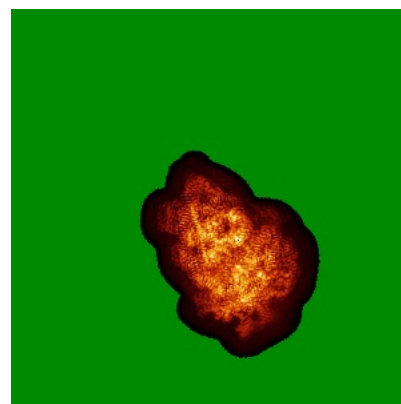
6.4.1 Primary map



X



Y

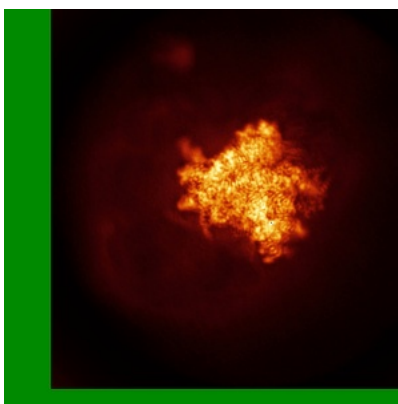


Z

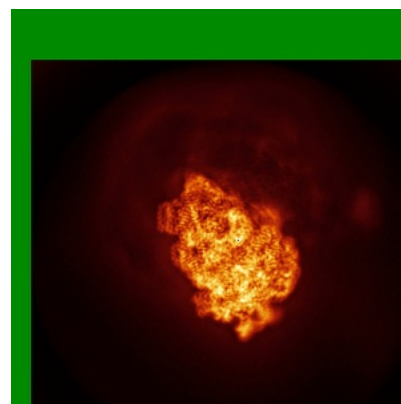
6.4.2 Raw map



X



Y

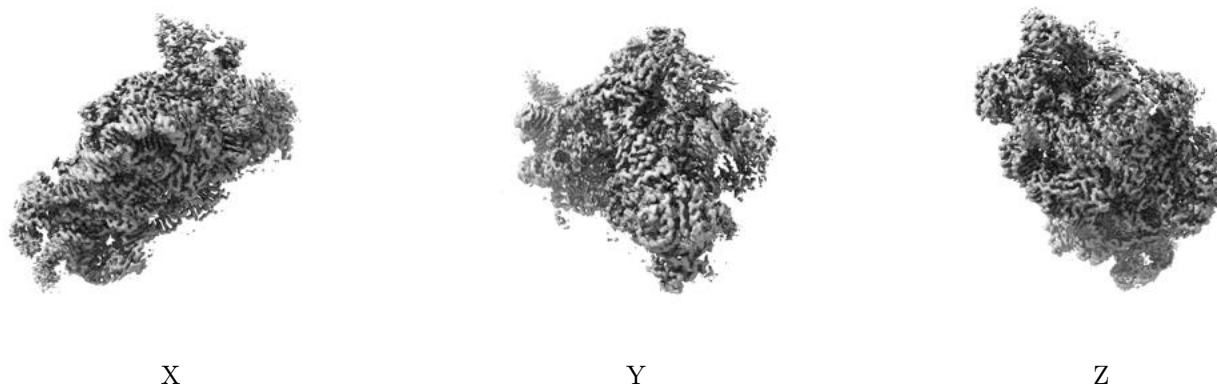


Z

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 0.05. 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.

