



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 11:38 PM UTC

PDB ID : 6ZOL / pdb_00006zol
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:

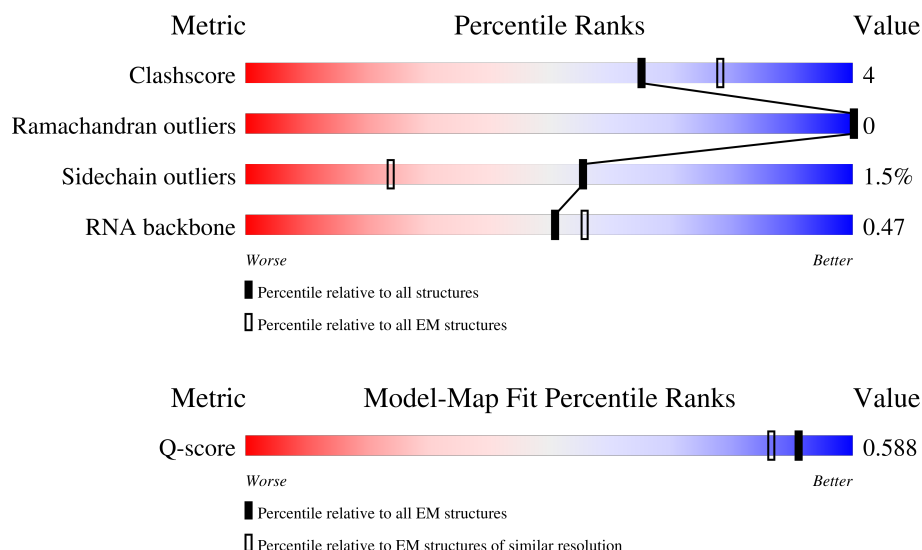
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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.



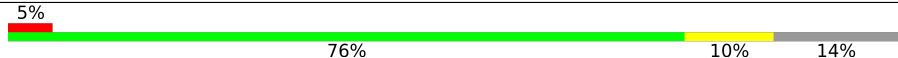
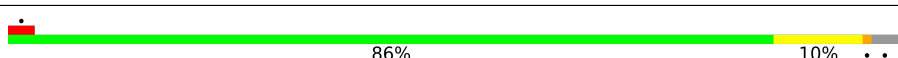
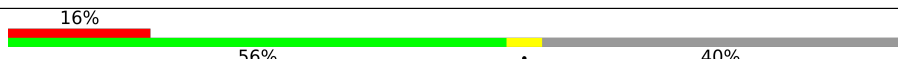
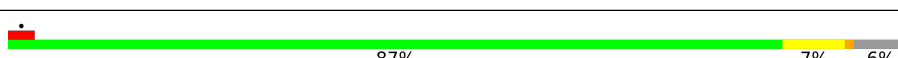
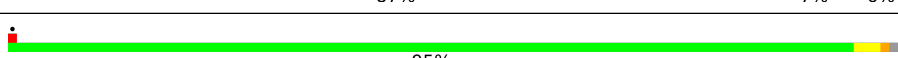
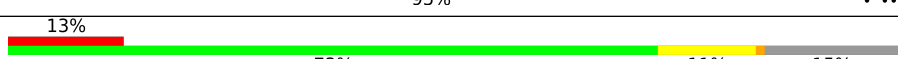
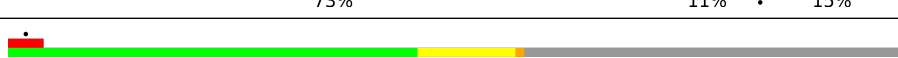
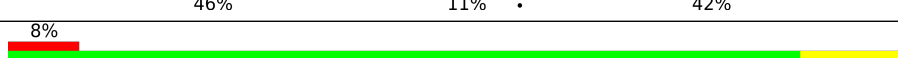
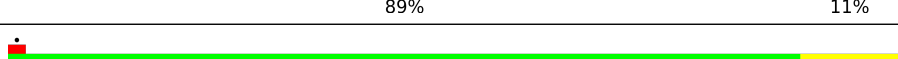
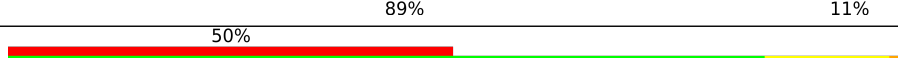
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	
2	D	243	
3	F	204	

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Mol	Chain	Length	Quality of chain
4	K	165	
5	M	132	
6	P	145	
7	Q	146	
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
1	2	472	Total	C	N	O	P	0	0
			10050	4484	1782	3312	472		

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

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

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

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

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

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

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

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

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

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

- 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.

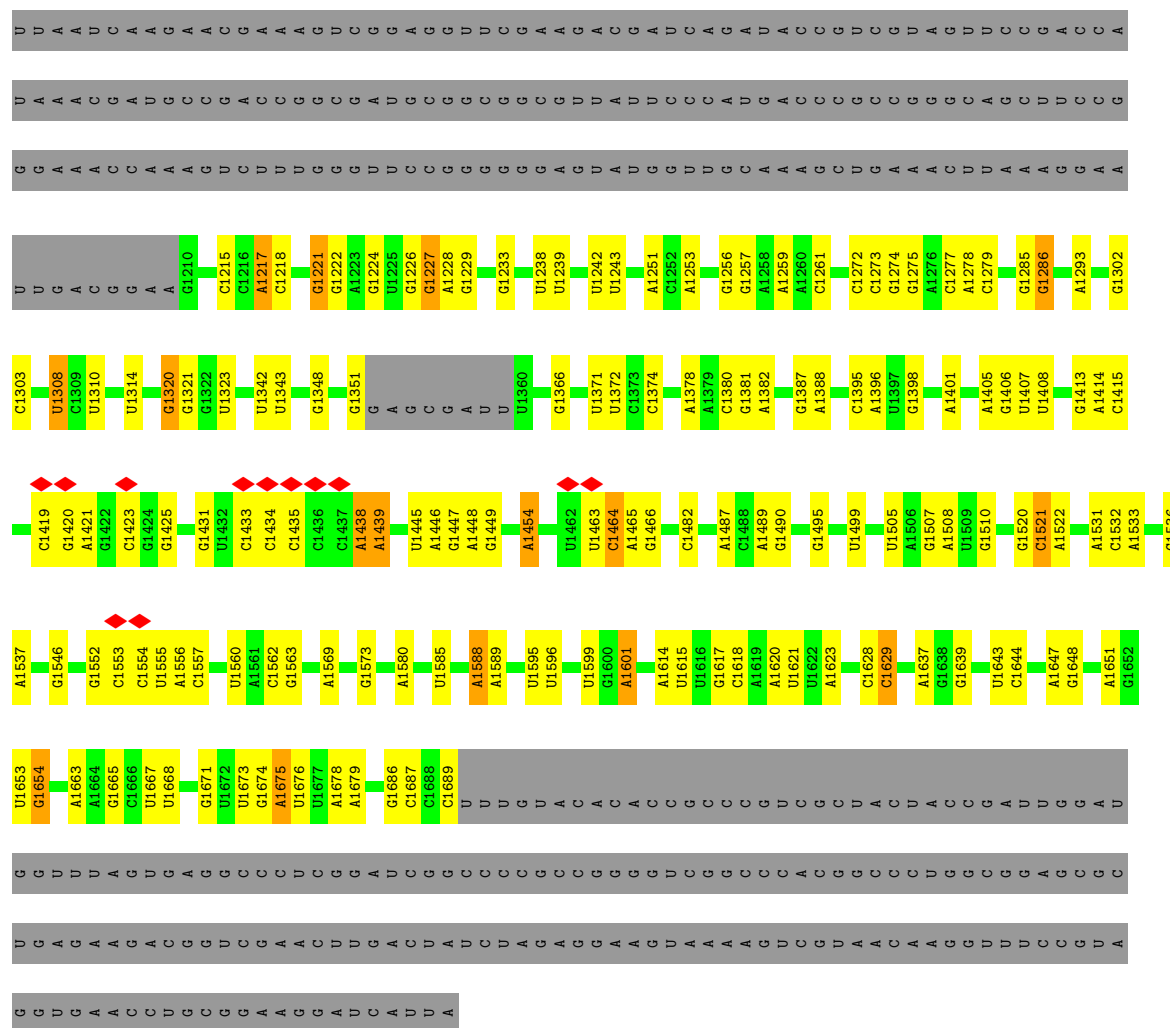
Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

