



# wwPDB EM Validation Summary Report ⓘ

Nov 12, 2024 – 09:54 am GMT

PDB ID : 8P6P  
EMDB ID : EMD-17133  
Title : Mycoplasma pneumoniae small ribosomal subunit in chloramphenicol-treated cells  
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.  
Deposited on : 2023-05-27  
Resolution : 3.20 Å (reported)  
Based on initial models : 7OOD, 7OOC

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
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

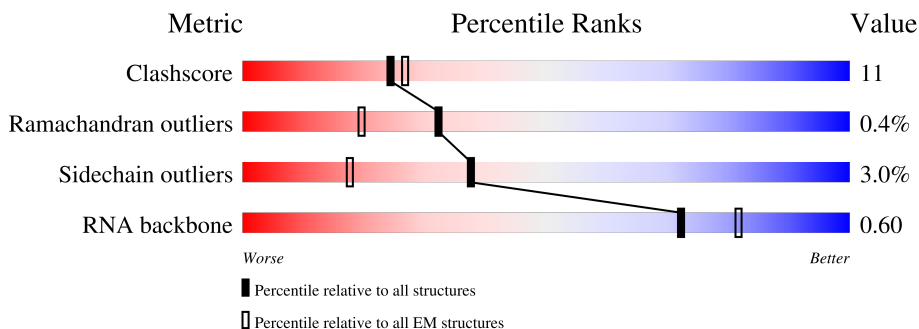
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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.








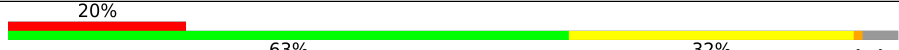
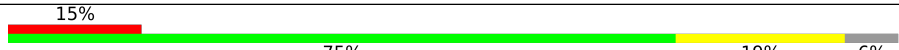

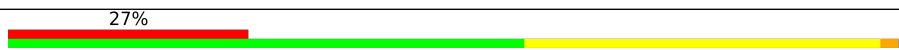





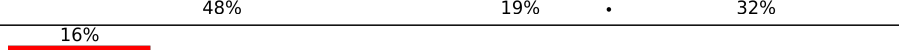
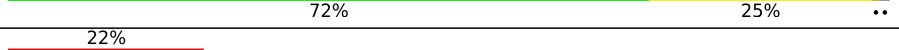


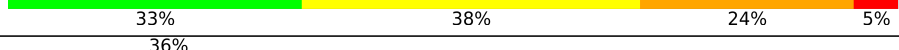
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	2907	99%
2	5	1520	8% (red), 52% (green), 41% (yellow), 6% (grey)
3	7	75	15% (red), 20% (green), 17% (yellow), 60% (grey)
4	8	76	26% (red), 20% (green), 18% (yellow), 61% (grey)
5	A	294	26% (red), 58% (green), 31% (yellow), 10% (grey)
6	B	273	11% (red), 67% (green), 17% (yellow), 15% (grey)
7	C	205	62% (red), 62% (green), 36% (yellow)

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Mol	Chain	Length	Quality of chain
8	D	219	
9	E	215	
10	F	155	
11	G	142	
12	H	132	
13	I	108	
14	J	121	
15	K	139	
16	L	124	
17	M	61	
18	N	86	
19	O	94	
20	P	85	
21	Q	104	
22	R	87	
23	S	87	
24	T	60	
25	Y	21	
26	x	97	

## 2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 55465 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3	24	512	229	93	166	24	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	1507	32258	14420	5847	10484	1507	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 3 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	7	30	640	285	112	213	30	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 4 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	8	30	639	286	114	209	30	0	0

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	266	Total	C	N	O	S	0	0
			2138	1359	376	394	9		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	232	Total	C	N	O	S	0	0
			1835	1158	343	329	5		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	204	Total	C	N	O	S	0	0
			1669	1057	316	292	4		

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	155	Total	C	N	O	S	0	0
			1191	753	228	207	3		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	184	Total	C	N	O	S	0	0
			1509	950	270	287	2		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	155	Total	C	N	O	S	0	0
			1254	790	240	217	7		

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	141	Total	C	N	O	S	0	0
			1110	723	193	192	2		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	129	Total	C	N	O	S	0	0
			1040	661	195	183	1		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	104	Total	C	N	O	S	0	0
			832	536	147	148	1		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	135	Total	C	N	O	S	0	0
			1071	677	212	180	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	L	123	Total	C	N	O	0	0
			991	618	200	173		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	N	85	Total	C	N	O	0	0
			689	436	130	123		

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	87	Total	C	N	O	S	0	0
			705	453	130	118	4		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	85	Total	C	N	O	S	0	0
			693	436	138	118	1		

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	71	Total	C	N	O	S	0	0
			590	378	115	93	4		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	86	Total	C	N	O	S	0	0
			700	444	132	122	2		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	S	79	Total	C	N	O	0	0
			643	391	138	114		

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	59	Total	C	N	O	S	0	0
			519	326	111	80	2		

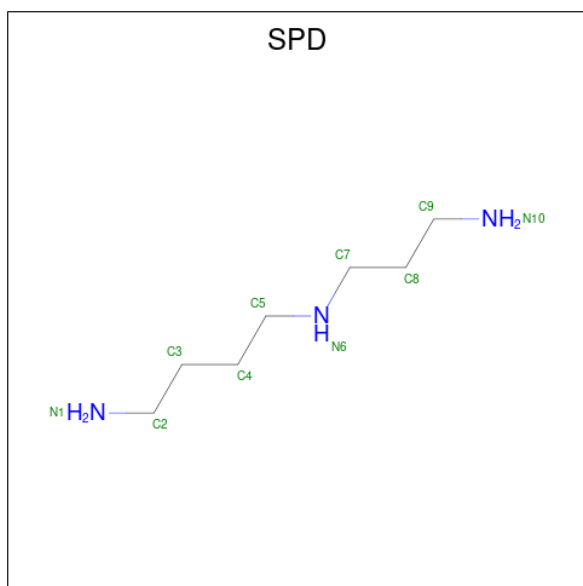
- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	21	Total	C	N	O	P	0	0
			446	200	79	146	21		

- Molecule 26 is a protein called 50S ribosomal protein L31.

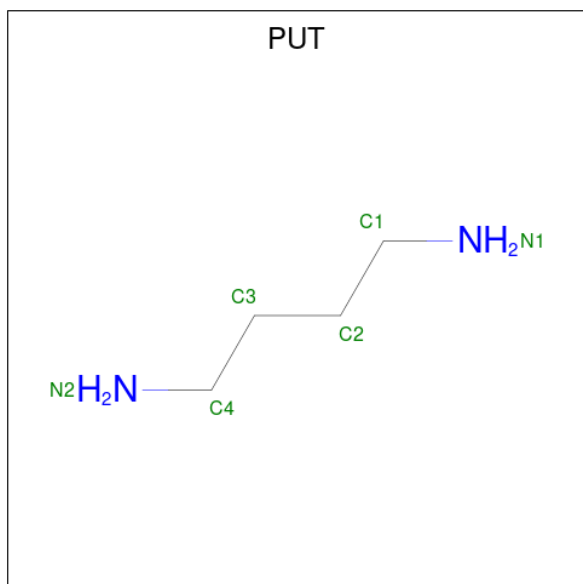
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	x	43	342	214	65	63	0	0

- Molecule 27 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
27	5	1	10	7	3	0
27	5	1	10	7	3	0

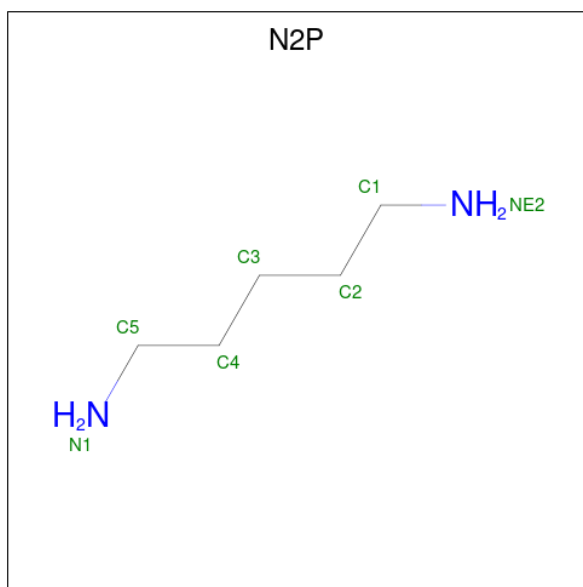
- Molecule 28 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula:  $C_4H_{12}N_2$ ).





Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	N	0
			6	4	2	
28	5	1	Total	C	N	0
			6	4	2	

- Molecule 29 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: C<sub>5</sub>H<sub>14</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
29	5	1	Total	C	N	0
			7	5	2	

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	5	96	Total	Mg	0
			96	96	
30	7	1	Total	Mg	0
			1	1	
30	8	1	Total	Mg	0
			1	1	
30	H	1	Total	Mg	0
			1	1	
30	K	1	Total	Mg	0
			1	1	
30	L	1	Total	Mg	0
			1	1	
30	P	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
30	Y	1	Total	Mg	0
			1	1	

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	M	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	