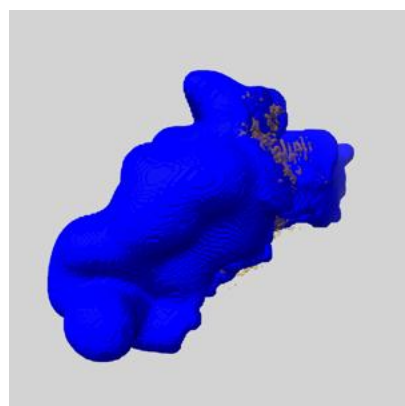
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

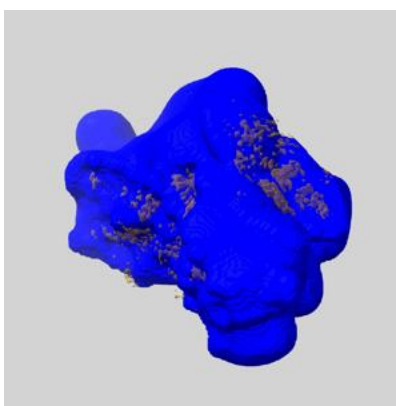
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

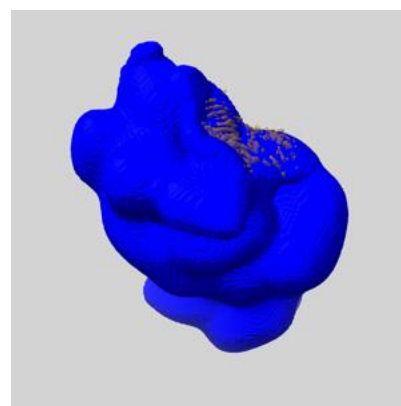
6.6.1 emd_10914_msk_1.map [i](#)



