



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2022 – 08:18 AM EDT

PDB ID : 5UZ4  
EMDB ID : EMD-8621  
Title : The cryo-EM structure of YjeQ bound to the 30S subunit suggests a fidelity checkpoint function for this protein in ribosome assembly  
Authors : Razi, A.; Guarne, A.; Ortega, J.  
Deposited on : 2017-02-24  
Resolution : 5.80 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:

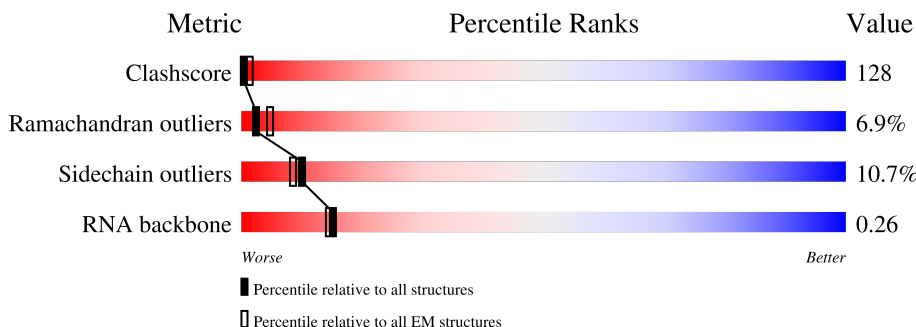
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 5.80 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.



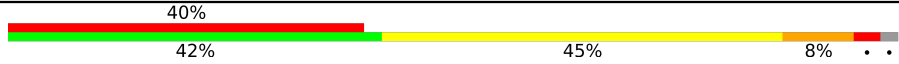

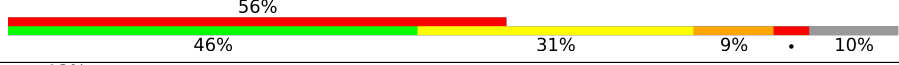
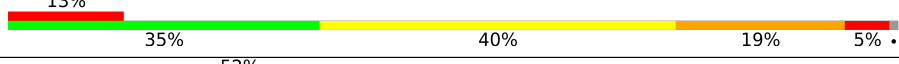
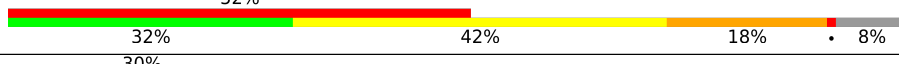
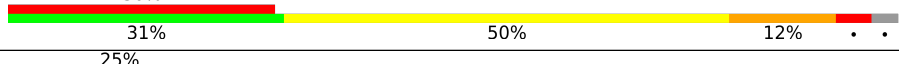
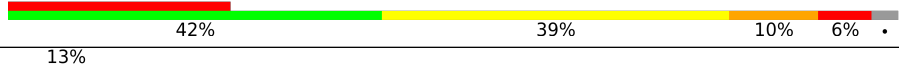
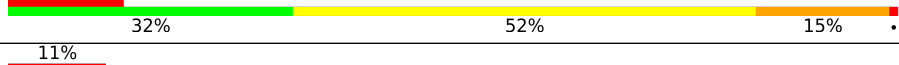
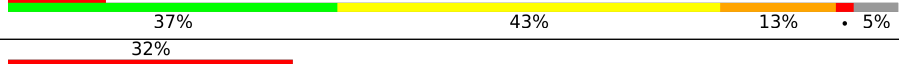
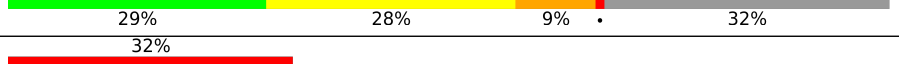
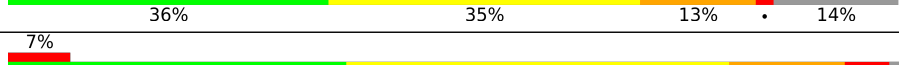


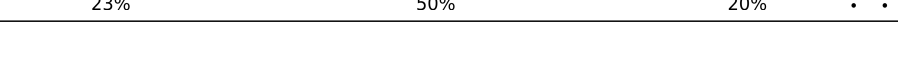
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1527	
2	C	233	
3	D	206	
4	E	167	
5	F	131	
6	G	179	
7	H	130	

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Mol	Chain	Length	Quality of chain
8	I	130	
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	S	92	
19	T	87	
20	B	241	
21	Z	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	GGM	Z	402	-	-	X	-