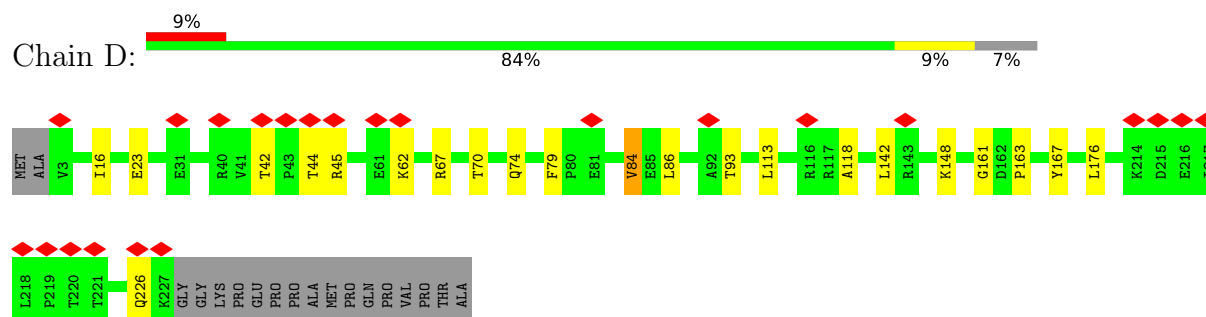
Mol	Chain	Residues	Atoms		AltConf
17	2	53	Total	Mg	0
			53	53	
17	F	1	Total	Mg	0
			1	1	
17	S	2	Total	Mg	0
			2	2	
17	T	1	Total	Mg	0
			1	1	

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

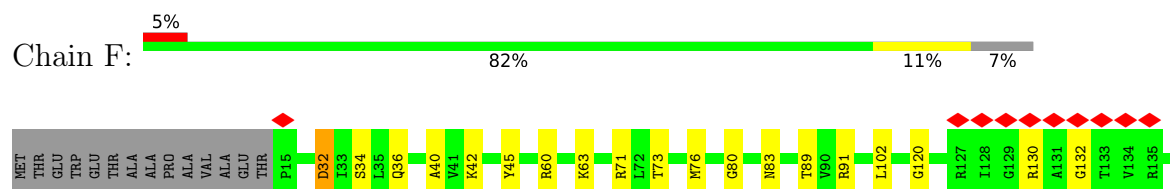
Mol	Chain	Residues	Atoms		AltConf
18	d	1	Total	Zn	0
			1	1	
18	f	1	Total	Zn	0
			1	1	



• Molecule 2: 40S ribosomal protein S3

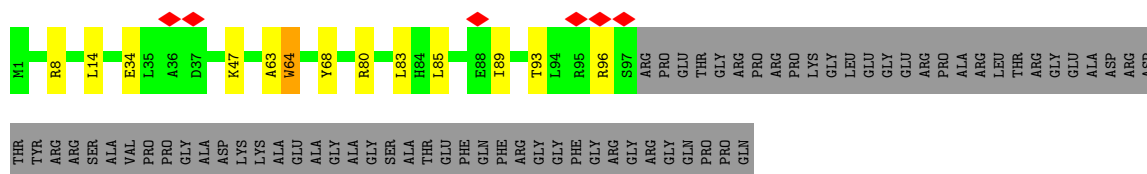


• Molecule 3: 40S ribosomal protein S5

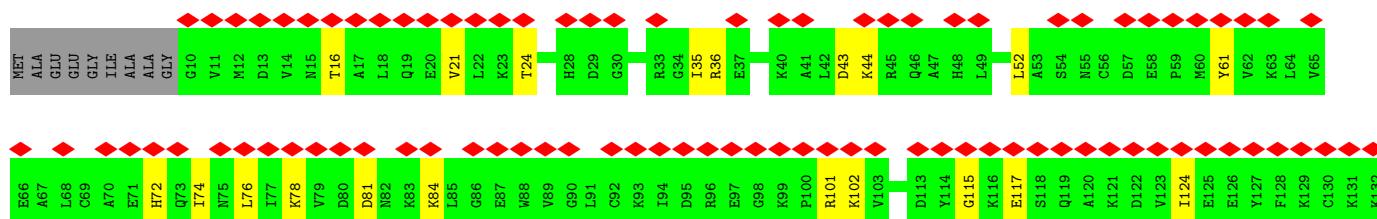
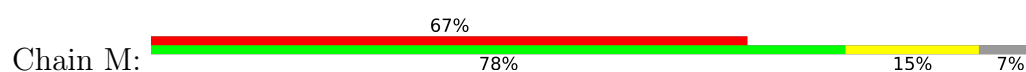




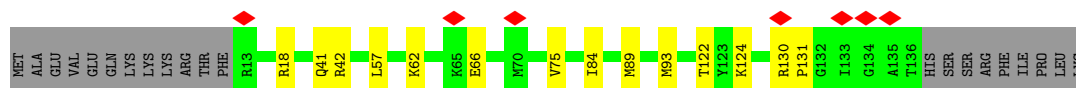
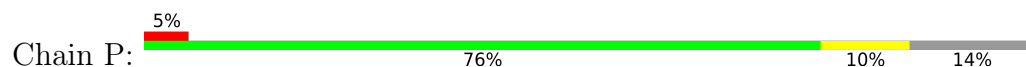
- Molecule 4: 40S ribosomal protein S10



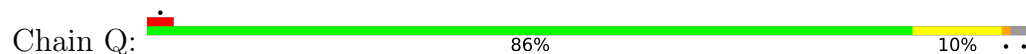
- Molecule 5: 40S ribosomal protein S12



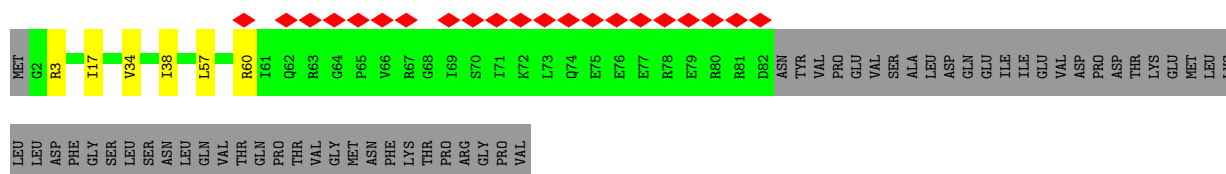
- Molecule 6: 40S ribosomal protein S15



- Molecule 7: 40S ribosomal protein S16



- Molecule 8: 40S ribosomal protein S17

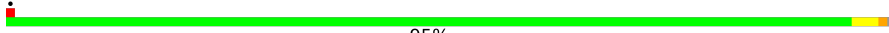


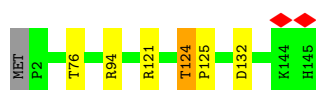
- Molecule 9: 40S ribosomal protein S18

Chain S:  87% 7% 6%



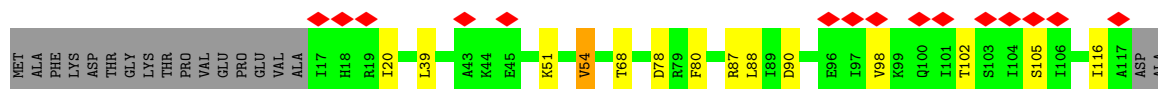
- Molecule 10: 40S ribosomal protein S19

Chain T:  95%

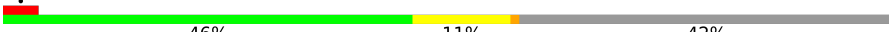


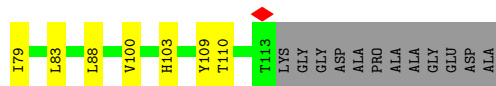
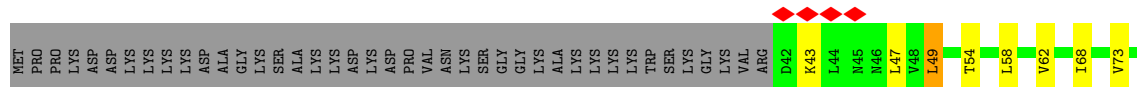
- Molecule 11: 40S ribosomal protein S20

Chain U:  13% 73% 11% 15%



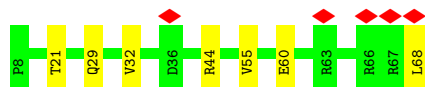
- Molecule 12: 40S ribosomal protein S25

Chain Z:  46% 11% 42%



- Molecule 13: 40S ribosomal protein S28

Chain c:  8% 89% 11%

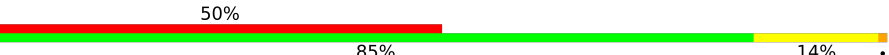


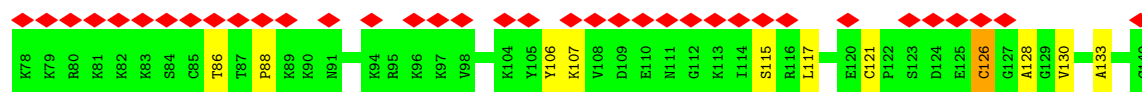
- Molecule 14: 40S ribosomal protein S29

