



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 09:02 am GMT

PDB ID : 6ZOK
EMDB ID : EMD-11321
Title : SARS-CoV-2-Nsp1-40S complex, focused on body
Authors : Schubert, K.; Karousis, E.D.; Jomaa, A.; Scaiola, A.; Echeverria, B.; Gurzeler, L.-A.; Leibundgut, M.; Thiel, V.; Muehlemann, O.; Ban, N.
Deposited on : 2020-07-07
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

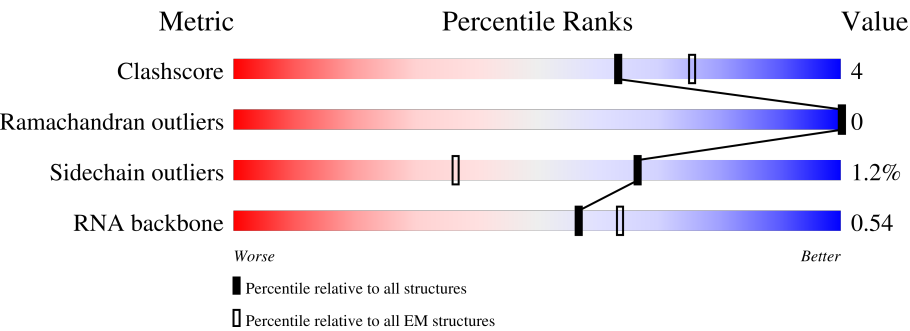
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1869	<div><div>8%</div><div>42%</div><div>21%</div><div>.</div><div>34%</div></div>
2	A	295	<div><div>7%</div><div>63%</div><div>11%</div><div>27%</div></div>
3	B	264	<div><div>.</div><div>69%</div><div>11%</div><div>19%</div></div>
4	C	293	<div><div>.</div><div>69%</div><div>6%</div><div>26%</div></div>
5	E	263	<div><div>.</div><div>89%</div><div>10%</div></div>
6	G	249	<div><div>10%</div><div>79%</div><div>14%</div><div>8%</div></div>
7	H	194	<div><div>53%</div><div>80%</div><div>16%</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	208	
9	J	194	
10	L	158	
11	N	151	
12	O	151	
13	R	135	
14	V	83	
15	W	130	
16	X	143	
17	Y	130	
18	a	101	
19	b	82	
20	e	56	
21	j	180	
22	h	25	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 50192 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1232	Total	C	N	O	P	0	0
			26317	11749	4744	8592	1232		

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 9 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 11 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 12 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	51	Total	C	N	O	S	0	0
			397	251	63	81	2		

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 15 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 18 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	a	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 19 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 20 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	56	Total	C	N	O	S	0	0
			441	273	96	71	1		

- Molecule 21 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	33	Total	C	N	O	S	0	0
			267	162	47	57	1		

- Molecule 22 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
23	2	106	Total	Mg	0
			106	106	
23	L	1	Total	Mg	0
			1	1	
23	X	2	Total	Mg	0
			2	2	

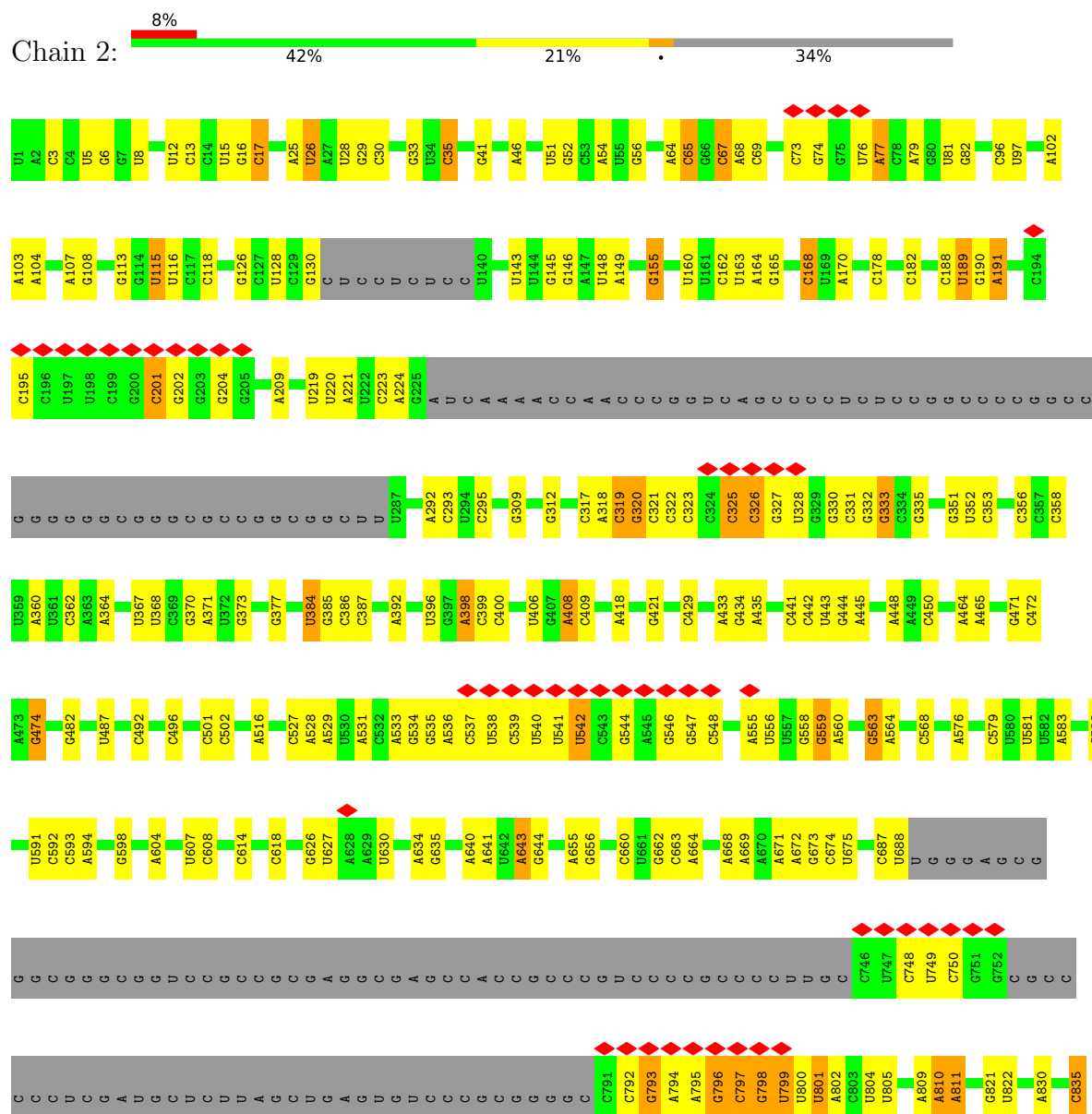
- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

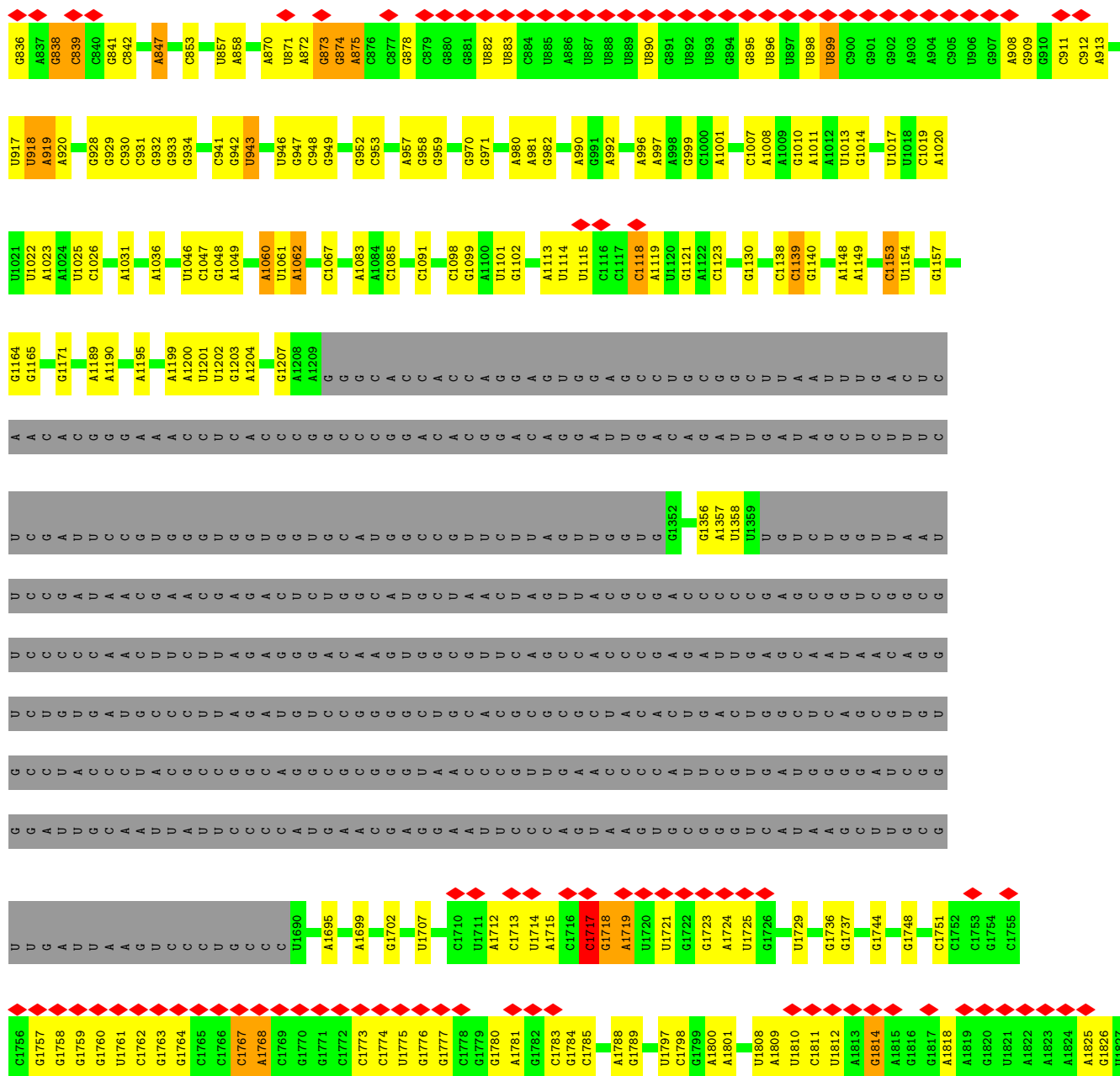
Mol	Chain	Residues	Atoms		AltConf
24	a	1	Total	Zn	0
			1	1	

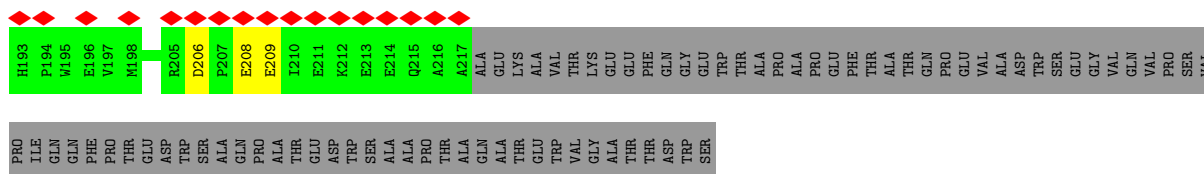
3 Residue-property plots

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.

