



## wwPDB EM Validation Summary Report ⓘ

Nov 4, 2023 – 12:16 PM EDT

PDB ID : 8EYT  
EMDB ID : EMD-28720  
Title : 30S\_delta\_ksgA+KsgA complex  
Authors : Sun, J.; Kinman, L.F.; Jahagirdar, D.; Ortega, J.; Davis, J.H.  
Deposited on : 2022-10-28  
Resolution : 2.80 Å(reported)

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:

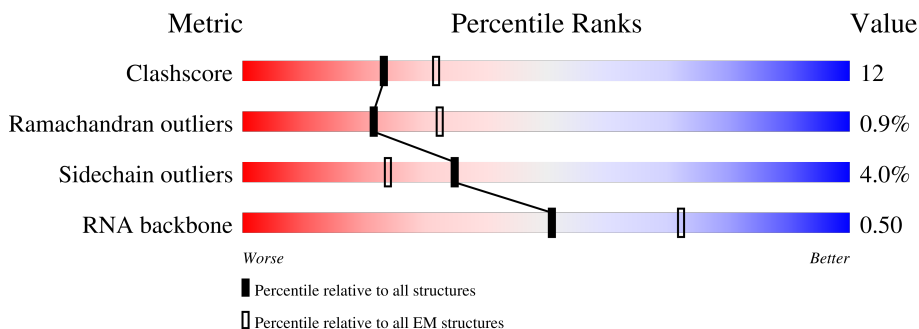
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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.



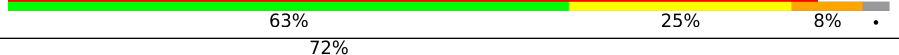

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	A	1415	
2	B	241	
3	D	206	
4	E	167	
5	H	130	
6	L	124	
7	P	82	

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Mol	Chain	Length	Quality of chain
8	Q	84	 77% 15% 5%
9	T	87	 89% 10%
10	F	233	 52% 70% 17% 12%
11	G	179	 83% 55% 28% 16%
12	I	130	 57% 65% 30%
13	J	103	 83% 55% 35% 6%
14	M	118	 91% 63% 25% 8%
15	N	101	 72% 73% 24%
16	S	92	 65% 52% 30% 5% 12%
17	O	135	 44% 54% 24% 21%
18	R	129	 33% 66% 21% 9%
19	U	89	 29% 80% 18%
20	V	75	 59% 59% 21% 19%
21	W	254	 40% 52% 42% 6%

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 50699 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1415	30367	13543	5577	9832	1415	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	A	deletion	GB 1776881223
A	?	-	G	deletion	GB 1776881223
A	?	-	A	deletion	GB 1776881223
A	?	-	U	deletion	GB 1776881223

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	205	1643	1026	315	298	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	155	1144	711	216	211	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	129	979	616	173	184	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	123	957	591	196	165	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P	82	649	406	128	114	1	0	0

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Q	80	648	411	121	113	3	0	0

- Molecule 9 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	T	86	670	414	138	115	3	0	0

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	206	1624	1028	305	288	3	0	0

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	151	1181	735	227	215	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 14 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 15 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 16 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	81	Total	C	N	O	S	0	0
			651	416	124	109	2		

- Molecule 17 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	88	714	439	144	130	1	0	0

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	V	61	496	312	93	91	0	0

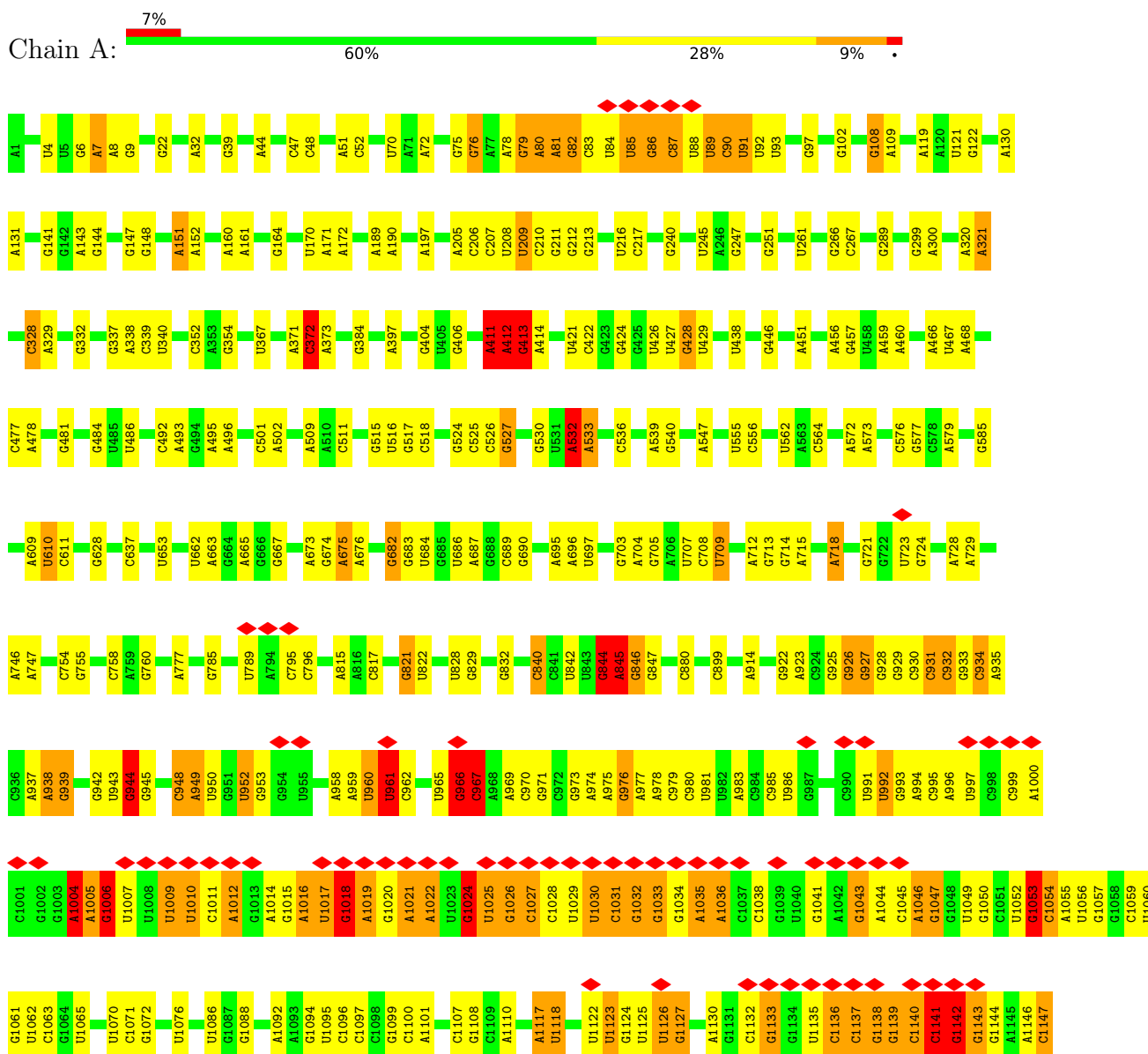
- Molecule 21 is a protein called Ribosomal RNA small subunit methyltransferase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	254	1979	1263	340	363	13	0	0

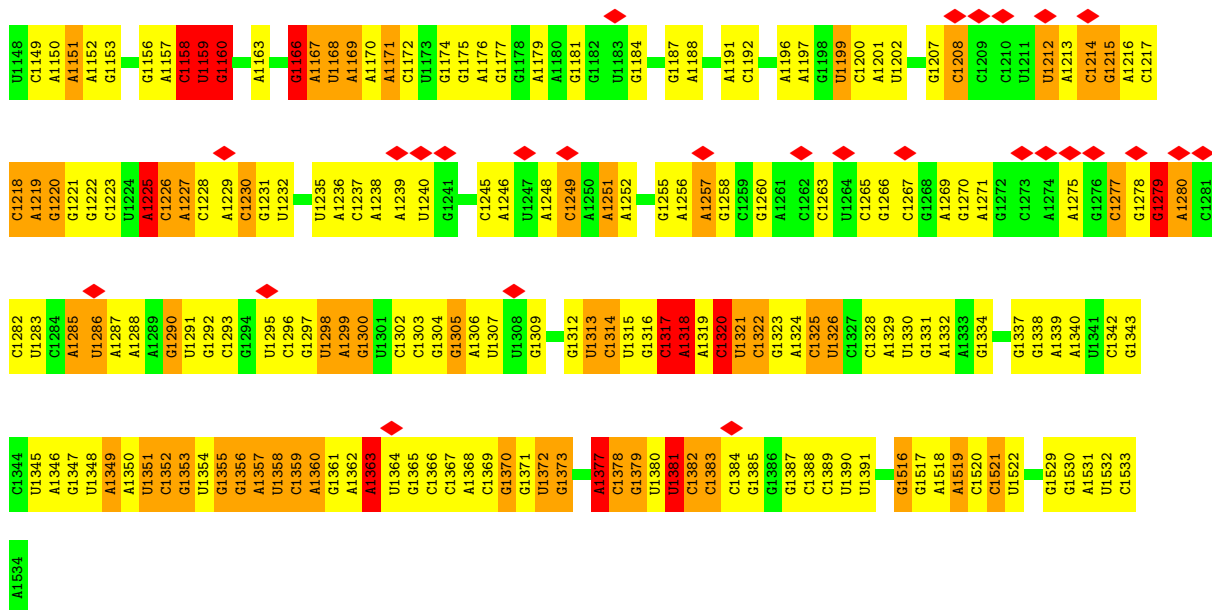
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