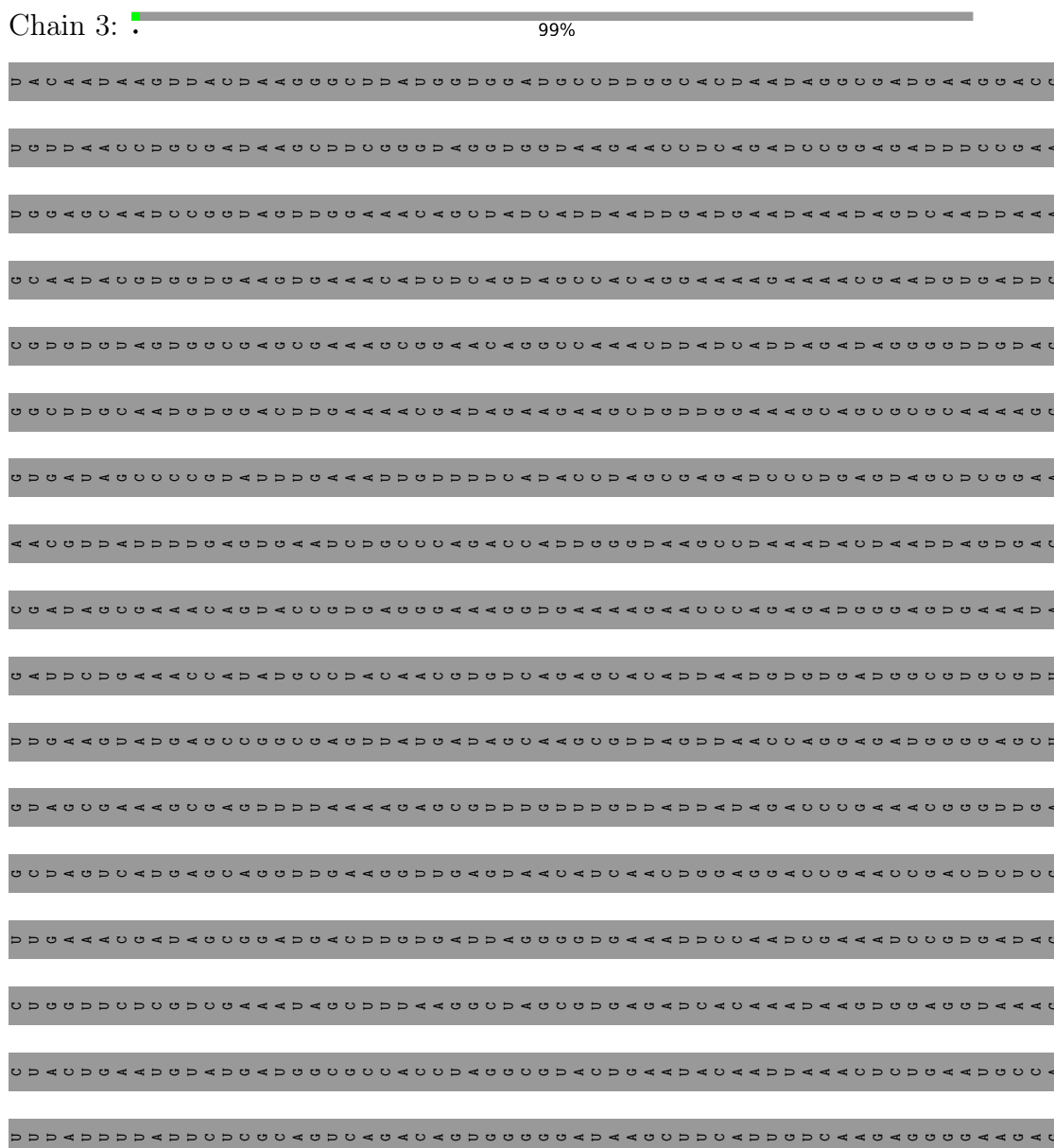
- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	5	1	Total	O	0
			1	1	
32	A	1	Total	O	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.

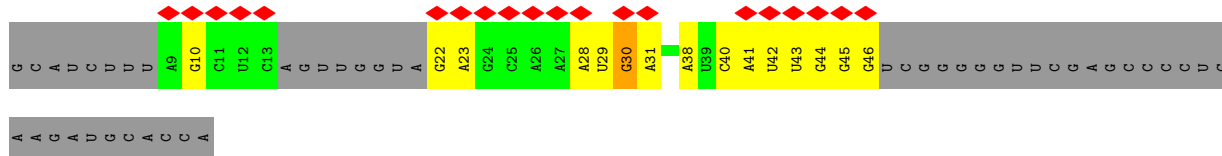
- Molecule 1: 23S ribosomal RNA



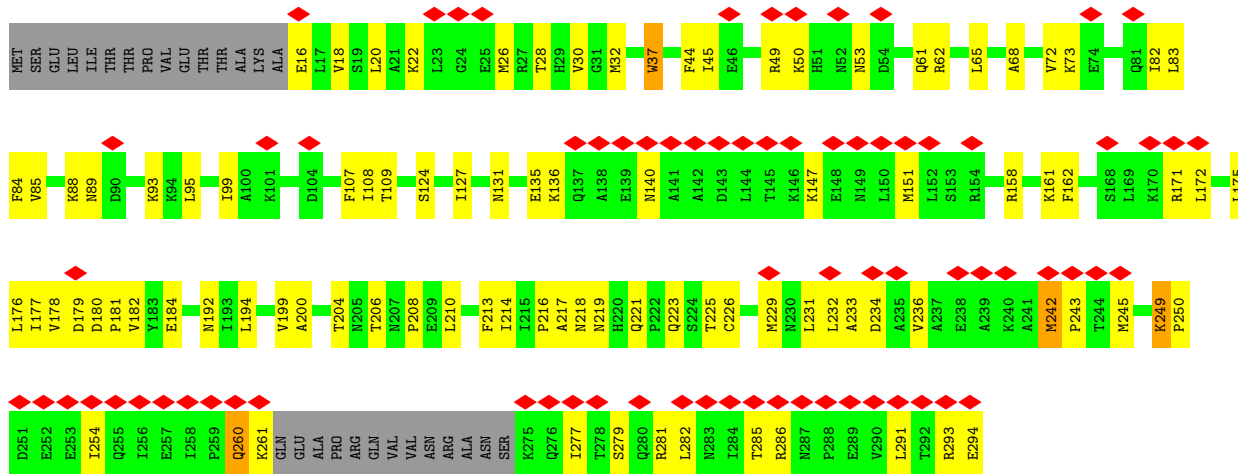




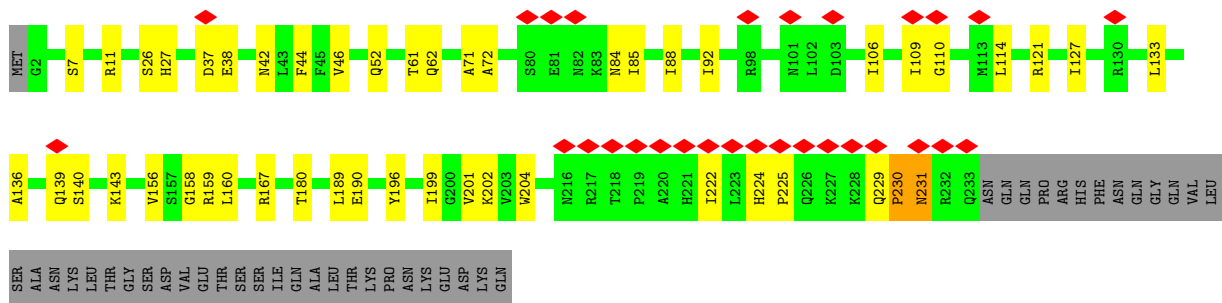




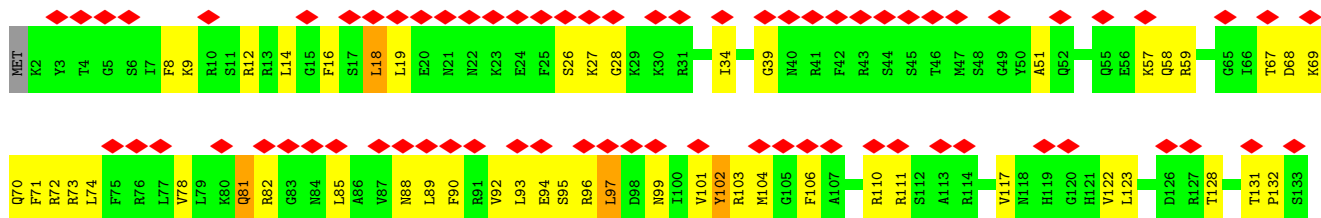
• Molecule 5: 30S ribosomal protein S2



• Molecule 6: 30S ribosomal protein S3



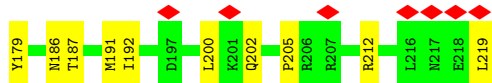
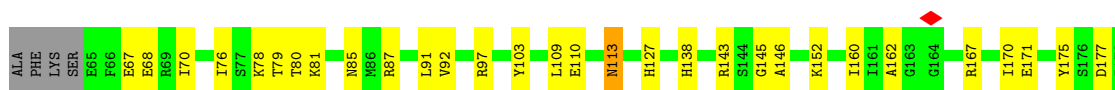
• Molecule 7: 30S ribosomal protein S4





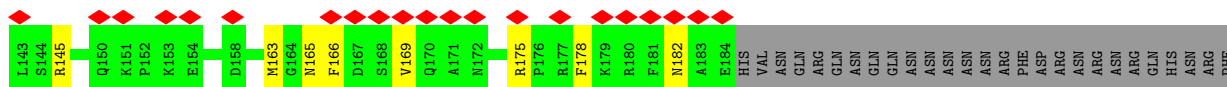
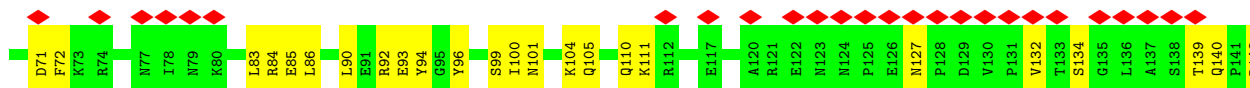
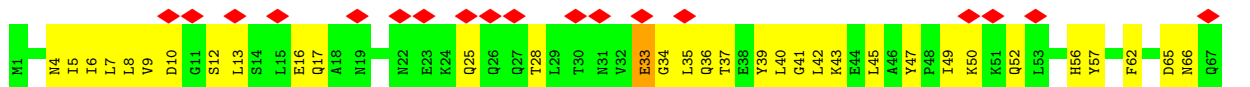
- Molecule 8: 30S ribosomal protein S5