Chain d:  89% 11%

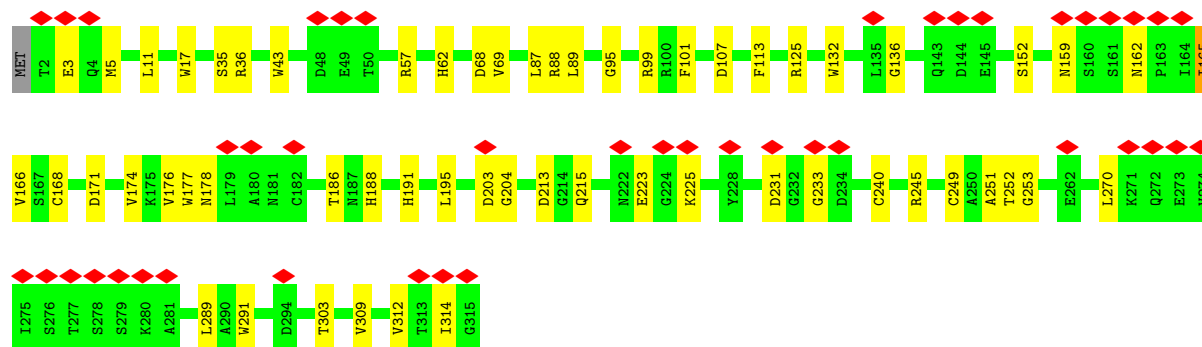
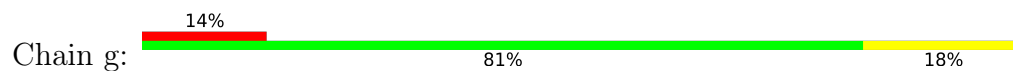


- Molecule 15: Ribosomal protein S27a

Chain f:  50% 85% 14%



- Molecule 16: Receptor of activated protein C kinase 1



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	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 ($\text{\AA}$)	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 ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/11228	0.29	0/17496
2	D	0.13	0/1780	0.32	0/2397
3	F	0.16	0/1523	0.36	0/2048
4	K	0.13	0/840	0.36	0/1133
5	M	0.11	0/963	0.31	0/1291
6	P	0.13	0/1035	0.30	0/1383
7	Q	0.17	0/1146	0.39	0/1534
8	R	0.13	0/678	0.34	0/902
9	S	0.15	0/1202	0.36	0/1610
10	T	0.13	0/1142	0.29	0/1530
11	U	0.15	0/813	0.36	0/1092
12	Z	0.13	0/580	0.33	0/780
13	c	0.15	0/481	0.36	0/643
14	d	0.14	0/469	0.34	0/623
15	f	0.11	0/595	0.34	0/785
16	g	0.12	0/2497	0.35	0/3399
All	All	0.14	0/26972	0.32	0/38646

There are no bond length outliers.

There are no bond angle outliers.

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	66	0
2	D	1752	0	1848	16	0
3	F	1501	0	1557	16	0
4	K	816	0	841	10	0
5	M	953	0	990	13	0
6	P	1016	0	1066	8	0
7	Q	1128	0	1195	11	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	8	0
12	Z	574	0	627	11	0
13	c	479	0	507	3	0
14	d	458	0	448	5	0
15	f	585	0	615	9	0
16	g	2440	0	2396	35	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	188	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 (188) 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)
16:g:87:LEU:HB2	16:g:101:PHE:HB2	1.72	0.71
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
16:g:223:GLU:OE1	16:g:225:LYS:NZ	2.26	0.69
11:U:80:PHE:HB3	14:d:52:PHE:HB3	1.74	0.68
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
16:g:165:ILE:HG13	16:g:177:TRP:HB2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:68:ILE:HB	12:Z:109:TYR:HB2	1.80	0.62
11:U:78:ASP:OD2	14:d:44:ARG:NH1	2.32	0.62
16:g:166:VAL:HG12	16:g:176:VAL:HG22	1.82	0.61
1:2:1277:C:H2'	1:2:1278:A:H8	1.64	0.61
1:2:1507:G:N2	15:f:86:THR:OG1	2.32	0.61
3:F:71:ARG:NH2	3:F:148:ASN:OD1	2.35	0.60
16:g:107:ASP:OD2	16:g:125:ARG:NH1	2.33	0.59
1:2:1396:A:O2'	1:2:1398:G:N7	2.36	0.58
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
3:F:120:GLY:O	3:F:193:LYS:NZ	2.38	0.57
5:M:44:LYS:HD3	15:f:128:ALA:HB3	1.86	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
15:f:107:LYS:HG2	15:f:115:SER:HB3	1.86	0.56
15:f:121:CYS:HB3	15:f:126:CYS:HB2	1.86	0.56
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
16:g:233:GLY:HA3	16:g:252:THR:HG21	1.86	0.56
16:g:174:VAL:HB	16:g:188:HIS:HB2	1.89	0.54
1:2:1438:A:H2'	1:2:1439:A:C8	2.43	0.54
16:g:162:ASN:ND2	16:g:178:ASN:OD1	2.30	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
16:g:62:HIS:CE1	16:g:88:ARG:HG3	2.43	0.54
14:d:19:ARG:HD2	14:d:32:ARG:HD3	1.90	0.53
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
16:g:159:ASN:HB2	16:g:204:GLY:HA3	1.90	0.53
16:g:3:GLU:HG3	16:g:314:ILE:HA	1.91	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
1:2:1522:A:O2'	9:S:145:THR:O	2.22	0.51
16:g:240:CYS:SG	16:g:249:CYS:HB3	2.50	0.51
1:2:1415:C:O2'	10:T:132:ASP:OD2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1310:U:H5''	15:f:130:VAL:HG13	1.92	0.50
2:D:142:LEU:HD12	2:D:148:LYS:HG3	1.93	0.50
16:g:3:GLU:OE1	16:g:245:ARG:NH2	2.33	0.50
1:2:1536:G:H2'	1:2:1537:A:H8	1.77	0.50
16:g:159:ASN:ND2	16:g:203:ASP:O	2.40	0.50
5:M:43:ASP:OD2	15:f:106:TYR:OH	2.29	0.50
13:c:21:THR:HG22	13:c:68:LEU:HD11	1.92	0.50
13:c:44:ARG:NH2	13:c:60:GLU:O	2.43	0.50
2:D:226:GLN:HG2	16:g:186:THR:HG23	1.93	0.49
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
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
16:g:191:HIS:CG	16:g:195:LEU:HD21	2.49	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
16:g:5:MET:HE1	16:g:291:TRP:HH2	1.80	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
16:g:215:GLN:NE2	16:g:231:ASP:OD1	2.45	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
1:2:1482:C:OP1	14:d:54:LYS:NZ	2.43	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
16:g:11:LEU:HB3	16:g:43:TRP:CZ3	2.50	0.46
16:g:17:TRP:CE2	16:g:303:THR:HG23	2.50	0.46
16:g:176:VAL:HB	16:g:186:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1507:G:N1	15:f:88:PRO:O	2.48	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
16:g:171:ASP:OD1	16:g:171:ASP:N	2.49	0.45
2:D:62:LYS:HD3	4:K:96:ARG:HD2	1.99	0.45
16:g:213:ASP:OD1	16:g:213:ASP:N	2.49	0.45
1:2:1395:C:O2'	1:2:1396:A:H5'	2.17	0.45
1:2:1554:C:OP2	1:2:1555:U:O2'	2.32	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
16:g:35:SER:OG	16:g:36:ARG:N	2.50	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
16:g:252:THR:HG22	16:g:253:GLY:H	1.81	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
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
16:g:5:MET:HB2	16:g:270:LEU:HD21	2.00	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
16:g:152:SER:HB2	16:g:168:CYS:SG	2.59	0.43
1:2:1464:C:O3'	8:R:60:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:18:ARG:NH1	9:S:88:LYS:O	2.52	0.43
16:g:249:CYS:SG	16:g:289:LEU:HD21	2.58	0.43
1:2:1686:G:H2'	1:2:1687:C:C6	2.52	0.43
7:Q:16:LYS:O	7:Q:17:LYS:C	2.62	0.43
3:F:34:SER:HA	13:c:55:VAL:HB	2.01	0.42
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
16:g:5:MET:HE2	16:g:312:VAL:HG22	2.00	0.42
16:g:57:ARG:HD3	16:g:95:GLY:HA3	2.00	0.42
11:U:20:ILE:HG12	11:U:116:ILE:HG13	2.01	0.42
16:g:101:PHE:CE2	16:g:136:GLY:HA2	2.54	0.42
6:P:57:LEU:HD21	6:P:89:MET:HE2	2.02	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
1:2:1308:U:O2'	15:f:133:ALA:HB1	2.20	0.41
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
16:g:89:LEU:HB3	16:g:99:ARG:HB3	2.01	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
1:2:1446:A:O2'	1:2:1447:G:H8	2.03	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
16:g:251:ALA:HB2	16:g:289:LEU:HD22	2.03	0.41
4:K:47:LYS:HD3	4:K:47:LYS:HA	1.86	0.41
16:g:68:ASP:OD1	16:g:69:VAL:N	2.54	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
2:D:16:ILE:HD11	14:d:36:LEU:HD23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:42:THR:HG22	2:D:44:THR:H	1.87	0.40
16:g:101:PHE:CD2	16:g:136:GLY:HA2	2.56	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
11:U:102:THR:O	11:U:105:SER:OG	2.35	0.40
15:f:107:LYS:HD3	15:f:117:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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 ⓘ