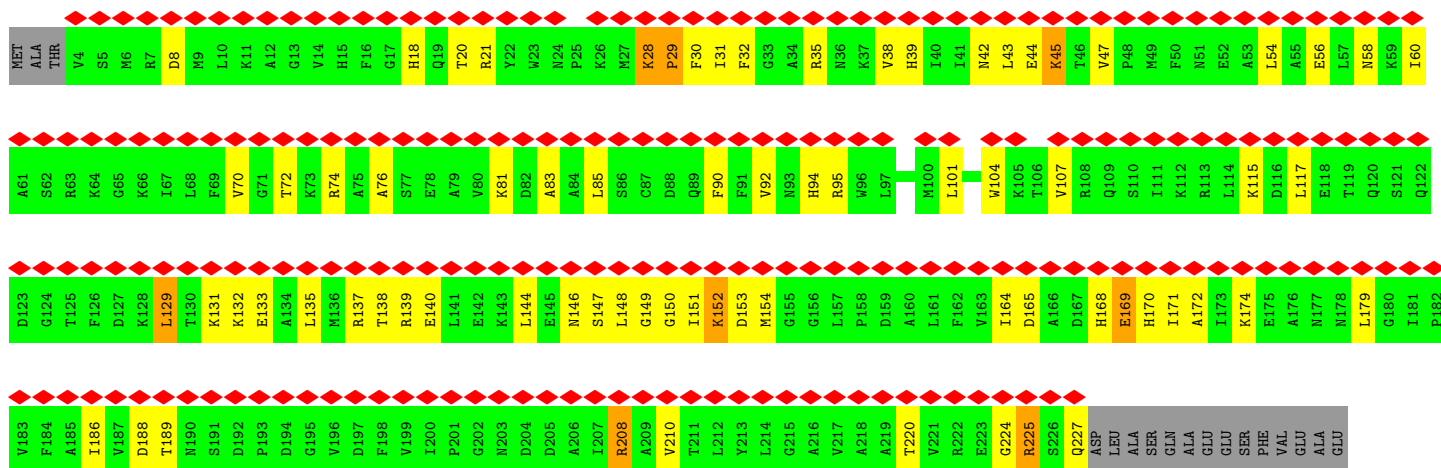
- Molecule 1: 16S rRNA



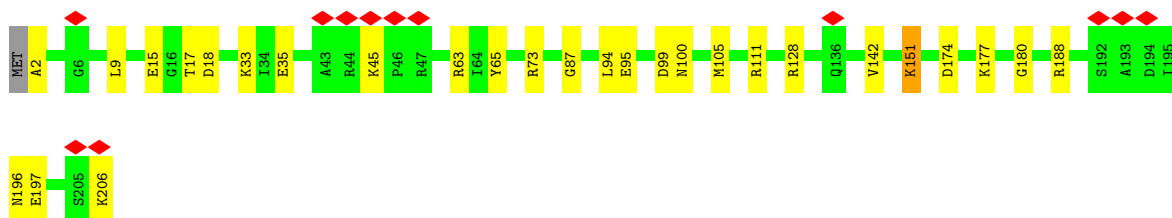
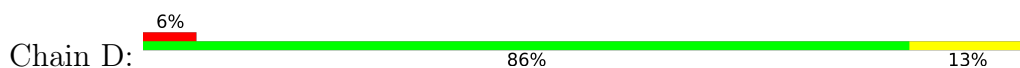