Chain D: 53% 18% 29%



- Molecule 9: 30S ribosomal protein S6

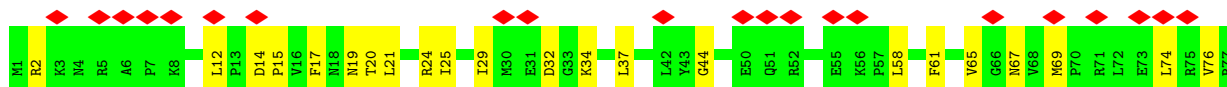
Chain E: 30% 55% 30% 14%



LYS  
ASP  
LYS  
GLN

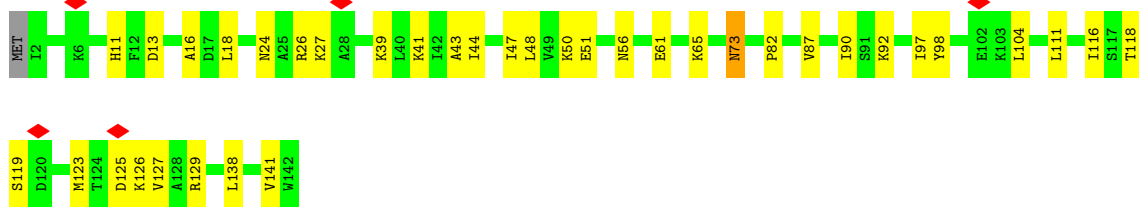
- Molecule 10: 30S ribosomal protein S7

Chain F: 26% 69% 29%

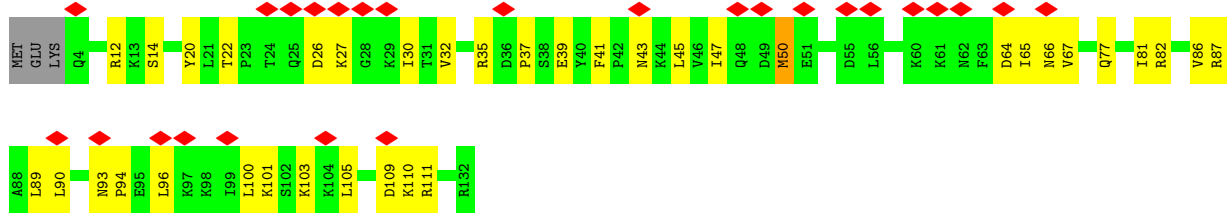


- Molecule 11: 30S ribosomal protein S8

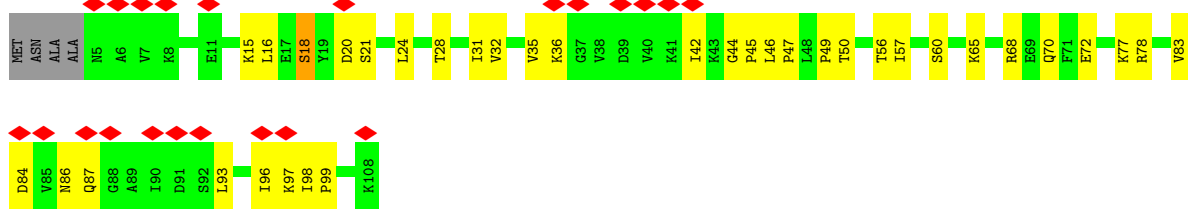




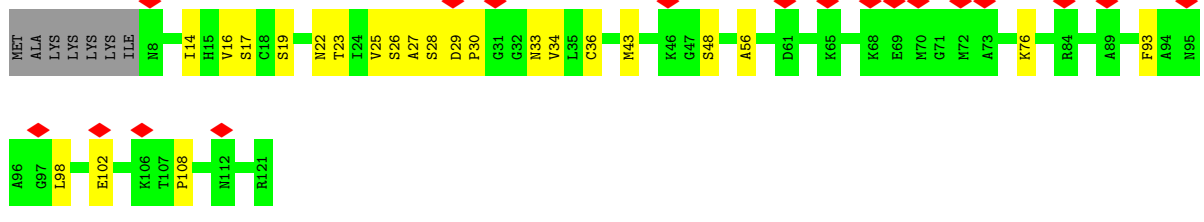
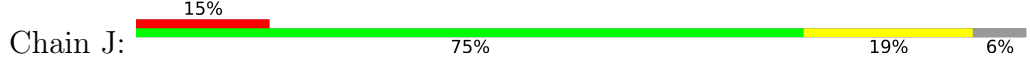
• Molecule 12: 30S ribosomal protein S9



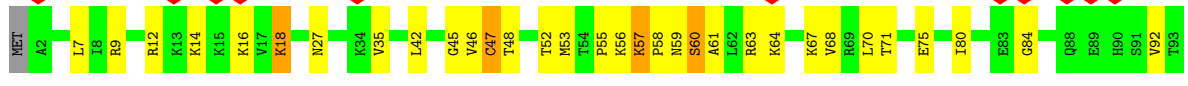
• Molecule 13: 30S ribosomal protein S10

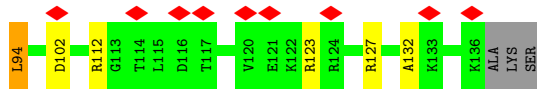


• Molecule 14: 30S ribosomal protein S11

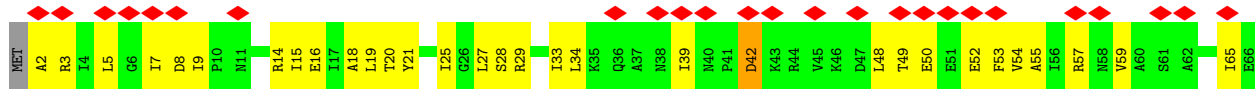


• Molecule 15: 30S ribosomal protein S12

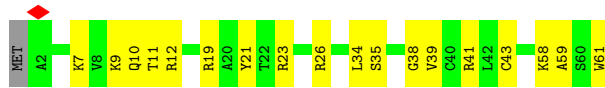




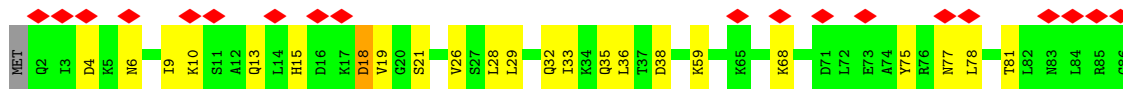
• Molecule 16: 30S ribosomal protein S13



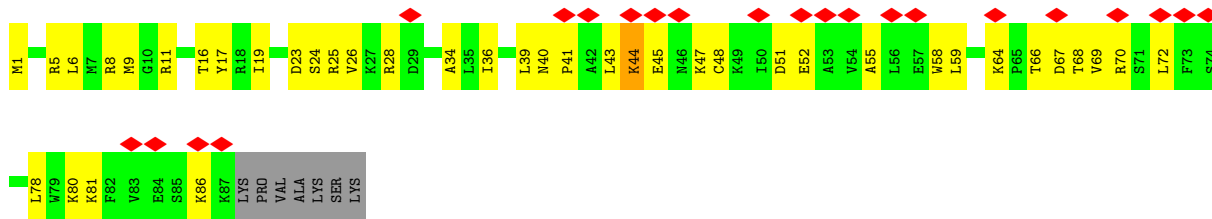
• Molecule 17: 30S ribosomal protein S14 type Z



• Molecule 18: 30S ribosomal protein S15



• Molecule 19: 30S ribosomal protein S16

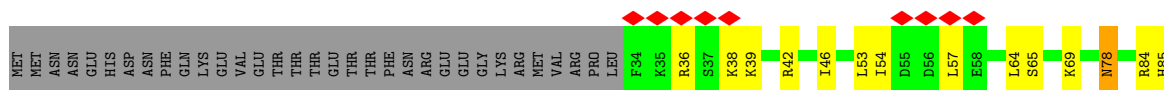


• Molecule 20: 30S ribosomal protein S17

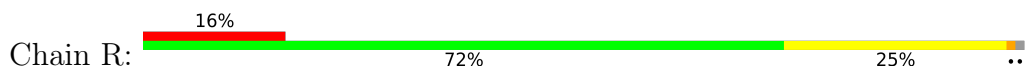




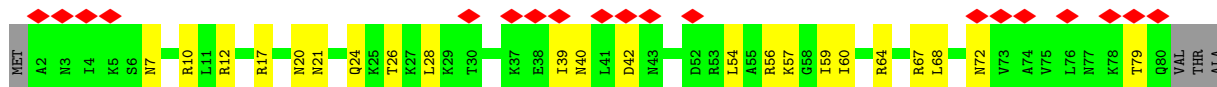
• Molecule 21: 30S ribosomal protein S18



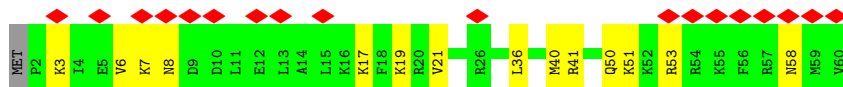
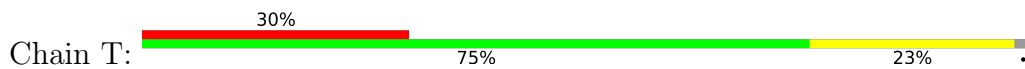
• Molecule 22: 30S ribosomal protein S19



• Molecule 23: 30S ribosomal protein S20



• Molecule 24: 30S ribosomal protein S21



• Molecule 25: mRNA



• Molecule 26: 50S ribosomal protein L31



MET	LYS	LYS	ASP	PHE	HIS	PHE	PRO	SER	GLN	SER	VAL	SER	PHE	LYS	CYS	ALA	SER	CYS	SER	ASN	SER	PHE	THR	ILE	GLU	SER	THR	LEU	LYS	GLN	LYS	GLU	ILE	THR	ILE	ASP	ILE	CYS	GLY	LYS	CYS	HIS	PRO	PHE	TYR	ILE	GLY	GLU	LEU	THR	LYS	GLN	THR	N55	H56	G57	H58	A59	E60
K61	L62	S63	G64	K65	F66	N67	A68	A71	F72	L73	E74	N75	K76	T77	F78	K79	R80	A81	R82	G83	R84	T85	E86	E87	T88	H91	R92	H98	E99	L100																													

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	30774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0022	Depositor
Map size ( $\text{\AA}$ )	539.574, 539.574, 539.574	wwPDB
Map dimensions	406, 406, 406	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.329, 1.329, 1.329	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: B8T, G7M, MA6, 5MC, PUT, MG, SPD, N2P, 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	3	0.24	0/572	0.76	0/889
2	5	0.30	0/35992	0.77	4/56111 (0.0%)
3	7	0.25	0/713	0.77	0/1107
4	8	0.20	0/713	0.77	0/1106
5	A	0.26	0/2172	0.51	0/2934
6	B	0.28	0/1863	0.56	0/2516
7	C	0.37	1/1700 (0.1%)	0.69	3/2278 (0.1%)
8	D	0.27	0/1206	0.55	1/1616 (0.1%)
9	E	0.27	0/1536	0.54	0/2072
10	F	0.26	0/1274	0.55	0/1710
11	G	0.27	0/1126	0.52	0/1517
12	H	0.28	0/1056	0.61	0/1409
13	I	0.27	0/843	0.55	0/1132
14	J	0.31	0/844	0.66	2/1136 (0.2%)
15	K	0.26	0/1089	0.58	0/1461
16	L	0.26	0/1002	0.61	0/1340
17	M	0.30	0/483	0.58	0/643
18	N	0.25	0/695	0.54	0/926
19	O	0.34	0/718	0.74	2/962 (0.2%)
20	P	0.24	0/702	0.56	0/934
21	Q	0.26	0/601	0.57	0/801
22	R	0.30	0/716	0.62	1/958 (0.1%)
23	S	0.27	0/645	0.54	0/857
24	T	0.28	0/524	0.58	0/685
25	Y	0.27	0/498	0.87	1/773 (0.1%)
26	x	0.25	0/347	0.53	0/457
All	All	0.29	1/59630 (0.0%)	0.71	14/88330 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	152	PRO	CG-CD	-10.24	1.16	1.50

