Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 07:42 pm GMT

PDB ID	:	6ZOL
EMDB ID	:	EMD-11322
Title	:	SARS-CoV-2-Nsp1-40S complex, focused on head
Authors	:	Schubert, K.; Karousis, E.D.; Jomaa, A.; Scaiola, A.; Echeverria, B.; Gurzeler, L.-A.; Leibundgut, M.L.; 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:

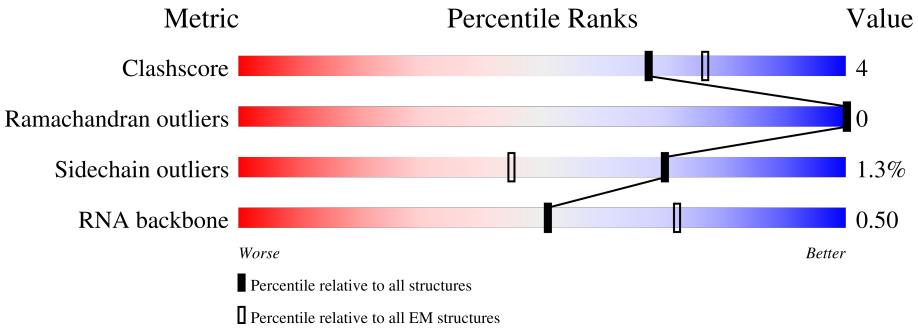
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	17% 7% 75%
2	D	243	9% 84% 8% 7%
3	F	204	5% 82% 11% 7%
4	K	165	51% 7% 41%
5	M	132	67% 80% 14% 7%
6	P	145	5% 77% 8% 14%
7	Q	146	86% 11%

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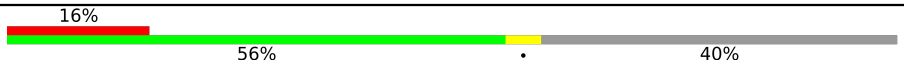
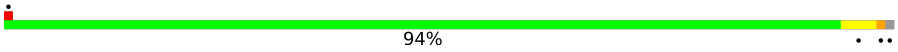
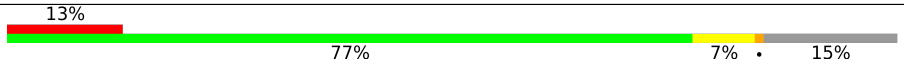
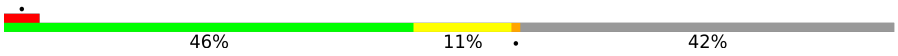
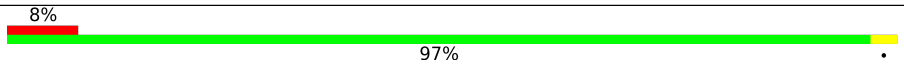
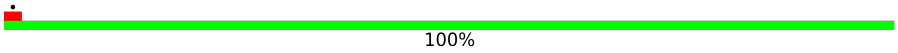
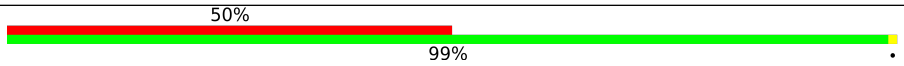
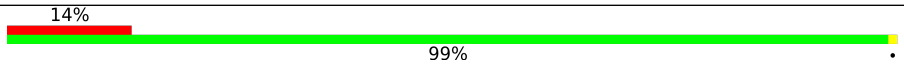
Mol	Chain	Length	Quality of chain
8	R	135	
9	S	152	
10	T	145	
11	U	119	
12	Z	125	
13	c	61	
14	d	55	
15	f	72	
16	g	315	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 25591 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
			Total	C	N	O	P		
1	2	472	10050	4484	1782	3312	472	0	0

- Molecule 2 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	225	1752	1117	315	313	7	0	0

- Molecule 3 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	190	1501	939	285	270	7	0	0

- Molecule 4 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	97	816	533	144	133	6	0	0

- Molecule 5 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	123	953	598	169	177	9	0	0

- Molecule 6 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	P	124	1016	644	192	173	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 8 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	81	Total	C	N	O	S	0	0
			671	419	136	114	2		

- Molecule 9 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 10 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 11 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 12 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 13 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 14 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 15 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	72	Total	C	N	O	S	0	0
			585	366	114	97	8		

- Molecule 16 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	2	53	Total	Mg	0
			53	53	
17	F	1	Total	Mg	0
			1	1	
17	S	2	Total	Mg	0
			2	2	
17	T	1	Total	Mg	0
			1	1	

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

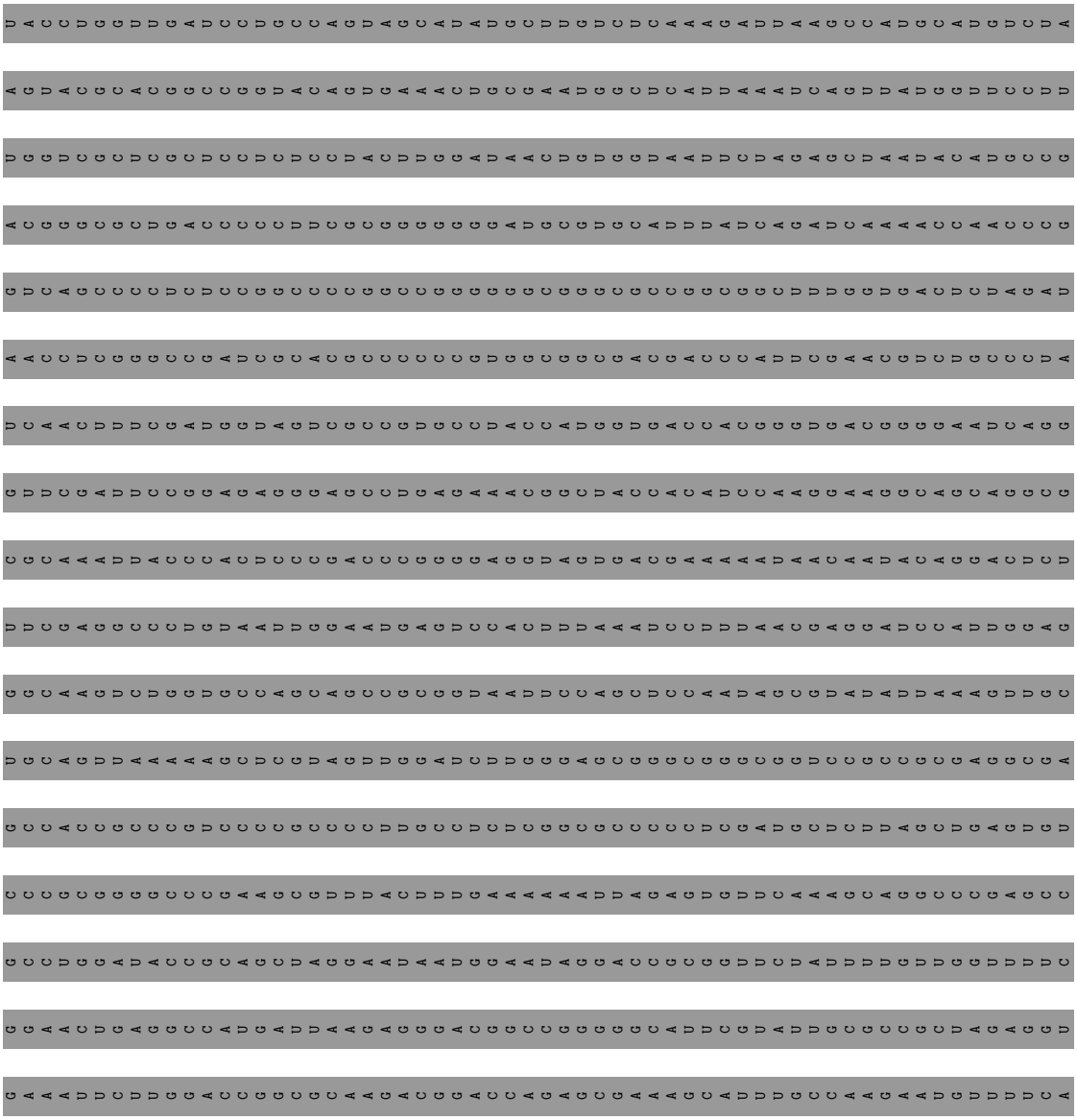
Mol	Chain	Residues	Atoms		AltConf
18	d	1	Total	Zn	0
			1	1	
18	f	1	Total	Zn	0
			1	1	