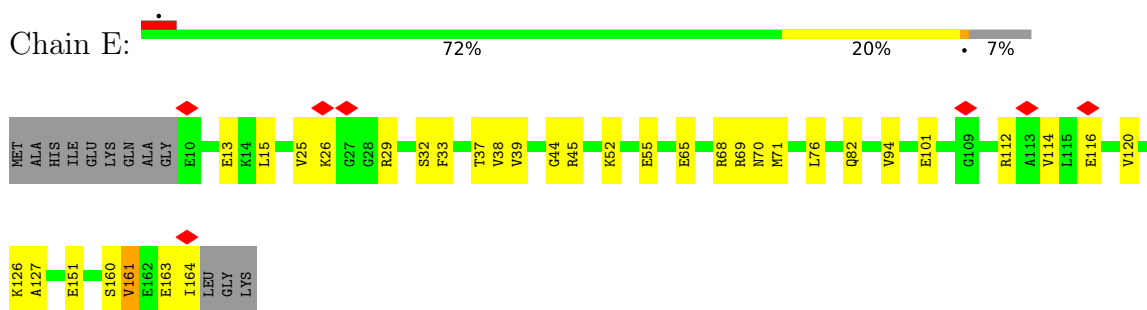
• Molecule 2: 30S ribosomal protein S2



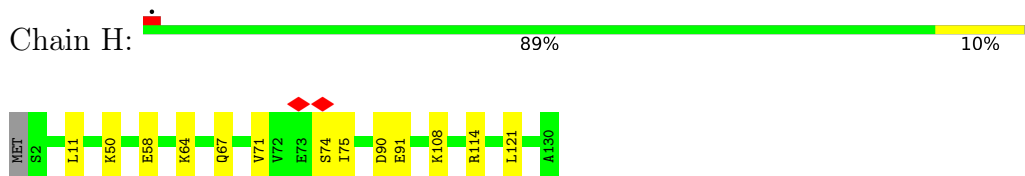
• Molecule 3: 30S ribosomal protein S4



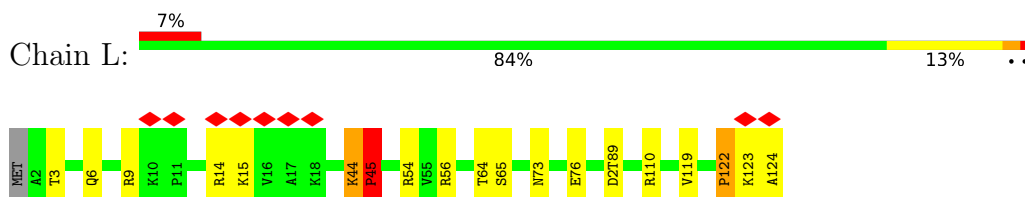
• Molecule 4: 30S ribosomal protein S5



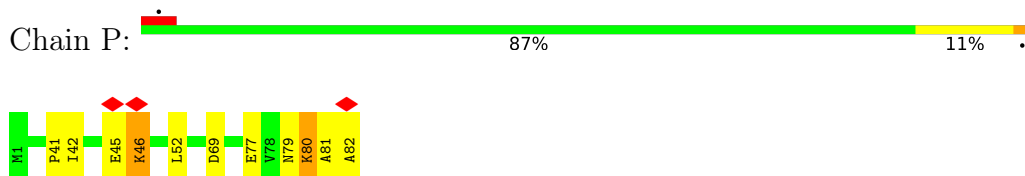
• Molecule 5: 30S ribosomal protein S8



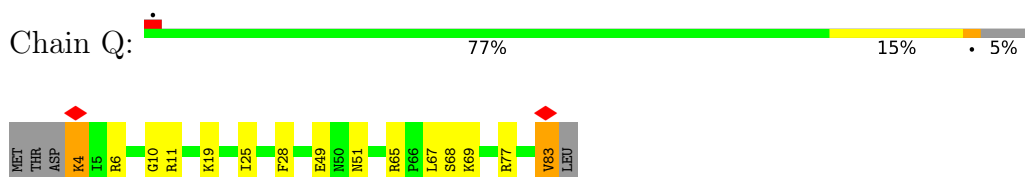
• Molecule 6: 30S ribosomal protein S12



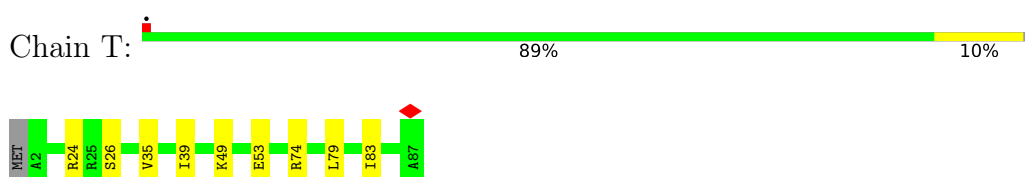
• Molecule 7: 30S ribosomal protein S16



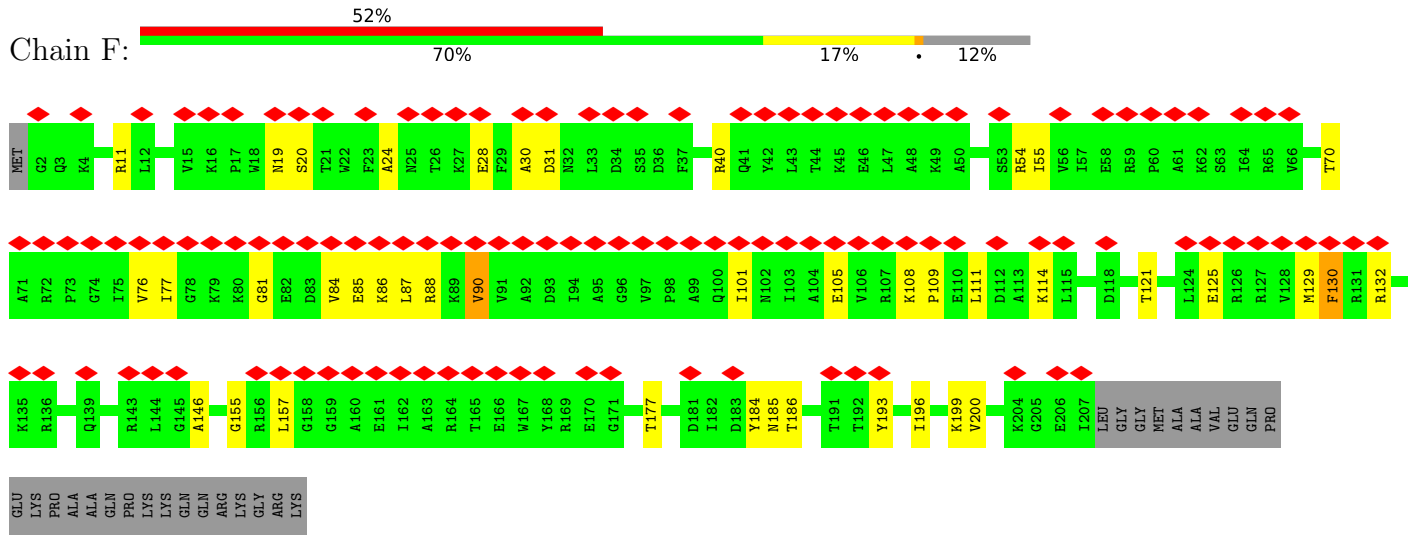
• Molecule 8: 30S ribosomal protein S17



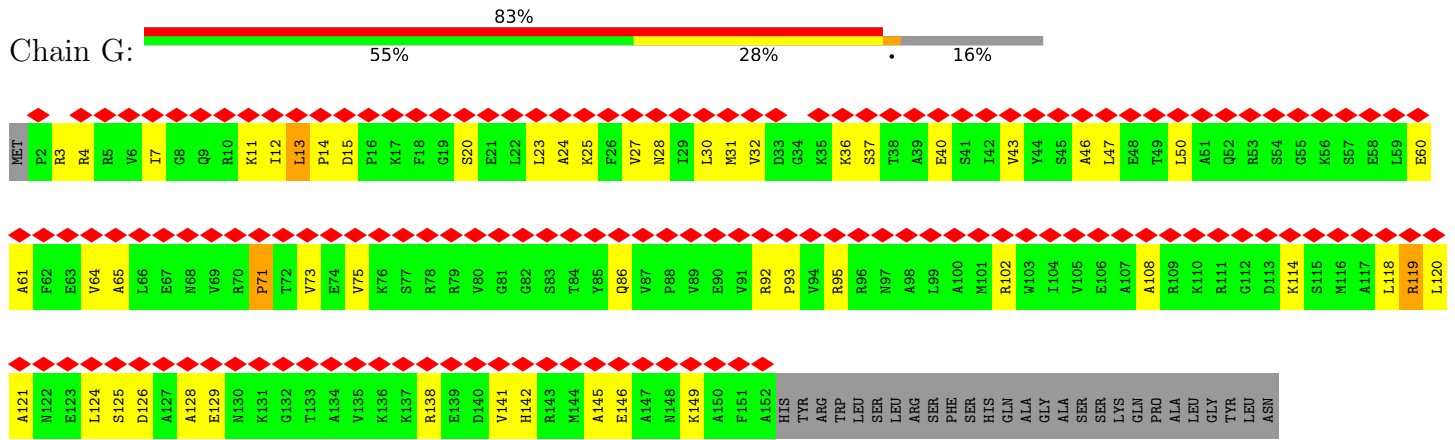
• Molecule 9: 30S ribosomal protein S20



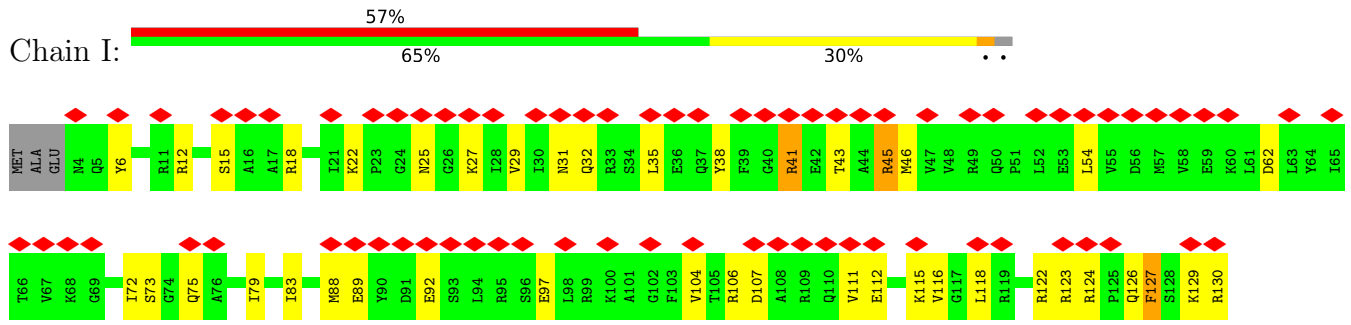
• Molecule 10: 30S ribosomal protein S3



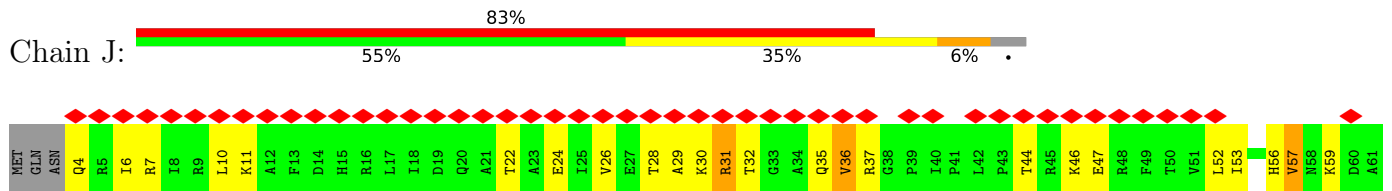
• Molecule 11: 30S ribosomal protein S7

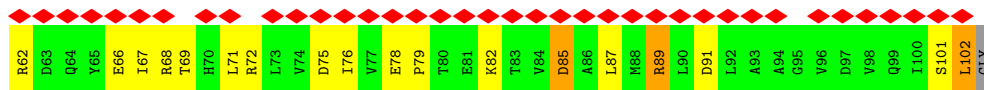


• Molecule 12: 30S ribosomal protein S9

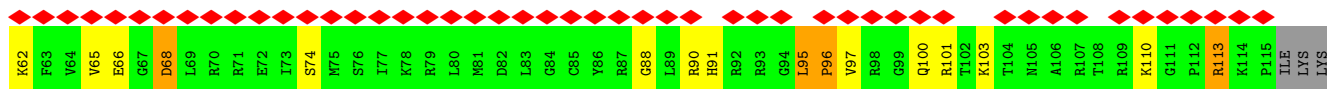
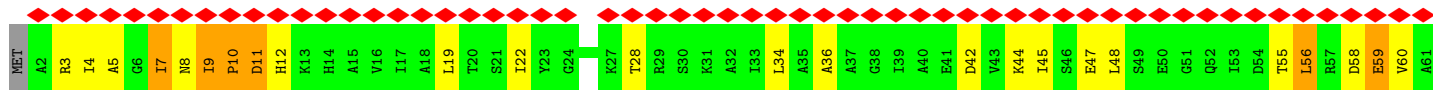


• Molecule 13: 30S ribosomal protein S10

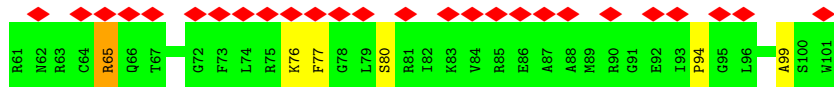
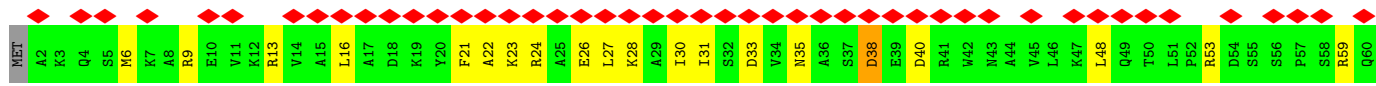
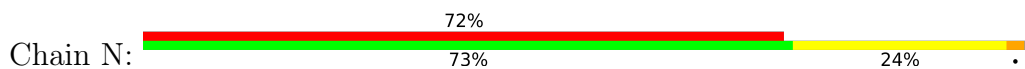




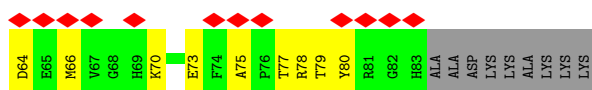
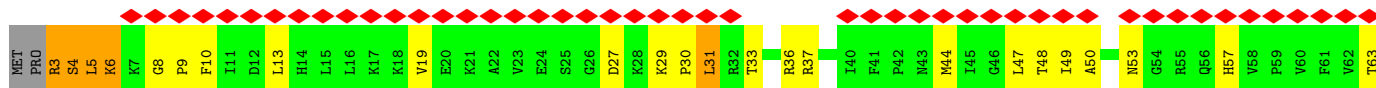
• Molecule 14: 30S ribosomal protein S13



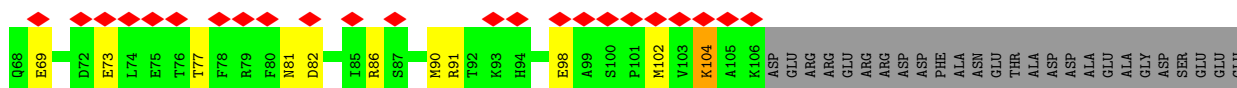
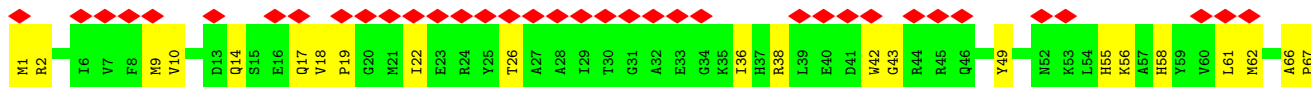
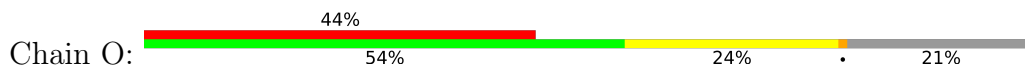
• Molecule 15: 30S ribosomal protein S14



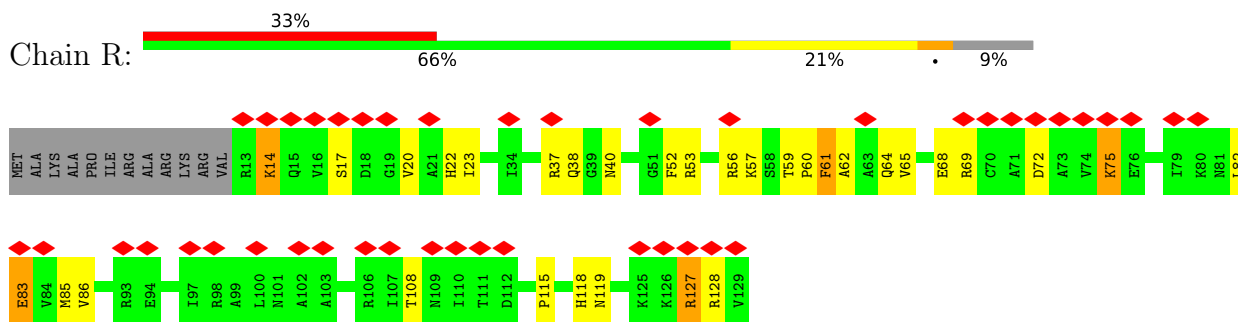
• Molecule 16: 30S ribosomal protein S19