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	152	PRO	N-CD-CG	-13.35	83.17	103.20
14	J	108	PRO	CA-N-CD	-12.03	94.65	111.50
22	R	76	PRO	CA-N-CD	-9.30	98.48	111.50
19	O	41	PRO	CA-N-CD	-8.45	99.67	111.50
19	O	41	PRO	N-CD-CG	-6.60	93.30	103.20

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	3	512	0	260	1	0
2	5	32258	0	16204	502	0
3	7	640	0	324	15	0
4	8	639	0	324	9	0
5	A	2138	0	2204	59	0
6	B	1835	0	1909	36	0
7	C	1669	0	1729	58	0
8	D	1191	0	1284	27	0
9	E	1509	0	1520	48	0
10	F	1254	0	1320	32	0
11	G	1110	0	1226	30	0
12	H	1040	0	1107	25	0
13	I	832	0	918	26	0
14	J	829	0	855	16	0
15	K	1071	0	1165	27	0
16	L	991	0	1061	39	0
17	M	474	0	505	16	0
18	N	689	0	746	13	0
19	O	705	0	755	30	0
20	P	693	0	753	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Q	590	0	625	23	0
22	R	700	0	709	15	0
23	S	643	0	694	18	0
24	T	519	0	578	8	0
25	Y	446	0	226	11	0
26	x	342	0	354	0	0
27	5	20	0	38	2	0
28	5	12	0	24	0	0
29	5	7	0	14	0	0
30	5	96	0	0	0	0
30	7	1	0	0	0	0
30	8	1	0	0	0	0
30	H	1	0	0	0	0
30	K	1	0	0	0	0
30	L	1	0	0	0	0
30	P	1	0	0	0	0
30	Y	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
32	5	1	0	0	0	0
32	A	1	0	0	0	0
All	All	55465	0	39431	976	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 11.

The worst 5 of 976 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)
3:7:34:G:H1	25:Y:42:U:H3	1.16	0.92
2:5:169:G:N2	2:5:219:A:O2'	2.13	0.81
2:5:983:G:H21	2:5:1012:A:H8	1.28	0.81
18:N:26:VAL:HG11	18:N:78:LEU:HD21	1.62	0.81
2:5:452:A:OP1	19:O:70:ARG:NH2	2.14	0.80

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	
5	A	262/294 (89%)	240 (92%)	22 (8%)	0	100	100
6	B	230/273 (84%)	215 (94%)	13 (6%)	2 (1%)	14	49
7	C	202/205 (98%)	171 (85%)	30 (15%)	1 (0%)	25	60
8	D	153/219 (70%)	148 (97%)	5 (3%)	0	100	100
9	E	182/215 (85%)	161 (88%)	20 (11%)	1 (0%)	25	60
10	F	153/155 (99%)	139 (91%)	13 (8%)	1 (1%)	19	54
11	G	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
12	H	127/132 (96%)	114 (90%)	12 (9%)	1 (1%)	16	51
13	I	102/108 (94%)	90 (88%)	12 (12%)	0	100	100
14	J	112/121 (93%)	104 (93%)	8 (7%)	0	100	100
15	K	133/139 (96%)	122 (92%)	9 (7%)	2 (2%)	8	38
16	L	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
17	M	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
18	N	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
19	O	85/94 (90%)	82 (96%)	2 (2%)	1 (1%)	11	43
20	P	83/85 (98%)	73 (88%)	9 (11%)	1 (1%)	11	43
21	Q	69/104 (66%)	64 (93%)	5 (7%)	0	100	100
22	R	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
23	S	77/87 (88%)	75 (97%)	2 (3%)	0	100	100
24	T	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	x	41/97 (42%)	30 (73%)	10 (24%)	1 (2%)	5	29
All	All	2553/2888 (88%)	2345 (92%)	197 (8%)	11 (0%)	32	64

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	230	PRO
20	P	54	LEU
15	K	56	LYS
7	C	81	GLN
6	B	231	ASN

### 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	
5	A	238/262 (91%)	228 (96%)	10 (4%)	25	58
6	B	195/232 (84%)	195 (100%)	0	100	100
7	C	182/183 (100%)	174 (96%)	8 (4%)	24	57
8	D	125/178 (70%)	123 (98%)	2 (2%)	58	79
9	E	165/196 (84%)	160 (97%)	5 (3%)	36	66
10	F	132/132 (100%)	125 (95%)	7 (5%)	19	52
11	G	123/124 (99%)	122 (99%)	1 (1%)	79	90
12	H	112/115 (97%)	111 (99%)	1 (1%)	75	89
13	I	97/99 (98%)	95 (98%)	2 (2%)	48	74
14	J	91/97 (94%)	88 (97%)	3 (3%)	33	64
15	K	117/120 (98%)	111 (95%)	6 (5%)	20	53
16	L	104/105 (99%)	98 (94%)	6 (6%)	17	49
17	M	47/48 (98%)	46 (98%)	1 (2%)	48	74
18	N	77/78 (99%)	73 (95%)	4 (5%)	19	52
19	O	76/82 (93%)	73 (96%)	3 (4%)	27	60
20	P	75/75 (100%)	73 (97%)	2 (3%)	40	69
21	Q	62/94 (66%)	61 (98%)	1 (2%)	58	79
22	R	76/77 (99%)	74 (97%)	2 (3%)	41	70
23	S	71/77 (92%)	71 (100%)	0	100	100
24	T	55/56 (98%)	52 (94%)	3 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	x	35/86 (41%)	34 (97%)	1 (3%)	37 67
All	All	2255/2516 (90%)	2187 (97%)	68 (3%)	37 66

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	O	48	CYS
20	P	49	ASN
24	T	19	LYS
9	E	178	PHE
9	E	175	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
16	L	100	GLN
26	x	98	ASN
8	D	193	HIS
9	E	17	GLN
9	E	25	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	23/2907 (0%)	1 (4%)	0
2	5	1503/1520 (98%)	234 (15%)	6 (0%)
25	Y	20/21 (95%)	11 (55%)	1 (5%)
3	7	28/75 (37%)	2 (7%)	1 (3%)
4	8	28/76 (36%)	4 (14%)	0
All	All	1602/4599 (34%)	252 (15%)	8 (0%)

5 of 252 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	1920	A
2	5	6	C
2	5	10	G
2	5	40	G
2	5	48	C

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	Y	51	C
3	7	10	G
2	5	1123	G
2	5	1024	U
2	5	1158	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	G7M	5	525	2	20,26,27	4.04	10 (50%)	17,39,42	1.02	1 (5%)
2	MA6	5	1494	2	18,26,27	1.08	2 (11%)	19,38,41	3.41	3 (15%)
2	B8T	5	1377	2	19,22,23	3.24	8 (42%)	26,31,34	0.84	1 (3%)
2	5MC	5	1375	2	18,22,23	4.02	7 (38%)	26,32,35	1.03	2 (7%)
2	MA6	5	1493	2	18,26,27	1.06	2 (11%)	19,38,41	3.40	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G7M	5	525	2	-	2/3/25/26	0/3/3/3
2	MA6	5	1494	2	-	2/7/29/30	0/3/3/3
2	B8T	5	1377	2	-	2/7/27/28	0/2/2/2
2	5MC	5	1375	2	-	2/7/25/26	0/2/2/2
2	MA6	5	1493	2	-	0/7/29/30	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	525	G7M	C8-N7	10.07	1.51	1.33
2	5	1375	5MC	C6-C5	9.87	1.50	1.34
2	5	525	G7M	C8-N9	9.85	1.51	1.33
2	5	1375	5MC	C4-N3	7.42	1.46	1.34
2	5	1377	B8T	C4-N3	7.11	1.45	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1493	MA6	N1-C6-N6	-12.42	103.98	117.06
2	5	1494	MA6	N1-C6-N6	-12.35	104.06	117.06
2	5	1494	MA6	N3-C2-N1	-5.58	119.96	128.68
2	5	1494	MA6	C1'-N9-C4	5.50	136.30	126.64
2	5	1493	MA6	C1'-N9-C4	5.44	136.19	126.64

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5	525	G7M	O4'-C4'-C5'-O5'
2	5	525	G7M	C3'-C4'-C5'-O5'
2	5	1494	MA6	O4'-C4'-C5'-O5'
2	5	1377	B8T	O4'-C4'-C5'-O5'
2	5	1494	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	525	G7M	1	0
2	5	1493	MA6	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 105 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	SPD	5	1601	-	9,9,9	0.32	0	8,8,8	0.91	0
29	N2P	5	1603	-	6,6,6	0.24	0	5,5,5	0.64	0
28	PUT	5	1605	-	5,5,5	0.24	0	4,4,4	0.52	0
27	SPD	5	1604	-	9,9,9	0.32	0	8,8,8	0.88	0
28	PUT	5	1602	-	5,5,5	0.24	0	4,4,4	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SPD	5	1601	-	-	1/7/7/7	-
29	N2P	5	1603	-	-	0/4/4/4	-
28	PUT	5	1605	-	-	0/3/3/3	-
27	SPD	5	1604	-	-	0/7/7/7	-
28	PUT	5	1602	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	5	1601	SPD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	5	1601	SPD	1	0
27	5	1604	SPD	1	0

## 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.

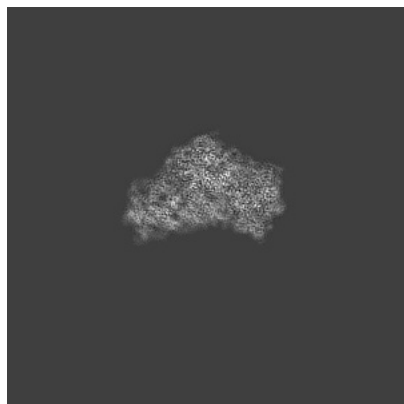
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17133. These allow visual inspection of the internal detail of the map and identification of artifacts.