X



Y

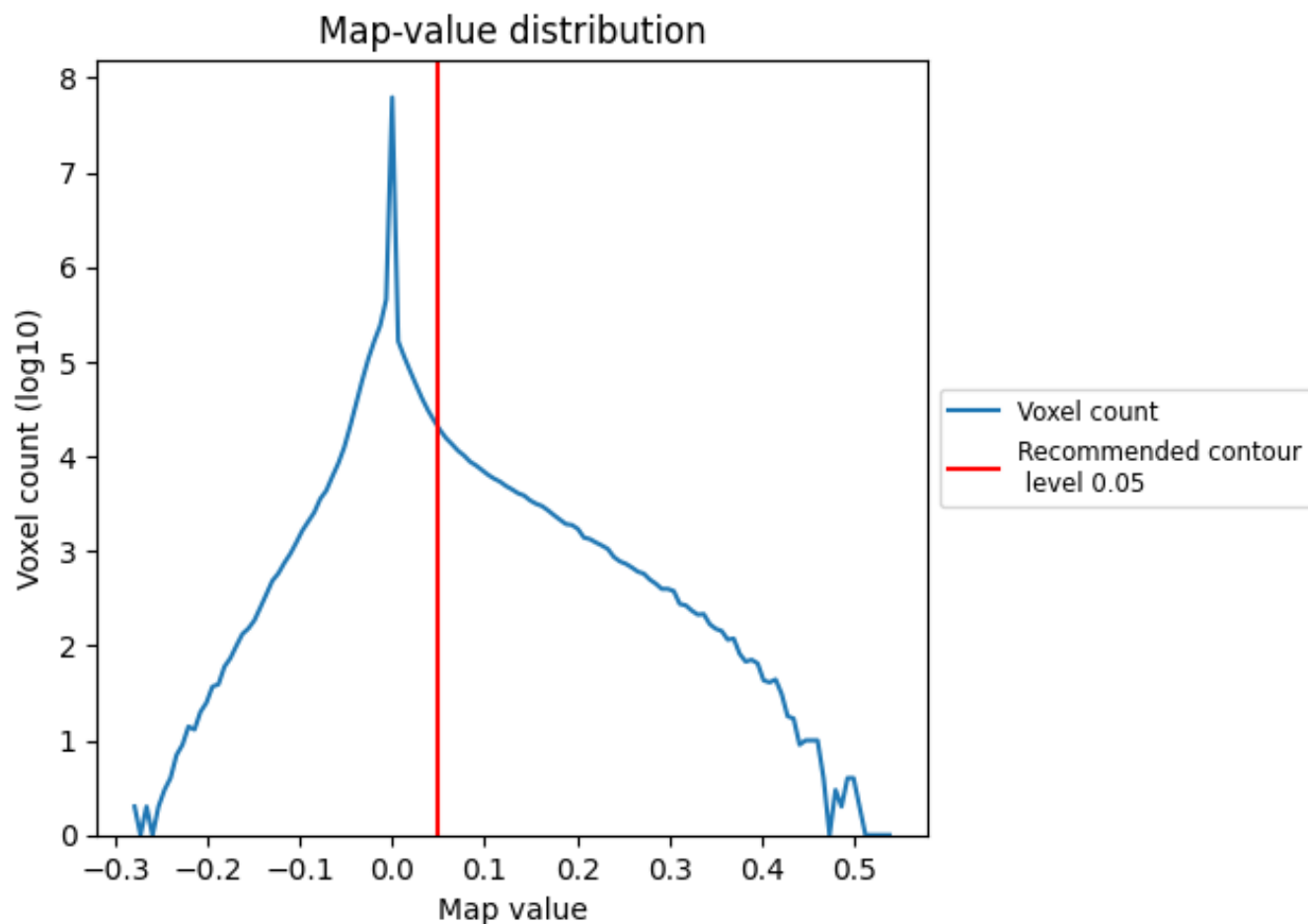


Z

7 Map analysis [i](#)