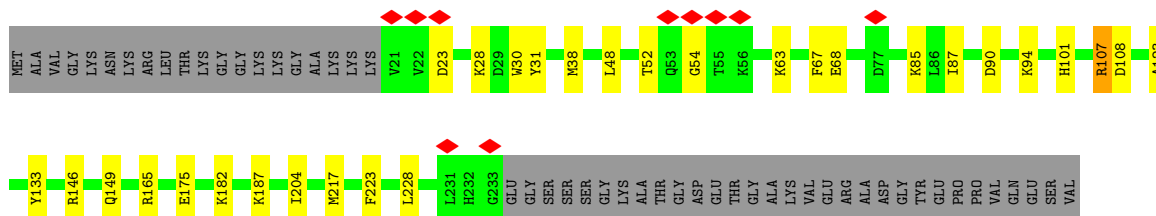
• Molecule 1: 18S ribosomal RNA



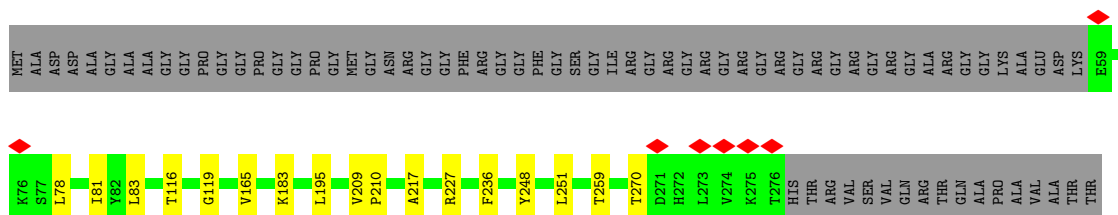




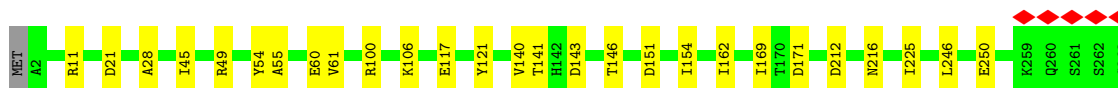
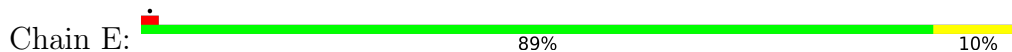
- Molecule 3: 40S ribosomal protein S3a



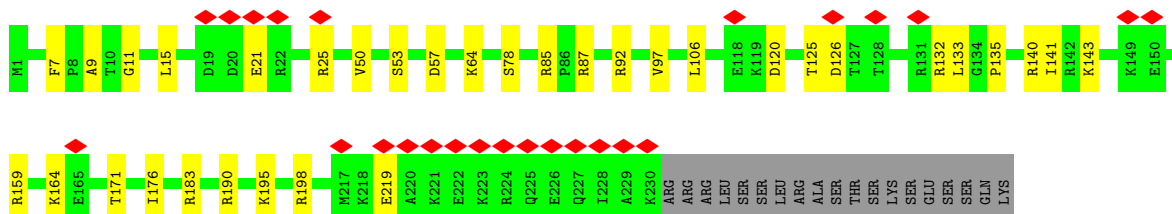
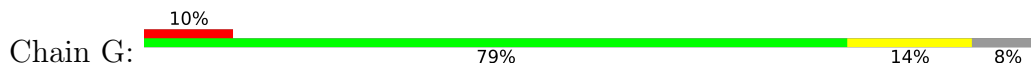
- Molecule 4: 40S ribosomal protein S2



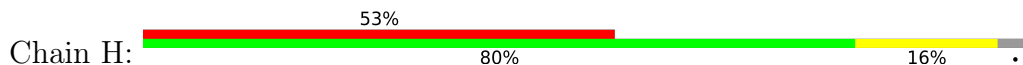
- Molecule 5: 40S ribosomal protein S4, X isoform



- Molecule 6: 40S ribosomal protein S6

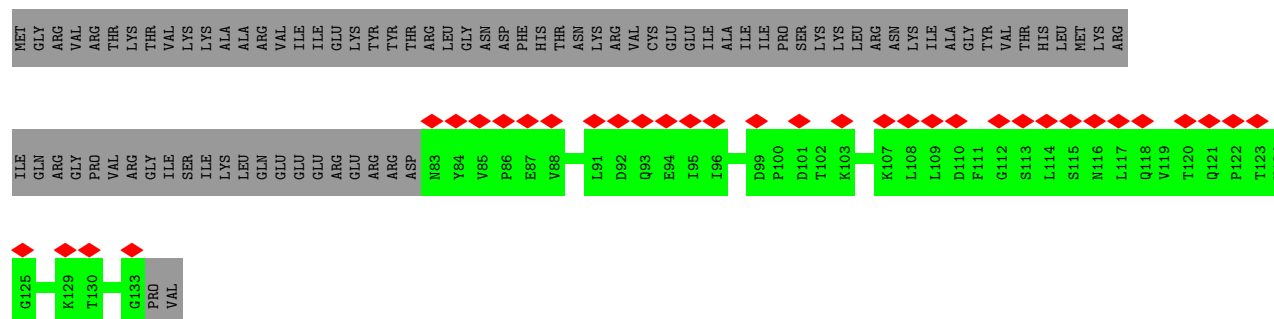


- Molecule 7: 40S ribosomal protein S7





- Chain R:  25% 38% 62%



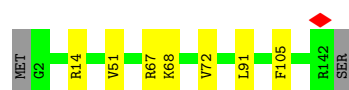
- Chain V:  94% 6%



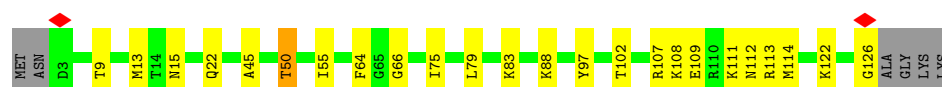
- Chain W: 85% 14%



- Chain X:  94% 5%



- Chain Y: 77% 18% 5%



-
- Diagram illustrating a 16x16 grid structure. A 4x4 subgrid is highlighted in red. The subgrid contains labels M1, R17, R18, K19, M20, R21, Q22, R23, S24, and K25. Red diamonds are placed above the subgrid labels.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118765	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.113	Depositor
Minimum map value	-3.485	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.143	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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, 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	0.27	0/29435	0.80	18/45875 (0.0%)
2	A	0.24	0/1742	0.40	0/2367
3	B	0.23	0/1756	0.42	0/2350
4	C	0.25	0/1726	0.43	0/2332
5	E	0.25	0/2118	0.44	0/2849
6	G	0.24	0/1885	0.41	0/2510
7	H	0.24	0/1524	0.40	0/2042
8	I	0.24	0/1711	0.43	0/2282
9	J	0.25	0/1524	0.41	0/2035
10	L	0.25	0/1250	0.44	0/1673
11	N	0.24	0/1226	0.39	0/1649
12	O	0.24	0/1023	0.45	0/1372
13	R	0.24	0/403	0.39	0/547
14	V	0.24	0/643	0.41	0/860
15	W	0.25	0/1051	0.43	0/1406
16	X	0.25	0/1116	0.43	0/1490
17	Y	0.24	0/1031	0.42	0/1370
18	a	0.24	0/828	0.40	0/1109
19	b	0.23	0/653	0.42	0/876
20	e	0.26	0/446	0.42	0/587
21	j	0.23	0/272	0.37	0/366
22	h	0.22	0/240	0.38	0/305
All	All	0.26	0/53603	0.67	18/78252 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	C2-N1-C1'	8.34	127.98	118.80
1	2	356	C	C2-N1-C1'	7.00	126.50	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1717	C	C2-N1-C1'	6.83	126.31	118.80
1	2	501	C	N1-C2-O2	6.64	122.89	118.90
1	2	293	C	N1-C2-O2	6.58	122.85	118.90
1	2	293	C	C2-N1-C1'	6.50	125.95	118.80
1	2	356	C	N1-C2-O2	6.41	122.74	118.90
1	2	1022	U	C2-N1-C1'	6.38	125.36	117.70
1	2	501	C	C6-N1-C1'	-6.16	113.41	120.80
1	2	630	U	C2-N1-C1'	6.05	124.95	117.70
1	2	1123	C	N1-C2-O2	5.97	122.48	118.90
1	2	853	C	C2-N1-C1'	5.75	125.12	118.80
1	2	1123	C	N3-C2-O2	-5.72	117.89	121.90
1	2	1751	C	N1-C2-O2	5.63	122.28	118.90
1	2	1751	C	N3-C2-O2	-5.56	118.00	121.90
1	2	630	U	N1-C2-O2	5.28	126.50	122.80
1	2	293	C	N3-C2-O2	-5.17	118.28	121.90
1	2	356	C	N3-C2-O2	-5.03	118.38	121.90

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	26317	0	13285	179	0
2	A	1705	0	1706	17	0
3	B	1729	0	1803	18	0
4	C	1690	0	1777	8	0
5	E	2076	0	2177	16	0
6	G	1862	0	2018	25	0
7	H	1501	0	1593	21	0
8	I	1682	0	1769	16	0
9	J	1499	0	1618	11	0
10	L	1229	0	1302	9	0
11	N	1202	0	1289	9	0
12	O	1010	0	1034	11	0
13	R	397	0	396	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	V	636	0	637	5	0
15	W	1034	0	1080	11	0
16	X	1098	0	1167	4	0
17	Y	1014	0	1082	14	0
18	a	814	0	863	0	0
19	b	640	0	663	0	0
20	e	441	0	487	0	0
21	j	267	0	238	0	0
22	h	239	0	289	0	0
23	2	106	0	0	0	0
23	L	1	0	0	0	0
23	X	2	0	0	0	0
24	a	1	0	0	0	0
All	All	50192	0	38273	327	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 4.