## 2 Entry composition i

There are 23 unique types of molecules in this entry. The entry contains 53225 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 RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1527	32767	14614	6014	10613	1526	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	A	G	conflict	GB 1095872043

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	206	1624	1028	305	288	3	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	1639	1023	314	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	150	1105	687	211	201	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	100	817	515	148	148	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	149	Total	C	N	O	S	0	0
			1160	721	222	213	4		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	129	Total	C	N	O	S	0	0
			975	613	172	184	6		

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			951	587	195	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	109	Total	C	N	O	S	0	0
			845	522	169	151	3		

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	98	Total	C	N	O	S	0	0
			759	472	157	127	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	86	Total	C	N	O	S	0	0
			700	431	144	124	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	51	Total	C	N	O	0	0
			414	264	77	73		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	79	Total	C	N	O	S	0	0
			619	393	117	107	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	B	233	1830	1154	328	340	8	2	0

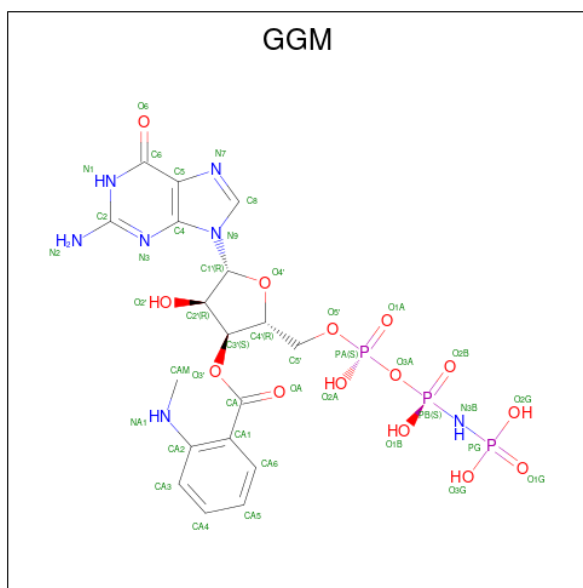
- Molecule 21 is a protein called Small ribosomal subunit biogenesis GTPase RsgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Z	323	2348	1463	397	479	9	0	0

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	Z	1	1	1	0

- Molecule 23 is 3'-O-(N-methylanthraniloyl)-beta:gamma-imidoguanosine-5'-triphosphate (three-letter code: GGM) (formula: C<sub>18</sub>H<sub>24</sub>N<sub>7</sub>O<sub>14</sub>P<sub>3</sub>).