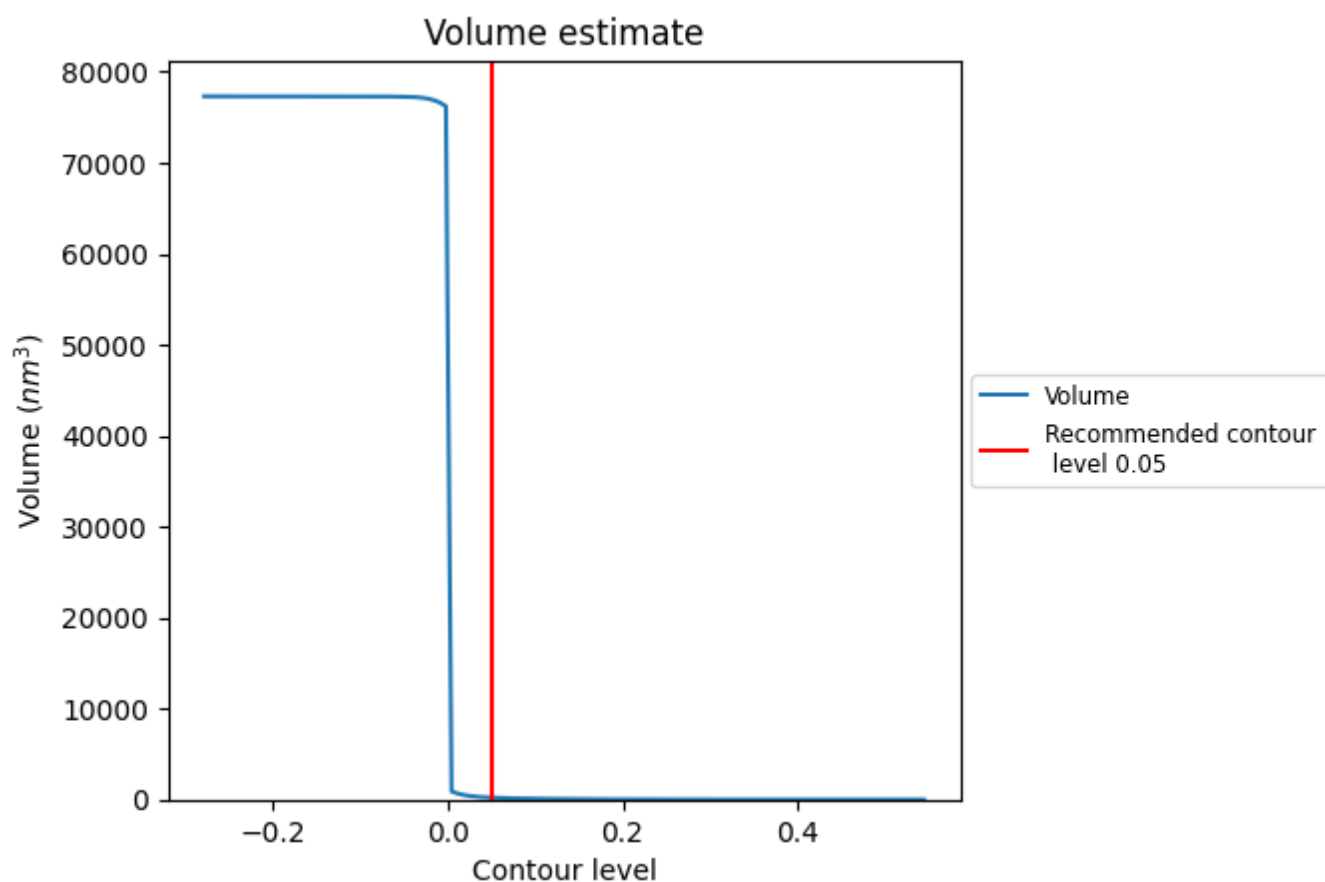
This section contains the results of statistical analysis of the map.