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%)	65	87
3	F	160/170 (94%)	159 (99%)	1 (1%)	78	92
4	K	88/136 (65%)	87 (99%)	1 (1%)	65	87
5	M	104/108 (96%)	103 (99%)	1 (1%)	68	88
6	P	110/130 (85%)	109 (99%)	1 (1%)	70	89
7	Q	117/121 (97%)	115 (98%)	2 (2%)	53	83
8	R	72/122 (59%)	72 (100%)	0	100	100
9	S	124/132 (94%)	120 (97%)	4 (3%)	34	70
10	T	114/115 (99%)	113 (99%)	1 (1%)	70	89
11	U	93/107 (87%)	90 (97%)	3 (3%)	34	70
12	Z	64/103 (62%)	62 (97%)	2 (3%)	35	70
13	c	54/54 (100%)	52 (96%)	2 (4%)	30	65
14	d	48/48 (100%)	48 (100%)	0	100	100
15	f	65/65 (100%)	64 (98%)	1 (2%)	57	84
16	g	272/273 (100%)	268 (98%)	4 (2%)	57	84
All	All	1674/1886 (89%)	1649 (98%)	25 (2%)	55	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	84	VAL
2	D	93	THR
3	F	32	ASP
4	K	64	TRP
5	M	16	THR
6	P	122	THR
7	Q	72	VAL
7	Q	100	VAL
9	S	53	THR
9	S	104	ASP
9	S	117	ILE
9	S	131	VAL
10	T	124	THR
11	U	39	LEU
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
16	g	165	ILE
16	g	309	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	95	HIS
3	F	203	ASN
4	K	66	HIS
6	P	32	GLN
6	P	54	HIS
7	Q	11	GLN
8	R	74	GLN
10	T	12	GLN
12	Z	64	ASN
12	Z	106	GLN
15	f	111	ASN
16	g	26	GLN

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Mol	Chain	Res	Type
16	g	226	HIS
16	g	296	GLN
16	g	311	GLN

5.3.3 RNA ⓘ

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [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 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.

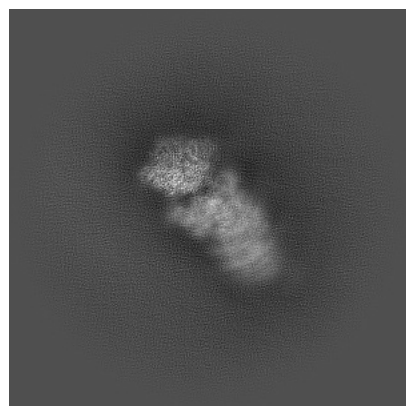
6 Map visualisation [i](#)

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.

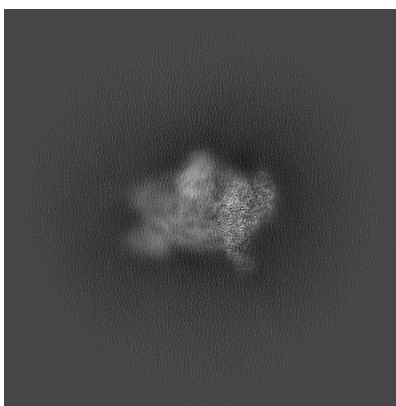
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

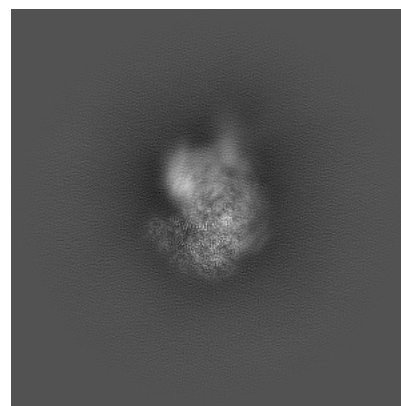
6.1.1 Primary map



X

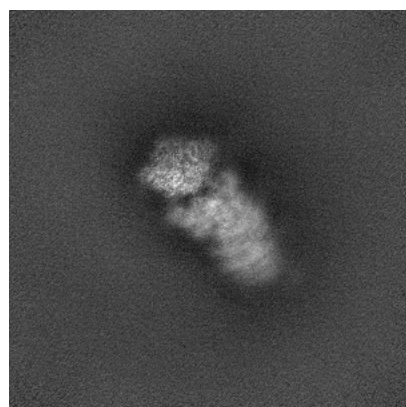


Y

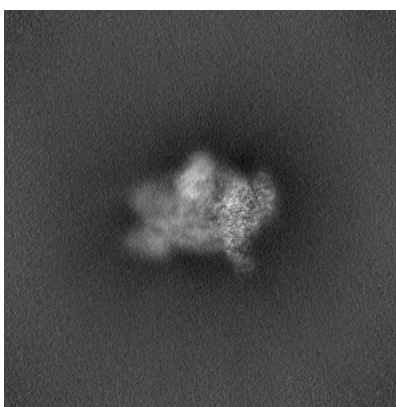


Z

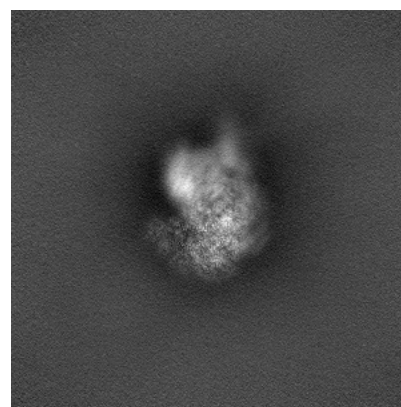
6.1.2 Raw map



X



Y

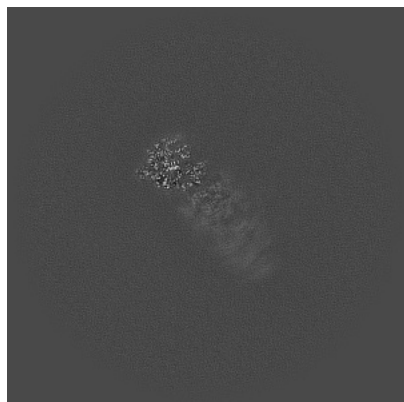


Z

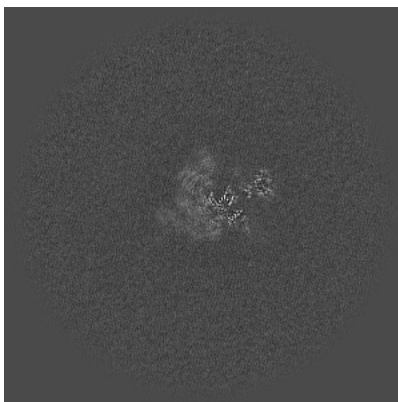
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