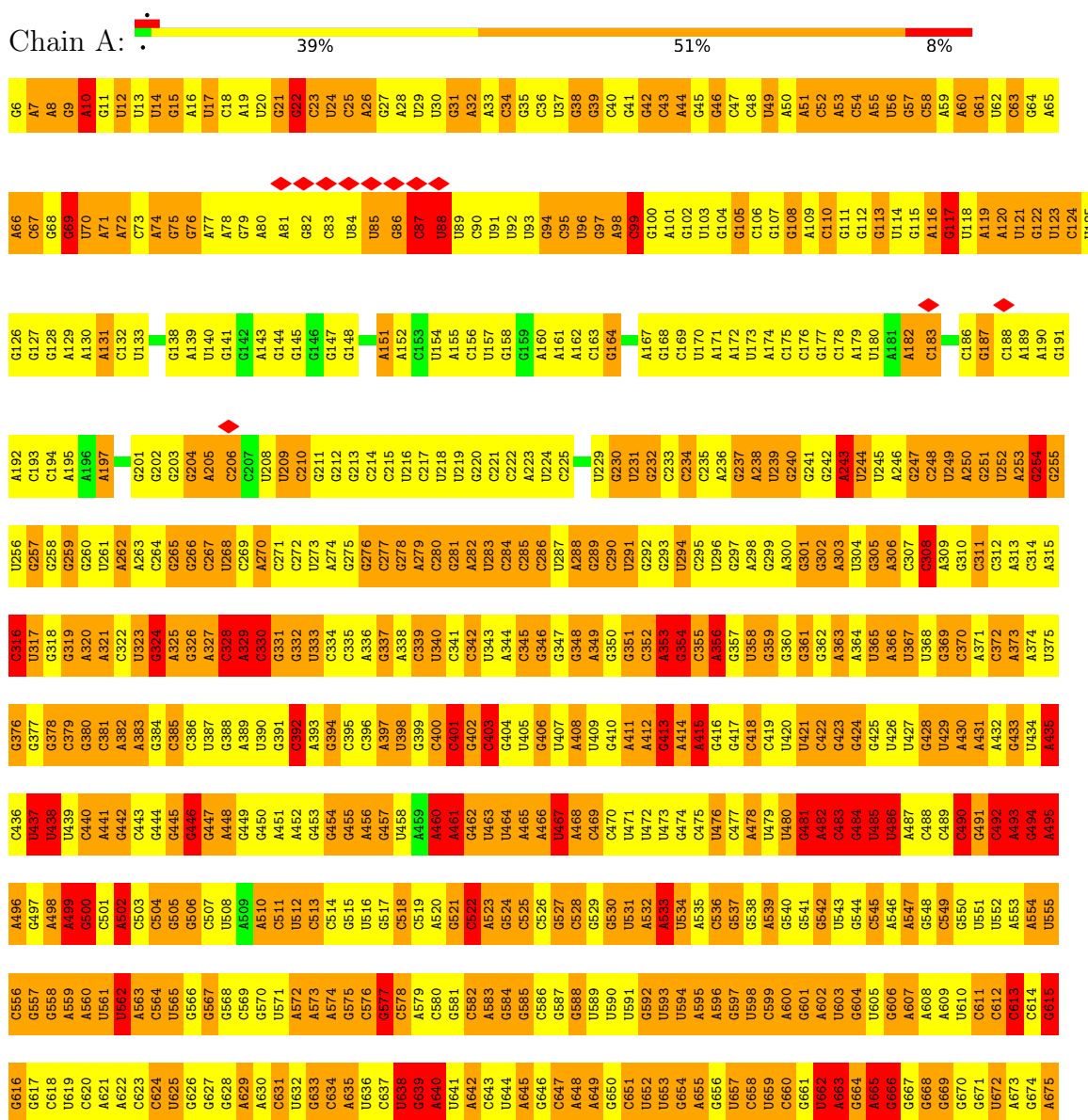


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	Z	1	32	10	6	13	3	0

### 3 Residue-property plots

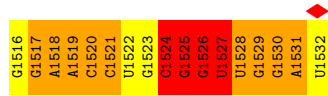
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