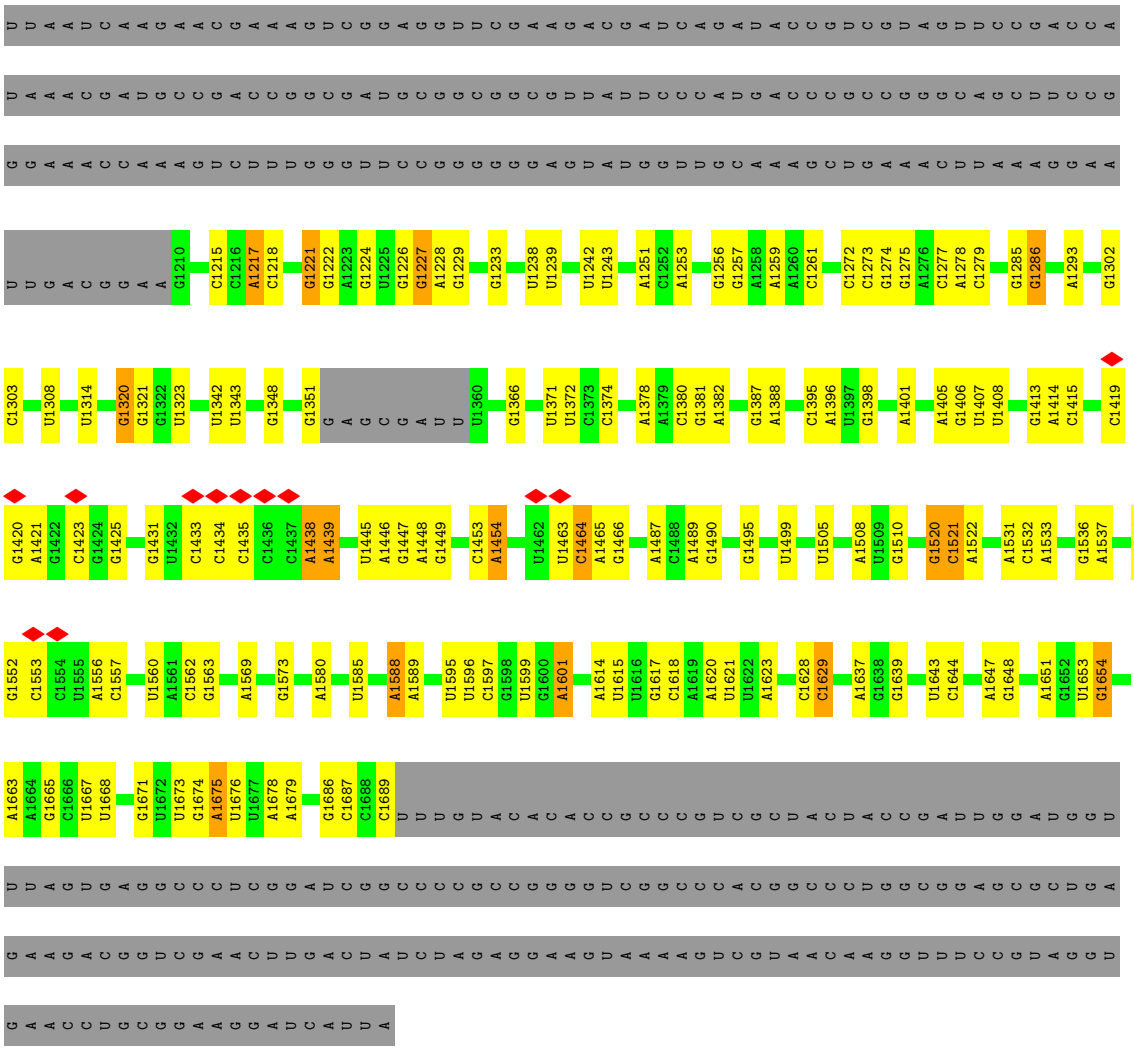
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

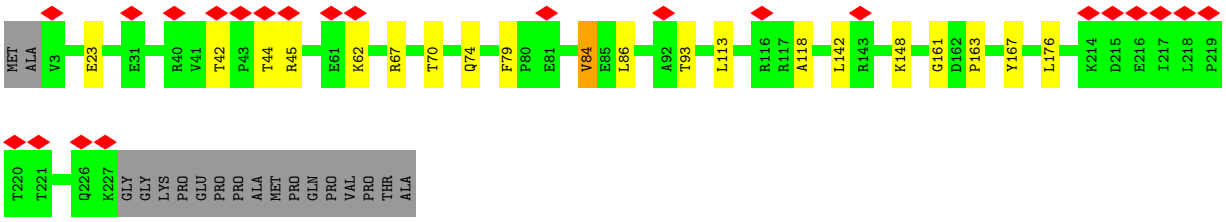
Chain 2: 





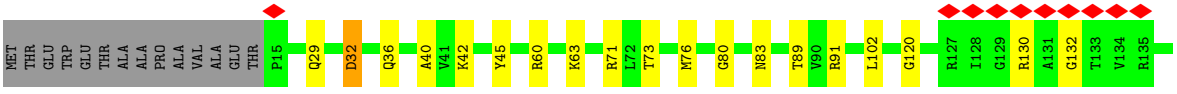
• Molecule 2: 40S ribosomal protein S3

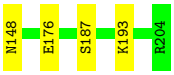
Chain D:



• Molecule 3: 40S ribosomal protein S5

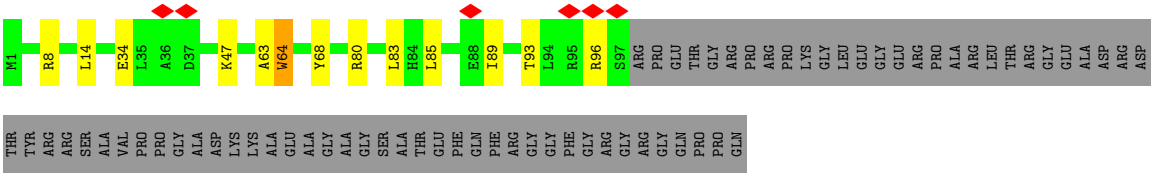
Chain F:





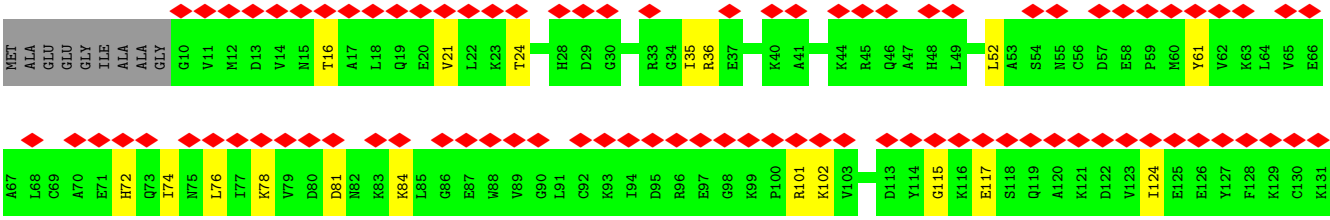
• Molecule 4: 40S ribosomal protein S10

Chain K:



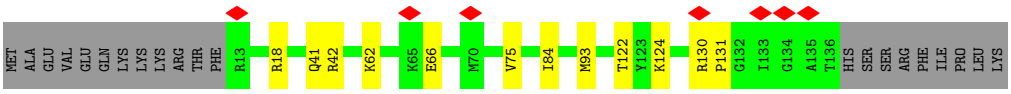
• Molecule 5: 40S ribosomal protein S12

Chain M:



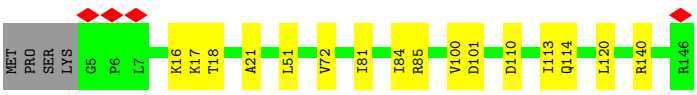
• Molecule 6: 40S ribosomal protein S15

Chain P:



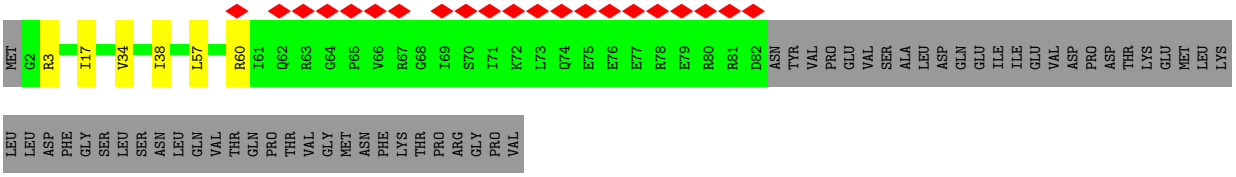
• Molecule 7: 40S ribosomal protein S16

Chain Q:



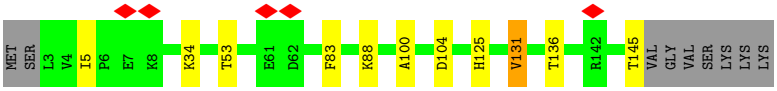
• Molecule 8: 40S ribosomal protein S17

Chain R:



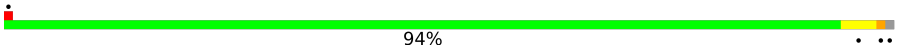
• Molecule 9: 40S ribosomal protein S18

Chain S:



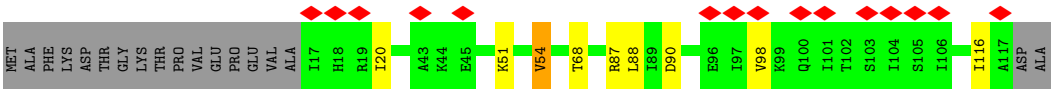
• Molecule 10: 40S ribosomal protein S19

Chain T:



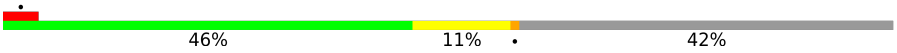
• Molecule 11: 40S ribosomal protein S20

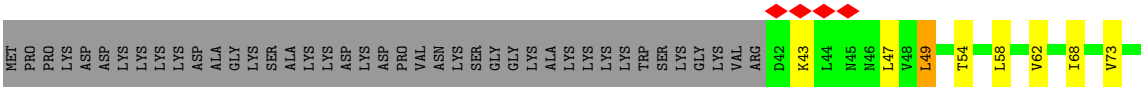
Chain U:

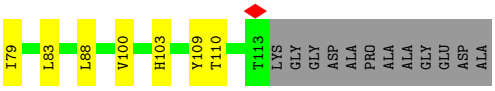


• Molecule 12: 40S ribosomal protein S25

Chain Z:

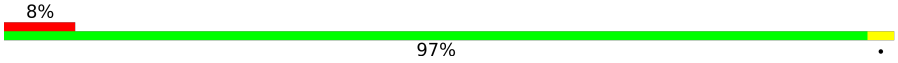


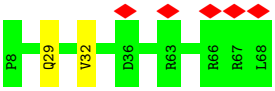




• Molecule 13: 40S ribosomal protein S28

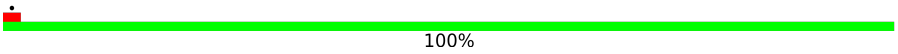
Chain c:





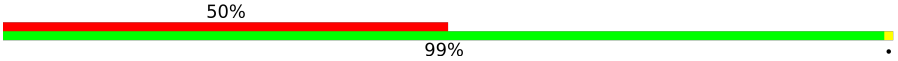
• Molecule 14: 40S ribosomal protein S29

Chain d:



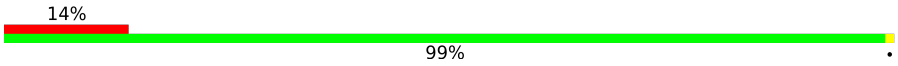
• Molecule 15: Ribosomal protein S27a

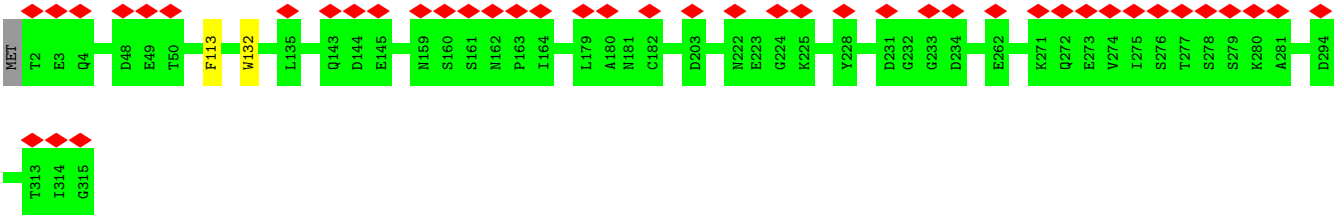
Chain f:



• Molecule 16: Receptor of activated protein C kinase 1

Chain g:





4 Experimental information (i)

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 ($e^-/Å^2$)	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	6.601	Depositor
Minimum map value	-3.122	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	2	0.31	0/11228	0.80	6/17496 (0.0%)
2	D	0.25	0/1780	0.42	0/2397
3	F	0.25	0/1523	0.42	0/2048
4	K	0.26	0/840	0.42	0/1133
5	M	0.24	0/963	0.42	0/1291
6	P	0.26	0/1035	0.40	0/1383
7	Q	0.27	0/1146	0.45	0/1534
8	R	0.23	0/678	0.38	0/902
9	S	0.25	0/1202	0.43	0/1610
10	T	0.24	0/1142	0.39	0/1530
11	U	0.23	0/813	0.42	0/1092
12	Z	0.24	0/580	0.43	0/780
13	c	0.23	0/481	0.44	0/643
14	d	0.25	0/469	0.39	0/623
15	f	0.24	0/595	0.44	0/785
16	g	0.24	0/2497	0.45	0/3399
All	All	0.27	0/26972	0.63	6/38646 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1453	C	C2-N1-C1'	7.13	126.64	118.80
1	2	1453	C	N1-C2-O2	6.67	122.90	118.90
1	2	1597	C	N3-C2-O2	-6.21	117.55	121.90
1	2	1597	C	N1-C2-O2	5.54	122.22	118.90
1	2	1520	G	C4-N9-C1'	5.21	133.27	126.50
1	2	1453	C	N3-C2-O2	-5.10	118.33	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	10050	0	5087	60	0
2	D	1752	0	1848	14	0
3	F	1501	0	1557	15	0
4	K	816	0	841	10	0
5	M	953	0	990	11	0
6	P	1016	0	1066	7	0
7	Q	1128	0	1195	10	0
8	R	671	0	724	4	0
9	S	1184	0	1244	6	0
10	T	1122	0	1153	4	0
11	U	803	0	873	5	0
12	Z	574	0	627	11	0
13	c	479	0	507	0	0
14	d	458	0	448	0	0
15	f	585	0	615	0	0
16	g	2440	0	2396	0	0
17	2	53	0	0	0	0
17	F	1	0	0	0	0
17	S	2	0	0	0	0
17	T	1	0	0	0	0
18	d	1	0	0	0	0
18	f	1	0	0	0	0
All	All	25591	0	21171	132	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 (132) 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)
1:2:1239:U:H5"	6:P:124:LYS:HD3	1.72	0.71
11:U:54:VAL:HG13	11:U:88:LEU:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1314:U:O2'	4:K:8:ARG:NH1	2.27	0.67
1:2:1228:A:H2'	1:2:1229:G:C8	2.29	0.66
10:T:76:THR:HG22	10:T:94:ARG:HB3	1.75	0.66
1:2:1521:C:OP2	9:S:136:THR:OG1	2.15	0.65
7:Q:51:LEU:HD13	7:Q:81:ILE:HG23	1.79	0.64
1:2:1588:A:H2'	1:2:1589:A:C8	2.34	0.62
12:Z:68:ILE:HB	12:Z:109:TYR:HB2	1.80	0.62
1:2:1277:C:H2'	1:2:1278:A:H8	1.64	0.61
3:F:71:ARG:NH2	3:F:148:ASN:OD1	2.35	0.60
6:P:41:GLN:HG3	6:P:84:ILE:HD13	1.84	0.58
5:M:52:LEU:HB2	5:M:76:LEU:HD11	1.85	0.58
1:2:1446:A:HO2'	1:2:1447:G:H8	1.53	0.57
3:F:120:GLY:O	3:F:193:LYS:NZ	2.38	0.57
1:2:1388:A:H61	2:D:161:GLY:HA3	1.69	0.57
6:P:130:ARG:HD3	6:P:131:PRO:HD2	1.87	0.57
12:Z:54:THR:HG21	12:Z:79:ILE:HD11	1.86	0.57
1:2:1563:G:OP1	10:T:121:ARG:NH1	2.39	0.56
1:2:1228:A:H2'	1:2:1229:G:H8	1.69	0.56
1:2:1438:A:H2'	1:2:1439:A:C8	2.43	0.54
2:D:79:PHE:HE2	2:D:84:VAL:HG13	1.73	0.54
5:M:52:LEU:HD22	5:M:78:LYS:HE3	1.90	0.54
1:2:1463:U:H4'	1:2:1464:C:H5"	1.90	0.53
4:K:80:ARG:NH2	4:K:89:ILE:O	2.41	0.53
1:2:1536:G:H2'	1:2:1537:A:C8	2.44	0.53
1:2:1522:A:O2'	9:S:145:THR:O	2.22	0.53
1:2:1413:G:H2'	1:2:1414:A:H8	1.74	0.52
1:2:1277:C:H2'	1:2:1278:A:C8	2.43	0.52
1:2:1217:A:H2'	1:2:1218:C:C6	2.44	0.52
7:Q:16:LYS:HG3	7:Q:17:LYS:H	1.73	0.52
1:2:1447:G:OP1	11:U:87:ARG:NH2	2.28	0.52
2:D:79:PHE:CE2	2:D:84:VAL:HG13	2.44	0.52
1:2:1415:C:O2'	10:T:132:ASP:OD2	2.23	0.51
2:D:142:LEU:HD12	2:D:148:LYS:HG3	1.93	0.50
1:2:1396:A:O2'	1:2:1398:G:N7	2.36	0.50
1:2:1536:G:H2'	1:2:1537:A:H8	1.77	0.50
12:Z:47:LEU:HB2	12:Z:79:ILE:HD13	1.95	0.49
1:2:1562:C:H2'	1:2:1563:G:H8	1.77	0.49
7:Q:100:VAL:HG12	7:Q:101:ASP:H	1.78	0.49
2:D:70:THR:HB	2:D:86:LEU:HG	1.94	0.49
7:Q:81:ILE:O	7:Q:85:ARG:HG3	2.14	0.48
9:S:125:HIS:CD2	9:S:131:VAL:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1286:G:O6	5:M:36:ARG:HB3	2.14	0.48
1:2:1595:U:H2'	1:2:1596:U:H6	1.78	0.48
11:U:51:LYS:HB2	11:U:90:ASP:HB2	1.95	0.48
1:2:1628:C:H2'	1:2:1629:C:H6	1.79	0.47
1:2:1217:A:H2'	1:2:1218:C:H6	1.80	0.47
1:2:1407:U:H2'	1:2:1408:U:C6	2.49	0.47
1:2:1679:A:H2'	3:F:60:ARG:HD2	1.95	0.47
1:2:1546:G:H5'	7:Q:18:THR:HG21	1.96	0.47
9:S:5:ILE:HB	12:Z:49:LEU:HB3	1.96	0.47
2:D:44:THR:HG22	2:D:45:ARG:HG3	1.96	0.47
5:M:81:ASP:HB2	5:M:84:LYS:HE2	1.96	0.47
1:2:1628:C:H2'	1:2:1629:C:C6	2.49	0.47
10:T:124:THR:HG22	10:T:125:PRO:HD2	1.97	0.47
2:D:163:PRO:O	2:D:167:TYR:HB2	2.15	0.47
11:U:20:ILE:HD12	11:U:98:VAL:HG21	1.97	0.47
1:2:1227:G:C2	1:2:1228:A:C8	3.03	0.46
1:2:1614:A:OP2	6:P:42:ARG:NH1	2.48	0.46
3:F:32:ASP:O	3:F:36:GLN:HG3	2.14	0.46
9:S:34:LYS:HB3	9:S:100:ALA:HA	1.97	0.46
1:2:1667:U:H2'	1:2:1668:U:C6	2.51	0.46
2:D:74:GLN:HB2	2:D:84:VAL:HG21	1.98	0.46
3:F:76:MET:HB3	3:F:89:THR:HG23	1.97	0.46
3:F:91:ARG:HD2	12:Z:103:HIS:CE1	2.50	0.46
12:Z:58:LEU:HD12	12:Z:62:VAL:HG21	1.98	0.46
1:2:1595:U:H2'	1:2:1596:U:C6	2.51	0.45
1:2:1413:G:H2'	1:2:1414:A:C8	2.49	0.45
1:2:1499:U:H4'	2:D:176:LEU:HD13	1.98	0.45
2:D:62:LYS:HD3	4:K:96:ARG:HD2	1.99	0.45
1:2:1395:C:O2'	1:2:1396:A:H5'	2.17	0.45
4:K:63:ALA:HB3	4:K:68:TYR:CE1	2.51	0.45
4:K:63:ALA:HB3	4:K:68:TYR:HE1	1.81	0.45
1:2:1374:C:O2'	1:2:1464:C:O2	2.35	0.45
3:F:73:THR:O	3:F:89:THR:HG21	2.17	0.45
1:2:1531:A:H2'	1:2:1532:C:C6	2.52	0.44
12:Z:73:VAL:HG21	12:Z:88:LEU:HD11	1.99	0.44
1:2:1648:G:N2	1:2:1675:A:OP2	2.34	0.44
7:Q:110:ASP:O	7:Q:114:GLN:HG2	2.18	0.44
1:2:1285:G:H5'	5:M:35:ILE:HG22	2.00	0.44
6:P:75:VAL:HG22	6:P:93:MET:HB3	2.00	0.44
1:2:1653:U:H2'	1:2:1654:G:C8	2.53	0.43
8:R:17:ILE:HD12	8:R:57:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1278:A:H2'	1:2:1279:C:C6	2.53	0.43
1:2:1643:U:H2'	1:2:1644:C:C6	2.53	0.43
1:2:1448:A:H2'	1:2:1449:G:O4'	2.18	0.43
5:M:24:THR:HB	5:M:115:GLY:HA3	2.00	0.43
8:R:34:VAL:O	8:R:38:ILE:HG12	2.18	0.43
1:2:1226:G:N1	1:2:1639:G:OP2	2.42	0.43
3:F:63:LYS:HD2	3:F:71:ARG:HH12	1.82	0.43
1:2:1454:A:H5"	8:R:3:ARG:HD2	2.00	0.43
7:Q:72:VAL:HG21	7:Q:84:ILE:HD11	2.00	0.43
2:D:23:GLU:HG2	4:K:64:TRP:CD1	2.53	0.43
1:2:1464:C:O3'	8:R:60:ARG:NH1	2.52	0.43
6:P:18:ARG:NH1	9:S:88:LYS:O	2.52	0.43
1:2:1686:G:H2'	1:2:1687:C:C6	2.52	0.43
3:F:130:ARG:O	3:F:132:GLY:N	2.51	0.42
1:2:1678:A:O2'	1:2:1679:A:H5'	2.19	0.42
11:U:20:ILE:HG12	11:U:116:ILE:HG13	2.01	0.42
7:Q:113:ILE:HG13	7:Q:120:LEU:HD12	2.02	0.42
1:2:1521:C:OP2	1:2:1521:C:H6	2.02	0.42
3:F:40:ALA:HB1	3:F:45:TYR:CG	2.55	0.42
3:F:102:LEU:HD11	12:Z:100:VAL:HG21	2.02	0.42
1:2:1320:G:H2'	1:2:1321:G:O4'	2.20	0.42
1:2:1601:A:OP1	12:Z:43:LYS:NZ	2.49	0.42
3:F:42:LYS:HD3	3:F:42:LYS:HA	1.84	0.42
5:M:35:ILE:HB	5:M:61:TYR:CZ	2.55	0.41
1:2:1617:G:N1	1:2:1620:A:OP2	2.53	0.41
6:P:62:LYS:NZ	6:P:66:GLU:OE1	2.34	0.41
5:M:101:ARG:HG3	5:M:102:LYS:N	2.35	0.41
5:M:24:THR:HG21	5:M:117:GLU:HG3	2.03	0.41
5:M:72:HIS:O	5:M:74:ILE:HG13	2.21	0.41
5:M:21:VAL:HG21	5:M:124:ILE:HD12	2.03	0.41
1:2:1221:G:O2'	1:2:1676:U:O2	2.35	0.41
1:2:1272:C:H2'	1:2:1273:C:C6	2.56	0.41
4:K:83:LEU:HB2	4:K:85:LEU:HG	2.03	0.41
1:2:1673:U:H2'	1:2:1674:G:O4'	2.21	0.41
3:F:176:GLU:OE1	3:F:187:SER:HB2	2.20	0.41
4:K:47:LYS:HD3	4:K:47:LYS:HA	1.86	0.41
2:D:67:ARG:HD2	4:K:93:THR:O	2.21	0.41
3:F:102:LEU:HD23	3:F:102:LEU:HA	1.92	0.41
4:K:14:LEU:HD21	4:K:34:GLU:HG2	2.01	0.41
7:Q:21:ALA:HB2	7:Q:72:VAL:HG13	2.03	0.40
1:2:1438:A:H2'	1:2:1439:A:H8	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:THR:HG22	2:D:44:THR:H	1.87	0.40
1:2:1221:G:H2'	1:2:1222:G:C8	2.57	0.40
2:D:113:LEU:HD23	2:D:118:ALA:HB2	2.04	0.40
3:F:80:GLY:HA2	3:F:83:ASN:OD1	2.20	0.40
12:Z:79:ILE:HG23	12:Z:83:LEU:HD23	2.02	0.40
1:2:1644:C:H4'	7:Q:140:ARG:HB2	2.03	0.40
12:Z:49:LEU:HD12	12:Z:49:LEU:HA	1.88	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	D	223/243 (92%)	220 (99%)	3 (1%)	0	100	100
3	F	188/204 (92%)	180 (96%)	8 (4%)	0	100	100
4	K	95/165 (58%)	91 (96%)	4 (4%)	0	100	100
5	M	121/132 (92%)	116 (96%)	5 (4%)	0	100	100
6	P	122/145 (84%)	121 (99%)	1 (1%)	0	100	100
7	Q	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
8	R	79/135 (58%)	79 (100%)	0	0	100	100
9	S	141/152 (93%)	138 (98%)	3 (2%)	0	100	100
10	T	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
11	U	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
12	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
13	c	59/61 (97%)	59 (100%)	0	0	100	100
14	d	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
15	f	70/72 (97%)	64 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	g	312/315 (99%)	293 (94%)	19 (6%)	0	100	100
All	All	1914/2214 (86%)	1856 (97%)	58 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	189/202 (94%)	187 (99%)	2 (1%)	73	92
3	F	160/170 (94%)	158 (99%)	2 (1%)	69	91
4	K	88/136 (65%)	87 (99%)	1 (1%)	73	92
5	M	104/108 (96%)	103 (99%)	1 (1%)	76	93
6	P	110/130 (85%)	109 (99%)	1 (1%)	78	94
7	Q	117/121 (97%)	117 (100%)	0	100	100
8	R	72/122 (59%)	72 (100%)	0	100	100
9	S	124/132 (94%)	120 (97%)	4 (3%)	39	73
10	T	114/115 (99%)	112 (98%)	2 (2%)	59	86
11	U	93/107 (87%)	91 (98%)	2 (2%)	52	83
12	Z	64/103 (62%)	62 (97%)	2 (3%)	40	74
13	c	54/54 (100%)	52 (96%)	2 (4%)	34	68
14	d	48/48 (100%)	48 (100%)	0	100	100
15	f	65/65 (100%)	64 (98%)	1 (2%)	65	89
16	g	272/273 (100%)	270 (99%)	2 (1%)	84	95
All	All	1674/1886 (89%)	1652 (99%)	22 (1%)	70	91

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	84	VAL

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Mol	Chain	Res	Type
2	D	93	THR
3	F	29	GLN
3	F	32	ASP
4	K	64	TRP
5	M	16	THR
6	P	122	THR
9	S	53	THR
9	S	83	PHE
9	S	104	ASP
9	S	131	VAL
10	T	85	ASN
10	T	124	THR
11	U	54	VAL
11	U	68	THR
12	Z	49	LEU
12	Z	110	THR
13	c	29	GLN
13	c	32	VAL
15	f	126	CYS
16	g	113	PHE
16	g	132	TRP

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	470/1869 (25%)	91 (19%)	0

All (91) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1233	G
1	2	1238	U
1	2	1242	U

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Mol	Chain	Res	Type
1	2	1243	U
1	2	1251	A
1	2	1253	A
1	2	1256	G
1	2	1257	G
1	2	1259	A
1	2	1261	C
1	2	1274	G
1	2	1275	G
1	2	1286	G
1	2	1293	A
1	2	1302	G
1	2	1303	C
1	2	1308	U
1	2	1320	G
1	2	1323	U
1	2	1342	U
1	2	1343	U
1	2	1348	G
1	2	1351	G
1	2	1366	G
1	2	1371	U
1	2	1372	U
1	2	1378	A
1	2	1380	C
1	2	1381	G
1	2	1382	A
1	2	1387	G
1	2	1401	A
1	2	1405	A
1	2	1406	G
1	2	1419	C
1	2	1420	G
1	2	1421	A
1	2	1423	C
1	2	1425	G
1	2	1431	G
1	2	1433	C
1	2	1434	C
1	2	1435	C
1	2	1438	A
1	2	1439	A

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Mol	Chain	Res	Type
1	2	1445	U
1	2	1454	A
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1495	G
1	2	1505	U
1	2	1508	A
1	2	1510	G
1	2	1520	G
1	2	1521	C
1	2	1533	A
1	2	1552	G
1	2	1553	C
1	2	1556	A
1	2	1557	C
1	2	1560	U
1	2	1569	A
1	2	1573	G
1	2	1580	A
1	2	1585	U
1	2	1588	A
1	2	1599	U
1	2	1601	A
1	2	1615	U
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1629	C
1	2	1637	A
1	2	1647	A
1	2	1651	A
1	2	1654	G
1	2	1663	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1689	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 59 ligands modelled in this entry, 59 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.