All (327) 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)
1:2:1091:C:HO2'	15:W:2:VAL:N	1.77	0.82
1:2:190:G:O2'	1:2:209:A:N6	2.17	0.76
1:2:1153:C:OP2	15:W:71:LYS:NZ	2.22	0.73
1:2:164:A:H3'	1:2:165:G:H21	1.55	0.71
4:C:259:THR:HG21	14:V:16:LYS:H	1.57	0.70
6:G:64:LYS:HB2	6:G:97:VAL:HG11	1.74	0.68
7:H:93:VAL:HG11	7:H:133:LEU:HD12	1.74	0.68
7:H:147:LYS:HD2	7:H:151:SER:HB2	1.76	0.68
9:J:136:ARG:NH1	9:J:159:PHE:O	2.28	0.67
6:G:85:ARG:O	6:G:87:ARG:NH1	2.28	0.67
3:B:107:ARG:NH2	12:O:133:THR:O	2.28	0.66
1:2:1717:C:H3'	1:2:1718:G:H8	1.61	0.65
12:O:98:ARG:NH1	12:O:99:ALA:O	2.31	0.64
1:2:640:A:H2'	1:2:641:A:C8	2.34	0.63
15:W:80:ASP:OD1	15:W:124:LYS:NZ	2.30	0.63
1:2:981:A:H2'	1:2:982:G:C8	2.33	0.63
5:E:246:LEU:HB3	5:E:250:GLU:HG3	1.79	0.63
1:2:96:C:H1'	1:2:474:G:H5'	1.81	0.62
2:A:184:ARG:HD2	2:A:191:ARG:HG2	1.80	0.62
4:C:116:THR:OG1	4:C:119:GLY:O	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:89:GLU:OE2	8:I:92:ARG:NH2	2.31	0.62
1:2:797:C:O3'	7:H:109:ARG:NH1	2.30	0.61
10:L:125:ILE:HB	10:L:146:THR:HG23	1.80	0.61
4:C:83:LEU:O	14:V:15:ARG:NH1	2.34	0.61
1:2:126:G:OP1	6:G:198:ARG:NH1	2.34	0.61
2:A:184:ARG:HG2	2:A:189:ILE:HG13	1.82	0.61
1:2:895:G:H2'	1:2:896:U:C6	2.36	0.60
7:H:46:THR:HG23	7:H:65:PRO:HD3	1.83	0.60
1:2:835:C:N4	17:Y:9:THR:O	2.34	0.60
5:E:140:VAL:HG22	5:E:146:THR:HG22	1.83	0.60
1:2:496:C:OP1	5:E:49:ARG:NH2	2.34	0.60
1:2:563:G:H1	1:2:592:C:H5	1.48	0.60
12:O:53:ILE:HG23	12:O:88:LEU:HD12	1.83	0.60
1:2:1010:G:H2'	1:2:1011:A:H8	1.67	0.59
1:2:373:G:H4'	10:L:85:THR:HG21	1.84	0.59
1:2:1762:C:H2'	1:2:1763:G:H8	1.66	0.58
1:2:581:U:H4'	17:Y:66:GLY:HA2	1.84	0.58
7:H:69:LEU:O	7:H:73:GLN:HG2	2.03	0.58
11:N:55:ARG:NH1	11:N:56:ASP:OD1	2.36	0.58
1:2:527:C:H2'	1:2:528:A:H8	1.69	0.58
2:A:38:ILE:HD11	2:A:47:TYR:HB3	1.86	0.58
1:2:528:A:H2'	1:2:529:A:H8	1.68	0.58
1:2:898:U:H2'	1:2:899:U:H5''	1.85	0.57
1:2:1856:C:H2'	1:2:1857:G:C8	2.39	0.57
1:2:145:G:H2'	1:2:146:G:C8	2.39	0.57
7:H:144:ILE:HB	15:W:52:ILE:HB	1.86	0.57
17:Y:55:ILE:HG13	17:Y:75:ILE:HG12	1.87	0.57
1:2:641:A:OP1	9:J:40:LYS:NZ	2.33	0.57
1:2:797:C:O2	7:H:109:ARG:NH2	2.37	0.57
1:2:1098:C:H2'	1:2:1099:G:C8	2.40	0.57
6:G:135:PRO:HG2	6:G:141:ILE:HD13	1.87	0.57
1:2:792:C:O2'	1:2:793:G:H8	1.87	0.57
7:H:119:SER:OG	7:H:120:ARG:NH1	2.38	0.56
5:E:100:ARG:NH2	5:E:121:TYR:O	2.37	0.56
16:X:68:LYS:HB3	16:X:91:LEU:HD22	1.86	0.56
1:2:220:U:H2'	1:2:221:A:H8	1.71	0.56
8:I:101:ILE:HD12	8:I:190:LEU:HD11	1.88	0.56
1:2:1780:G:H2'	1:2:1781:A:N3	2.21	0.56
1:2:1713:C:H2'	1:2:1714:U:C6	2.41	0.55
8:I:57:ALA:HB2	8:I:183:GLY:HA2	1.87	0.55
1:2:387:C:OP2	8:I:10:LYS:NZ	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:857:U:H2'	1:2:858:A:C8	2.42	0.55
1:2:107:A:H2'	1:2:108:G:C8	2.42	0.55
1:2:126:G:OP2	6:G:195:LYS:NZ	2.38	0.55
1:2:54:A:OP1	17:Y:111:LYS:NZ	2.35	0.55
15:W:30:CYS:SG	15:W:31:SER:N	2.81	0.54
1:2:319:C:H2'	1:2:320:G:C8	2.43	0.53
1:2:527:C:H4'	9:J:121:LYS:HD2	1.89	0.53
1:2:377:G:H5'	8:I:98:LYS:HB3	1.90	0.53
3:B:146:ARG:HB2	3:B:149:GLN:HB2	1.90	0.53
1:2:1010:G:H2'	1:2:1011:A:C8	2.43	0.53
4:C:183:LYS:HA	4:C:195:LEU:O	2.08	0.53
7:H:51:ILE:HG21	7:H:179:LYS:HG2	1.90	0.53
9:J:136:ARG:HD3	9:J:160:SER:HA	1.91	0.53
1:2:35:C:H5'	1:2:579:C:H5''	1.91	0.53
1:2:558:G:H2'	1:2:559:G:C8	2.44	0.53
1:2:980:A:H2'	1:2:981:A:C8	2.43	0.53
17:Y:113:ARG:NH2	17:Y:126:GLY:O	2.41	0.53
1:2:1763:G:H2'	1:2:1764:G:C8	2.44	0.53
1:2:1828:C:H2'	1:2:1829:G:O4'	2.09	0.53
1:2:847:A:O2'	5:E:106:LYS:NZ	2.42	0.52
2:A:77:ILE:HG12	2:A:99:ILE:HB	1.90	0.52
2:A:132:GLN:NE2	2:A:136:GLU:OE2	2.41	0.52
1:2:118:C:H1'	1:2:445:A:C5	2.45	0.52
1:2:325:C:O2'	1:2:326:C:O4'	2.26	0.52
1:2:367:U:H4'	1:2:371:A:C8	2.45	0.52
1:2:1856:C:H2'	1:2:1857:G:H8	1.75	0.52
10:L:91:ASP:HB3	10:L:104:LYS:HE2	1.92	0.52
1:2:69:C:OP2	6:G:164:LYS:NZ	2.43	0.51
1:2:528:A:H2'	1:2:529:A:C8	2.44	0.51
1:2:115:U:H2'	1:2:116:U:C6	2.45	0.51
1:2:220:U:H2'	1:2:221:A:C8	2.45	0.51
1:2:223:C:H2'	1:2:224:A:C8	2.46	0.51
1:2:674:C:H2'	1:2:675:U:C6	2.45	0.51
2:A:144:THR:OG1	2:A:156:TYR:O	2.26	0.51
1:2:1714:U:H2'	1:2:1715:A:H8	1.76	0.51
11:N:99:ARG:NH2	11:N:119:GLU:OE1	2.44	0.51
1:2:919:A:OP2	11:N:64:ARG:NH2	2.38	0.51
1:2:928:G:H1	1:2:1013:U:H3	1.57	0.51
3:B:68:GLU:HG2	3:B:85:LYS:HG2	1.92	0.51
3:B:108:ASP:OD1	3:B:108:ASP:N	2.41	0.51
1:2:1808:U:H2'	1:2:1809:A:H8	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:52:THR:HG22	3:B:54:GLY:H	1.75	0.51
15:W:86:LEU:HD21	15:W:113:HIS:HB2	1.93	0.51
1:2:384:U:O4	8:I:5:ARG:NH2	2.40	0.50
1:2:1139:C:H5	1:2:1149:A:H62	1.60	0.50
1:2:190:G:H5'	1:2:191:A:OP1	2.11	0.50
4:C:165:VAL:HG21	4:C:217:ALA:HB1	1.93	0.50
6:G:57:ASP:HA	6:G:106:LEU:HA	1.92	0.50
7:H:9:VAL:HG12	7:H:11:PRO:HD3	1.93	0.50
1:2:957:A:H2'	1:2:958:G:H8	1.77	0.50
1:2:1714:U:H2'	1:2:1715:A:C8	2.47	0.50
8:I:141:ARG:HB2	8:I:146:GLN:HG2	1.93	0.50
8:I:11:ARG:NH1	8:I:15:GLY:O	2.45	0.50
1:2:29:G:H2'	1:2:30:C:C6	2.46	0.50
1:2:996:A:H2'	1:2:997:A:C8	2.47	0.50
6:G:120:ASP:HB2	6:G:125:THR:HB	1.94	0.50
3:B:30:TRP:CD2	12:O:19:PRO:HG3	2.47	0.49
1:2:16:G:H2'	1:2:17:C:C6	2.47	0.49
2:A:206:ASP:O	2:A:209:GLU:N	2.44	0.49
1:2:1808:U:H2'	1:2:1809:A:C8	2.47	0.49
5:E:212:ASP:OD1	5:E:216:ASN:N	2.46	0.49
2:A:206:ASP:O	2:A:208:GLU:N	2.45	0.49
17:Y:102:THR:HG23	17:Y:107:ARG:HH11	1.78	0.49
1:2:201:C:H3'	1:2:202:G:H8	1.77	0.49
7:H:69:LEU:HD22	7:H:96:ALA:HB2	1.95	0.48
7:H:145:ARG:NH2	15:W:51:GLU:OE1	2.46	0.48
10:L:103:GLU:OE2	16:X:14:ARG:NH2	2.46	0.48
1:2:1717:C:H3'	1:2:1718:G:C8	2.46	0.48
7:H:163:GLN:NE2	7:H:167:GLU:OE1	2.46	0.48
1:2:527:C:H2'	1:2:528:A:C8	2.47	0.48
1:2:942:G:H2'	1:2:943:U:C6	2.48	0.48
1:2:1713:C:H2'	1:2:1714:U:H6	1.76	0.48
1:2:1845:A:H2'	1:2:1846:G:C8	2.49	0.48
3:B:30:TRP:CE2	3:B:48:LEU:HD13	2.48	0.48
1:2:1201:U:H2'	1:2:1202:U:C6	2.49	0.48
15:W:6:VAL:HG12	15:W:34:ILE:HD11	1.96	0.48
1:2:560:A:OP2	9:J:177:ASN:ND2	2.39	0.48
15:W:104:LEU:HD23	15:W:125:ILE:HA	1.96	0.48
11:N:83:ASP:N	11:N:83:ASP:OD1	2.44	0.48
1:2:656:G:H5'	1:2:662:G:N2	2.29	0.48
1:2:1736:G:H2'	1:2:1737:G:C8	2.48	0.48
1:2:1139:C:H2'	1:2:1140:G:O4'	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:874:G:H2'	1:2:875:A:H8	1.78	0.47
1:2:164:A:H3'	1:2:165:G:N2	2.27	0.47
1:2:795:A:H2'	1:2:796:G:C8	2.49	0.47
12:O:34:PHE:HB3	12:O:41:PHE:HB2	1.95	0.47
1:2:798:G:H3'	1:2:799:U:H3'	1.96	0.47
8:I:10:LYS:O	8:I:18:ARG:NH1	2.47	0.47
15:W:28:ARG:HB3	15:W:60:LYS:HG2	1.97	0.47
1:2:496:C:P	5:E:49:ARG:HH22	2.38	0.47
1:2:656:G:N2	1:2:663:C:H5''	2.30	0.47
1:2:189:U:H2'	1:2:190:G:O4'	2.14	0.47
1:2:322:C:H2'	1:2:323:C:C6	2.50	0.47
1:2:928:G:H2'	1:2:929:G:C8	2.49	0.47
17:Y:88:LYS:HD2	17:Y:97:TYR:CD1	2.50	0.47
7:H:57:ARG:HE	7:H:91:HIS:CD2	2.32	0.47
1:2:882:U:H2'	1:2:883:U:C6	2.50	0.46
11:N:110:ASP:O	11:N:114:ARG:HG2	2.15	0.46
1:2:77:A:H1'	6:G:176:ILE:HG13	1.97	0.46
1:2:429:C:O2'	1:2:811:A:N1	2.46	0.46
1:2:1797:U:H2'	1:2:1798:C:C6	2.50	0.46
8:I:130:THR:HG22	8:I:131:PRO:HD2	1.98	0.46
6:G:21:GLU:O	6:G:25:ARG:HG2	2.15	0.46
7:H:78:ARG:HH21	7:H:81:ARG:HH22	1.64	0.46
1:2:1036:A:H4'	1:2:1855:G:N2	2.30	0.46
2:A:78:SER:HB2	2:A:87:VAL:HG21	1.97	0.46
8:I:133:GLU:OE1	8:I:133:GLU:N	2.48	0.46
1:2:67:C:H41	6:G:164:LYS:H	1.63	0.46
1:2:1717:C:O2	1:2:1717:C:H2'	2.16	0.46
7:H:76:GLN:HG2	7:H:135:PHE:CD2	2.50	0.46
1:2:1060:A:O2'	1:2:1062:A:N7	2.34	0.46
1:2:406:U:O2'	1:2:408:A:OP1	2.25	0.46
7:H:9:VAL:HG23	7:H:24:SER:HB3	1.97	0.46
1:2:398:A:OP1	1:2:399:C:O2'	2.26	0.45
5:E:11:ARG:HA	5:E:28:ALA:HB2	1.98	0.45
1:2:674:C:H2'	1:2:675:U:H6	1.82	0.45
1:2:1121:G:O2'	3:B:204:ILE:O	2.25	0.45
3:B:38:MET:HE1	3:B:182:LYS:HA	1.98	0.45
1:2:65:C:C2	6:G:133:LEU:HD22	2.52	0.45
1:2:1736:G:H2'	1:2:1737:G:H8	1.81	0.45
4:C:78:LEU:HD12	4:C:81:ILE:HD12	1.99	0.45
11:N:102:LEU:HD13	11:N:111:ALA:HB3	1.98	0.45
1:2:168:C:H4'	6:G:132:ARG:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1836:G:OP1	1:2:1839:U:H4'	2.17	0.45
2:A:151:ASP:OD1	2:A:151:ASP:N	2.49	0.45
1:2:1845:A:H2'	1:2:1846:G:H8	1.82	0.44
7:H:101:LEU:HD12	7:H:116:ARG:HG3	1.98	0.44