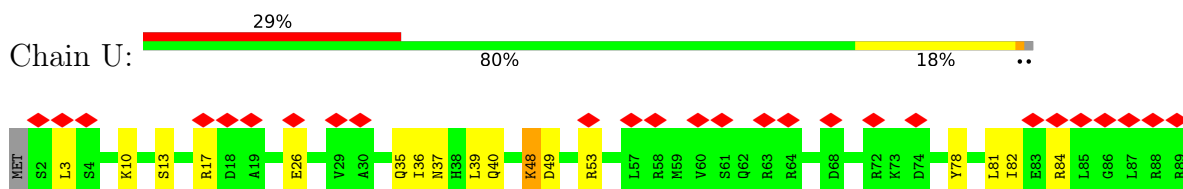
• Molecule 17: 30S ribosomal protein S6



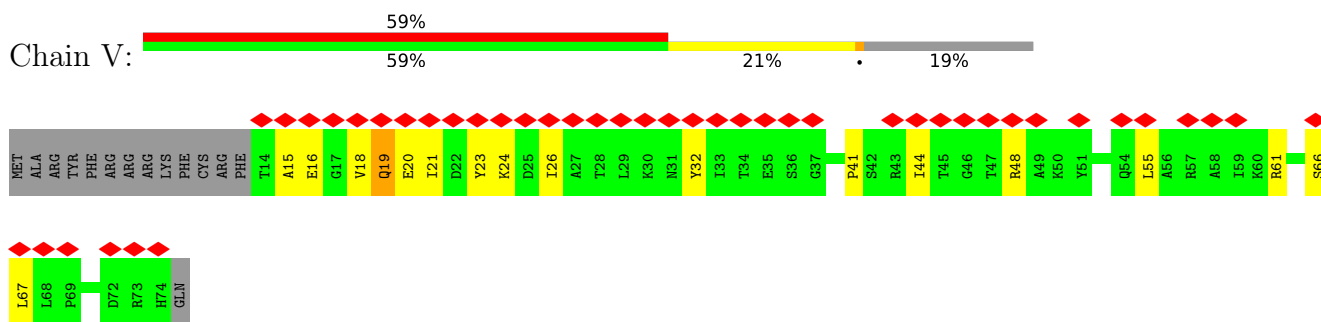
• Molecule 18: 30S ribosomal protein S11



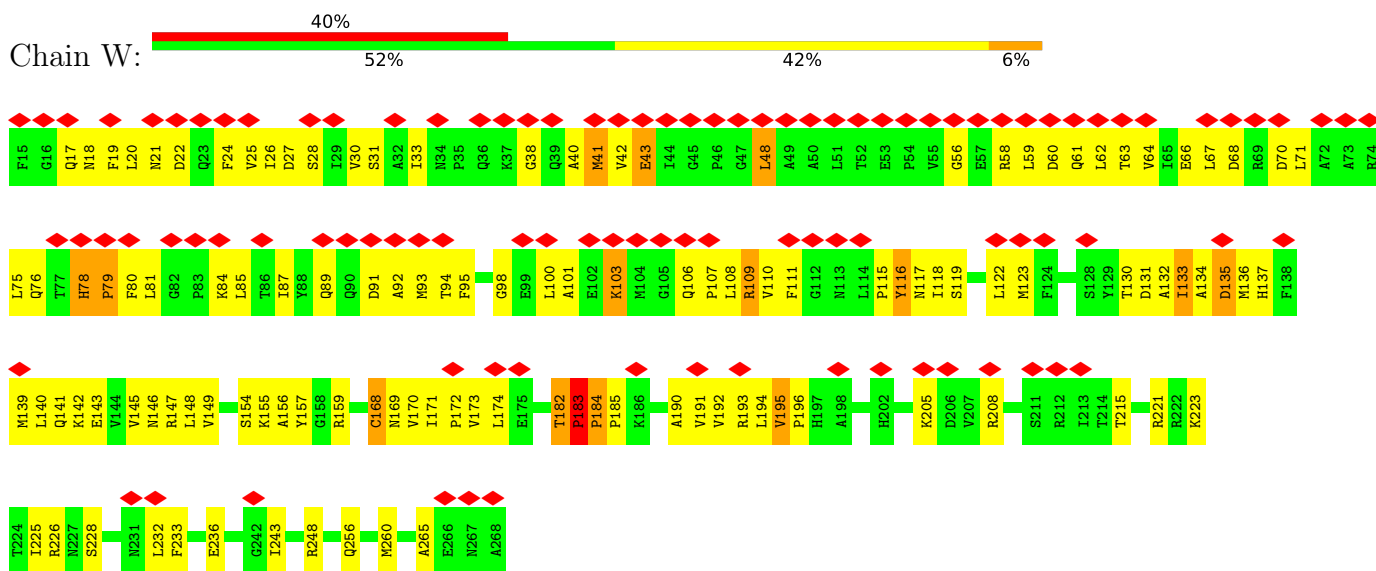
• Molecule 19: 30S ribosomal protein S15



• Molecule 20: 30S ribosomal protein S18



• Molecule 21: Ribosomal RNA small subunit methyltransferase A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	231280	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 ( $e^-/\text{\AA}^2$ )	72	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	326.61002, 326.61002, 326.61002	wwPDB
Map dimensions	382, 382, 382	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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: D2T

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	A	1.20	92/34002 (0.3%)	1.04	132/53040 (0.2%)
2	B	0.47	2/1784 (0.1%)	0.63	1/2403 (0.0%)
3	D	0.51	0/1665	0.61	0/2227
4	E	0.55	1/1157 (0.1%)	0.66	0/1557
5	H	0.55	0/989	0.63	0/1326
6	L	0.56	0/960	0.90	2/1286 (0.2%)
7	P	0.64	0/659	0.66	0/884
8	Q	0.55	0/657	0.67	0/881
9	T	0.43	0/676	0.58	0/895
10	F	0.44	0/1651	0.68	1/2225 (0.0%)
11	G	0.41	0/1195	0.80	0/1602
12	I	1.23	2/1034 (0.2%)	1.08	1/1375 (0.1%)
13	J	0.56	0/805	0.83	0/1089
14	M	5.61	1/892 (0.1%)	2.26	6/1193 (0.5%)
15	N	1.36	0/817	1.12	3/1088 (0.3%)
16	S	0.89	0/667	1.02	7/897 (0.8%)
17	O	0.37	0/881	0.64	0/1189
18	R	0.33	0/893	0.67	1/1205 (0.1%)
19	U	0.40	0/722	0.67	0/964
20	V	0.54	0/503	0.69	0/677
21	W	2.90	4/2023 (0.2%)	1.34	5/2751 (0.2%)
All	All	1.36	102/54632 (0.2%)	1.01	159/80754 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	I	0	1
15	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	10	PRO	N-CD	164.79	3.78	1.47
21	W	183	PRO	N-CD	128.11	3.27	1.47
1	A	949	A	O3'-P	-22.83	1.33	1.61
1	A	1320	C	O3'-P	-14.68	1.43	1.61
1	A	1214	C	O3'-P	14.02	1.77	1.61

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	10	PRO	N-CD-CG	-61.68	10.69	103.20
21	W	183	PRO	N-CD-CG	-51.38	26.13	103.20
14	M	10	PRO	CA-N-CD	-28.12	72.12	111.50
21	W	183	PRO	CA-N-CD	-19.61	84.05	111.50
6	L	44	LYS	C-N-CD	-19.44	77.83	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	I	31	ASN	Mainchain
15	N	80	SER	Mainchain

## 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	A	30367	0	15283	409	0
2	B	1753	0	1780	87	0
3	D	1643	0	1707	21	0
4	E	1144	0	1185	19	0
5	H	979	0	1031	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	957	0	1017	13	0
7	P	649	0	666	16	0
8	Q	648	0	691	10	0
9	T	670	0	719	4	0
10	F	1624	0	1696	35	0
11	G	1181	0	1238	80	0
12	I	1022	0	1070	35	0
13	J	795	0	836	46	0
14	M	883	0	941	57	0
15	N	805	0	844	23	0
16	S	651	0	675	33	0
17	O	862	0	864	43	0
18	R	877	0	887	41	0
19	U	714	0	734	13	0
20	V	496	0	516	30	0
21	W	1979	0	1989	147	0
All	All	50699	0	36369	1057	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 12.

The worst 5 of 1057 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:A:79:G:N2	1:A:91:U:C2	1.67	1.58
2:B:29:PRO:N	2:B:29:PRO:CA	1.69	1.47
2:B:72:THR:OG1	2:B:168:HIS:CE1	1.69	1.46
14:M:4:ILE:CD1	14:M:10:PRO:HD3	1.52	1.36
14:M:3:ARG:NH1	14:M:9:ILE:HD11	1.43	1.34

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	B	222/241 (92%)	202 (91%)	17 (8%)	3 (1%)	11	34
3	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
4	E	153/167 (92%)	147 (96%)	4 (3%)	2 (1%)	12	36
5	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
6	L	120/124 (97%)	114 (95%)	3 (2%)	3 (2%)	5	19
7	P	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
8	Q	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
9	T	84/87 (97%)	84 (100%)	0	0	100	100
10	F	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
11	G	149/179 (83%)	131 (88%)	14 (9%)	4 (3%)	5	17
12	I	125/130 (96%)	117 (94%)	7 (6%)	1 (1%)	19	49
13	J	97/103 (94%)	95 (98%)	1 (1%)	1 (1%)	15	44
14	M	112/118 (95%)	98 (88%)	11 (10%)	3 (3%)	5	17
15	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
16	S	79/92 (86%)	74 (94%)	5 (6%)	0	100	100
17	O	104/135 (77%)	97 (93%)	7 (7%)	0	100	100
18	R	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
19	U	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
20	V	59/75 (79%)	55 (93%)	3 (5%)	1 (2%)	9	29
21	W	252/254 (99%)	227 (90%)	19 (8%)	6 (2%)	6	20
All	All	2547/2759 (92%)	2392 (94%)	131 (5%)	24 (1%)	21	46

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	170	HIS
6	L	45	PRO
20	V	19	GLN
21	W	183	PRO
6	L	123	LYS

### 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	B	186/199 (94%)	177 (95%)	9 (5%)	25	58
3	D	172/173 (99%)	169 (98%)	3 (2%)	60	87
4	E	118/126 (94%)	115 (98%)	3 (2%)	47	80
5	H	104/105 (99%)	99 (95%)	5 (5%)	25	58
6	L	102/103 (99%)	99 (97%)	3 (3%)	42	76
7	P	65/65 (100%)	62 (95%)	3 (5%)	27	60
8	Q	74/78 (95%)	68 (92%)	6 (8%)	11	33
9	T	65/66 (98%)	63 (97%)	2 (3%)	40	74
10	F	170/190 (90%)	167 (98%)	3 (2%)	59	86
11	G	124/147 (84%)	124 (100%)	0	100	100
12	I	105/107 (98%)	97 (92%)	8 (8%)	13	36
13	J	87/90 (97%)	81 (93%)	6 (7%)	15	41
14	M	92/96 (96%)	85 (92%)	7 (8%)	13	36
15	N	83/84 (99%)	78 (94%)	5 (6%)	19	48
16	S	71/79 (90%)	67 (94%)	4 (6%)	21	51
17	O	92/116 (79%)	91 (99%)	1 (1%)	73	92
18	R	90/99 (91%)	85 (94%)	5 (6%)	21	51
19	U	76/77 (99%)	72 (95%)	4 (5%)	22	54
20	V	52/65 (80%)	52 (100%)	0	100	100
21	W	217/217 (100%)	209 (96%)	8 (4%)	34	68
All	All	2145/2282 (94%)	2060 (96%)	85 (4%)	35	65