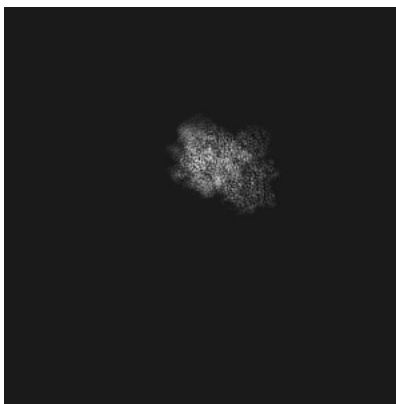
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

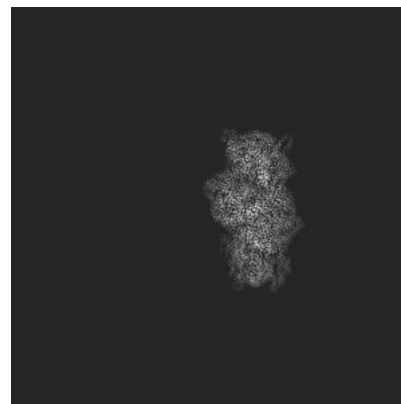
#### 6.1.1 Primary map



X

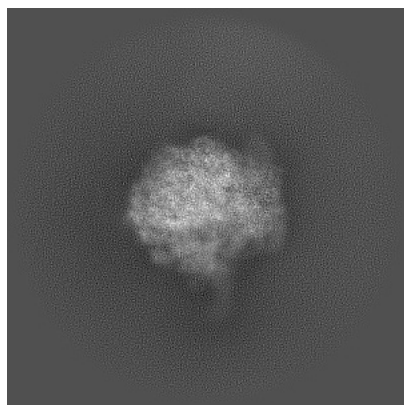


Y

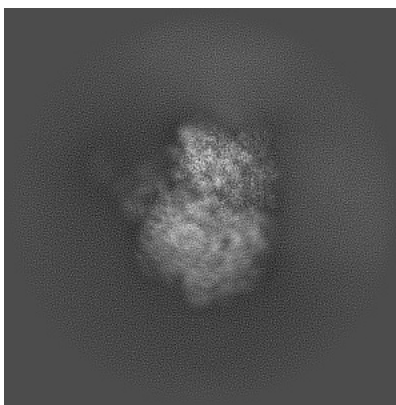


Z

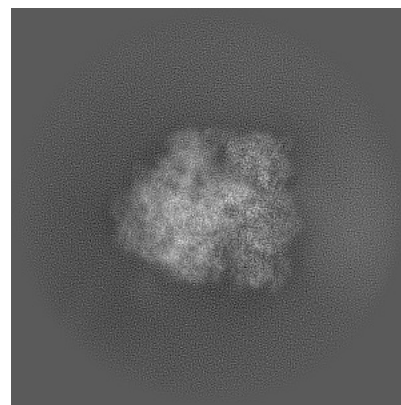
#### 6.1.2 Raw map



X



Y



Z

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

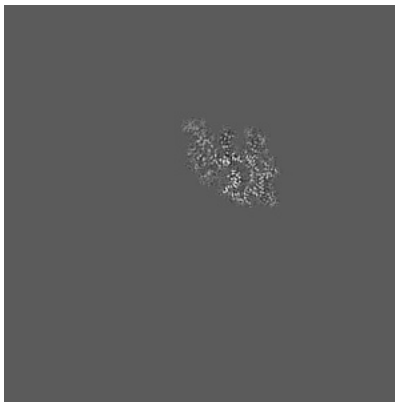


## 6.2 Central slices [i](#)

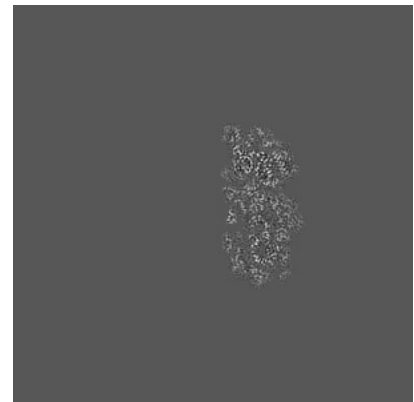
### 6.2.1 Primary map



X Index: 203

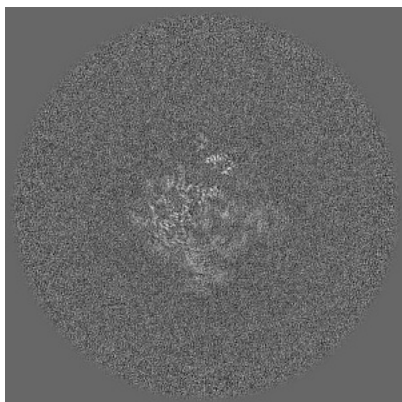


Y Index: 203

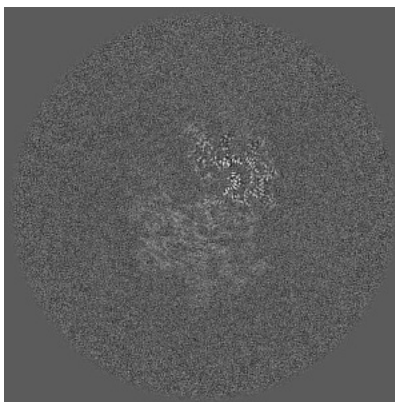


Z Index: 203

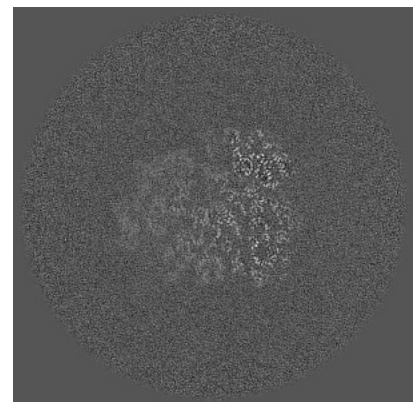
### 6.2.2 Raw map



X Index: 203



Y Index: 203

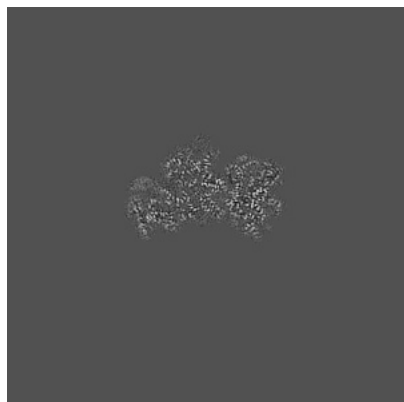


Z Index: 203

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

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

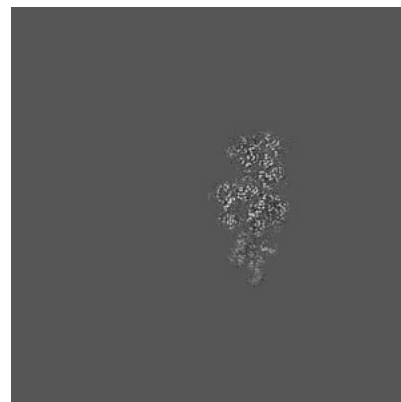
### 6.3.1 Primary map



X Index: 252

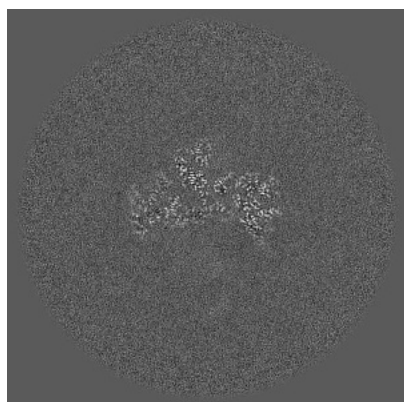


Y Index: 202

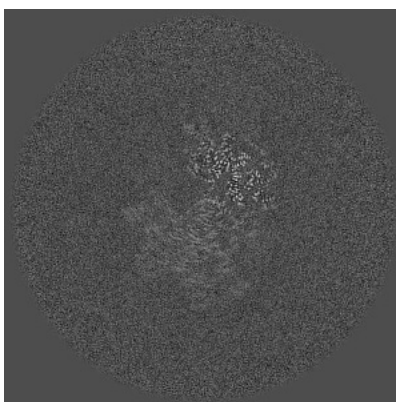


Z Index: 225

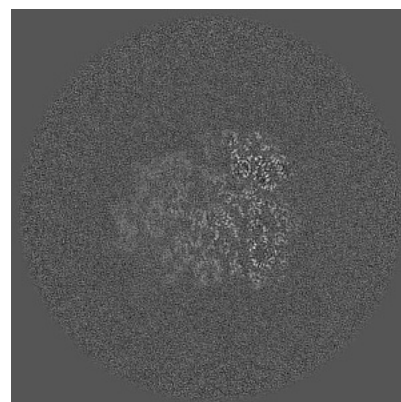
### 6.3.2 Raw map



X Index: 242



Y Index: 199

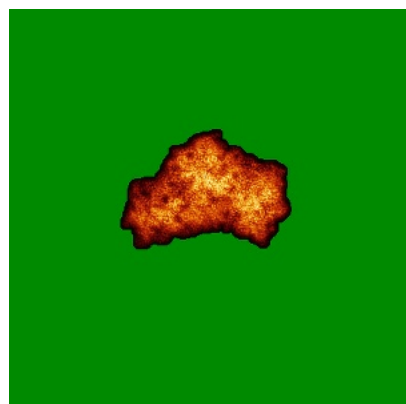


Z Index: 203

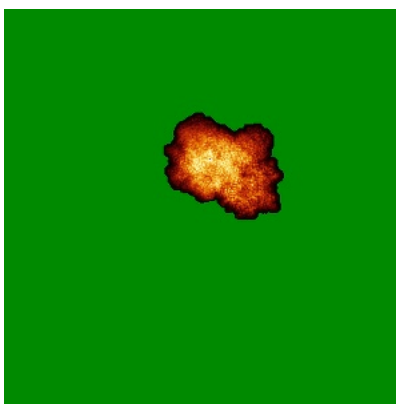
The images above show the largest variance slices of the map in three orthogonal directions.