1:2:911:C:O2'	1:2:912:C:H5'	2.17	0.44
2:A:103:PHE:CG	2:A:133:PRO:HG3	2.51	0.44
1:2:25:A:HO2'	1:2:26:U:H6	1.66	0.44
1:2:81:U:H2'	1:2:82:G:O4'	2.17	0.44
1:2:941:C:H2'	1:2:942:G:C8	2.53	0.44
1:2:1025:U:H2'	1:2:1026:C:O4'	2.18	0.44
1:2:1047:C:H2'	1:2:1048:G:O4'	2.17	0.44
1:2:1164:G:O2'	1:2:1165:G:H5'	2.17	0.44
1:2:51:U:H2'	1:2:52:G:C8	2.52	0.44
1:2:948:C:H2'	1:2:949:G:H8	1.82	0.44
1:2:1113:A:H2'	1:2:1114:U:C6	2.52	0.44
3:B:133:TYR:HD1	3:B:217:MET:HE1	1.82	0.44
1:2:96:C:H2'	1:2:97:U:C6	2.53	0.44
12:O:74:ALA:HB1	12:O:115:ALA:HB2	2.00	0.44
1:2:594:A:H61	1:2:643:A:H5''	1.83	0.44
5:E:11:ARG:HD3	5:E:21:ASP:O	2.17	0.44
9:J:140:GLN:NE2	17:Y:64:PHE:O	2.44	0.44
3:B:123:ALA:HB2	3:B:165:ARG:HG3	1.99	0.43
1:2:28:U:H2'	1:2:29:G:H8	1.84	0.43
1:2:804:U:H2'	1:2:805:U:C6	2.53	0.43
2:A:30:LEU:HD21	2:A:35:GLU:HG3	2.00	0.43
8:I:3:ILE:O	8:I:30:GLY:N	2.49	0.43
17:Y:79:LEU:HG	17:Y:83:LYS:HE3	2.01	0.43
1:2:1046:U:H1'	12:O:140:THR:HB	1.99	0.43
6:G:143:LYS:HE3	6:G:143:LYS:HB2	1.85	0.43
1:2:1712:A:H2'	1:2:1713:C:C6	2.54	0.43
1:2:155:G:H4'	6:G:15:LEU:HD22	2.00	0.43
1:2:1189:A:H2'	1:2:1190:A:C8	2.53	0.43
3:B:31:TYR:CD2	3:B:94:LYS:HA	2.52	0.43
9:J:48:PHE:CZ	9:J:52:LYS:HE3	2.54	0.43
17:Y:13:MET:HG3	17:Y:22:GLN:HG3	1.99	0.43
1:2:170:A:OP2	6:G:140:ARG:NH1	2.52	0.43
1:2:396:U:OP2	10:L:79:LYS:NZ	2.35	0.43
1:2:1007:C:H2'	1:2:1008:A:C8	2.54	0.43
10:L:30:LYS:HG3	10:L:32:LYS:HB2	2.01	0.43
17:Y:108:LYS:O	17:Y:112:ASN:ND2	2.39	0.43
1:2:1203:G:H2'	1:2:1204:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:76:VAL:HG12	2:A:123:VAL:HB	2.01	0.43
3:B:28:LYS:HB3	3:B:48:LEU:HD11	2.00	0.43
6:G:120:ASP:N	6:G:120:ASP:OD1	2.46	0.43
1:2:102:A:H4'	1:2:104:A:C8	2.54	0.43
1:2:160:U:O2'	1:2:162:C:OP2	2.32	0.43
2:A:149:ASN:OD1	2:A:150:THR:N	2.46	0.43
5:E:151:ASP:HB3	5:E:154:ILE:HG13	2.01	0.43
6:G:7:PHE:O	6:G:11:GLY:N	2.51	0.43
9:J:131:ARG:HD2	9:J:131:ARG:HA	1.85	0.43
14:V:51:LYS:HD2	14:V:78:ILE:HD11	2.01	0.43
1:2:333:G:OP2	6:G:190:ARG:NH1	2.52	0.42
1:2:563:G:O2'	1:2:564:A:H8	2.02	0.42
1:2:917:U:H2'	1:2:918:U:C6	2.54	0.42
10:L:111:VAL:HG12	10:L:140:PHE:HB2	2.01	0.42
15:W:47:ILE:HG13	15:W:48:GLY:H	1.84	0.42
1:2:882:U:H2'	1:2:883:U:H6	1.84	0.42
8:I:149:TYR:O	8:I:153:LYS:HG3	2.19	0.42
17:Y:114:MET:O	17:Y:122:LYS:NZ	2.50	0.42
1:2:352:U:H2'	1:2:353:C:C6	2.54	0.42
1:2:871:U:O2'	1:2:873:G:OP1	2.38	0.42
1:2:1101:U:H2'	1:2:1102:G:C8	2.54	0.42
12:O:39:ASP:OD1	12:O:40:THR:N	2.49	0.42
1:2:441:C:H2'	1:2:442:C:C6	2.54	0.42
8:I:81:VAL:HG22	8:I:102:VAL:HG12	2.01	0.42
2:A:33:GLN:HB3	2:A:154:LEU:HD12	2.01	0.42
1:2:533:A:H2'	1:2:534:G:H8	1.84	0.42
1:2:540:U:N3	1:2:542:U:OP1	2.45	0.42
1:2:946:U:H2'	1:2:947:G:H8	1.84	0.42
2:A:68:ILE:HD11	2:A:121:LEU:HB2	2.01	0.42
3:B:63:LYS:HE3	3:B:90:ASP:HA	2.01	0.42
1:2:1763:G:H2'	1:2:1764:G:H8	1.84	0.42
1:2:1118:C:H3'	1:2:1119:A:C8	2.55	0.42
1:2:1764:G:H1	1:2:1768:A:H62	1.67	0.42
1:2:1788:A:H2'	1:2:1789:G:O4'	2.20	0.42
10:L:23:VAL:HG23	10:L:26:GLY:H	1.84	0.42
11:N:4:MET:HG2	11:N:5:HIS:CD2	2.55	0.42
1:2:810:A:H5'	1:2:811:A:OP2	2.20	0.42
1:2:838:G:O2'	1:2:839:C:H4'	2.20	0.42
1:2:12:U:H2'	1:2:13:C:C6	2.55	0.42
3:B:223:PHE:HE1	3:B:228:LEU:HD12	1.83	0.42
6:G:78:SER:HB3	6:G:92:ARG:HG2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:86:LYS:NZ	12:O:122:SER:O	2.46	0.42
1:2:15:U:H2'	1:2:16:G:O4'	2.20	0.41
1:2:1714:U:C2	1:2:1715:A:C8	3.08	0.41
9:J:139:LYS:HA	9:J:139:LYS:HD3	1.57	0.41
1:2:219:U:H1'	8:I:184:ARG:HD2	2.02	0.41
1:2:946:U:C2	1:2:947:G:C8	3.08	0.41
1:2:958:G:H2'	1:2:959:G:C8	2.55	0.41
5:E:141:THR:OG1	5:E:143:ASP:OD1	2.26	0.41
1:2:406:U:H2'	1:2:408:A:H5''	2.02	0.41
1:2:793:G:H2'	1:2:794:A:H8	1.83	0.41
1:2:1767:C:H4'	1:2:1768:A:N3	2.36	0.41
1:2:957:A:H2'	1:2:958:G:C8	2.55	0.41
3:B:87:ILE:HG22	3:B:101:HIS:HB2	2.02	0.41
12:O:71:PRO:HB3	12:O:114:SER:OG	2.19	0.41
1:2:165:G:H4'	6:G:53:SER:HB3	2.01	0.41
1:2:801:U:H2'	1:2:802:A:H8	1.85	0.41
3:B:67:PHE:CE2	12:O:48:SER:HB3	2.55	0.41
5:E:55:ALA:HB1	5:E:60:GLU:HB2	2.02	0.41
4:C:209:VAL:HB	4:C:210:PRO:HD3	2.03	0.41
6:G:7:PHE:CE2	6:G:9:ALA:HB3	2.55	0.41
16:X:51:VAL:HA	16:X:72:VAL:HG12	2.02	0.41
1:2:1031:A:H4'	11:N:112:LYS:HE2	2.03	0.41
5:E:54:TYR:O	17:Y:15:ASN:ND2	2.54	0.41
7:H:134:VAL:HG12	7:H:173:PHE:CD2	2.56	0.41
10:L:75:GLY:HA3	10:L:88:ILE:HD12	2.03	0.41
1:2:5:U:H2'	1:2:6:G:H8	1.85	0.41
1:2:618:C:H41	16:X:67:ARG:NH2	2.19	0.41
1:2:749:U:H2'	1:2:750:C:C6	2.56	0.41
17:Y:45:ALA:HB1	17:Y:50:THR:O	2.21	0.41
1:2:443:U:H2'	1:2:444:G:O4'	2.21	0.41
1:2:795:A:H2'	1:2:796:G:H8	1.84	0.41
1:2:1019:C:H2'	1:2:1020:A:O4'	2.21	0.41
1:2:1719:A:H8	1:2:1814:G:H21	1.68	0.41
4:C:259:THR:HG21	14:V:16:LYS:N	2.31	0.41
8:I:105:ASP:OD1	8:I:106:SER:N	2.54	0.41
1:2:317:C:OP2	6:G:183:ARG:NH1	2.44	0.41
1:2:434:G:H2'	1:2:435:A:C8	2.56	0.41
1:2:952:G:H2'	1:2:953:C:C6	2.55	0.41
1:2:1762:C:H2'	1:2:1763:G:C8	2.52	0.41
6:G:126:ASP:OD1	6:G:126:ASP:N	2.53	0.41
14:V:51:LYS:NZ	14:V:76:ASP:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:433:A:H2'	1:2:434:G:C8	2.56	0.40
1:2:798:G:H3'	1:2:799:U:C3'	2.52	0.40
1:2:1199:A:H2'	1:2:1200:A:C8	2.56	0.40
5:E:162:ILE:HD11	5:E:169:ILE:HG12	2.03	0.40
5:E:171:ASP:OD1	5:E:171:ASP:N	2.54	0.40
9:J:174:LYS:HE3	9:J:174:LYS:HB3	1.94	0.40
11:N:100:LYS:O	11:N:103:GLU:HG2	2.21	0.40
1:2:5:U:H2'	1:2:6:G:C8	2.55	0.40
5:E:45:ILE:HG13	5:E:61:VAL:HG21	2.03	0.40
7:H:163:GLN:O	7:H:167:GLU:HB2	2.21	0.40
3:B:175:GLU:OE1	3:B:187:LYS:NZ	2.51	0.40
1:2:563:G:O2'	1:2:564:A:H5''	2.21	0.40
1:2:634:A:H2'	1:2:635:G:C8	2.56	0.40
1:2:931:C:H2'	1:2:932:G:C8	2.56	0.40
1:2:1013:U:C2	1:2:1014:G:C8	3.10	0.40
1:2:1356:G:H2'	1:2:1357:A:C8	2.56	0.40
9:J:93:LYS:HB2	9:J:96:TYR:CD2	2.56	0.40
2:A:170:SER:O	2:A:174:MET:HG2	2.21	0.40
6:G:159:ARG:HB3	6:G:171:THR:HG22	2.03	0.40
7:H:109:ARG:HD3	7:H:109:ARG:HA	1.90	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	A	214/295 (72%)	208 (97%)	6 (3%)	0	100	100
3	B	211/264 (80%)	208 (99%)	3 (1%)	0	100	100
4	C	216/293 (74%)	212 (98%)	4 (2%)	0	100	100
5	E	260/263 (99%)	258 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	228/249 (92%)	222 (97%)	6 (3%)	0	100	100
7	H	184/194 (95%)	175 (95%)	9 (5%)	0	100	100
8	I	203/208 (98%)	201 (99%)	2 (1%)	0	100	100
9	J	178/194 (92%)	173 (97%)	5 (3%)	0	100	100
10	L	149/158 (94%)	147 (99%)	2 (1%)	0	100	100
11	N	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
12	O	133/151 (88%)	129 (97%)	4 (3%)	0	100	100
13	R	49/135 (36%)	49 (100%)	0	0	100	100
14	V	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
15	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
16	X	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
17	Y	122/130 (94%)	120 (98%)	2 (2%)	0	100	100
18	a	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
19	b	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
20	e	54/56 (96%)	54 (100%)	0	0	100	100
21	j	31/180 (17%)	30 (97%)	1 (3%)	0	100	100
22	h	23/25 (92%)	23 (100%)	0	0	100	100
All	All	2928/3485 (84%)	2864 (98%)	64 (2%)	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	A	180/243 (74%)	180 (100%)	0	100	100
3	B	194/231 (84%)	192 (99%)	2 (1%)	73	91
4	C	184/225 (82%)	179 (97%)	5 (3%)	40	74
5	E	224/225 (100%)	222 (99%)	2 (1%)	75	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	200/218 (92%)	198 (99%)	2 (1%)	73	91
7	H	167/174 (96%)	167 (100%)	0	100	100
8	I	178/180 (99%)	174 (98%)	4 (2%)	47	79
9	J	160/168 (95%)	159 (99%)	1 (1%)	84	95
10	L	135/142 (95%)	132 (98%)	3 (2%)	47	79
11	N	130/131 (99%)	130 (100%)	0	100	100
12	O	105/119 (88%)	101 (96%)	4 (4%)	28	62
13	R	47/122 (38%)	47 (100%)	0	100	100
14	V	67/67 (100%)	67 (100%)	0	100	100
15	W	112/113 (99%)	112 (100%)	0	100	100
16	X	113/115 (98%)	112 (99%)	1 (1%)	75	92
17	Y	108/112 (96%)	106 (98%)	2 (2%)	52	82
18	a	88/88 (100%)	86 (98%)	2 (2%)	45	78
19	b	74/74 (100%)	72 (97%)	2 (3%)	40	74
20	e	45/45 (100%)	45 (100%)	0	100	100
21	j	29/151 (19%)	28 (97%)	1 (3%)	32	66
22	h	24/24 (100%)	24 (100%)	0	100	100
All	All	2564/2967 (86%)	2533 (99%)	31 (1%)	66	89