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	M	113	ARG
18	R	82	LEU
15	N	38	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	S	6	LYS
19	U	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
21	W	137	HIS
21	W	18	ASN
19	U	35	GLN
17	O	58	HIS
19	U	40	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1412/1415 (99%)	291 (20%)	43 (3%)

5 of 291 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	A
1	A	9	G
1	A	22	G
1	A	32	A

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1214	C
1	A	1325	C
1	A	1225	A
1	A	1257	A
1	A	1363	A

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

1 non-standard protein/DNA/RNA residue is 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
6	D2T	L	89	6	7,9,10	1.29	0	6,11,13	1.42	1 (16%)

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
6	D2T	L	89	6	-	3/7/12/14	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	89	D2T	CB-CA-N	2.05	113.47	109.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	89	D2T	CG-CB-SB-CB1
6	L	89	D2T	SB-CB-CG-OD1
6	L	89	D2T	SB-CB-CG-OD2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1391:U	O3'	1507:A	P	18.51
1	A	789:U	O3'	794:A	P	6.85
1	A	1214:C	O3'	1215:G	P	1.78
1	A	949:A	O3'	950:U	P	1.33

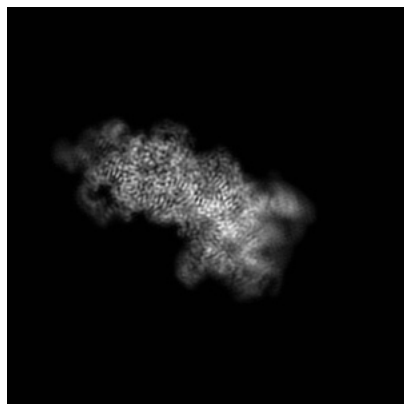
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28720. These allow visual inspection of the internal detail of the map and identification of artifacts.

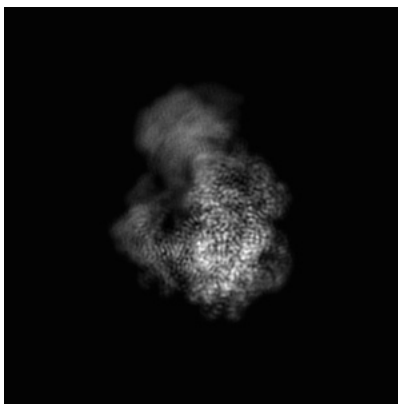
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

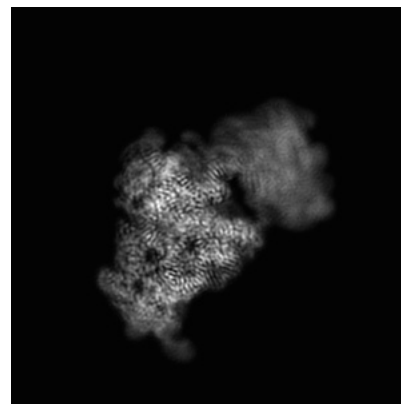
#### 6.1.1 Primary map



X

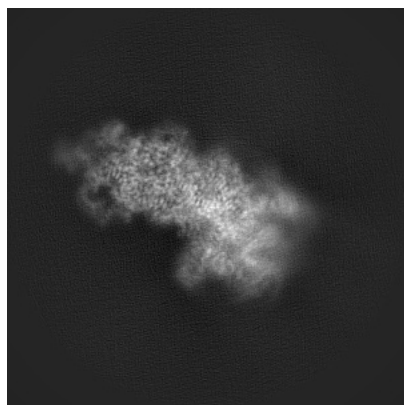


Y

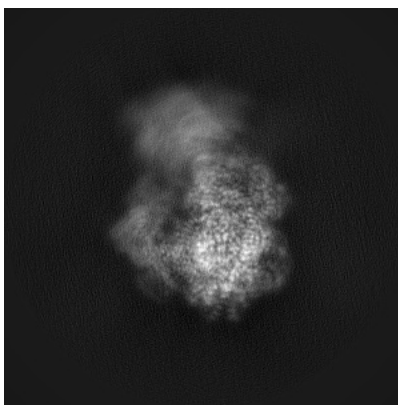


Z

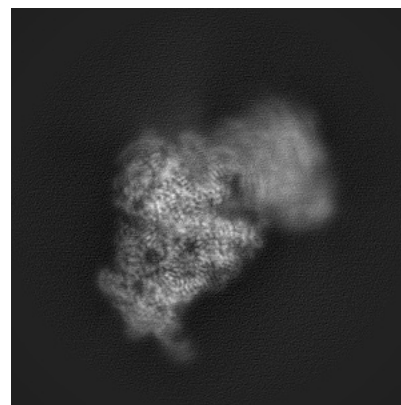
#### 6.1.2 Raw map



X



Y

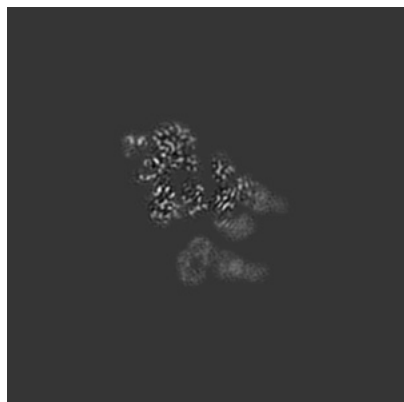


Z

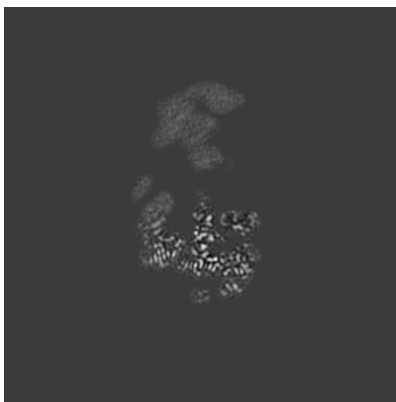
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