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

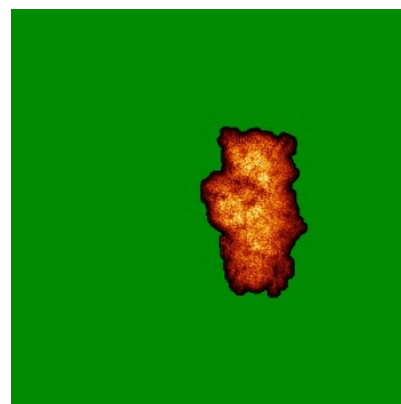
### 6.4.1 Primary map



X

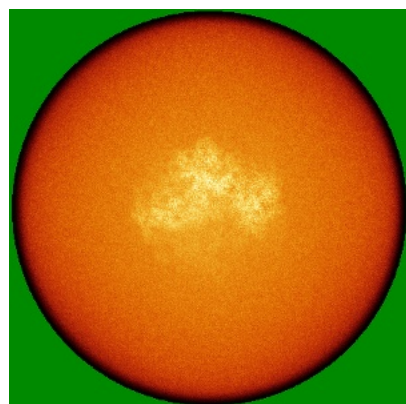


Y

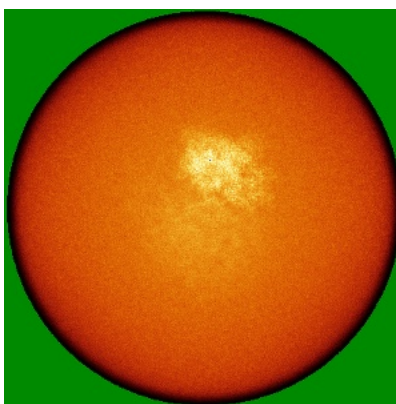


Z

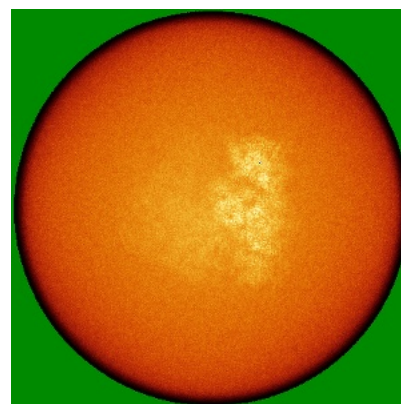
### 6.4.2 Raw map



X



Y

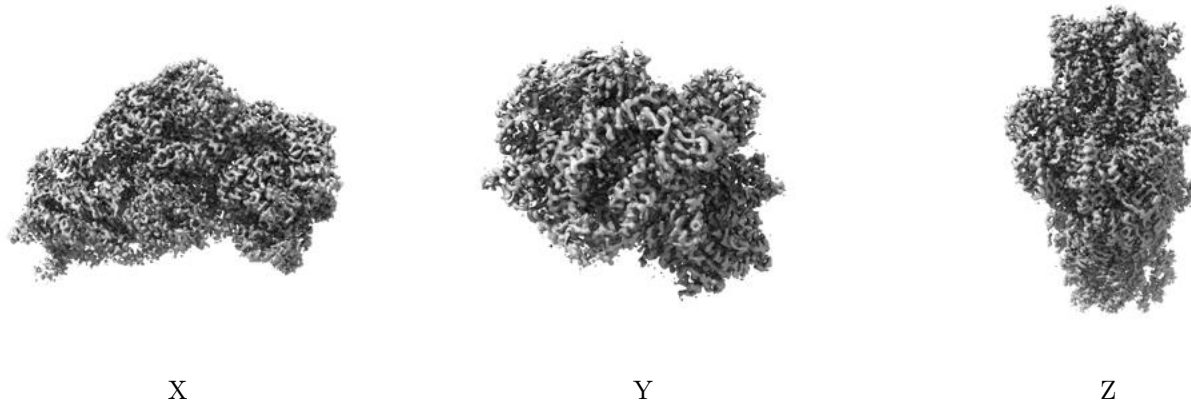


Z

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.

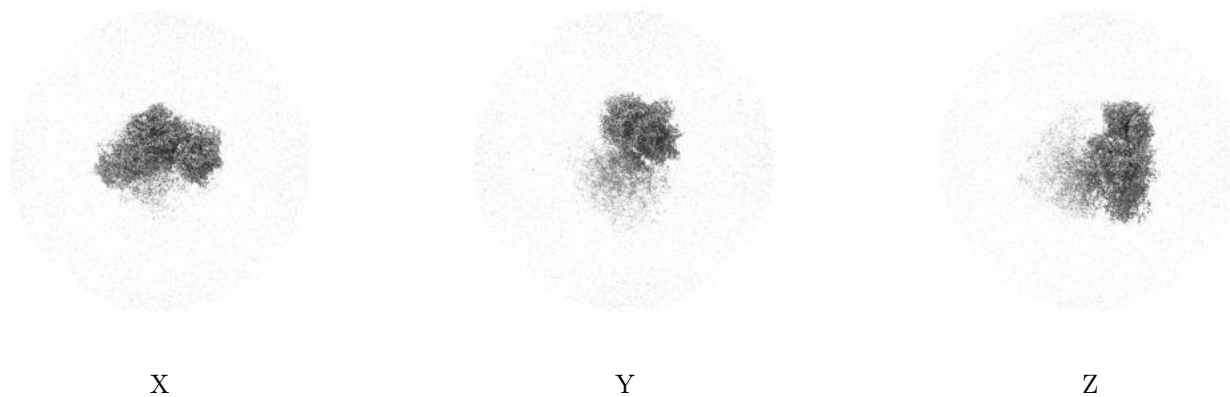
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0022. 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.

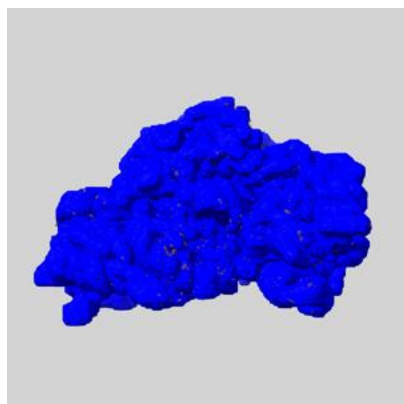
## 6.6 Mask visualisation [i](#)

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

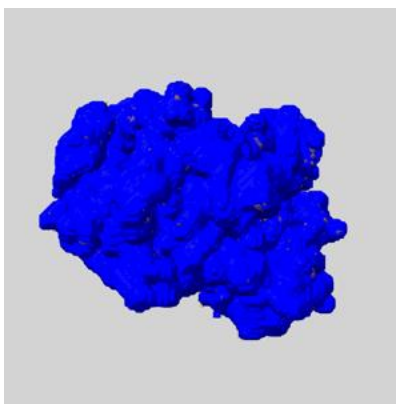
A mask typically either:

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

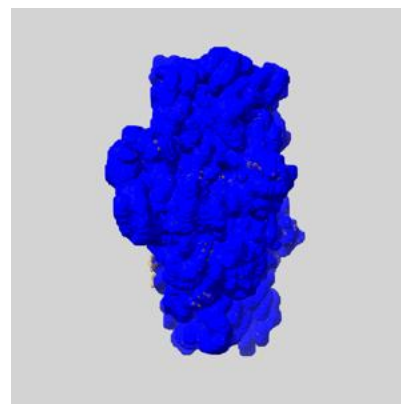
### 6.6.1 emd\_17133\_msk\_1.map [i](#)