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.

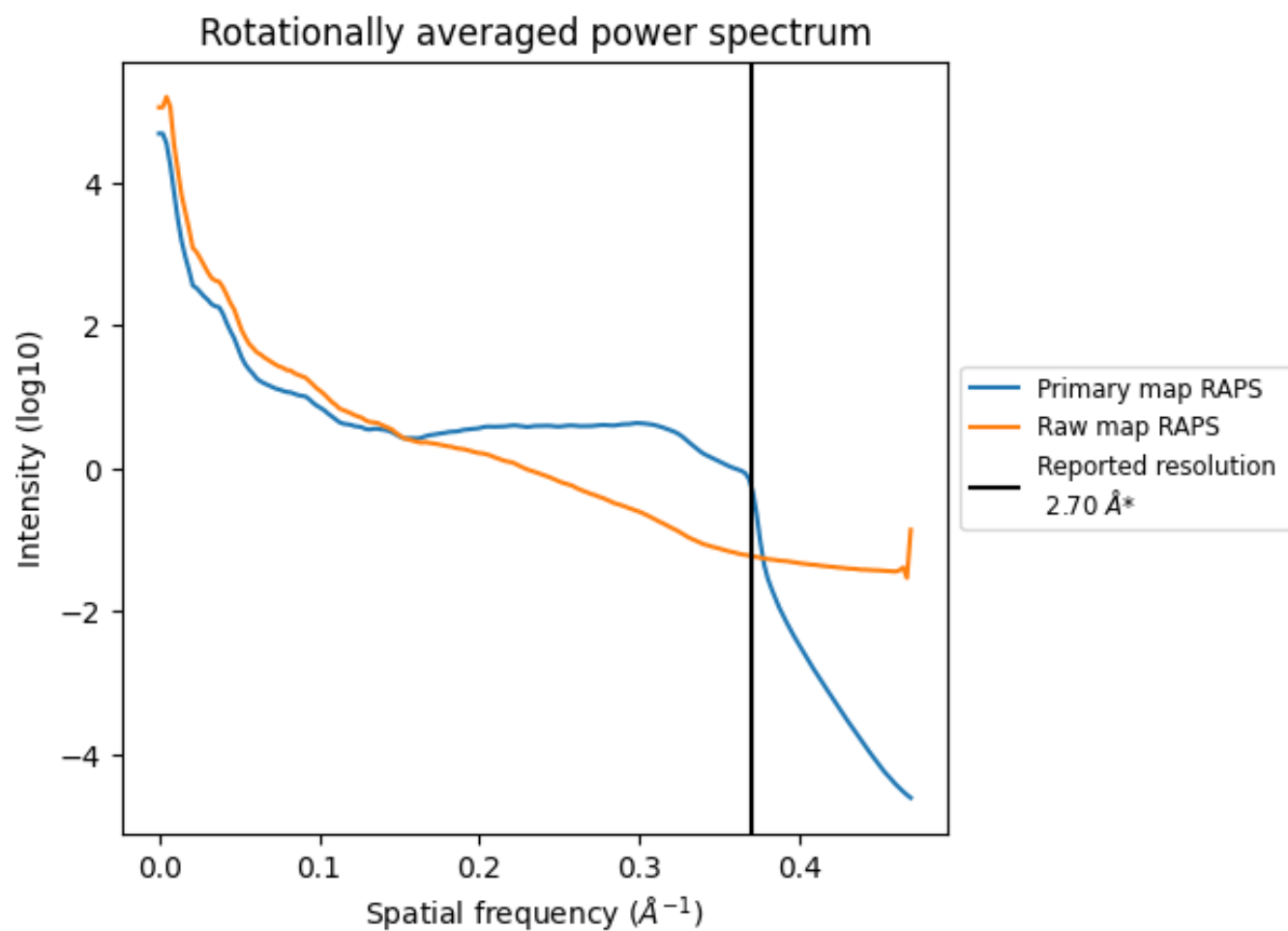
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm³; this corresponds to an approximate mass of 188 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 ⓘ