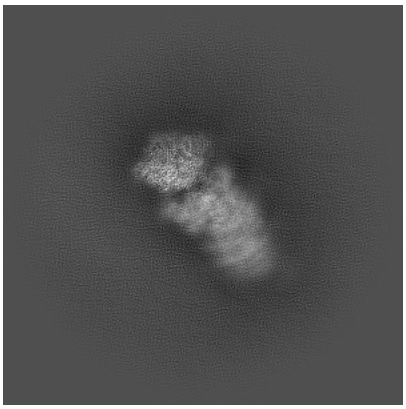
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11322. These allow visual inspection of the internal detail of the map and identification of artifacts.

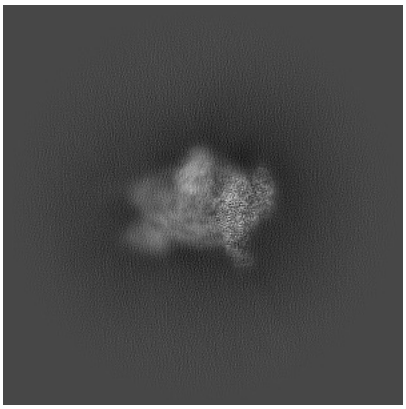
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

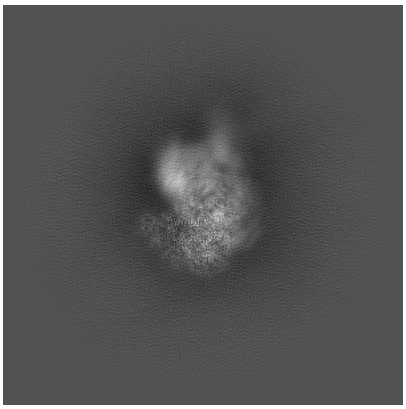
6.1.1 Primary map



X

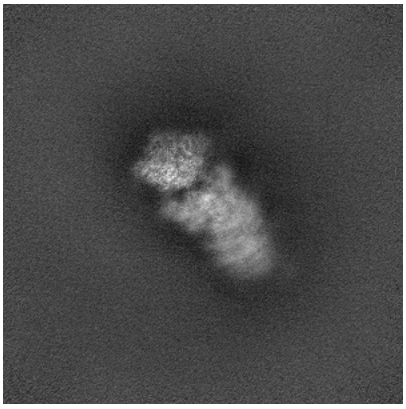


Y

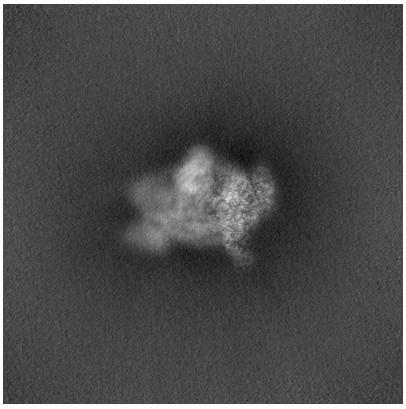


Z

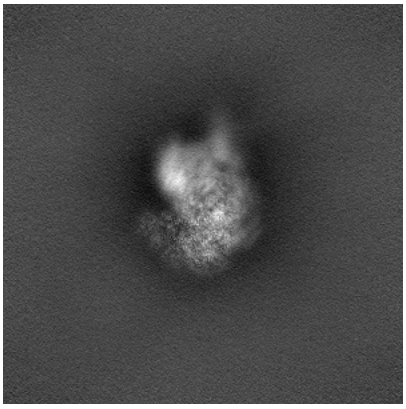
6.1.2 Raw map



X



Y

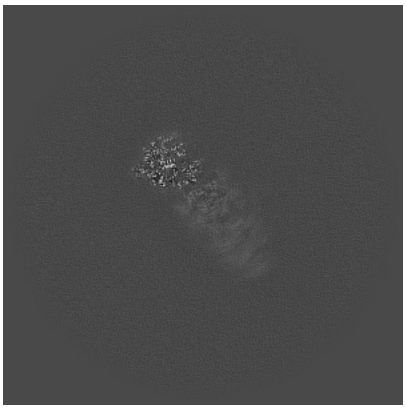


Z

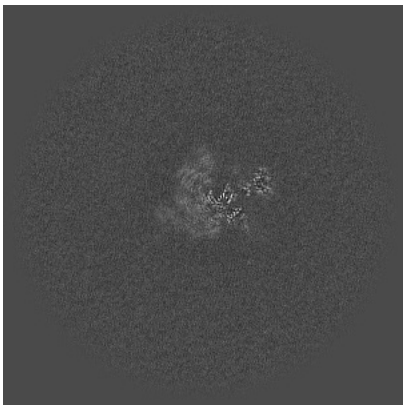
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

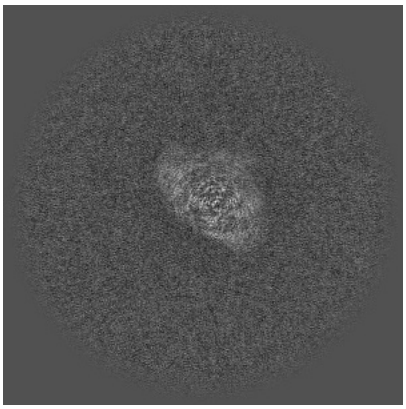
6.2.1 Primary map



X Index: 280

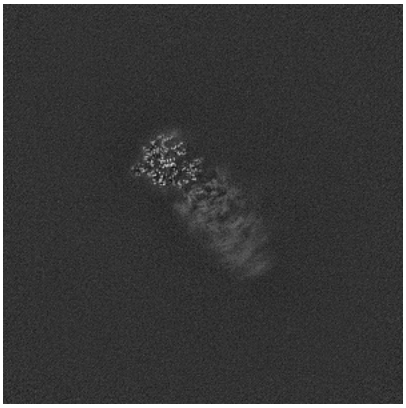


Y Index: 280

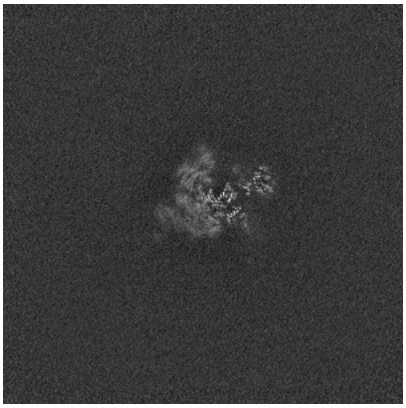


Z Index: 280

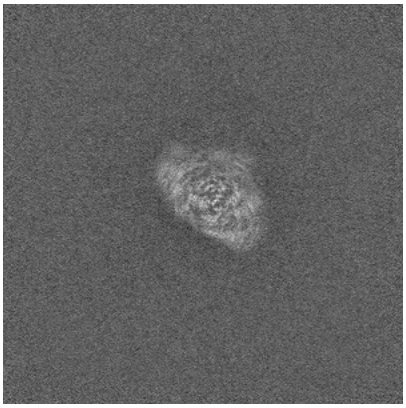
6.2.2 Raw map



X Index: 280



Y Index: 280



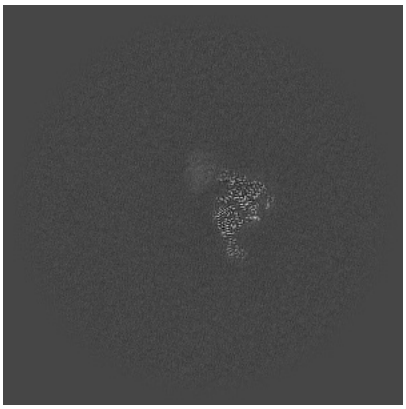
Z Index: 280

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

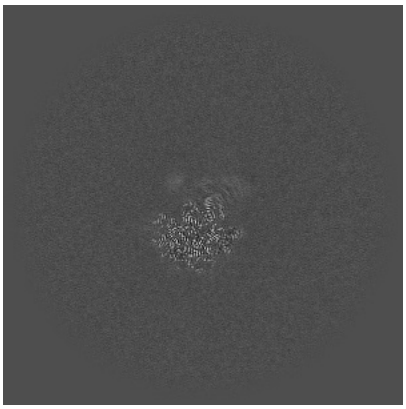
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 287