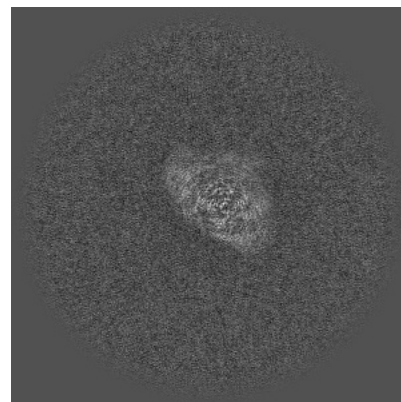
6.2.1 Primary map



X Index: 280

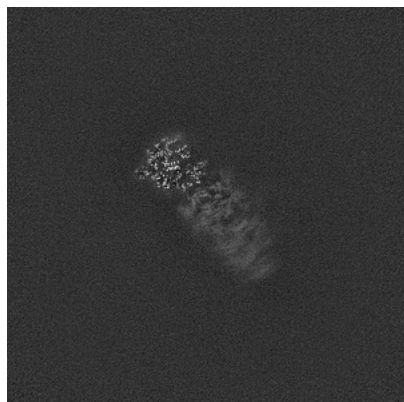


Y Index: 280

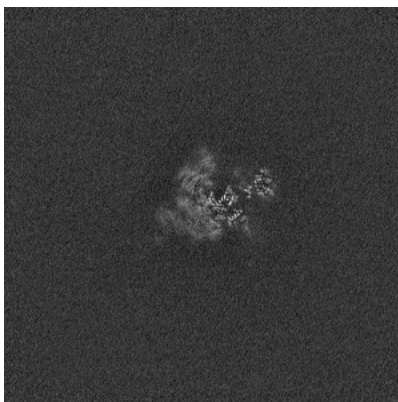


Z Index: 280

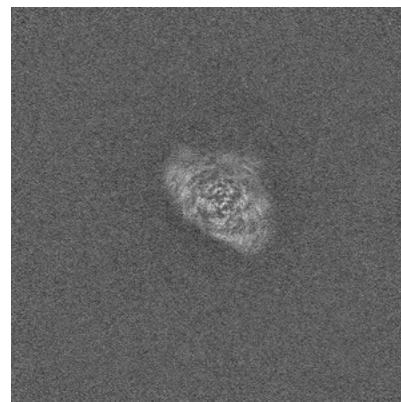
6.2.2 Raw map



X Index: 280



Y Index: 280

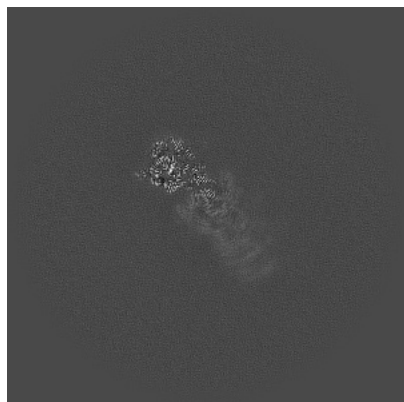


Z Index: 280

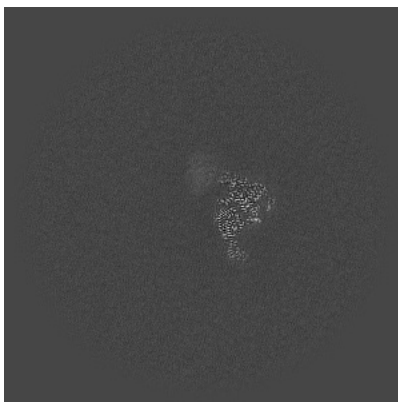
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

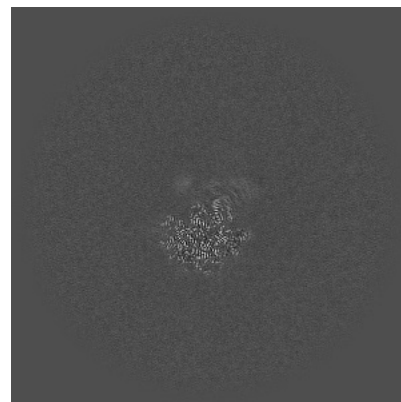
6.3.1 Primary map



X Index: 287



Y Index: 230



Z Index: 316

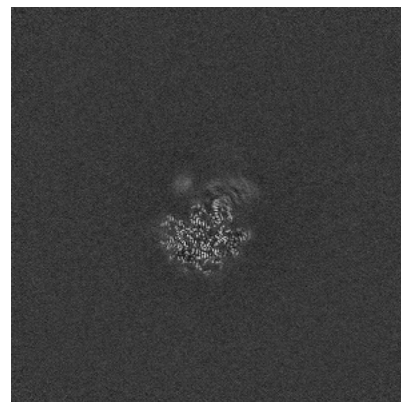
6.3.2 Raw map



X Index: 287



Y Index: 230

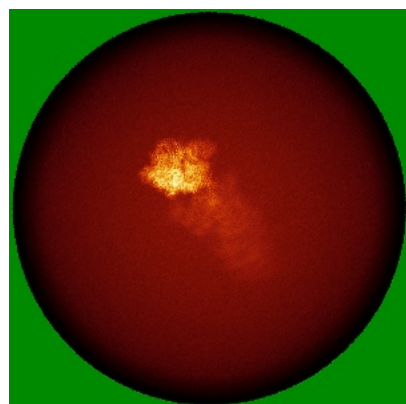


Z Index: 316

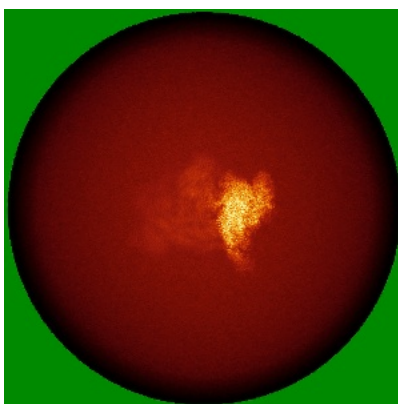
The images above show the largest variance slices of the map in three orthogonal directions.

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

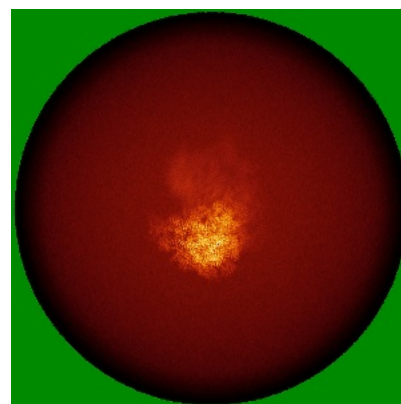
6.4.1 Primary map



X

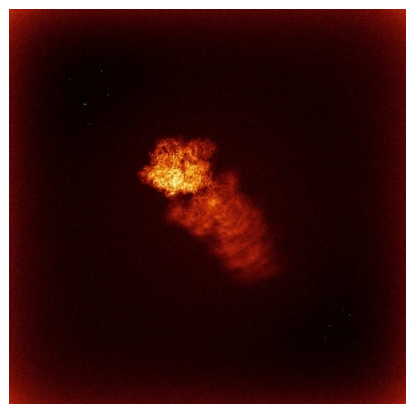


Y

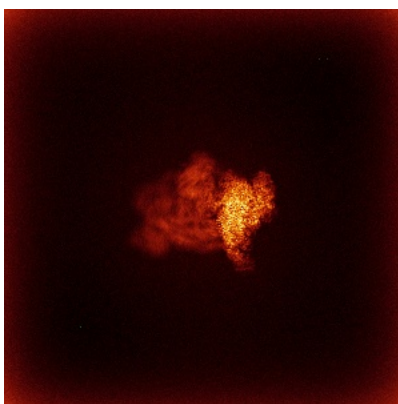


Z

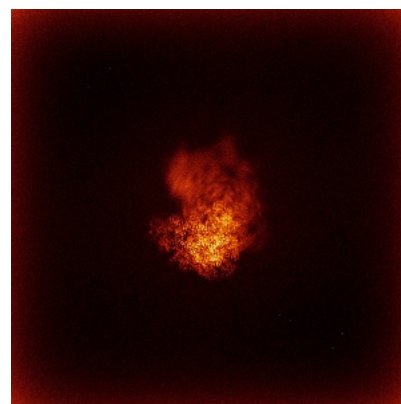
6.4.2 Raw map



X



Y



Z

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

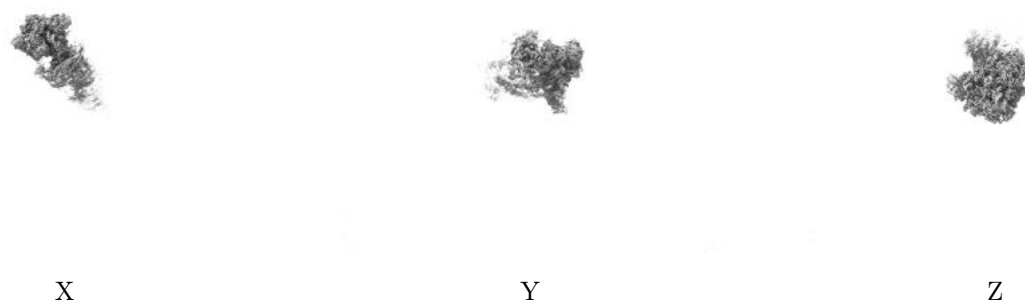
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

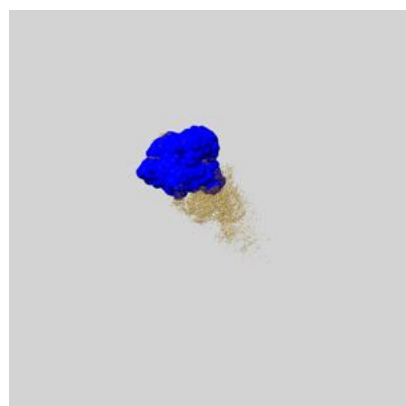
6.6 Mask visualisation [i](#)