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	23	ASP
3	B	107	ARG
4	C	227	ARG
4	C	236	PHE
4	C	248	TYR
4	C	251	LEU
4	C	270	THR
5	E	117	GLU
5	E	225	ILE
6	G	50	VAL
6	G	219	GLU
8	I	76	THR
8	I	107	THR
8	I	121	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	130	THR
9	J	106	LEU
10	L	69	ARG
10	L	85	THR
10	L	146	THR
12	O	34	PHE
12	O	98	ARG
12	O	100	THR
12	O	138	ASP
16	X	105	PHE
17	Y	50	THR
17	Y	109	GLU
18	a	30	VAL
18	a	67	LEU
19	b	17	ARG
19	b	40	CYS
21	j	163	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1225/1869 (65%)	246 (20%)	0

All (246) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	8	U
1	2	17	C
1	2	26	U
1	2	33	G
1	2	35	C
1	2	41	G
1	2	46	A
1	2	56	G
1	2	64	A
1	2	65	C
1	2	67	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	68	A
1	2	73	C
1	2	74	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	103	A
1	2	113	G
1	2	115	U
1	2	128	U
1	2	130	G
1	2	143	U
1	2	148	U
1	2	149	A
1	2	155	G
1	2	163	U
1	2	168	C
1	2	178	C
1	2	182	C
1	2	188	C
1	2	189	U
1	2	191	A
1	2	195	C
1	2	201	C
1	2	204	G
1	2	292	A
1	2	295	C
1	2	309	G
1	2	312	G
1	2	318	A
1	2	319	C
1	2	320	G
1	2	321	C
1	2	325	C
1	2	326	C
1	2	327	G
1	2	328	U
1	2	330	G
1	2	331	C
1	2	332	G
1	2	333	G
1	2	335	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	351	G
1	2	358	C
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	370	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	392	A
1	2	398	A
1	2	400	C
1	2	408	A
1	2	409	C
1	2	418	A
1	2	421	G
1	2	448	A
1	2	450	C
1	2	464	A
1	2	465	A
1	2	471	G
1	2	472	C
1	2	474	G
1	2	482	G
1	2	487	U
1	2	492	C
1	2	502	C
1	2	516	A
1	2	531	A
1	2	535	G
1	2	536	A
1	2	537	C
1	2	538	U
1	2	539	C
1	2	541	U
1	2	542	U
1	2	544	G
1	2	546	G
1	2	547	G
1	2	548	C
1	2	555	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	556	U
1	2	559	G
1	2	563	G
1	2	568	C
1	2	576	A
1	2	583	A
1	2	588	G
1	2	591	U
1	2	593	C
1	2	598	G
1	2	604	A
1	2	607	U
1	2	608	C
1	2	614	C
1	2	626	G
1	2	627	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	664	A
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	687	C
1	2	688	U
1	2	748	C
1	2	793	G
1	2	796	G
1	2	797	C
1	2	798	G
1	2	799	U
1	2	800	U
1	2	801	U
1	2	809	A
1	2	810	A
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	835	C
1	2	836	G
1	2	838	G
1	2	839	C
1	2	841	G
1	2	842	C
1	2	847	A
1	2	870	A
1	2	872	A
1	2	873	G
1	2	874	G
1	2	875	A
1	2	878	G
1	2	890	U
1	2	899	U
1	2	908	A
1	2	909	G
1	2	913	A
1	2	918	U
1	2	919	A
1	2	920	A
1	2	930	C
1	2	933	G
1	2	934	G
1	2	943	U
1	2	970	G
1	2	971	G
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1001	A
1	2	1017	U
1	2	1023	A
1	2	1049	A
1	2	1060	A
1	2	1061	U
1	2	1062	A
1	2	1067	C
1	2	1083	A
1	2	1085	C
1	2	1115	U
1	2	1118	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1130	G
1	2	1138	C
1	2	1139	C
1	2	1148	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1171	G
1	2	1195	A
1	2	1207	G
1	2	1358	U
1	2	1695	A
1	2	1699	A
1	2	1702	G
1	2	1707	U
1	2	1717	C
1	2	1718	G
1	2	1719	A
1	2	1721	U
1	2	1723	G
1	2	1724	A
1	2	1725	U
1	2	1729	U
1	2	1744	G
1	2	1748	G
1	2	1757	G
1	2	1758	G
1	2	1759	G
1	2	1760	G
1	2	1761	U
1	2	1767	C
1	2	1768	A
1	2	1773	C
1	2	1774	C
1	2	1775	U
1	2	1776	G
1	2	1777	G
1	2	1783	C
1	2	1784	G
1	2	1785	C
1	2	1800	A
1	2	1801	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	1810	U
1	2	1811	C
1	2	1812	U
1	2	1814	G
1	2	1818	A
1	2	1825	A
1	2	1826	G
1	2	1829	G
1	2	1831	A
1	2	1835	A
1	2	1836	G
1	2	1838	U
1	2	1849	G
1	2	1851	A
1	2	1852	C
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1864	U
1	2	1865	C
1	2	1866	A
1	2	1868	U
1	2	1869	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 110 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

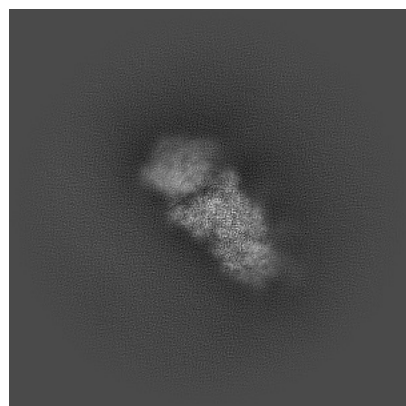
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11321. These allow visual inspection of the internal detail of the map and identification of artifacts.

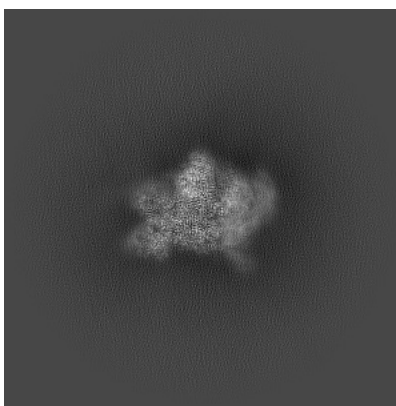
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

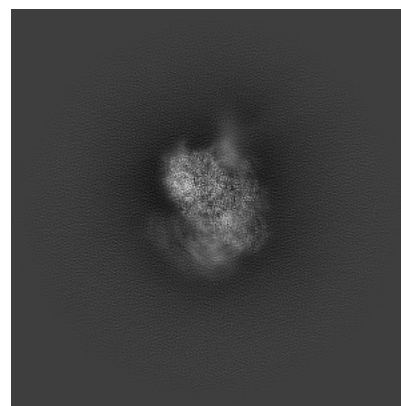
6.1.1 Primary map



X

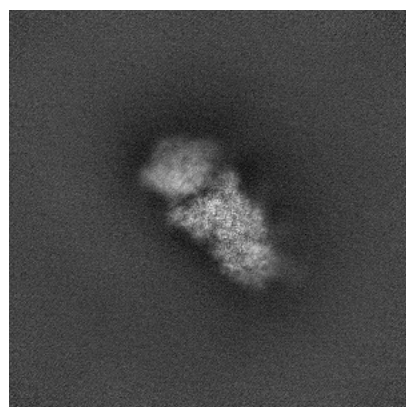


Y

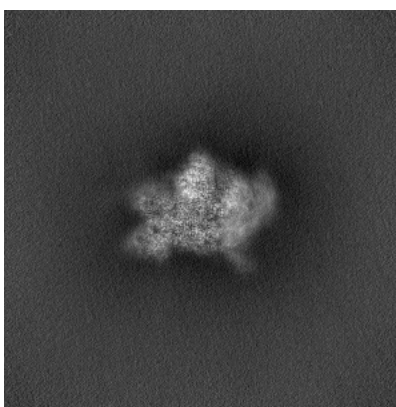


Z

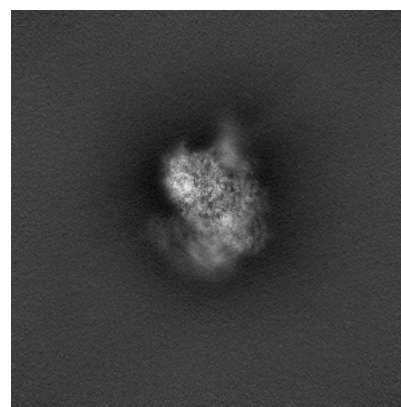
6.1.2 Raw map



X



Y



Z

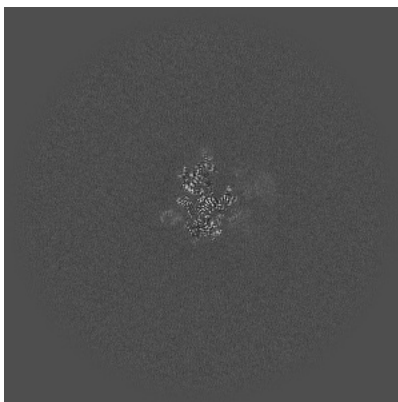
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