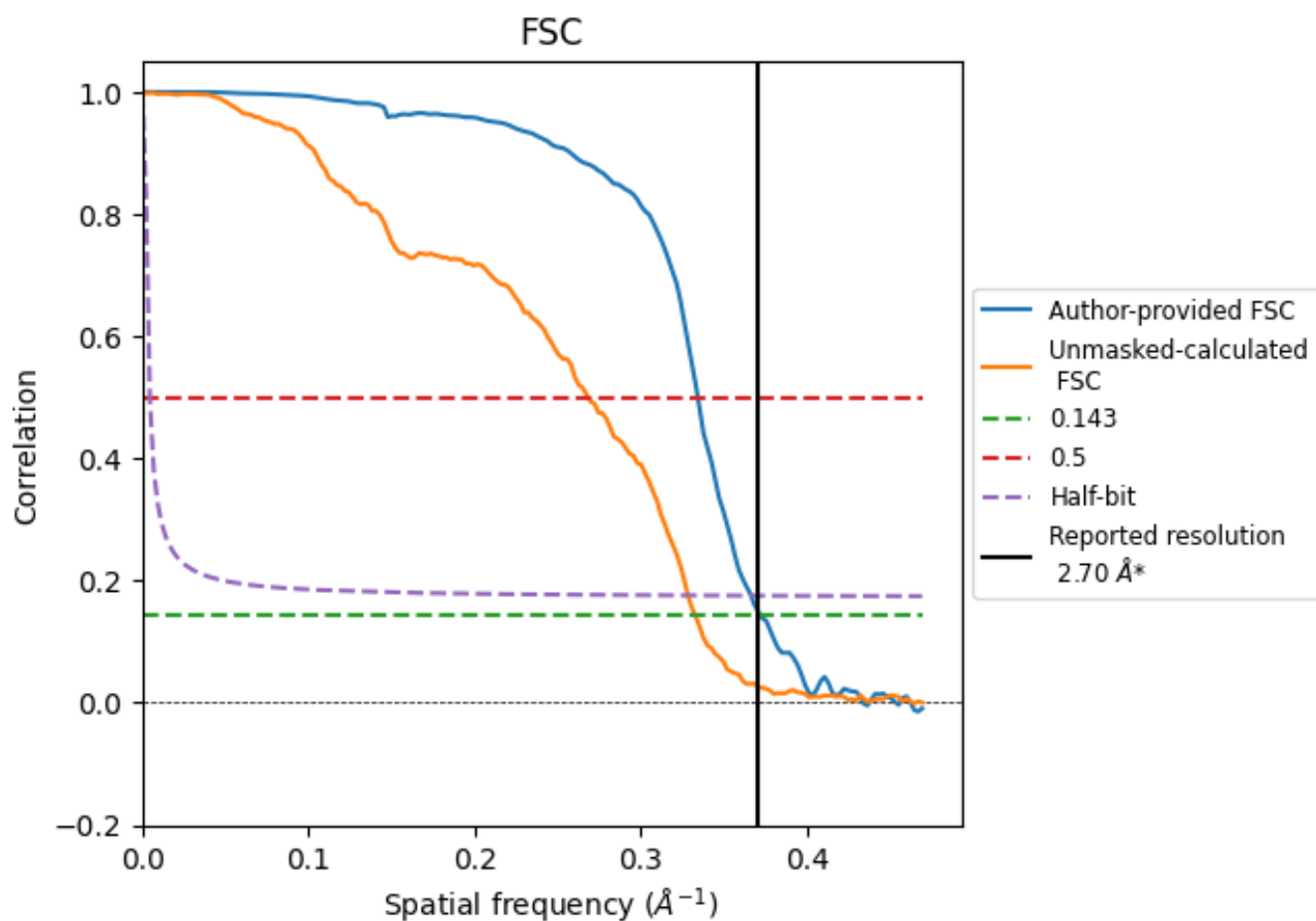


*Reported resolution corresponds to spatial frequency of $0.370 \text{ \AA}^{-1}$

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

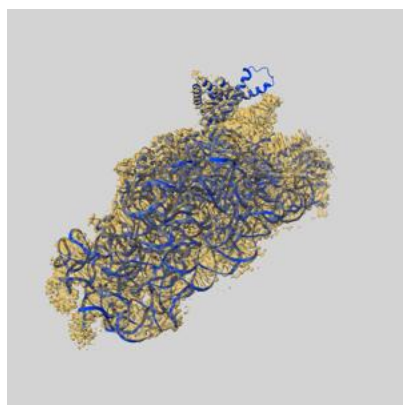
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	2.99	2.73
Unmasked-calculated*	3.00	3.72	3.04

*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 3.00 differs from the reported value 2.7 by more than 10 %

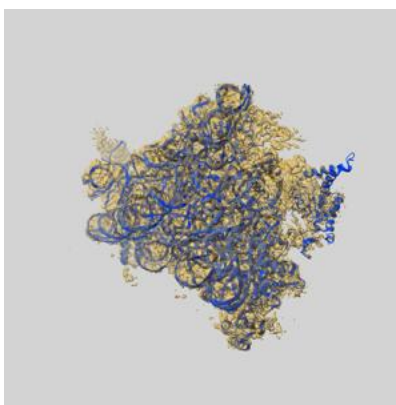
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10914 and PDB model 6YT9. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

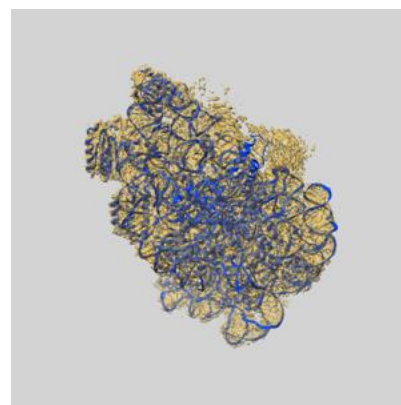
9.1 Map-model overlay [i](#)