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

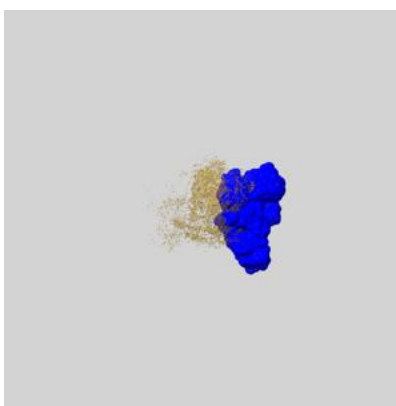
A mask typically either:

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

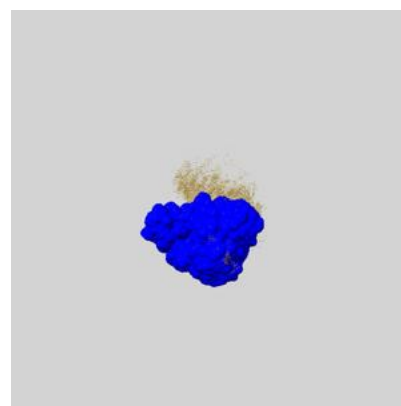
6.6.1 emd_11322_msk_1.map [i](#)



X



Y

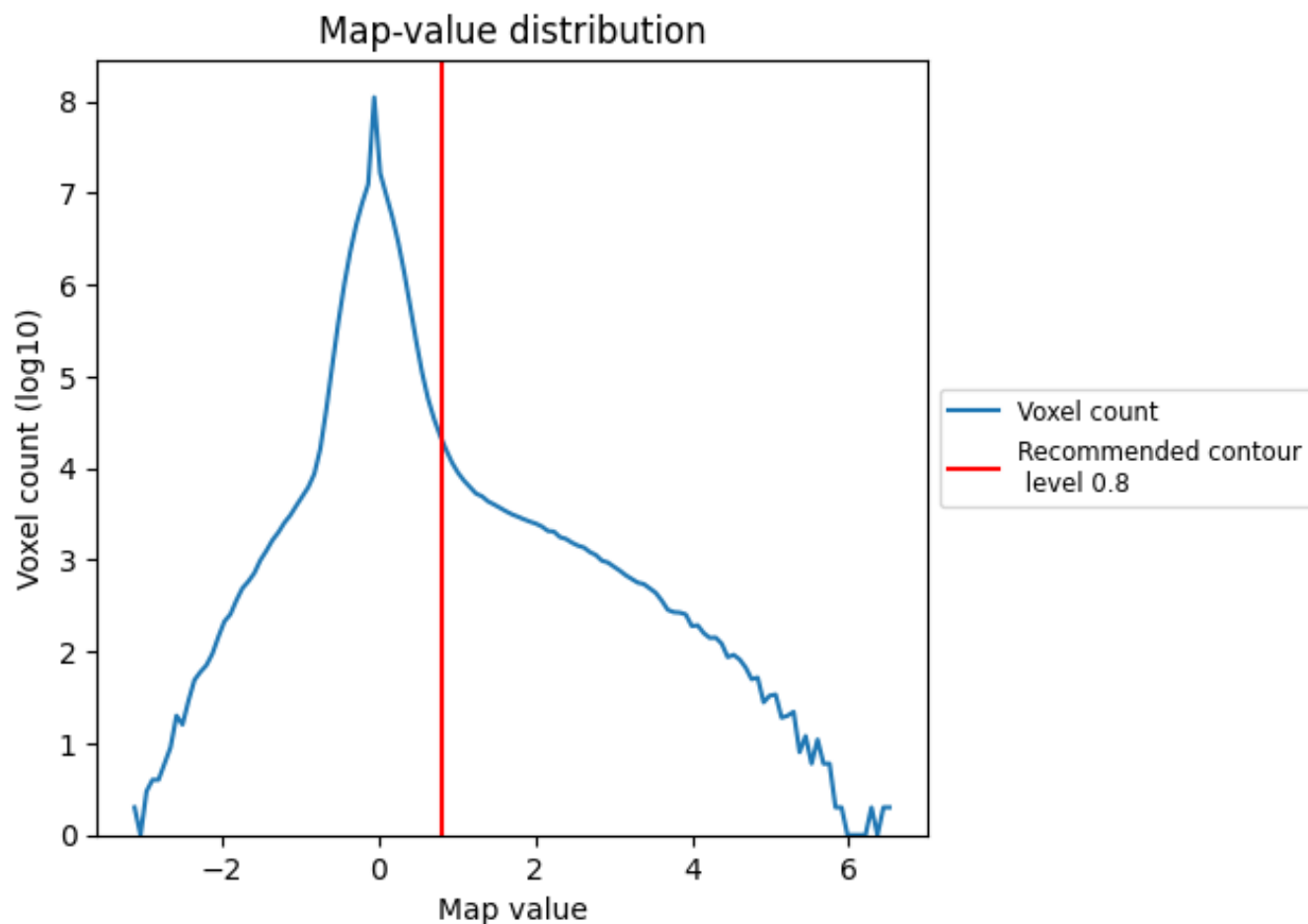


Z

7 Map analysis [i](#)

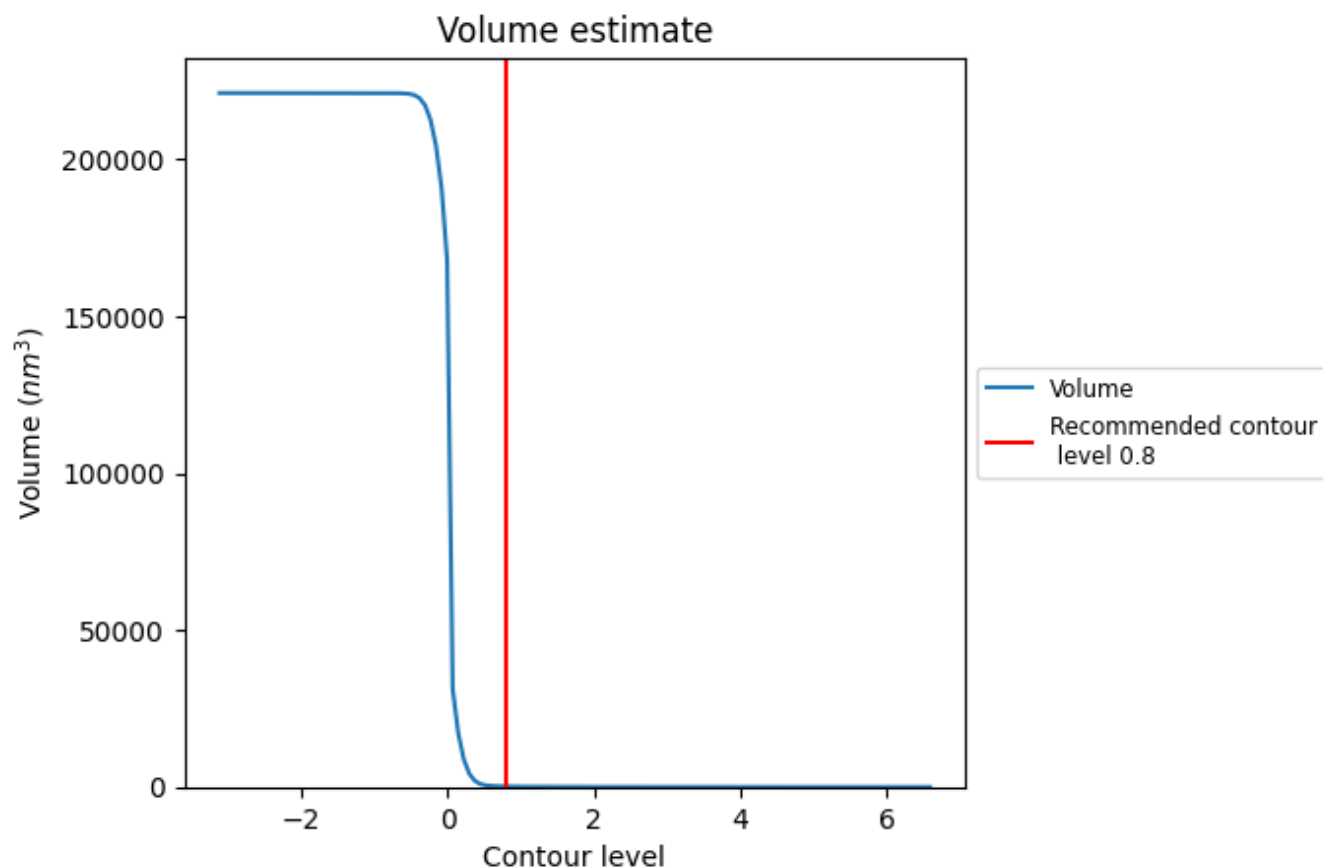
This section contains the results of statistical analysis of the map.

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.