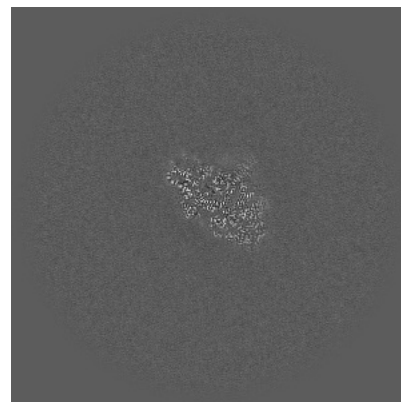
6.2.1 Primary map



X Index: 280



Y Index: 280



Z Index: 280

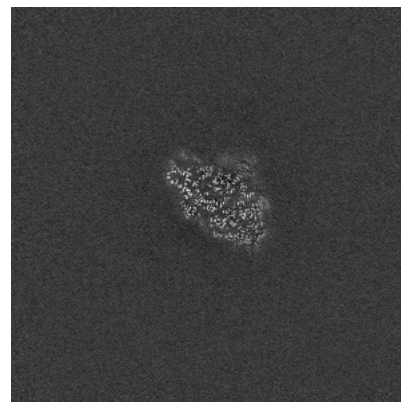
6.2.2 Raw map



X Index: 280



Y Index: 280



Z Index: 280

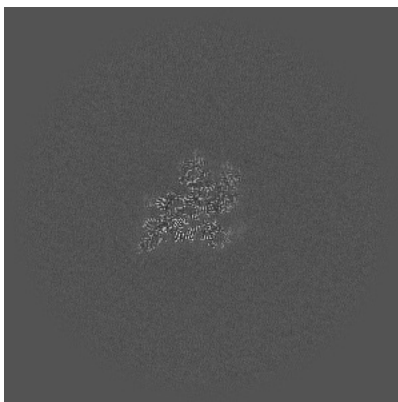
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

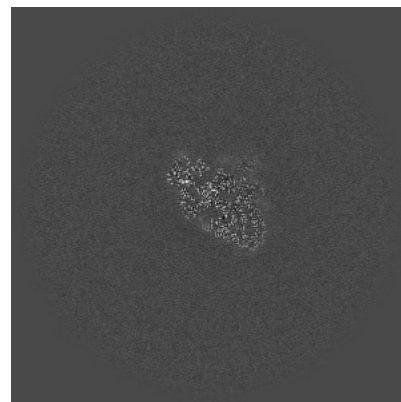
6.3.1 Primary map



X Index: 286



Y Index: 309



Z Index: 275

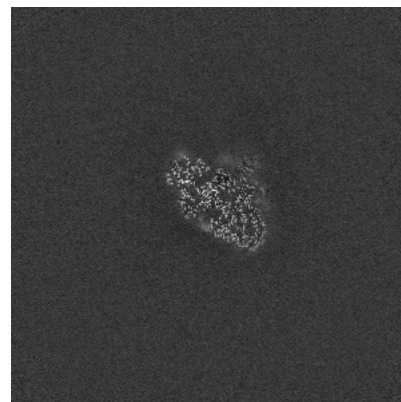
6.3.2 Raw map



X Index: 286



Y Index: 309

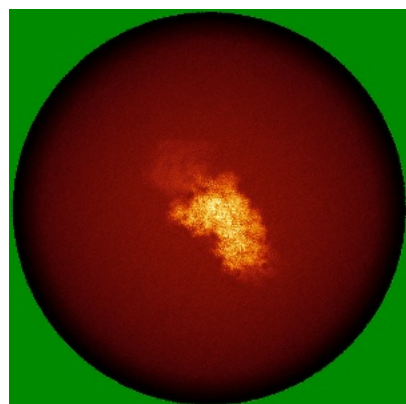


Z Index: 275

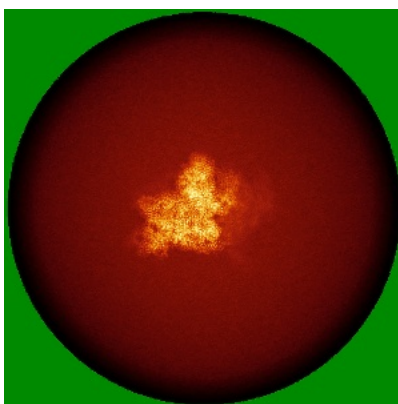
The images above show the largest variance slices of the map in three orthogonal directions.

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

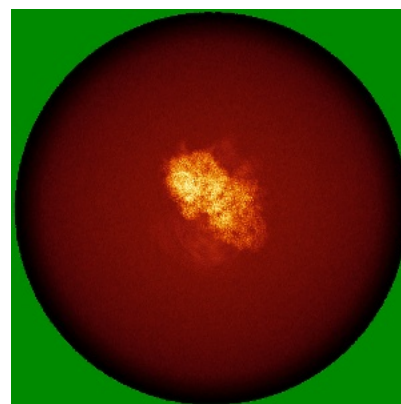
6.4.1 Primary map



X

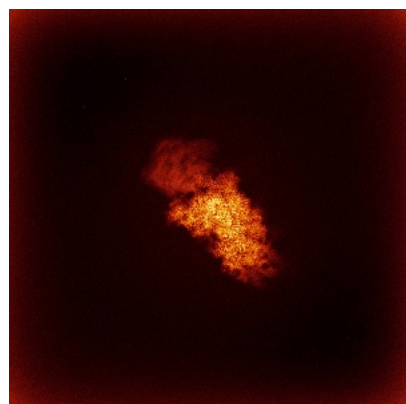


Y

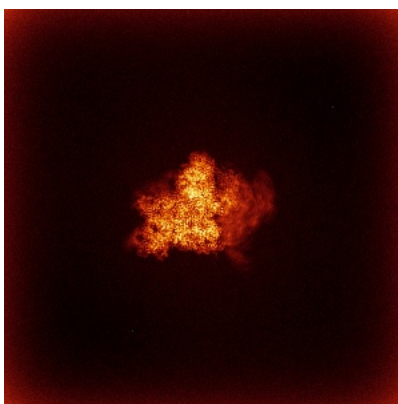


Z

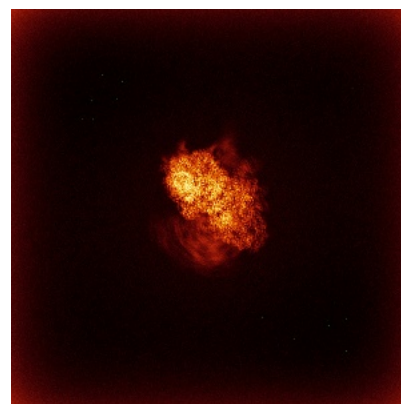
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. 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



X



Y



Z

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.

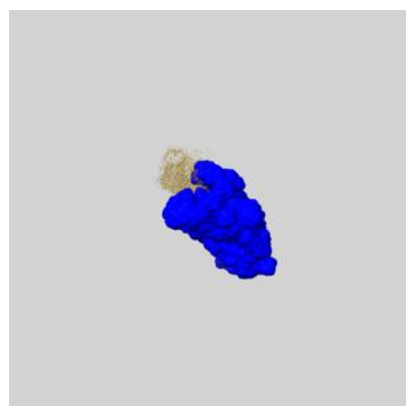
6.6 Mask visualisation [i](#)

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

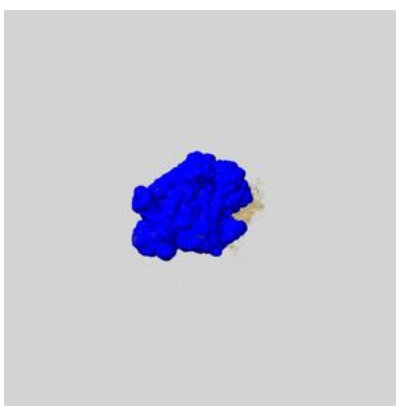
A mask typically either:

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

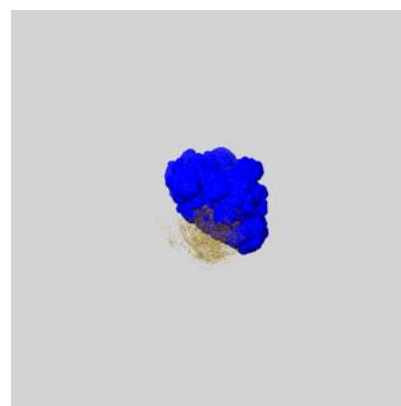
6.6.1 emd_11321_msk_1.map [i](#)