X



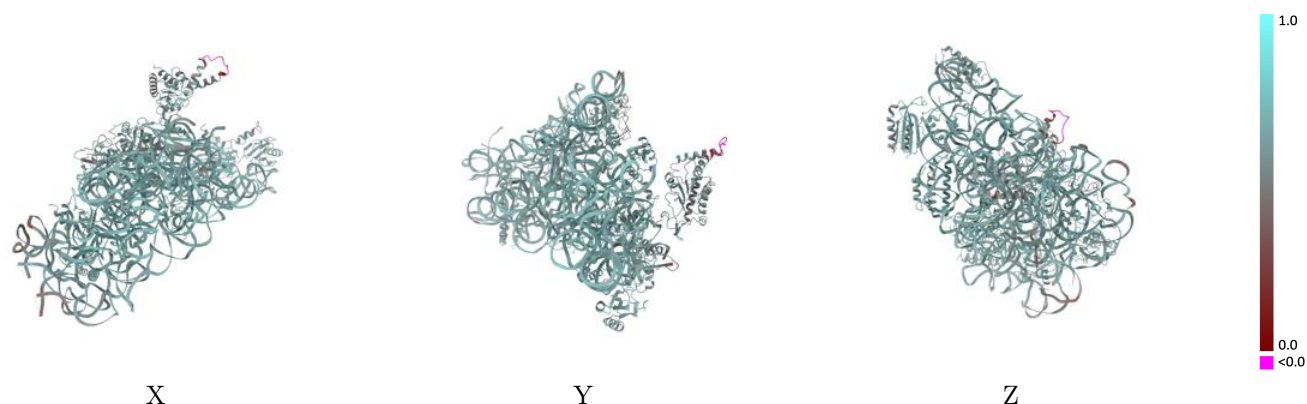
Y



Z

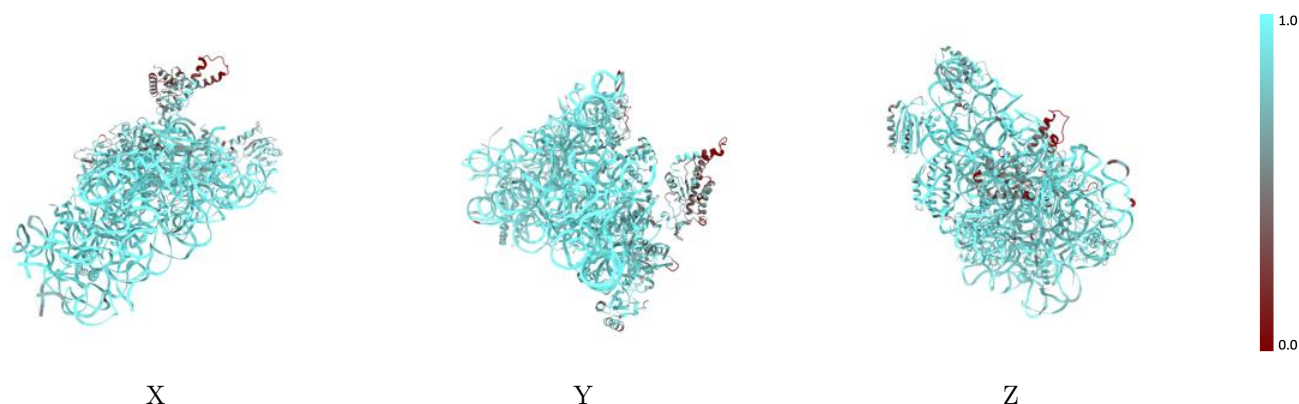
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