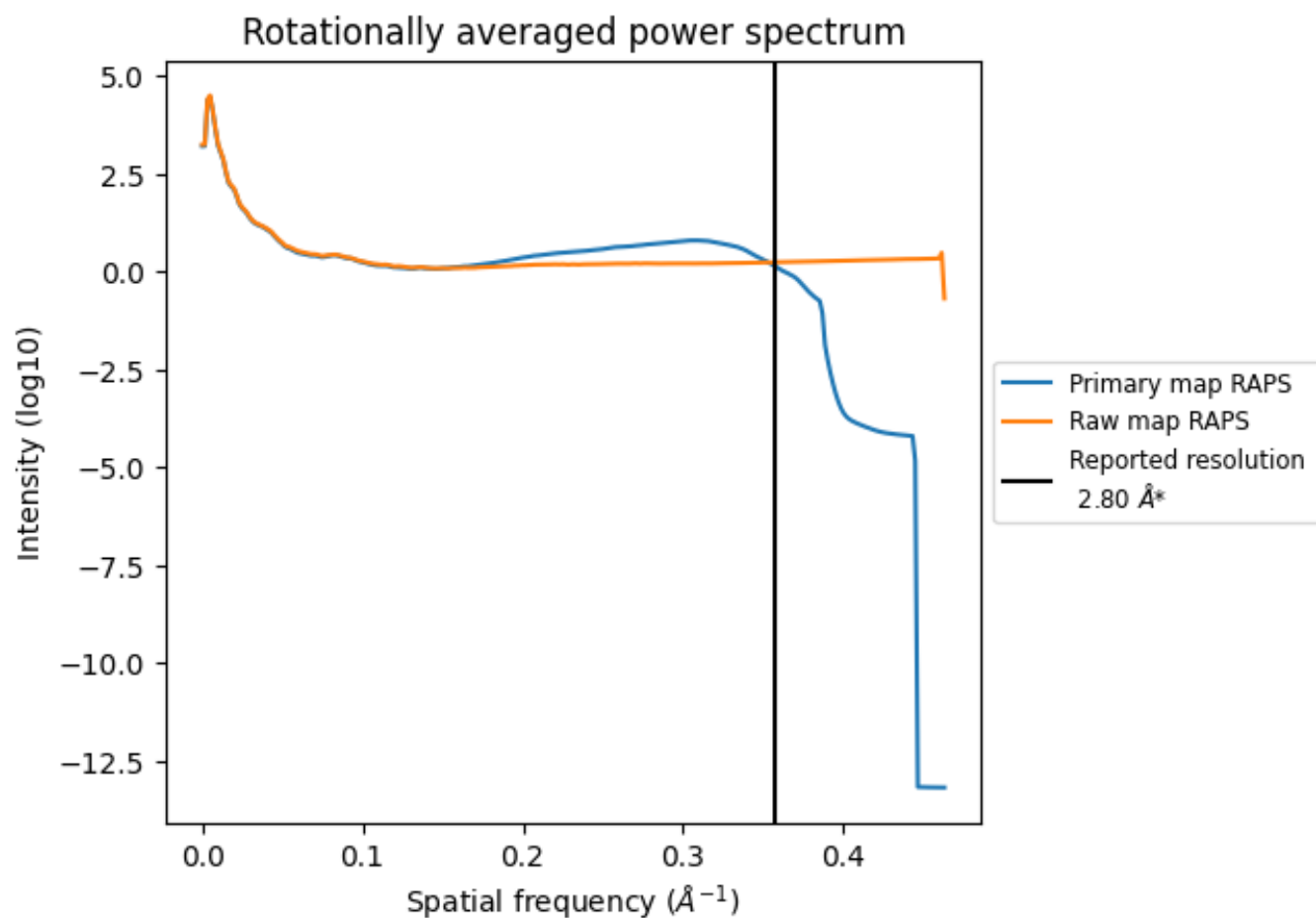
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 168 nm³; 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 ⓘ

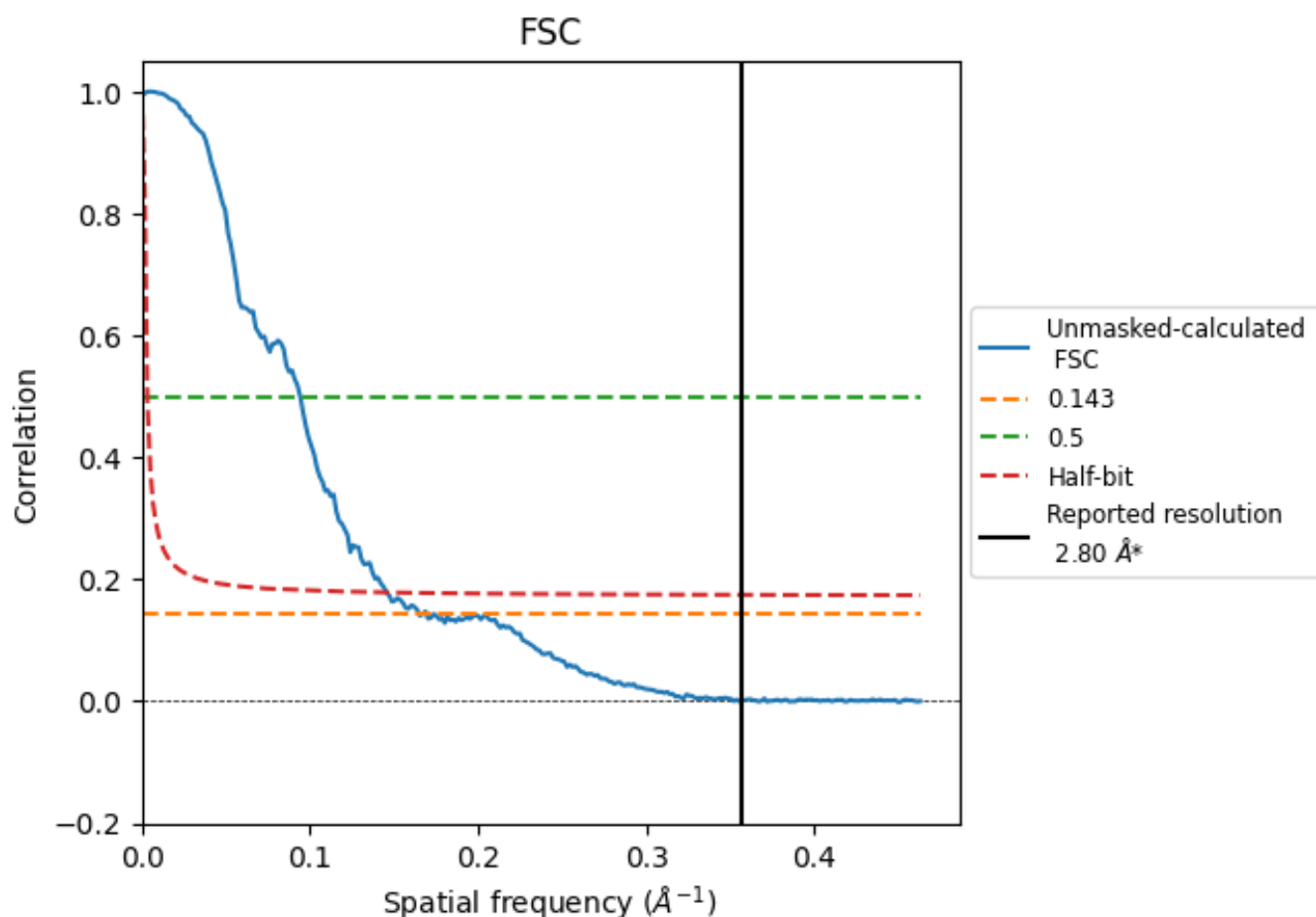


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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](#)

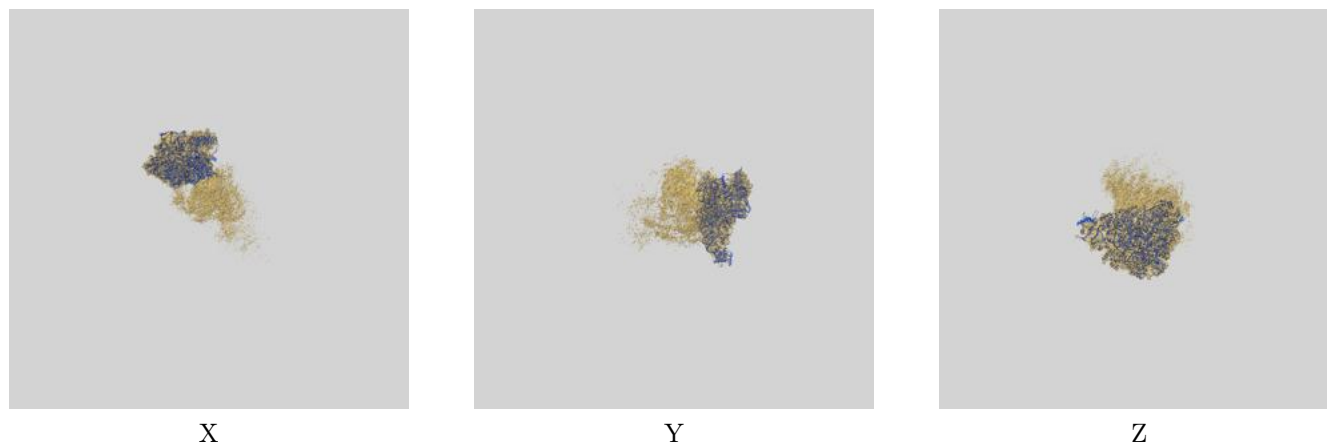
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.06	10.62	6.88