X



Y

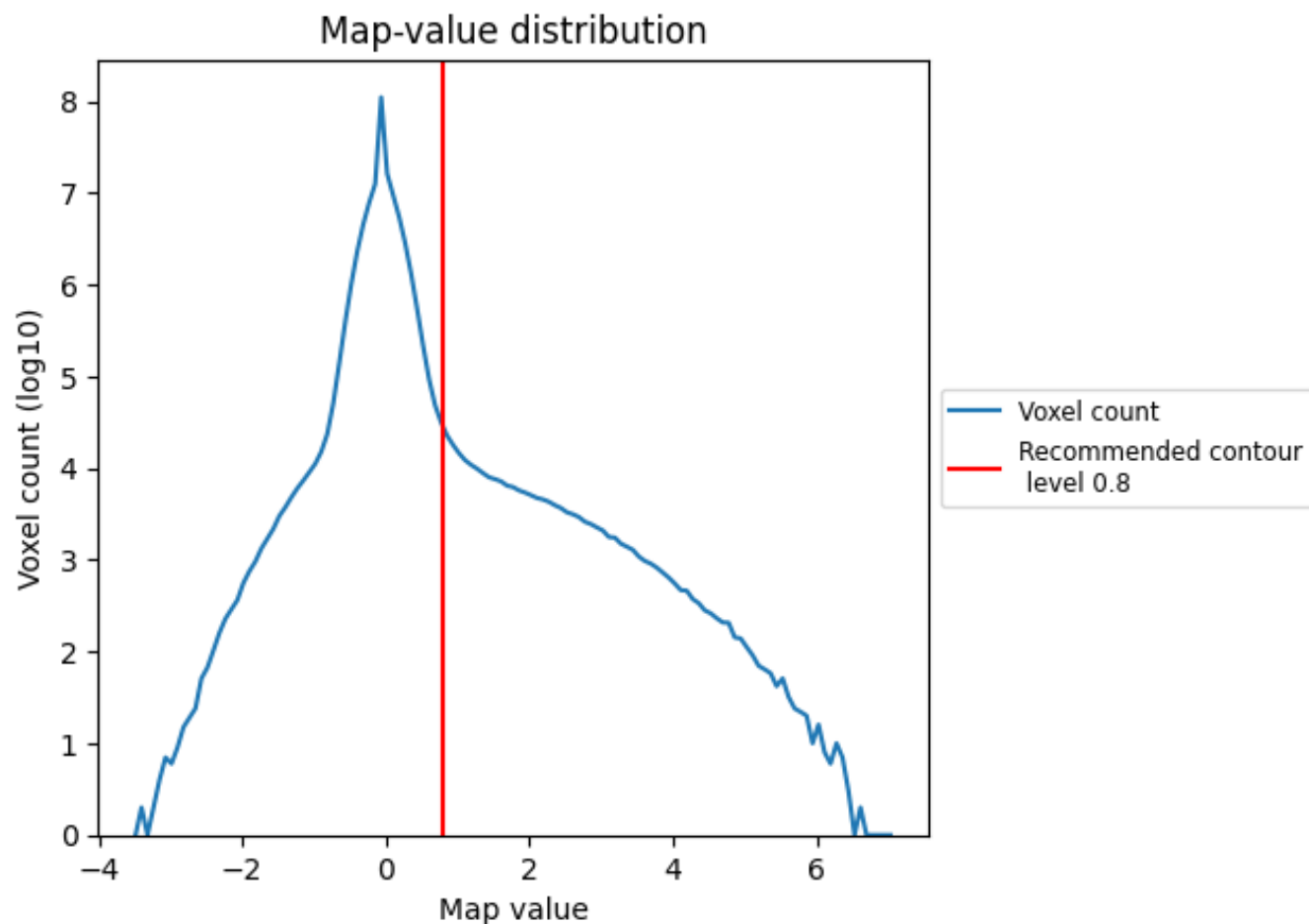


Z

7 Map analysis [i](#)

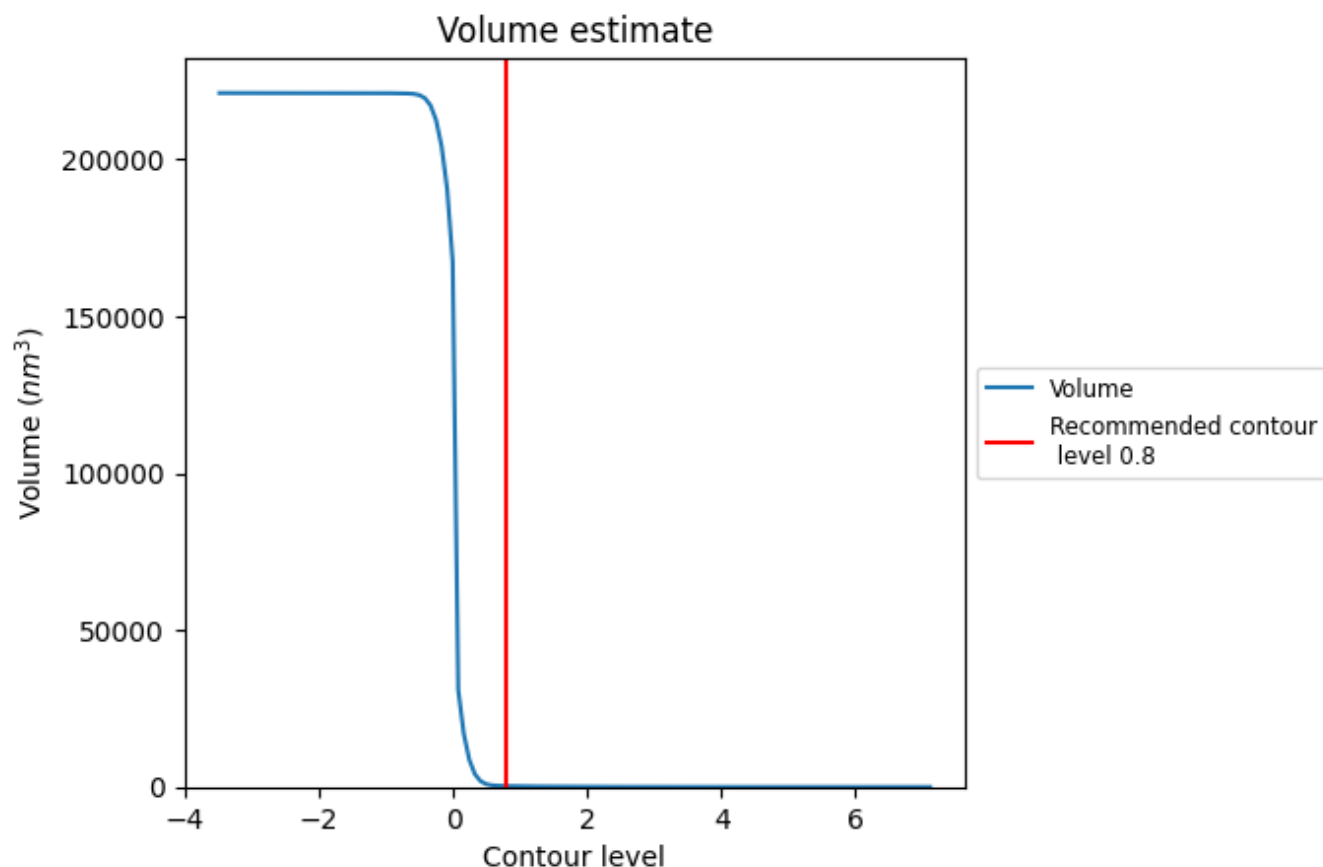
This section contains the results of statistical analysis of the map.

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.

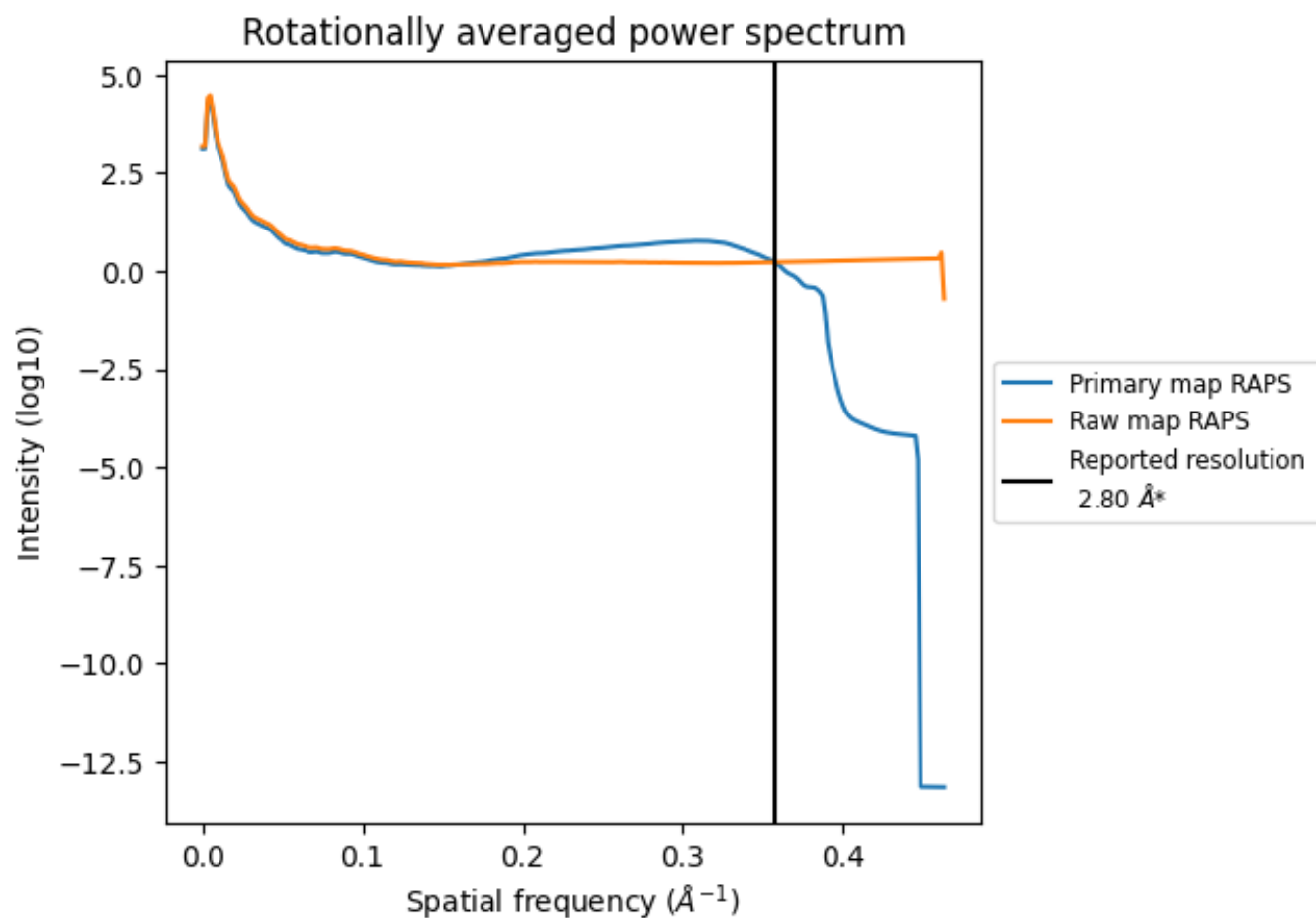
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm³; this corresponds to an approximate mass of 257 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 ⓘ