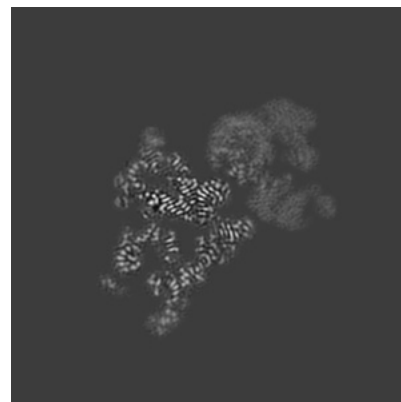
### 6.2.1 Primary map



X Index: 191

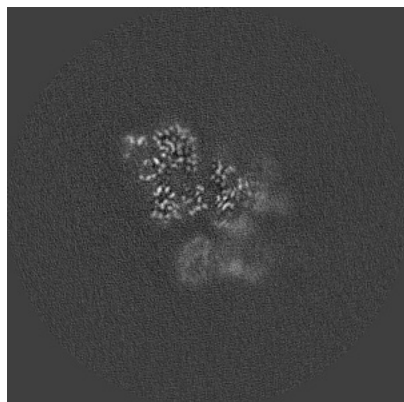


Y Index: 191

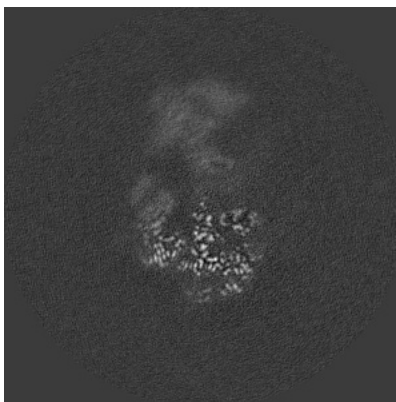


Z Index: 191

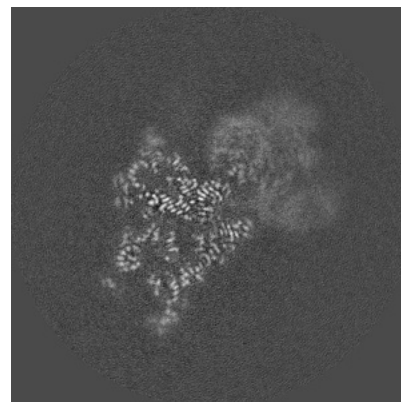
### 6.2.2 Raw map



X Index: 191



Y Index: 191



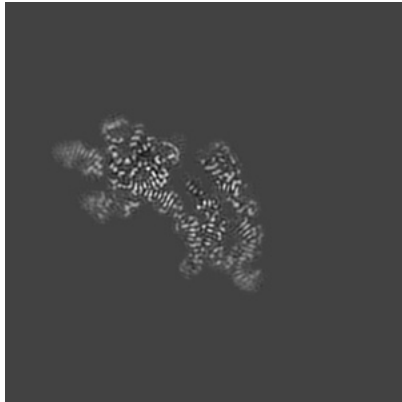
Z Index: 191

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

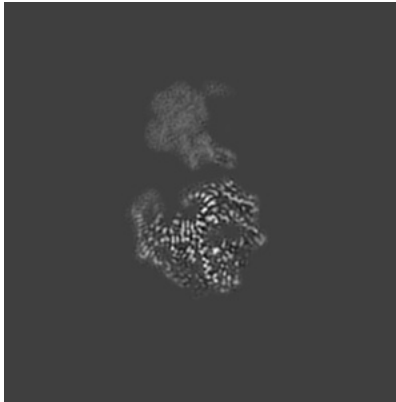


## 6.3 Largest variance slices [i](#)

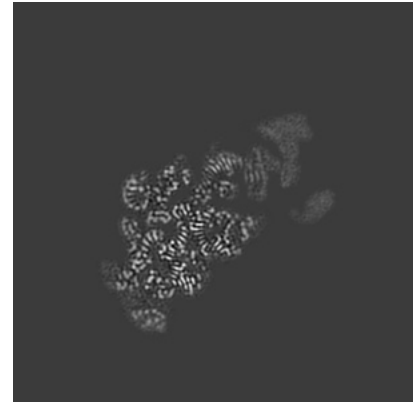
### 6.3.1 Primary map



X Index: 151

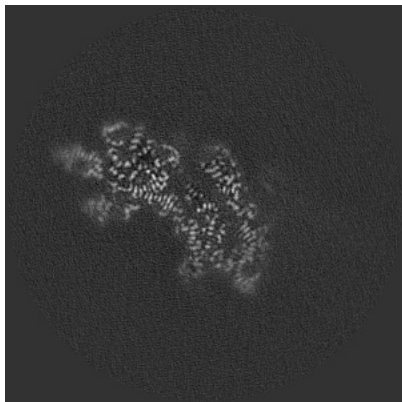


Y Index: 202

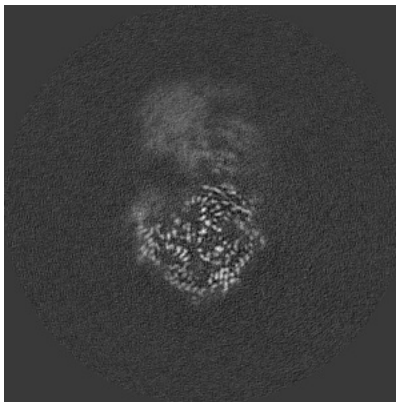


Z Index: 210

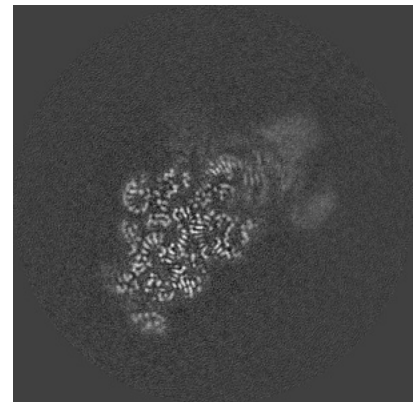
### 6.3.2 Raw map



X Index: 151



Y Index: 205

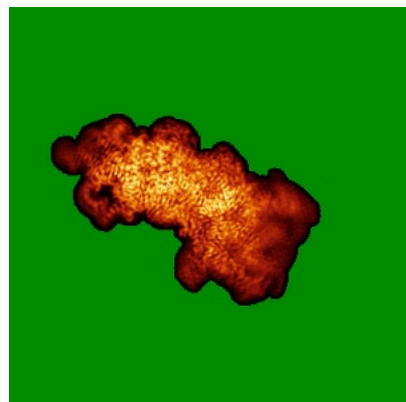


Z Index: 210

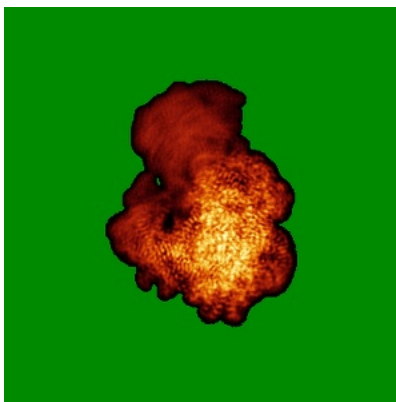
The images above show the largest variance slices of the map in three orthogonal directions.

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

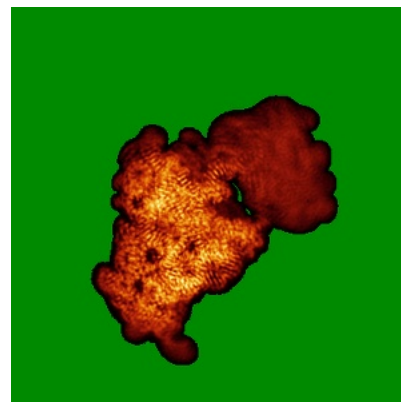
### 6.4.1 Primary map



X

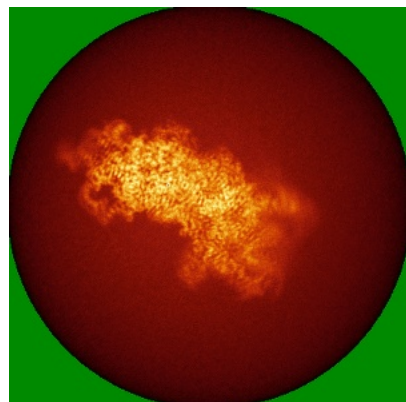


Y

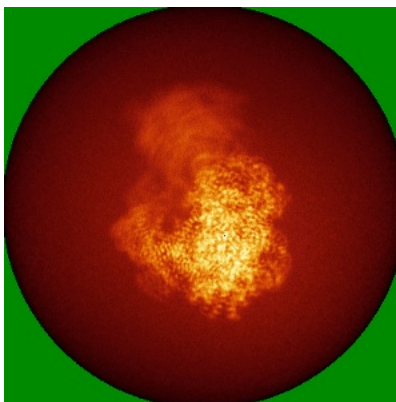


Z

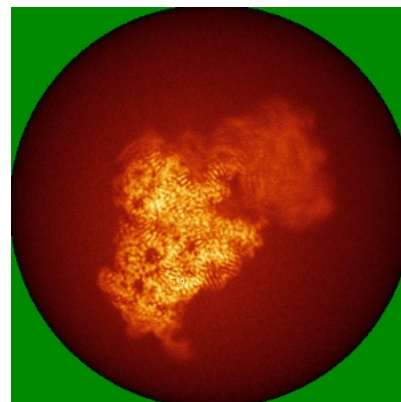
### 6.4.2 Raw map



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.

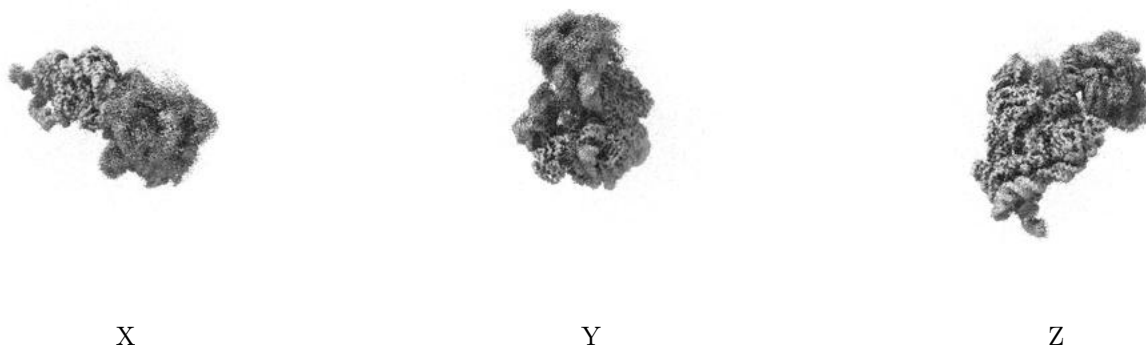
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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.

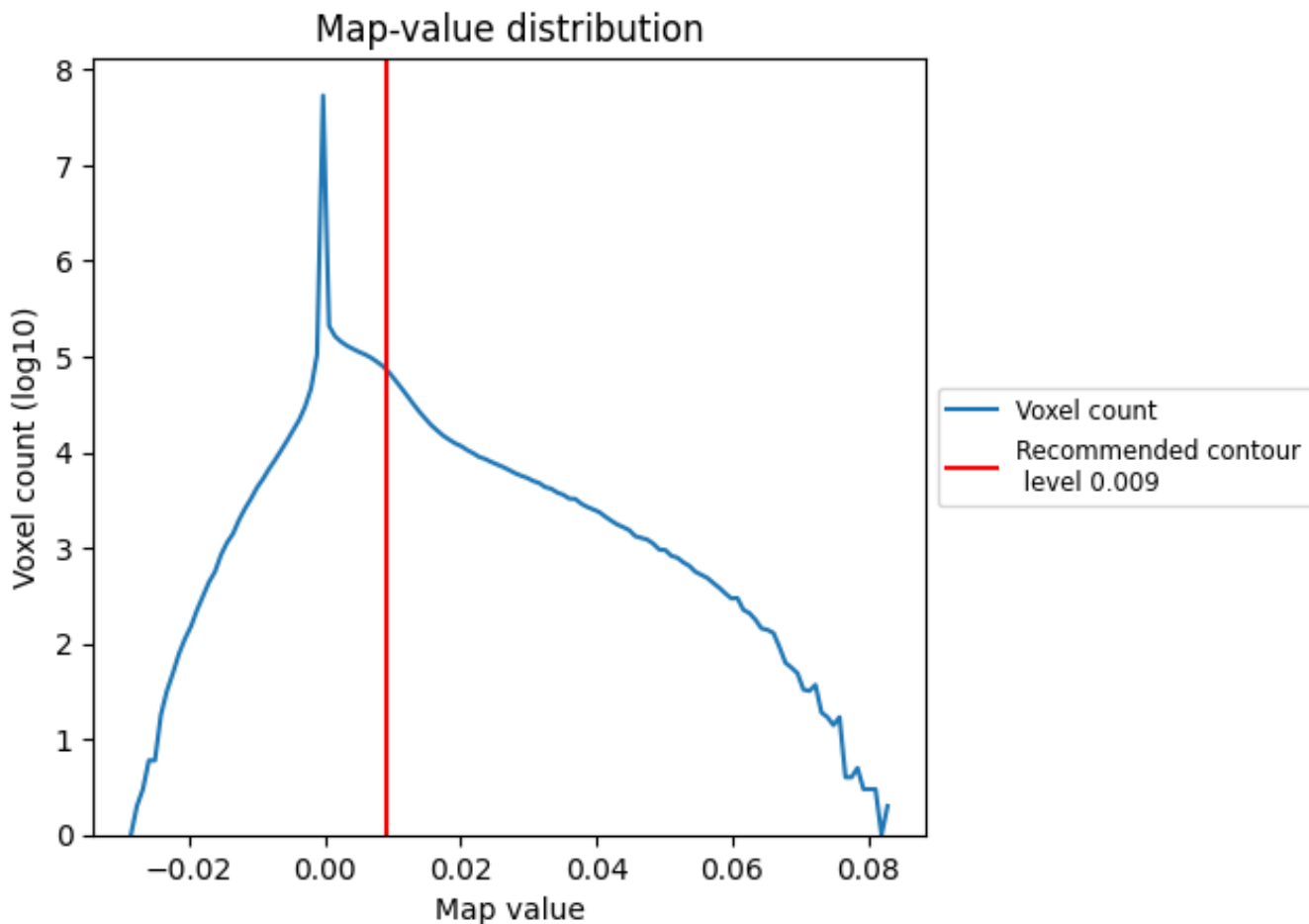
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