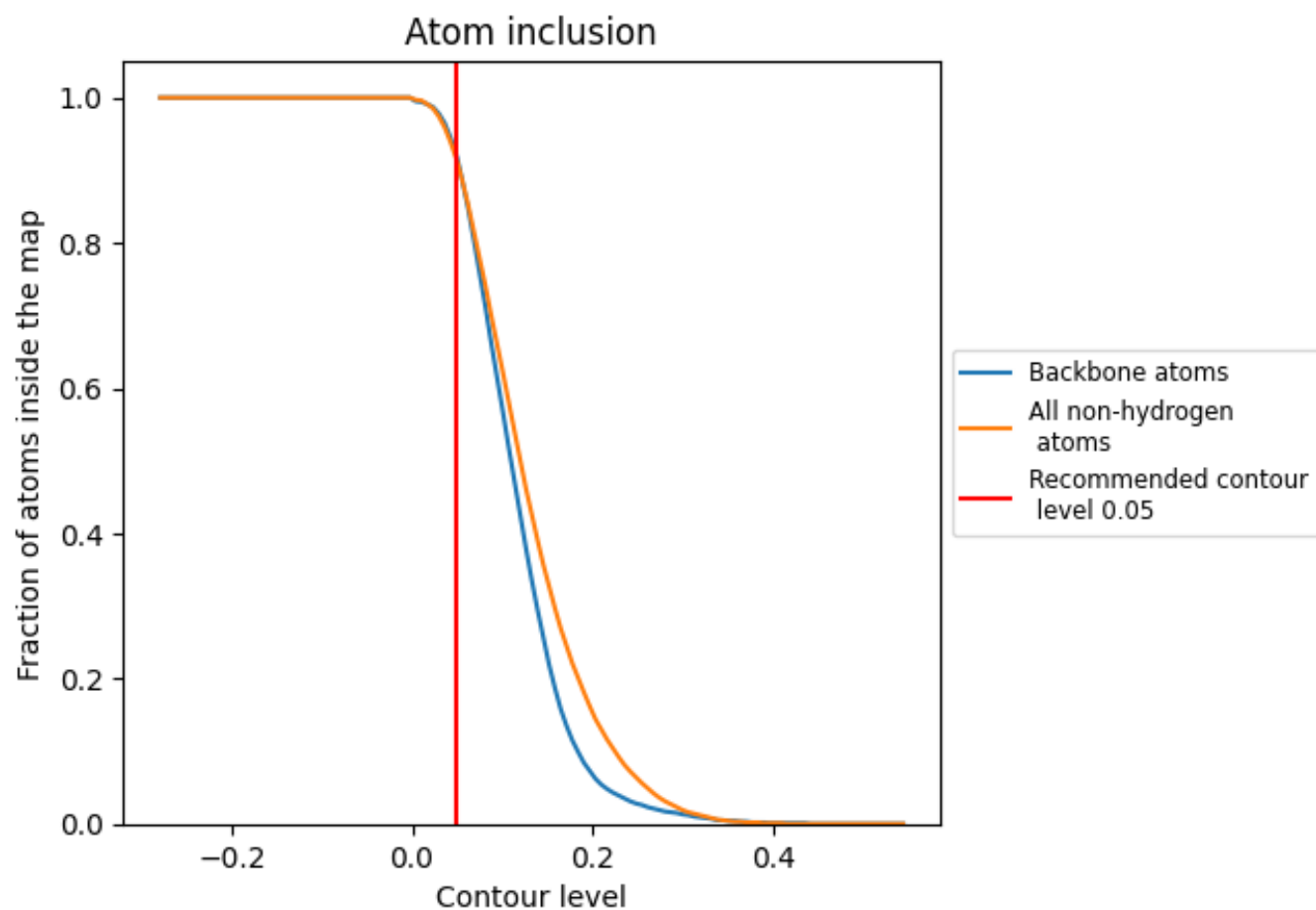
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.6290
2	0.9650	0.6390
4	0.9360	0.6290
c	0.5100	0.5180
e	0.7910	0.5940
f	0.8820	0.6400
g	0.7780	0.5940
i	0.8920	0.6430
l	0.7930	0.5950
m	0.8540	0.6390
p	0.8940	0.6320
q	0.9230	0.6490
r	0.8220	0.6140
s	0.8880	0.6350
u	0.9220	0.6410
v	0.7320	0.5990

1.0

0.0

<0.0