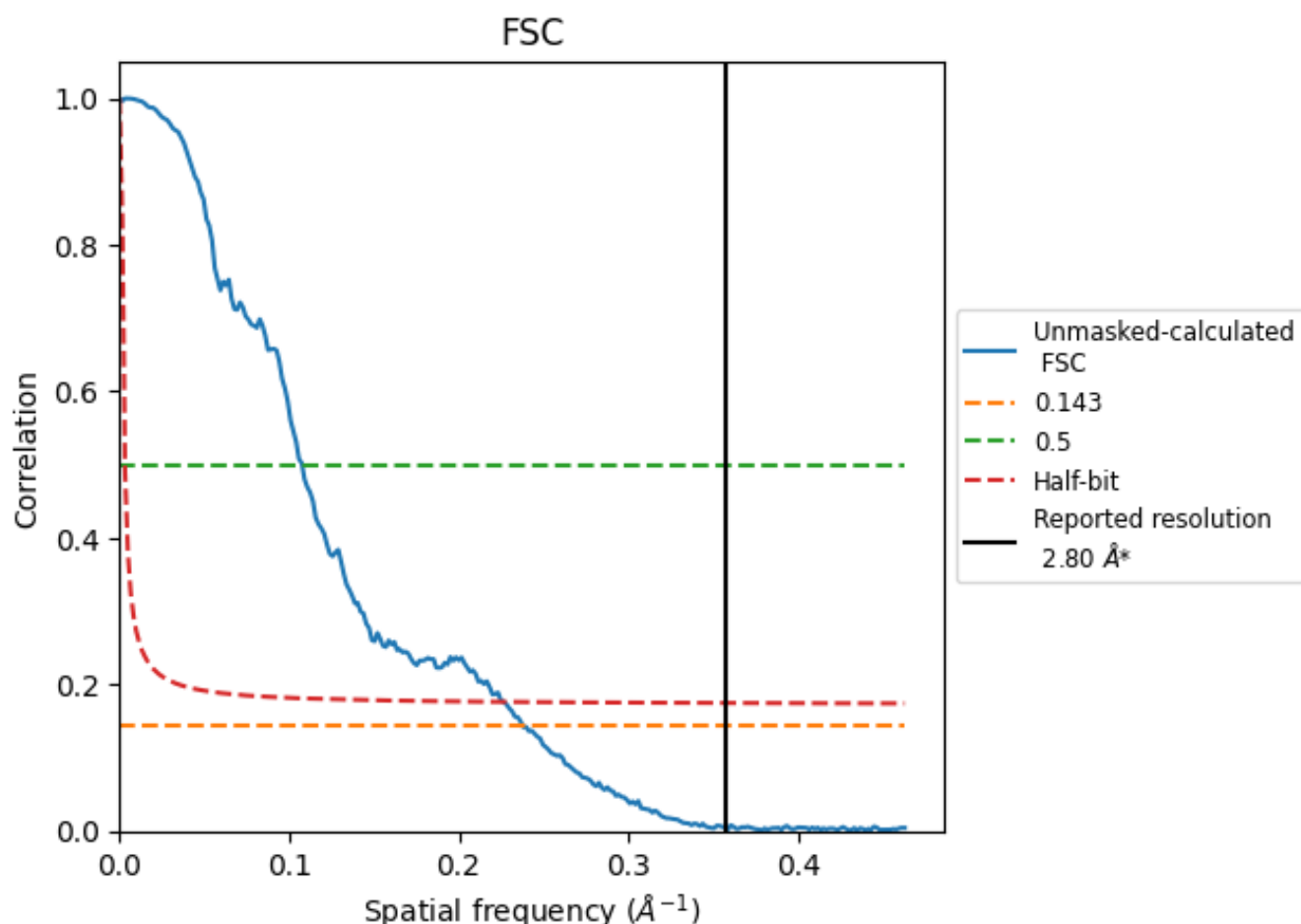


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

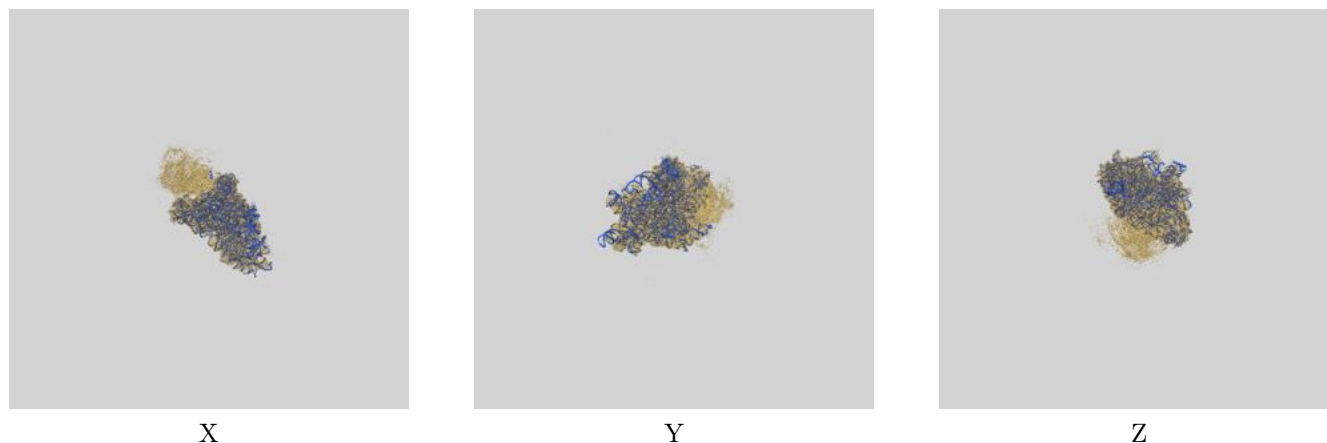
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.21	9.29	4.41

*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 4.21 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

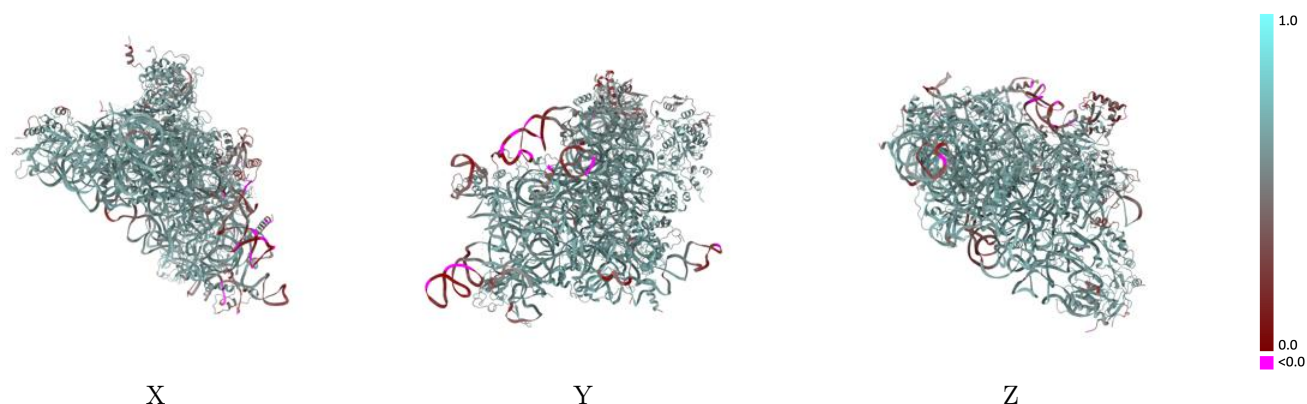
This section contains information regarding the fit between EMDB map EMD-11321 and PDB model 6ZOK. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



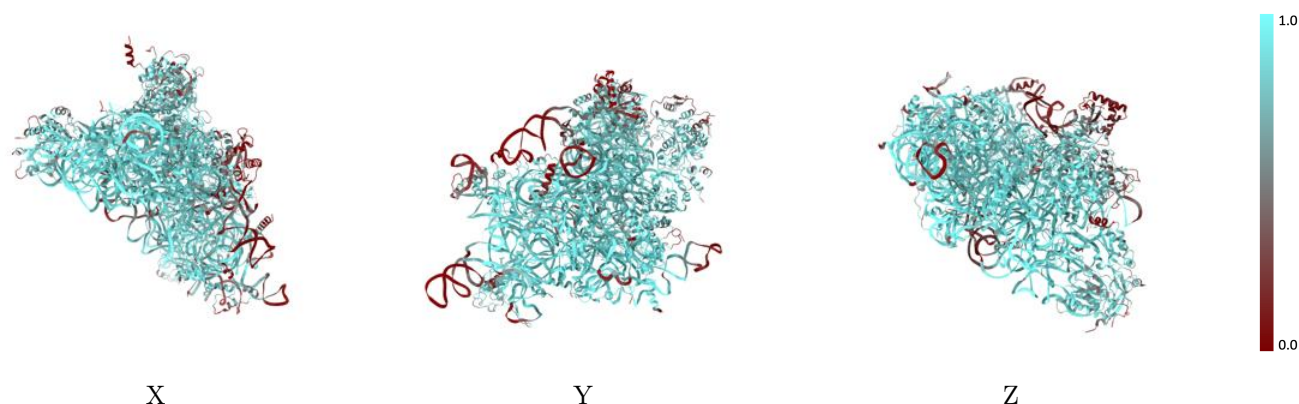
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



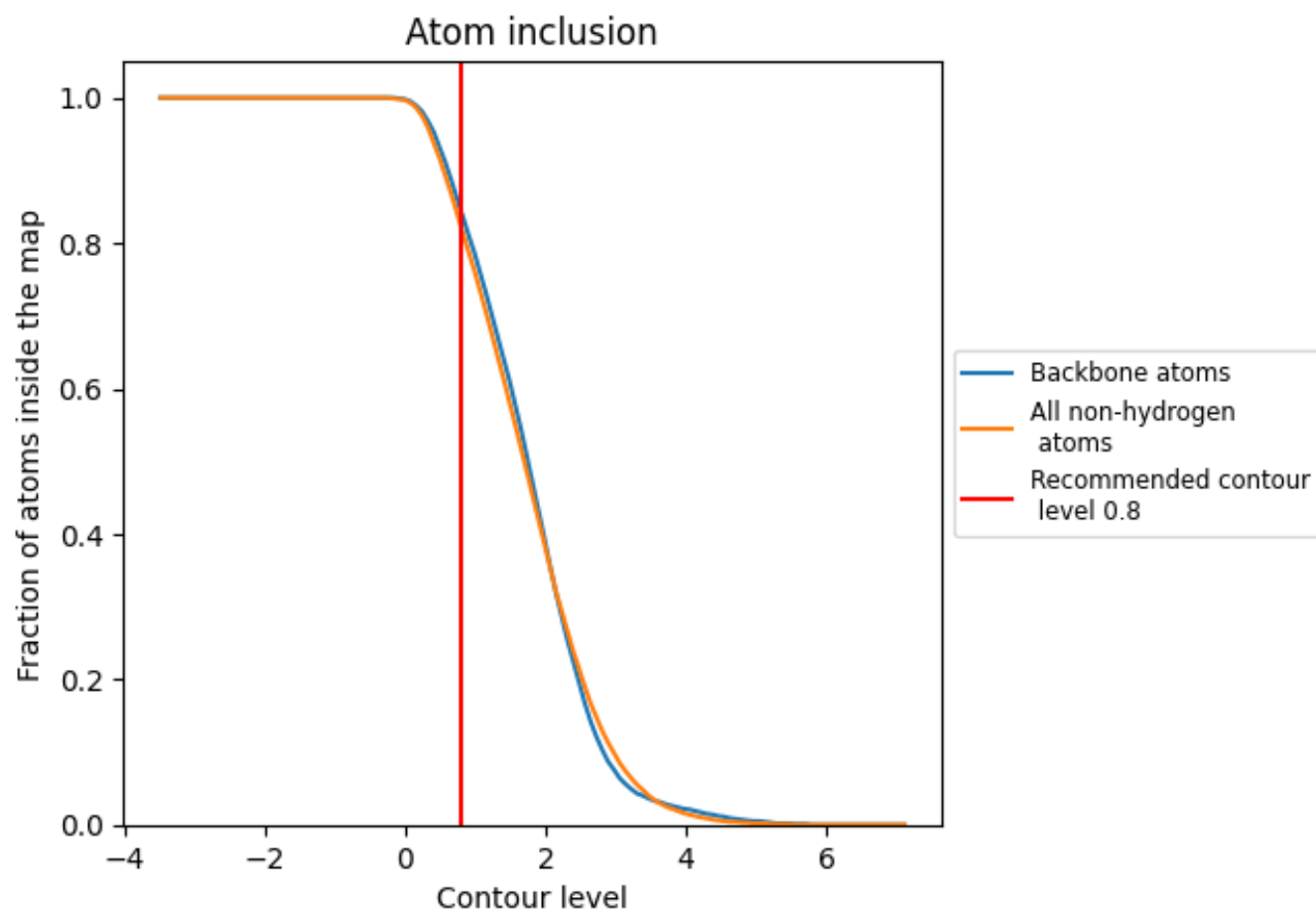
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.5830
2	 0.8480	 0.5730
A	 0.7560	 0.5860
B	 0.8060	 0.5960
C	 0.8660	 0.6260
E	 0.9060	 0.6330
G	 0.7590	 0.5730
H	 0.3910	 0.4480
I	 0.8130	 0.6000
J	 0.9170	 0.6330
L	 0.8300	 0.6100
N	 0.8080	 0.6010
O	 0.7880	 0.5840
R	 0.3400	 0.4600
V	 0.7880	 0.6000
W	 0.9210	 0.6420
X	 0.9160	 0.6430
Y	 0.8900	 0.6250
a	 0.8150	 0.5870
b	 0.6780	 0.5700
e	 0.7470	 0.5930
h	 0.5550	 0.5070
j	 0.7090	 0.5950