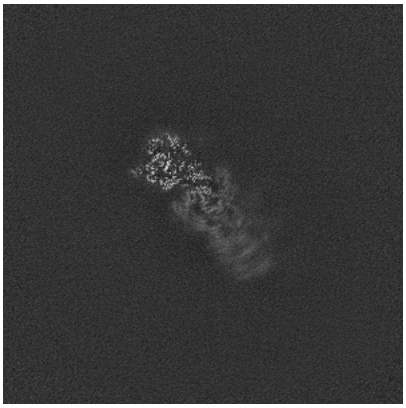


Y Index: 230

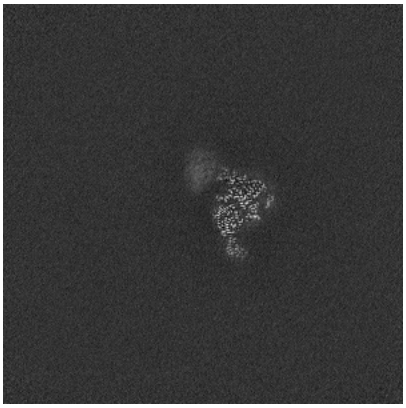


Z Index: 316

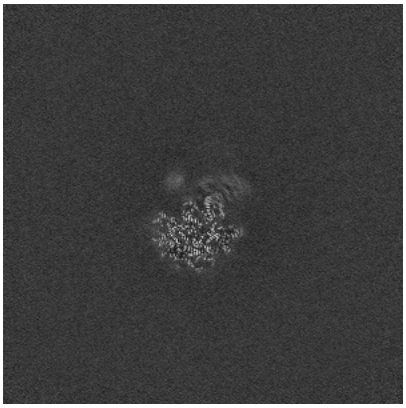
6.3.2 Raw map



X Index: 287



Y Index: 230



Z Index: 316

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

6.4 Orthogonal surface views (i)

6.4.1 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.

6.4.2 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.

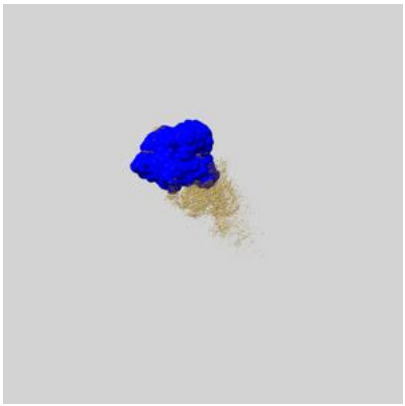
6.5 Mask visualisation (i)

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

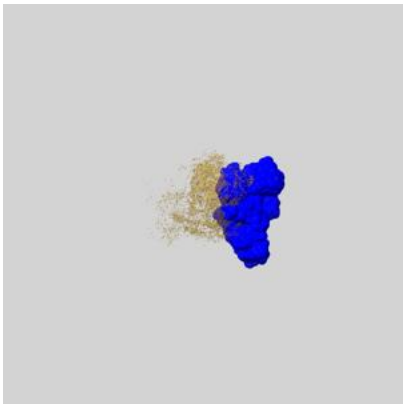
A mask typically either:

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

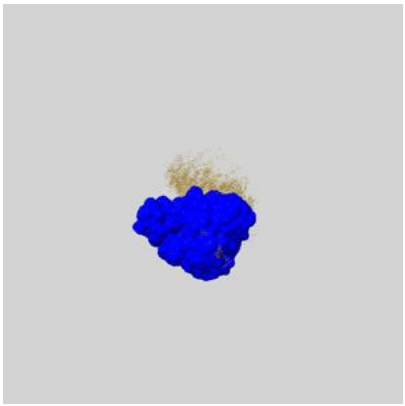
6.5.1 emd_11322_msk_1.map (i)



X



Y

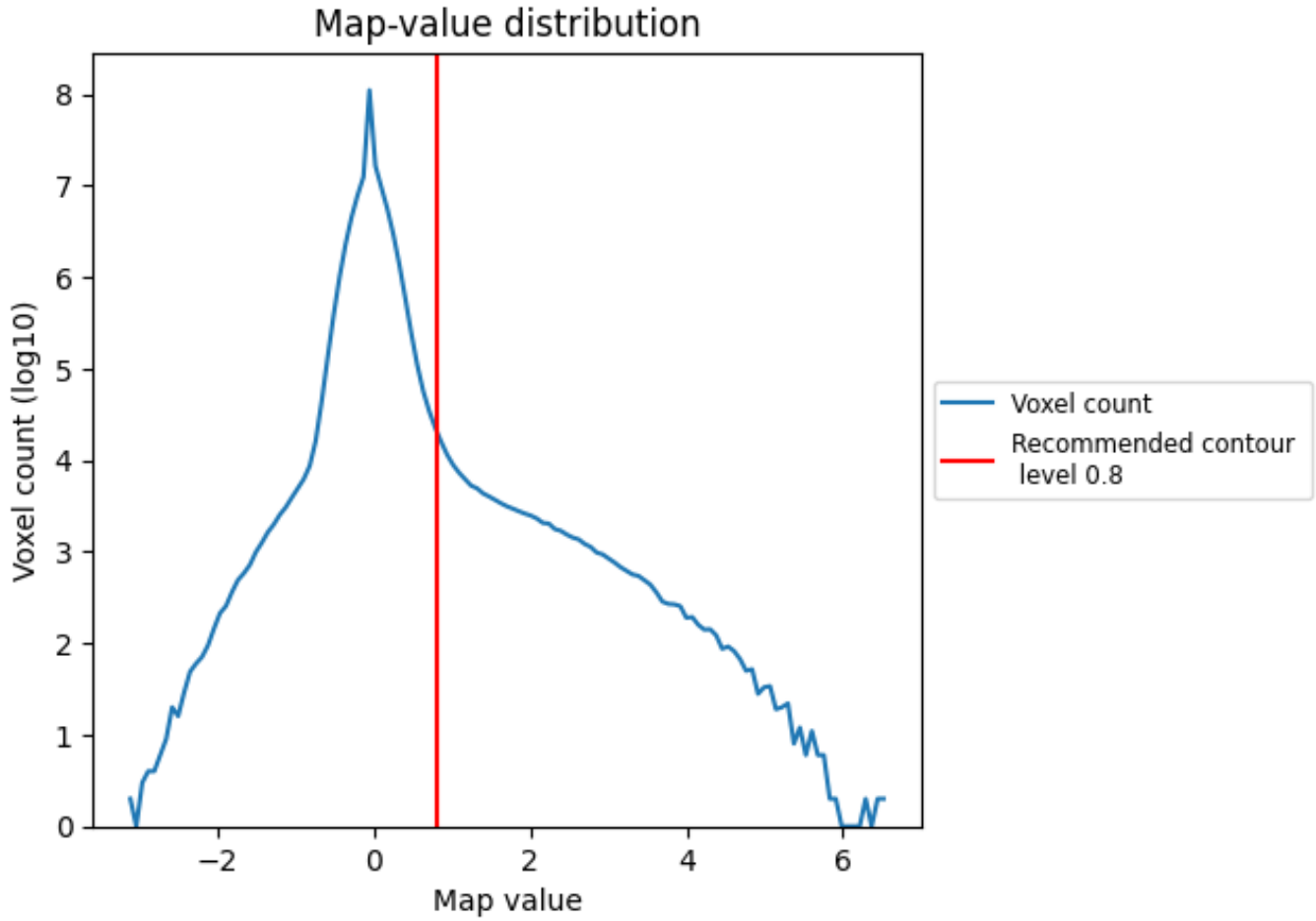


Z

7 Map analysis

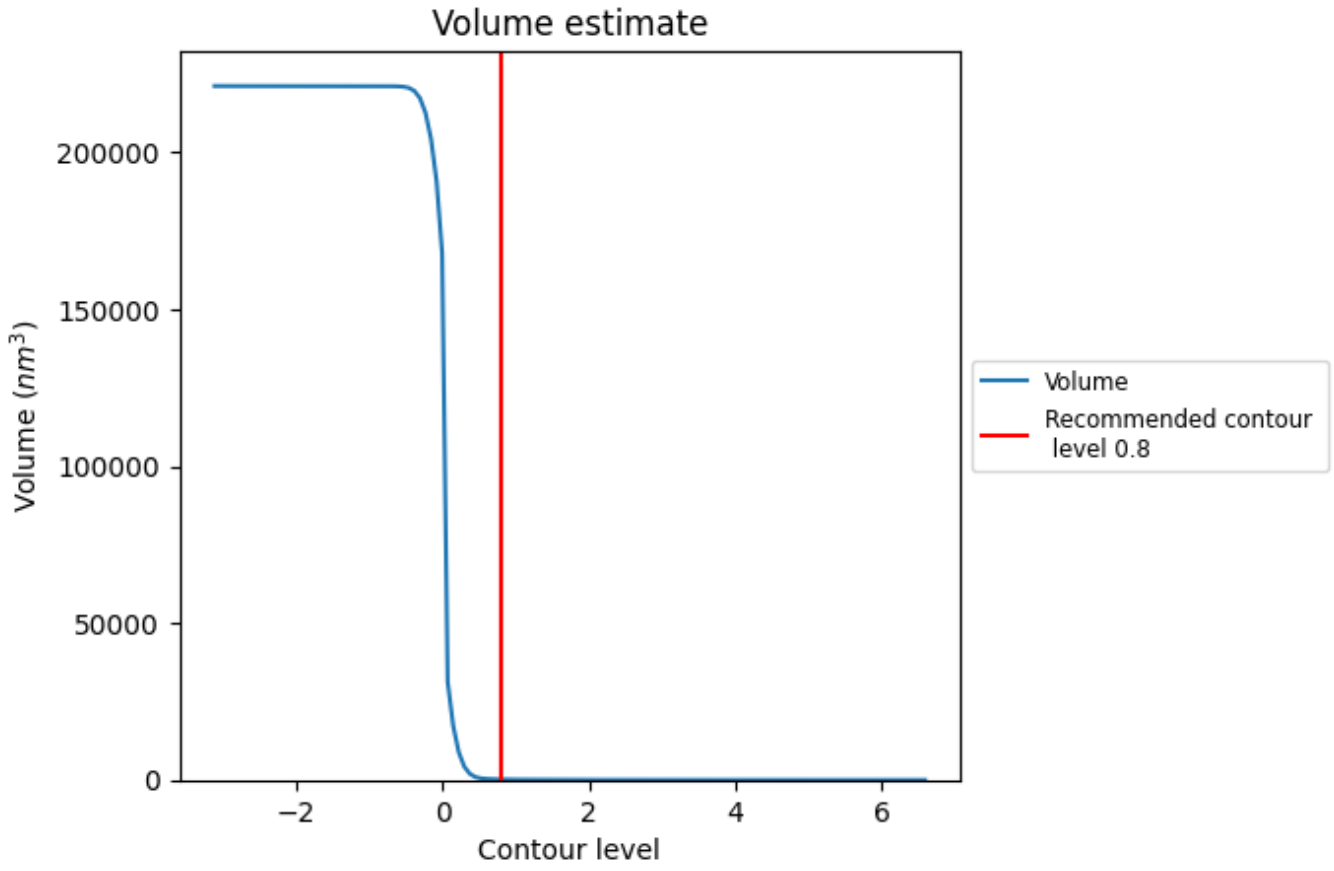
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