X



Y

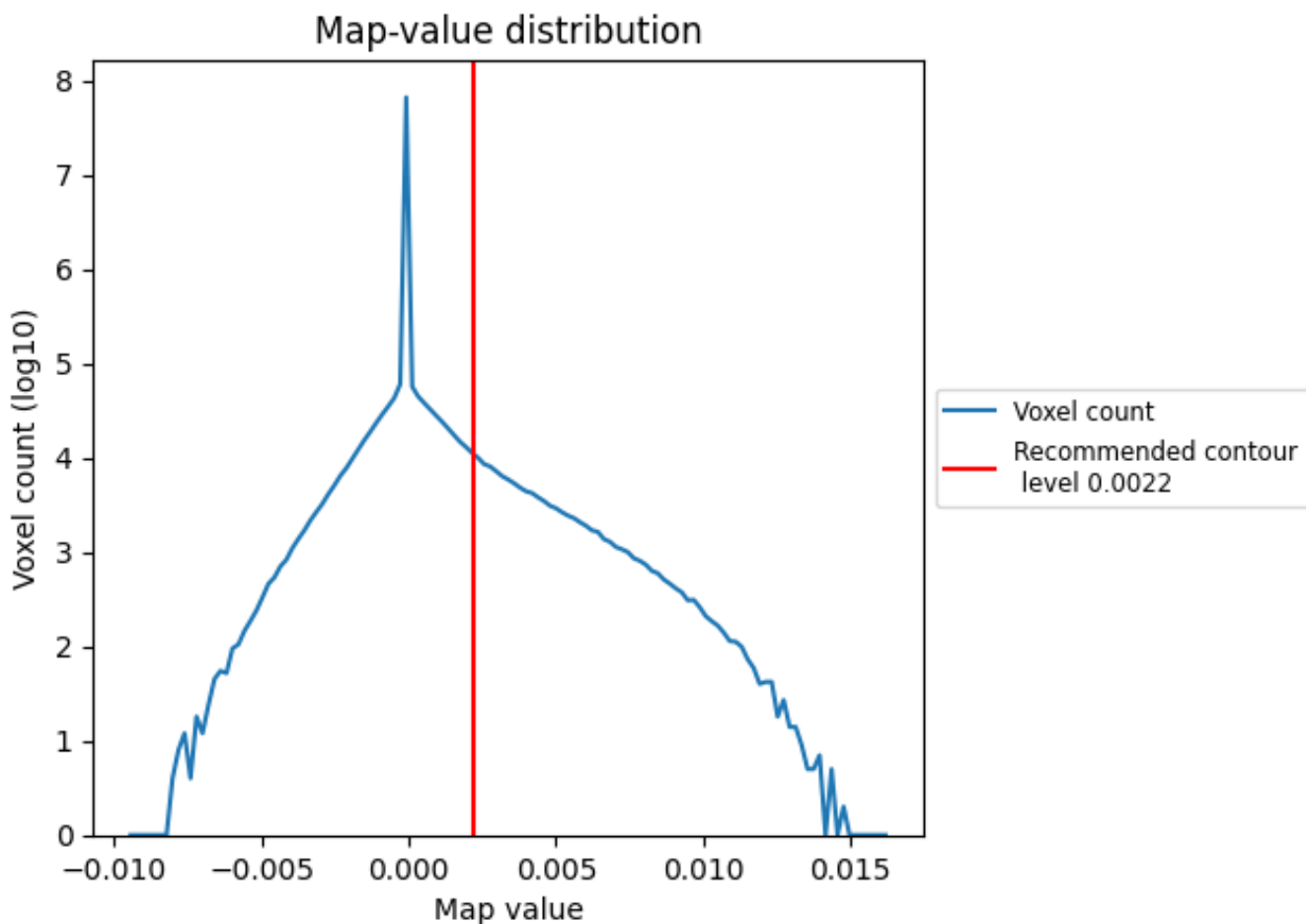


Z

## 7 Map analysis [i](#)

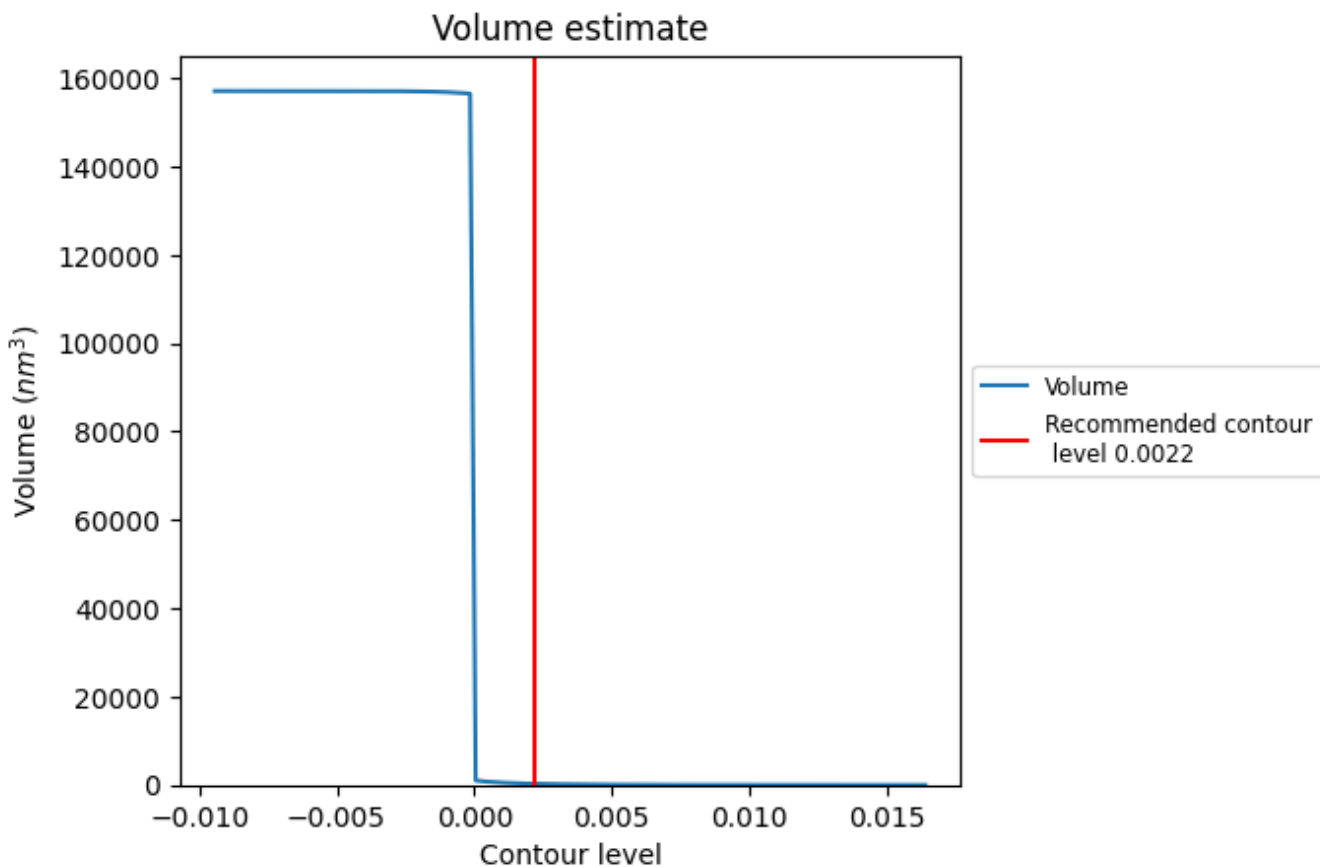
This section contains the results of statistical analysis of the map.

### 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.

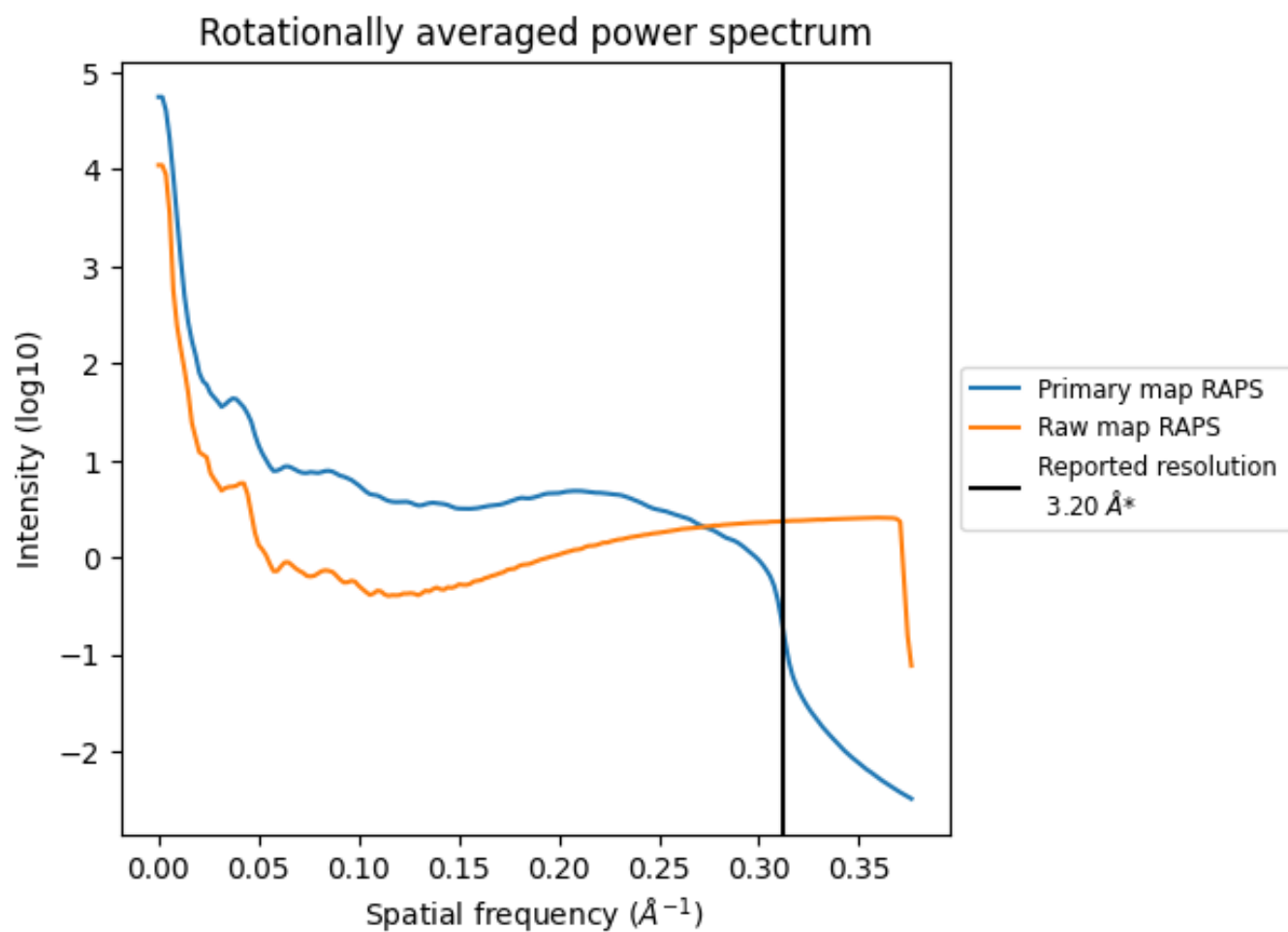
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 271 nm<sup>3</sup>; this corresponds to an approximate mass of 245 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



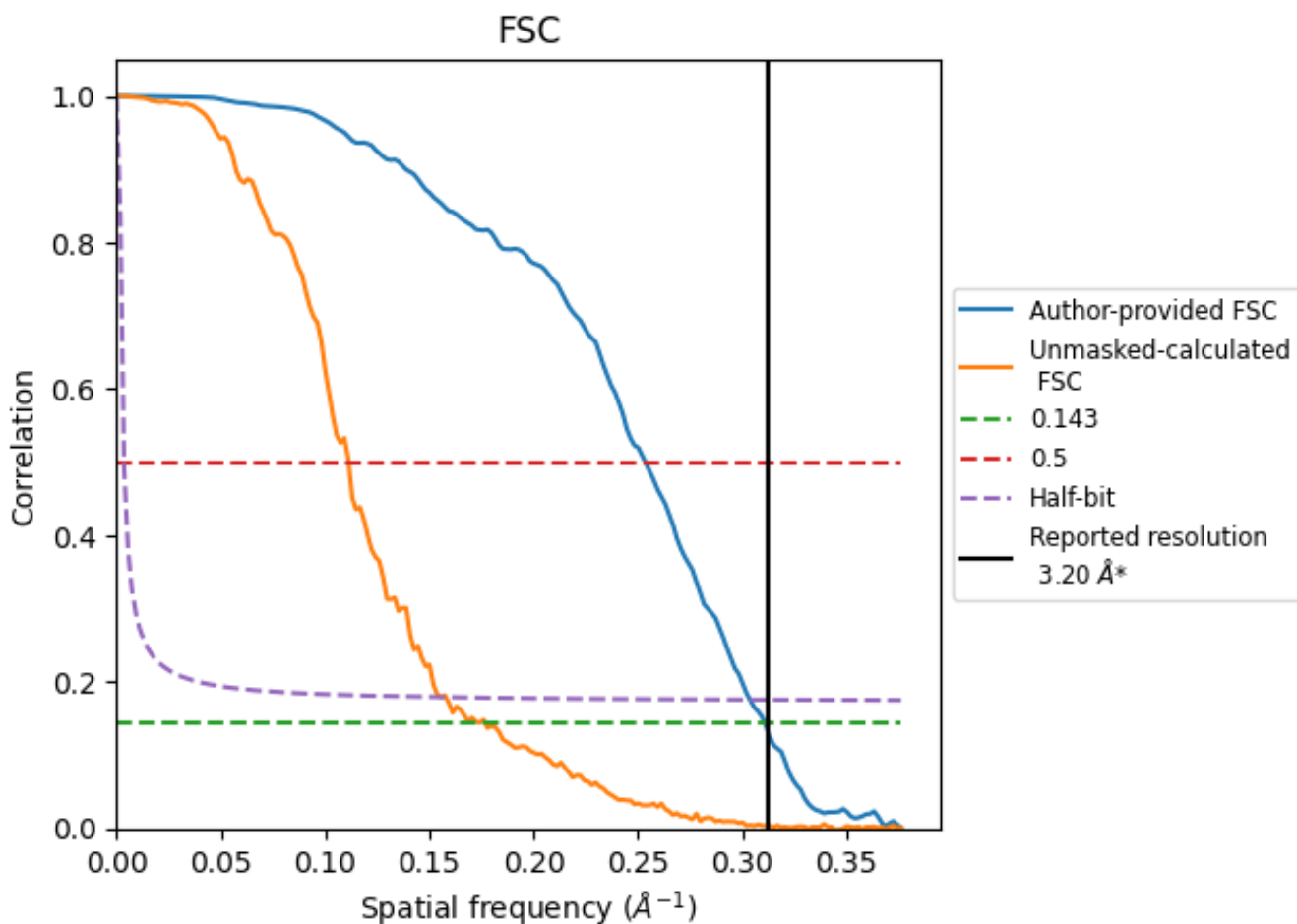
\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