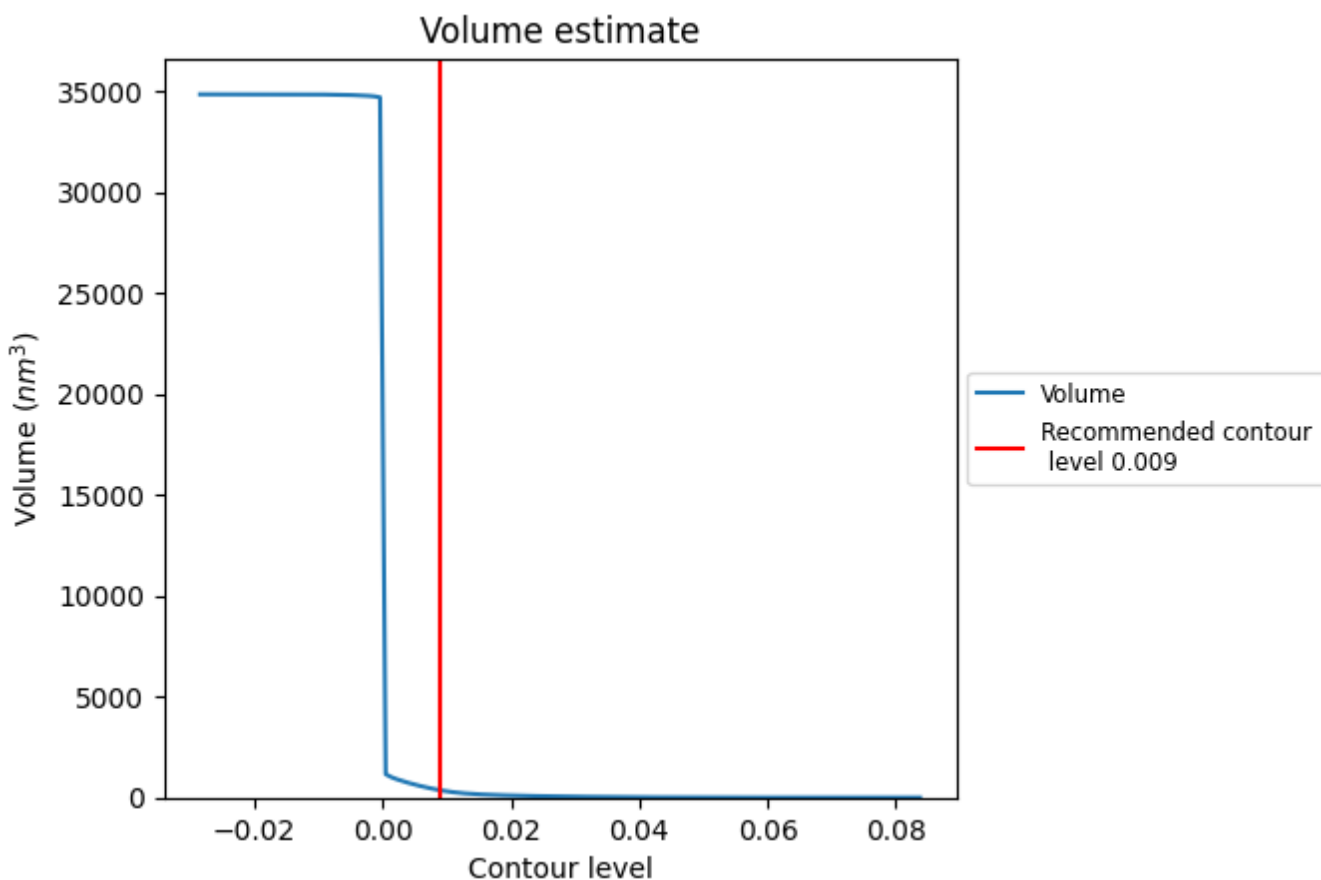
This section contains the results of statistical analysis of the map.

### 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.

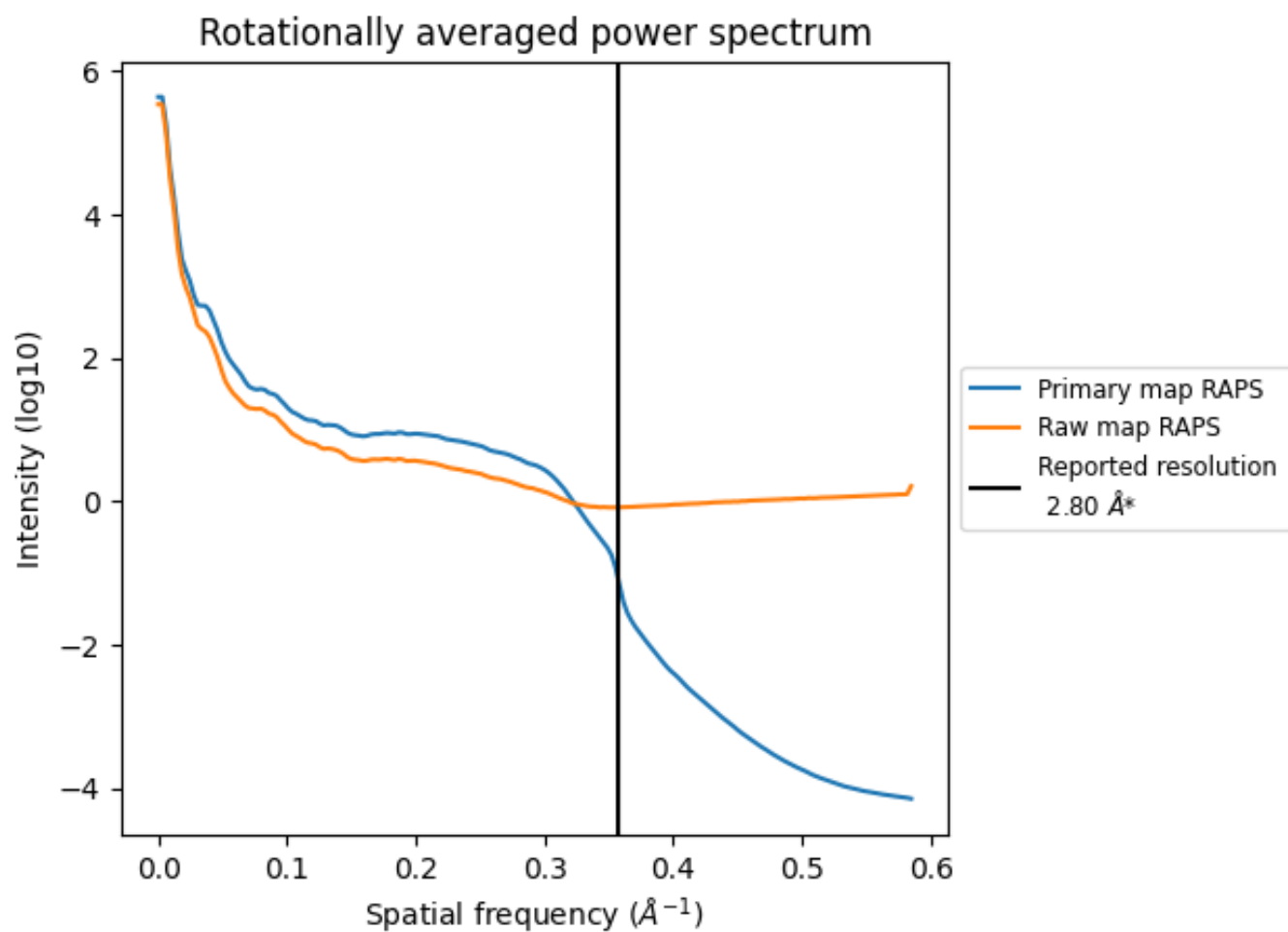
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 360  $\text{nm}^3$ ; this corresponds to an approximate mass of 326 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](#)

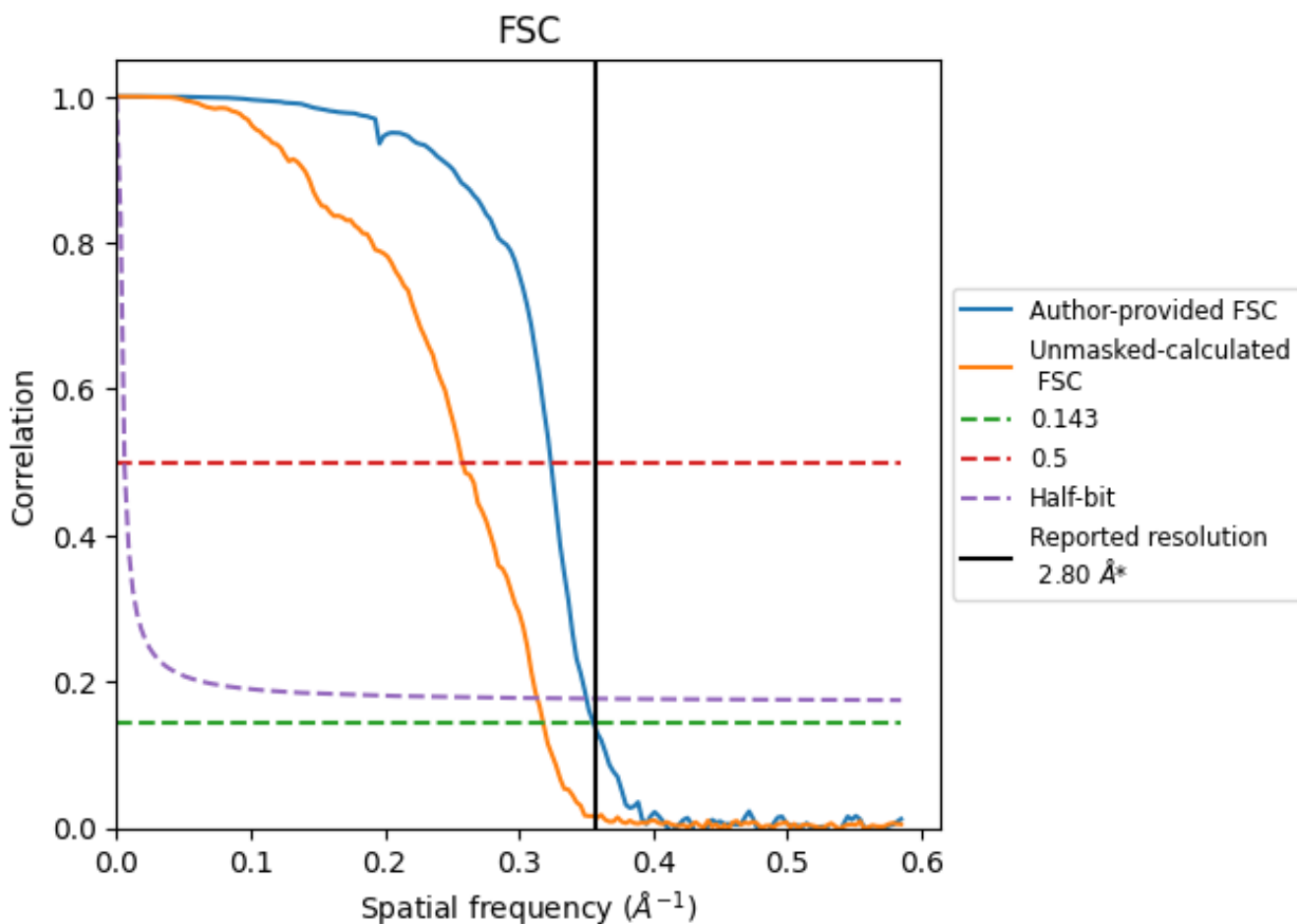


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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 0.357 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	2.80	-	-
Author-provided FSC curve	2.81	3.09	2.85
Unmasked-calculated*	3.14	3.88	3.19