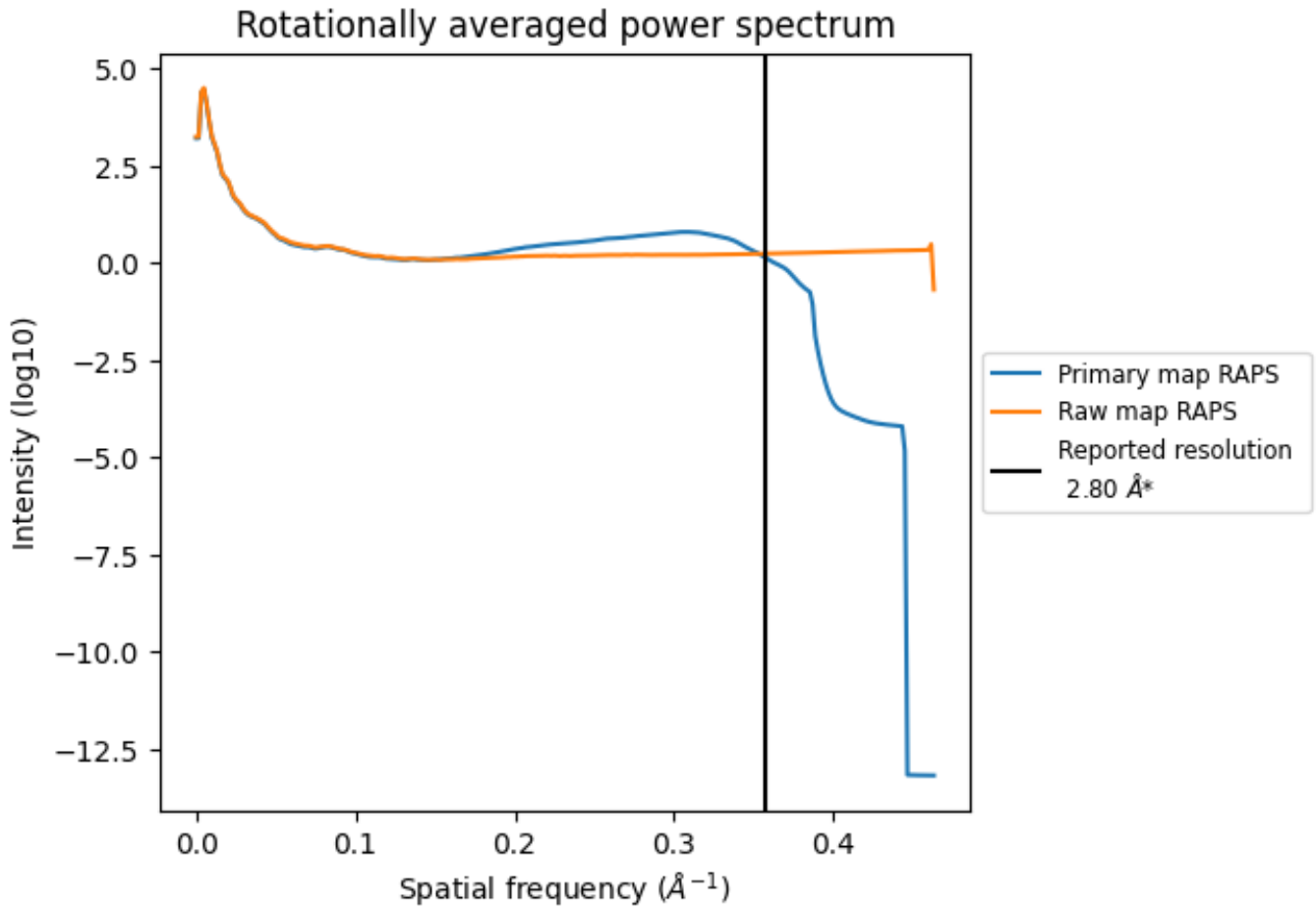
7.2 Volume estimate



The volume at the recommended contour level is 168 nm^3; this corresponds to an approximate mass of 152 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 (i)

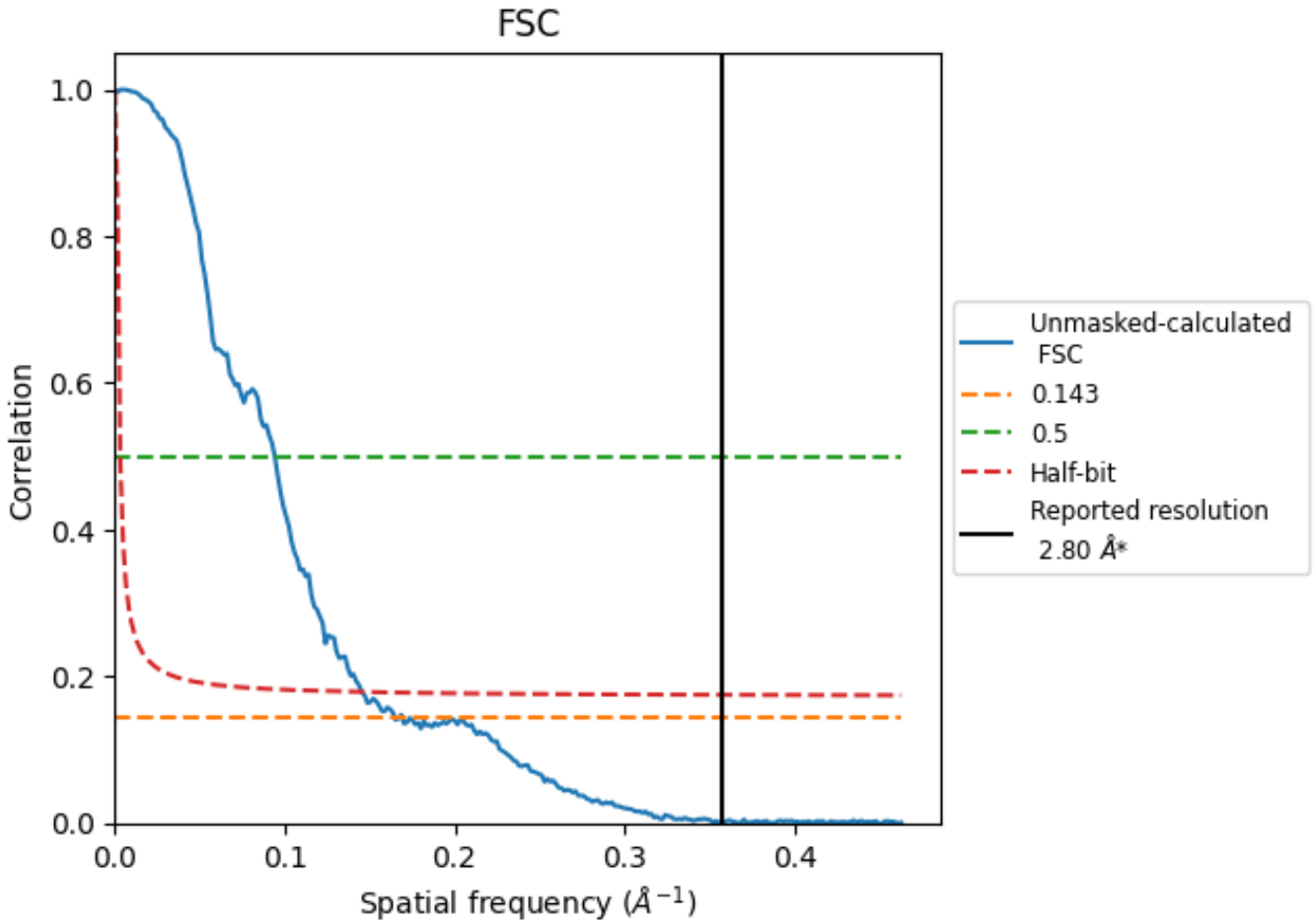


*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

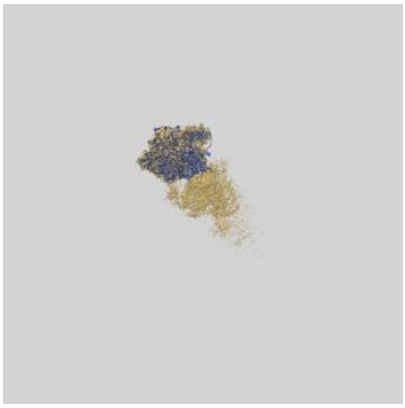
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.06	10.62	6.88

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

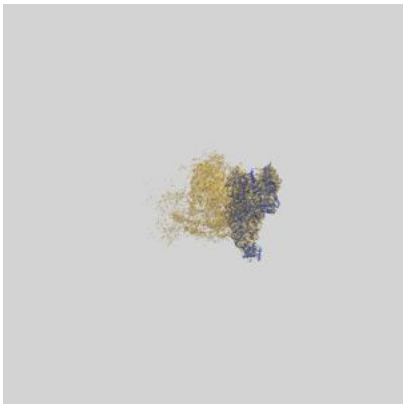
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11322 and PDB model 6ZOL. Per-residue inclusion information can be found in section 3 on page 7.