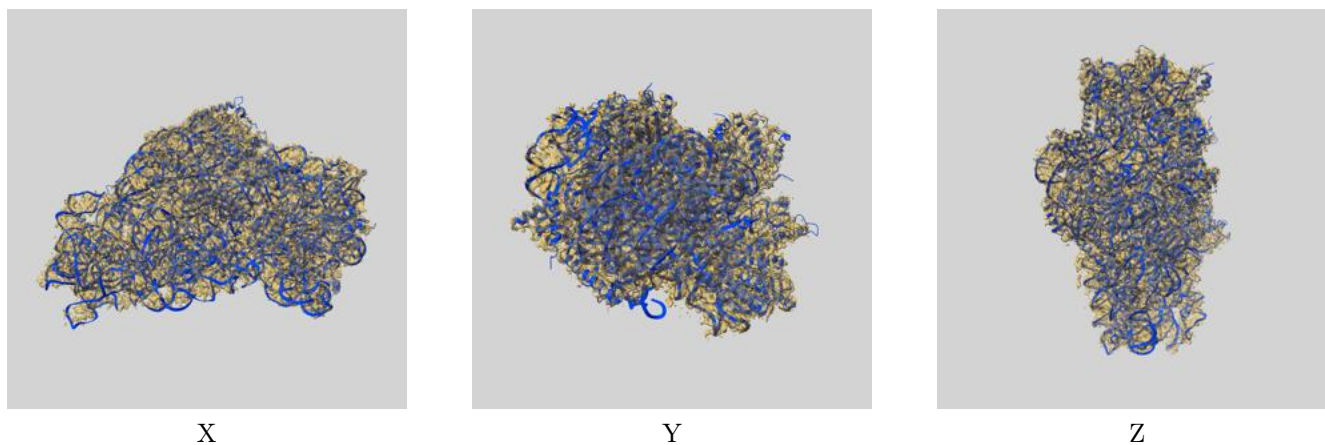
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.94	3.29
Unmasked-calculated*	5.66	8.98	6.33

\*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 5.66 differs from the reported value 3.2 by more than 10 %

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

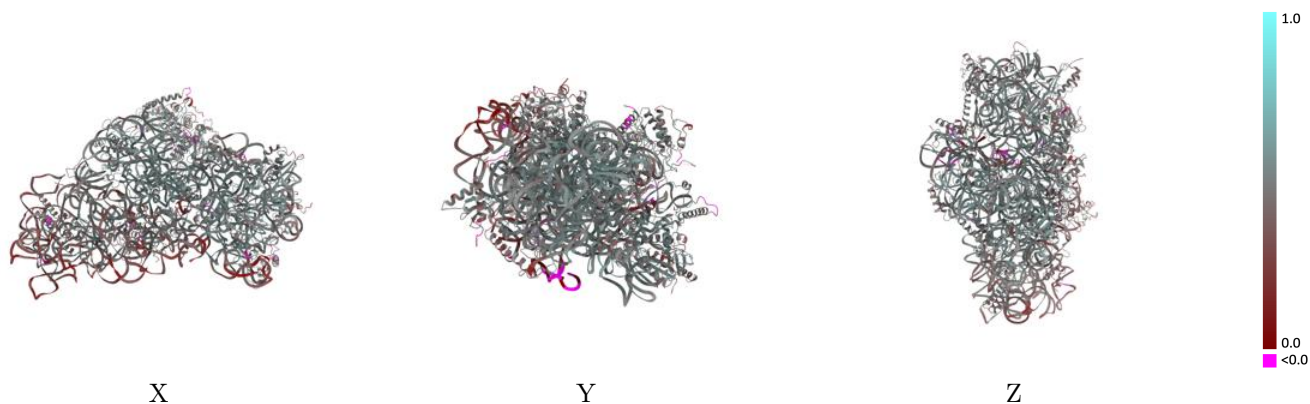
This section contains information regarding the fit between EMDB map EMD-17133 and PDB model 8P6P. Per-residue inclusion information can be found in section 3 on page 11.

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



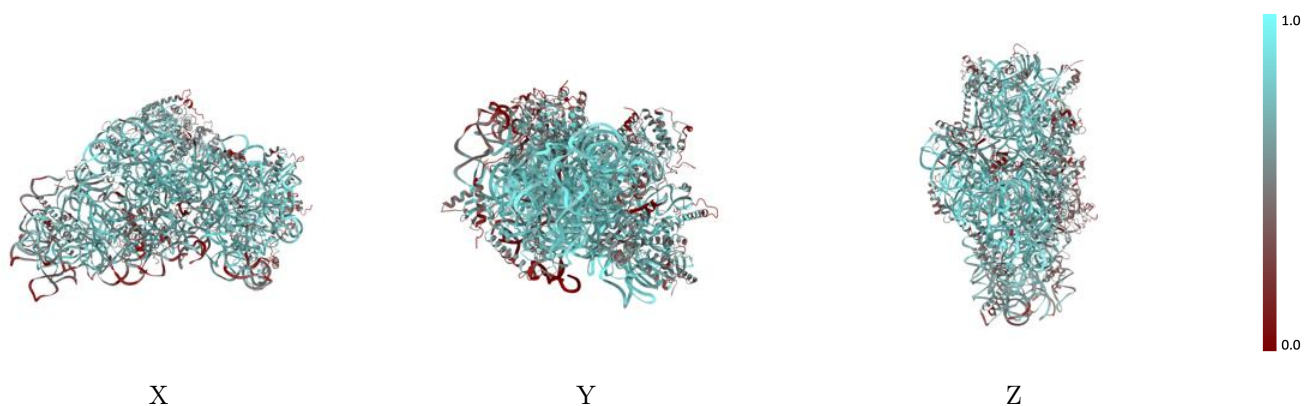
The images above show the 3D surface view of the map at the recommended contour level 0.0022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



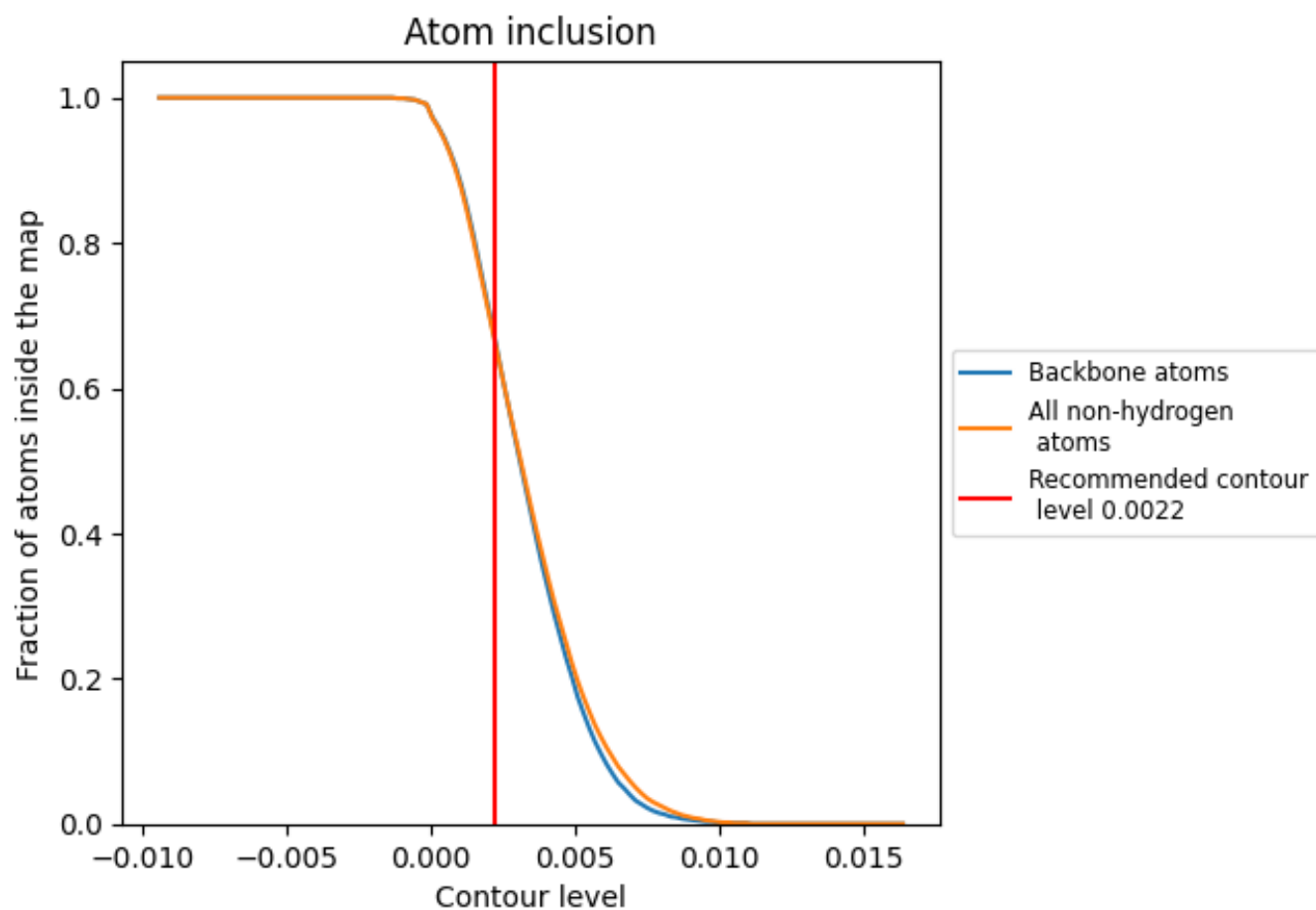
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0022).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 67% 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 (0.0022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.4630
3	 0.4300	 0.2790
5	 0.7580	 0.4690
7	 0.5410	 0.3330
8	 0.3390	 0.3170
A	 0.5220	 0.4550
B	 0.6360	 0.5010
C	 0.3500	 0.3660
D	 0.6850	 0.5220
E	 0.5090	 0.4450
F	 0.5180	 0.4640
G	 0.7040	 0.5260
H	 0.6300	 0.4890
I	 0.5980	 0.4840
J	 0.6320	 0.4950
K	 0.6140	 0.5100
L	 0.5580	 0.4570
M	 0.7850	 0.5460
N	 0.5990	 0.4890
O	 0.5540	 0.4410
P	 0.4820	 0.4580
Q	 0.6680	 0.4780
R	 0.6340	 0.5040
S	 0.5430	 0.4410
T	 0.4940	 0.4550
Y	 0.3980	 0.3460
x	 0.1900	 0.3060