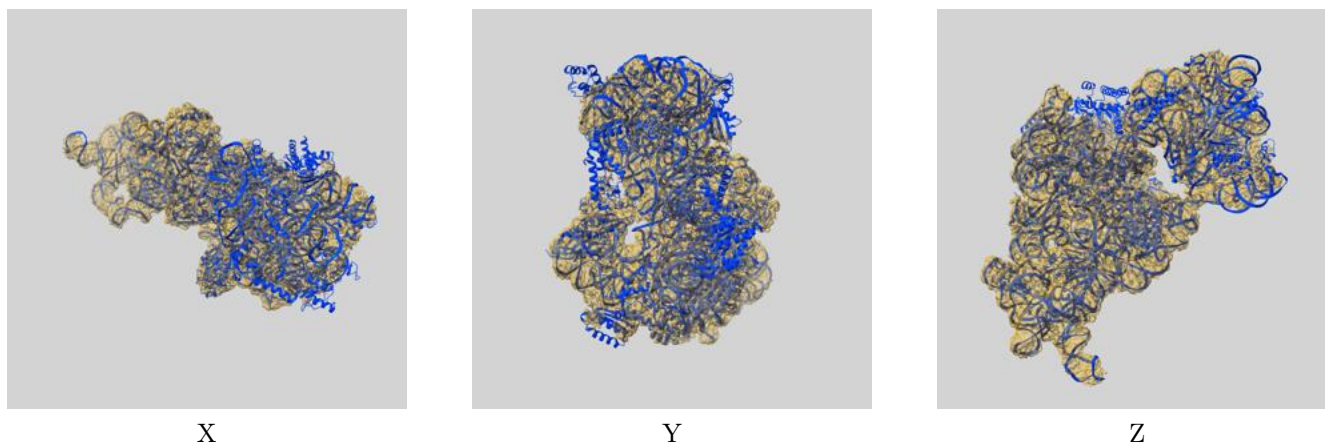
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.8 by more than 10 %



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

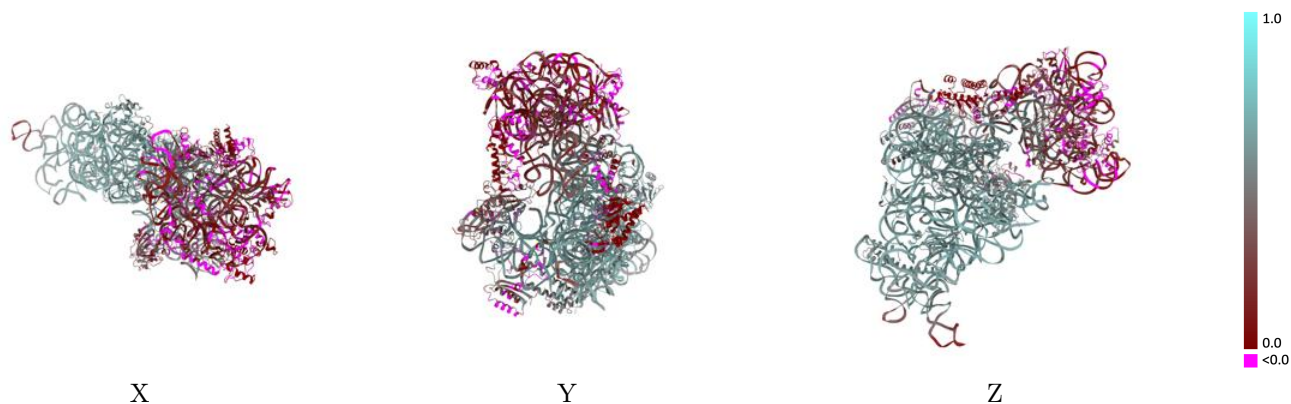
This section contains information regarding the fit between EMDB map EMD-28720 and PDB model 8EYT. Per-residue inclusion information can be found in section 3 on page 8.

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



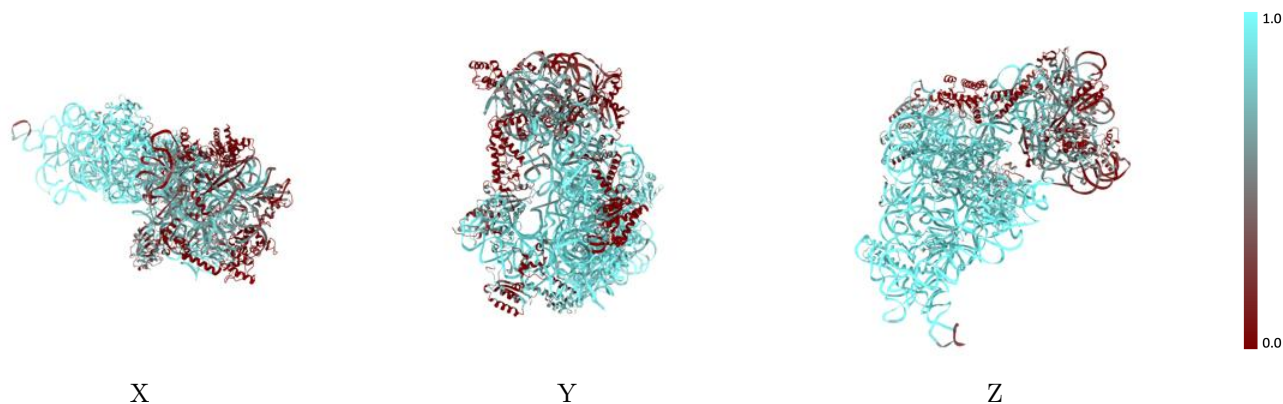
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



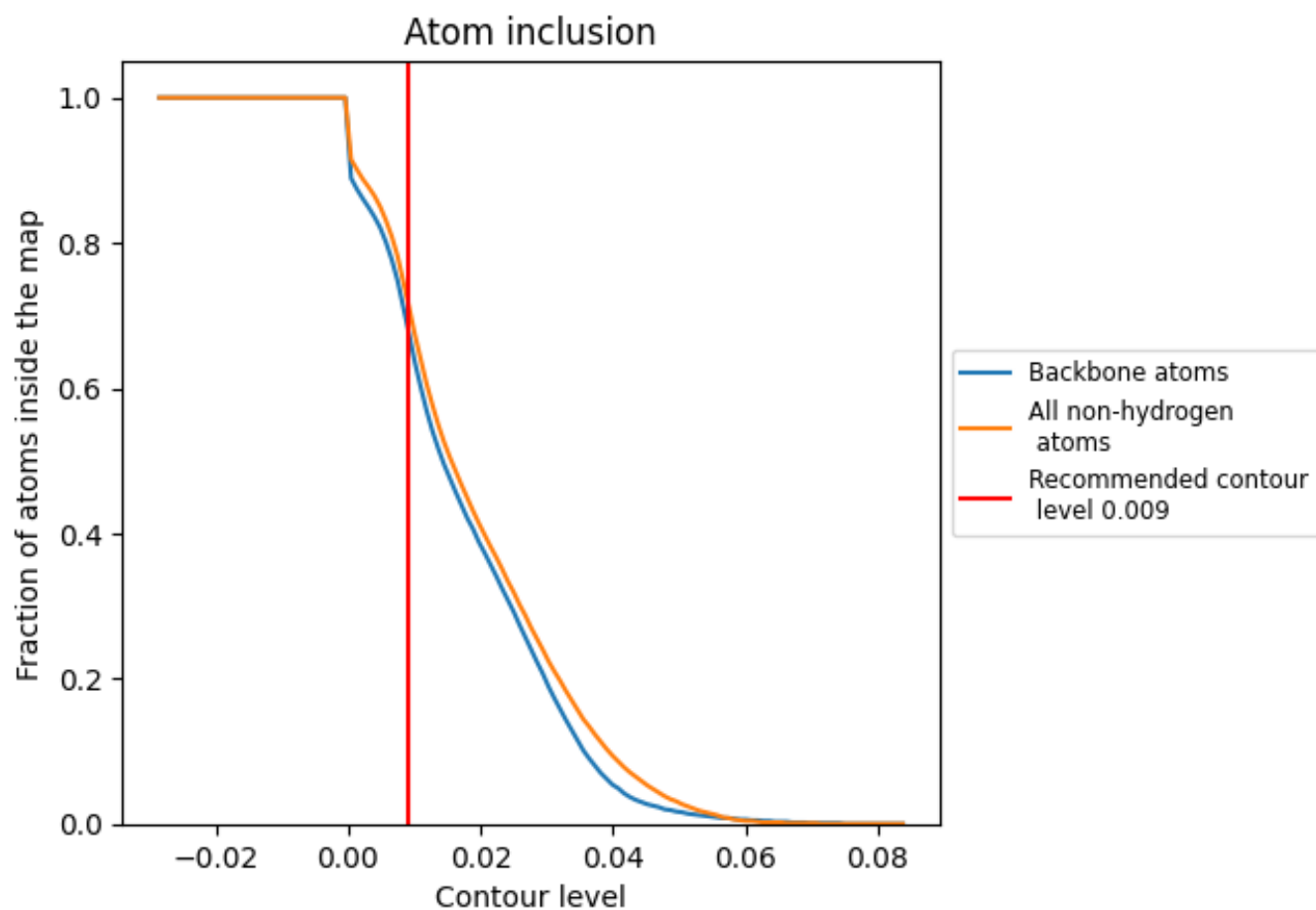
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 72% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.4070
A	 0.8750	 0.4750
B	 0.0190	 0.0300
D	 0.8480	 0.5530
E	 0.8860	 0.5740
F	 0.3630	 0.2400
G	 0.0120	 -0.0280
H	 0.9100	 0.5970
I	 0.3430	 0.1710
J	 0.1470	 0.0580
L	 0.8620	 0.5630
M	 0.0850	 0.0010
N	 0.2690	 0.1090
O	 0.3760	 0.3050
P	 0.9140	 0.6030
Q	 0.9070	 0.5810
R	 0.5170	 0.3160
S	 0.2020	 0.0530
T	 0.9340	 0.5730
U	 0.6090	 0.4570
V	 0.2560	 0.1850
W	 0.5150	 0.3290