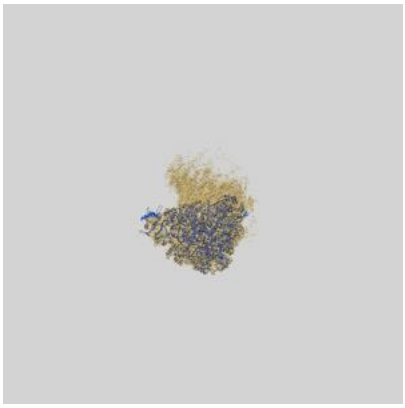
9.1 Map-model overlay



X



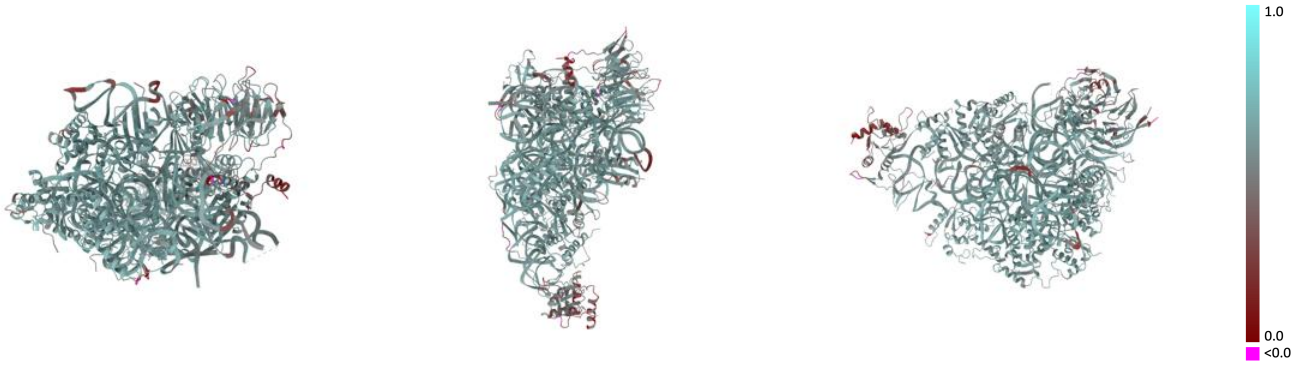
Y



Z

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.

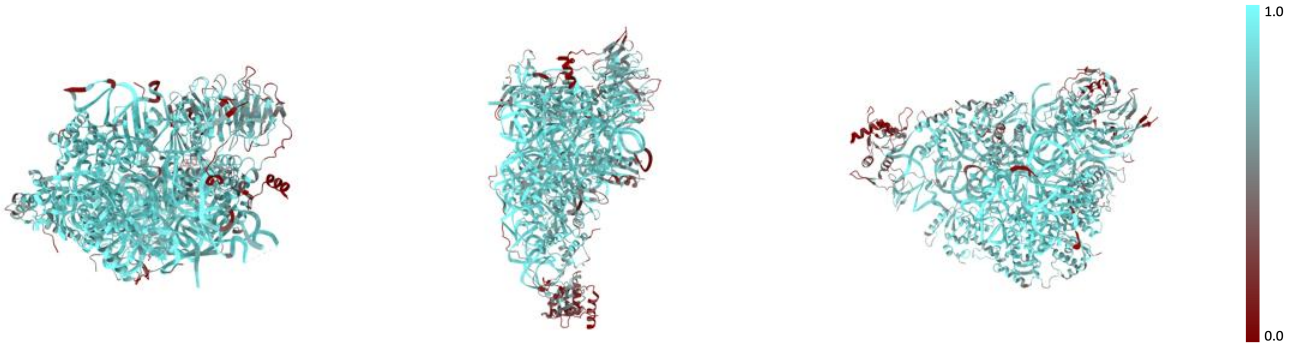
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

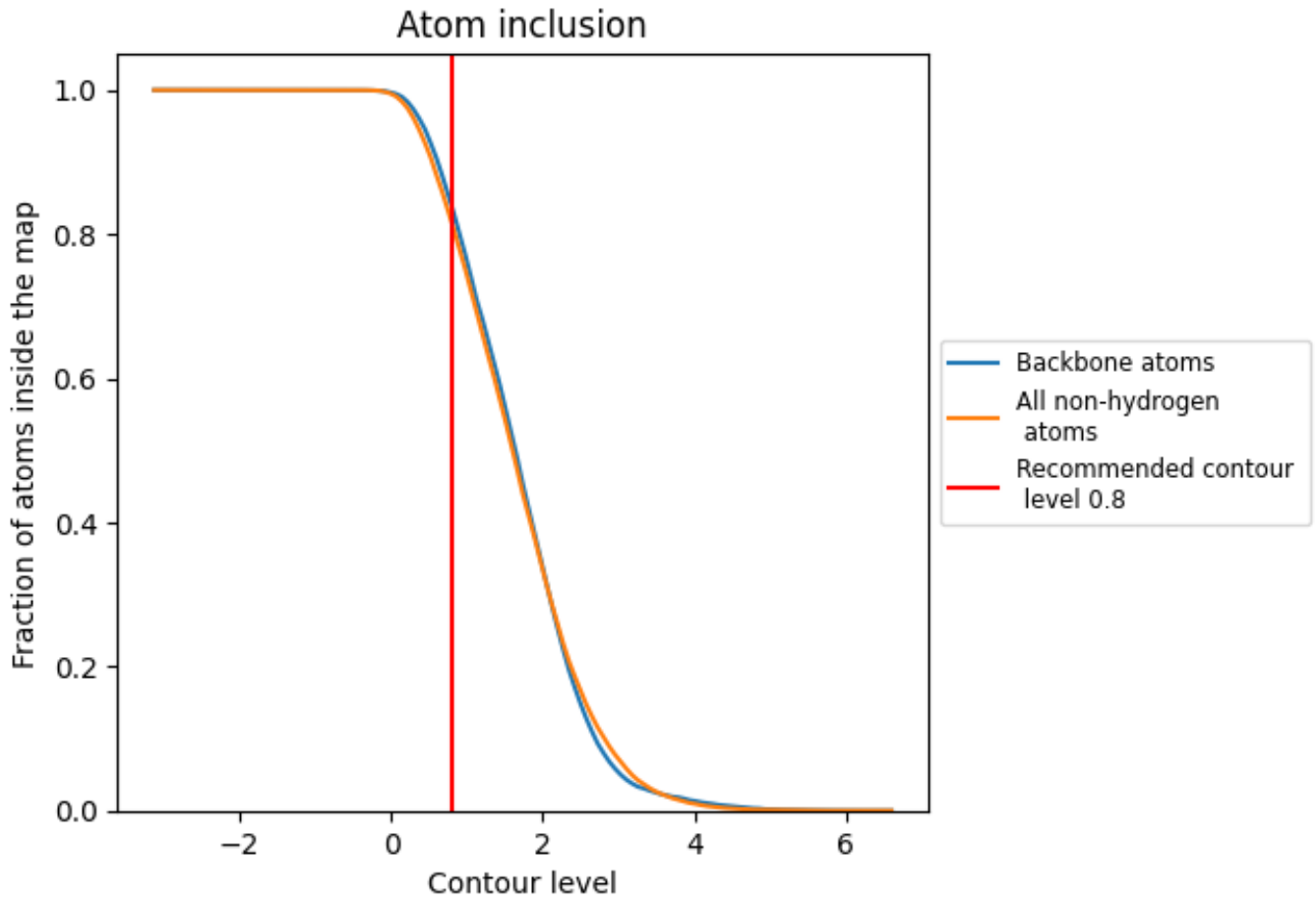
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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	0.8167	0.5880
2	0.9345	0.6140
D	0.7297	0.5730
F	0.8419	0.6020
K	0.8003	0.5970
M	0.2609	0.3880
P	0.8404	0.6060
Q	0.8965	0.6320
R	0.6351	0.5120
S	0.8440	0.6160
T	0.8939	0.6230
U	0.7340	0.5820
Z	0.7398	0.5860
c	0.7375	0.5810
d	0.8912	0.6390
f	0.4158	0.4410
g	0.6868	0.5510