*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 [i](#)

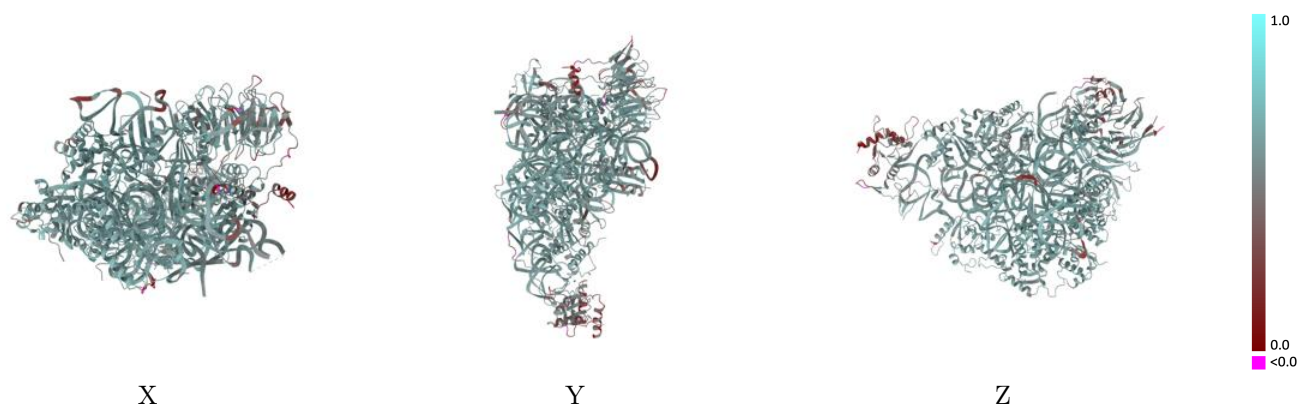
This section contains information regarding the fit between EMDB map EMD-11322 and PDB model 6ZOL. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



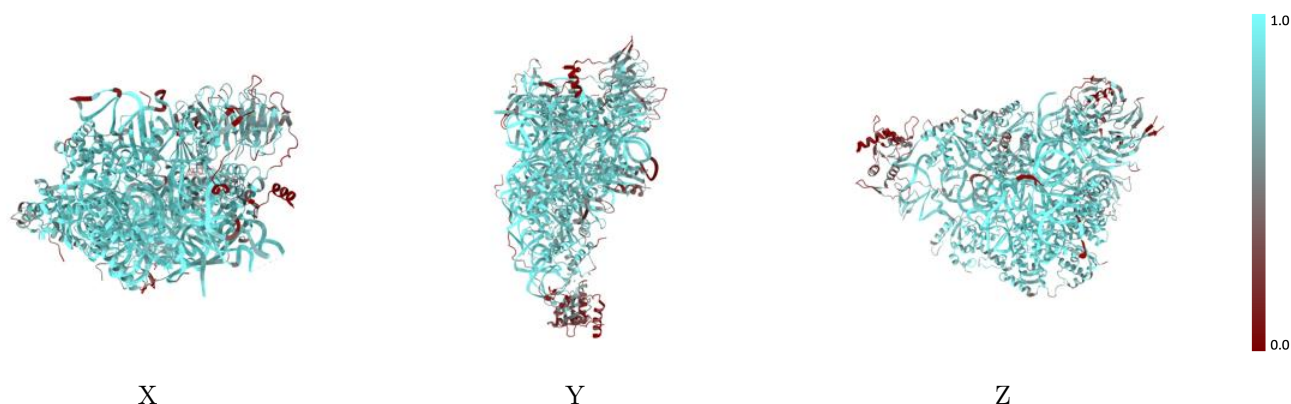
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



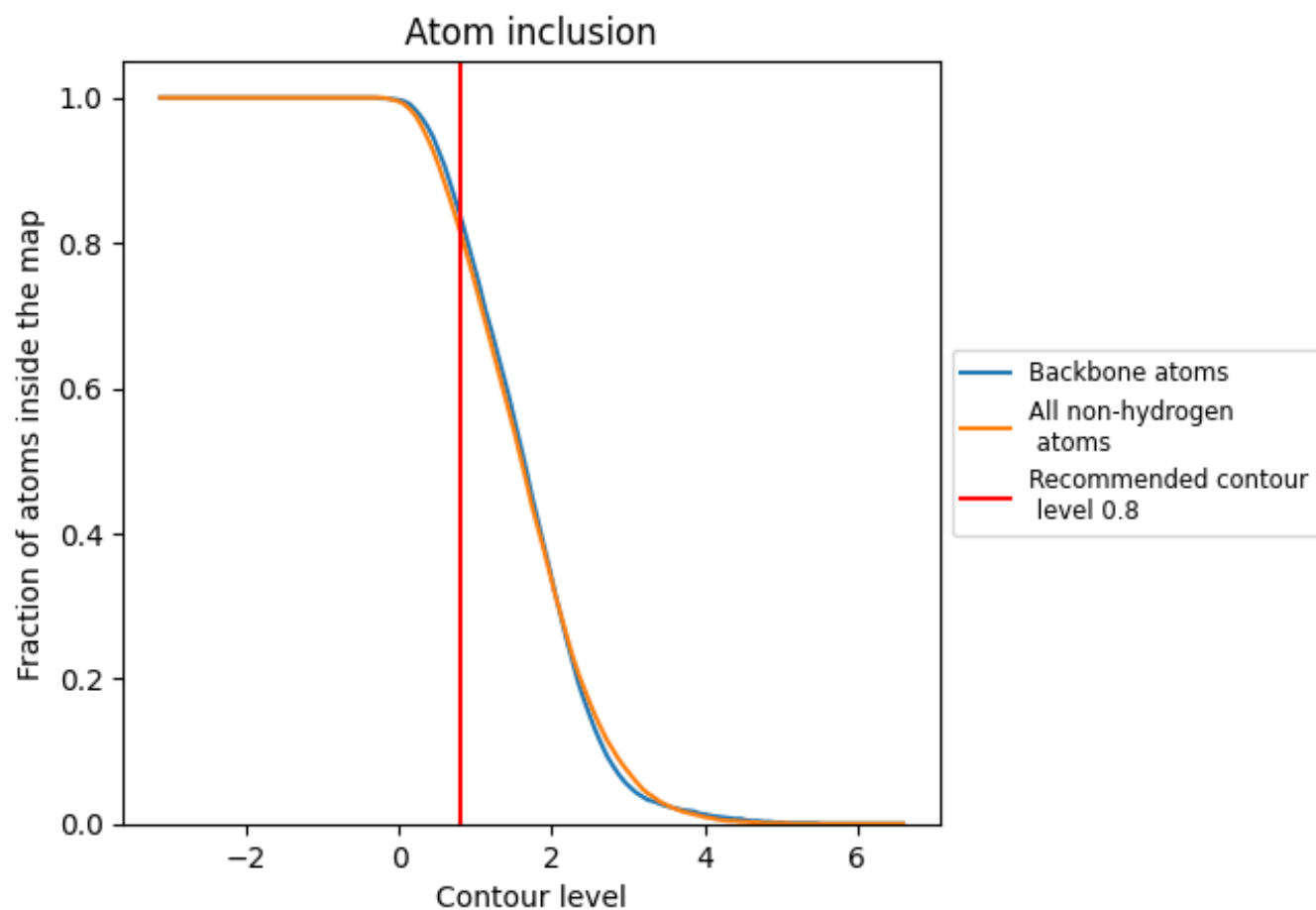
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

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	 0.8170	 0.5880
2	 0.9340	 0.6140
D	 0.7300	 0.5730
F	 0.8420	 0.6020
K	 0.8000	 0.5970
M	 0.2610	 0.3880
P	 0.8400	 0.6060
Q	 0.8960	 0.6320
R	 0.6350	 0.5120
S	 0.8440	 0.6160
T	 0.8940	 0.6230
U	 0.7340	 0.5820
Z	 0.7400	 0.5860
c	 0.7380	 0.5810
d	 0.8910	 0.6390
f	 0.4160	 0.4410
g	 0.6870	 0.5510