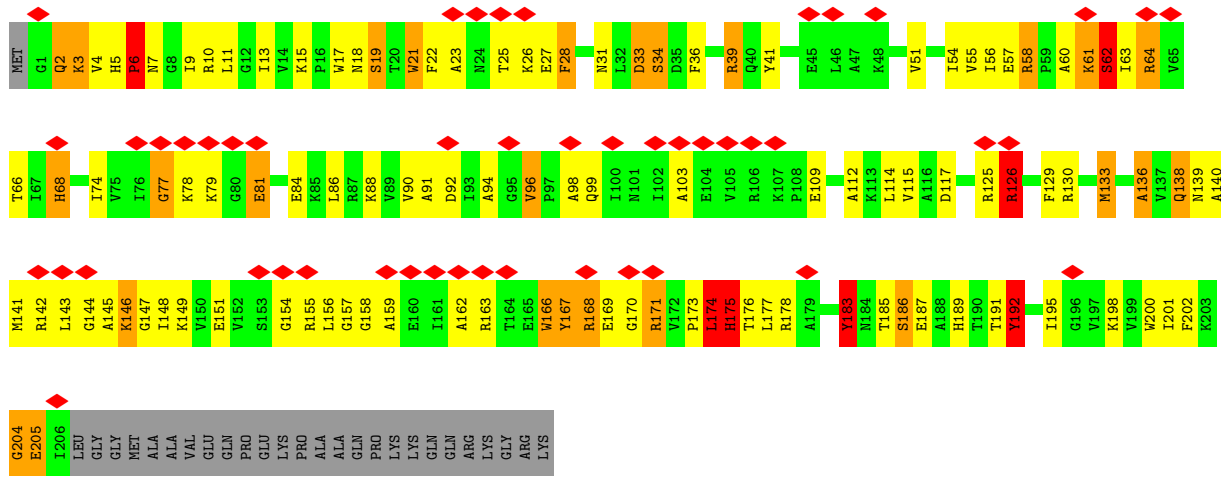




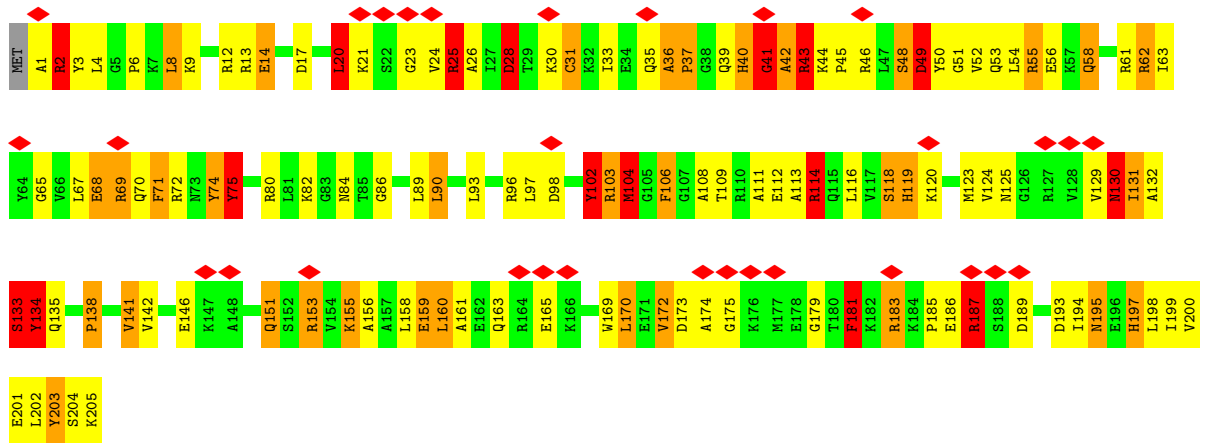




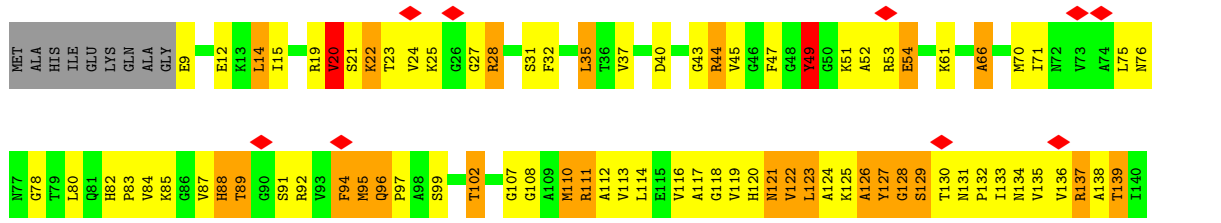
• Molecule 2: 30S ribosomal protein S3

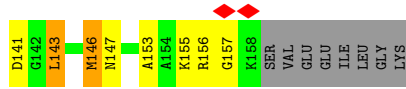


• Molecule 3: 30S ribosomal protein S4

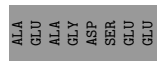
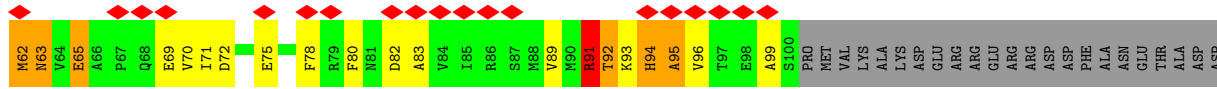
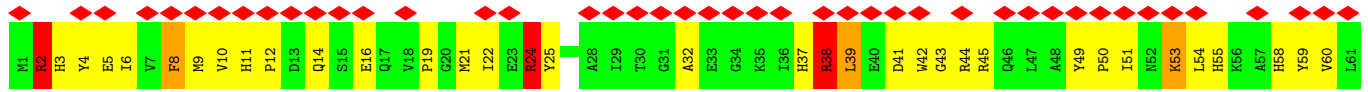


• Molecule 4: 30S ribosomal protein S5

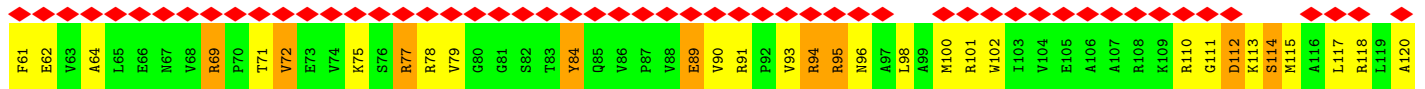




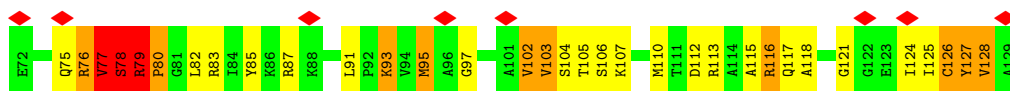
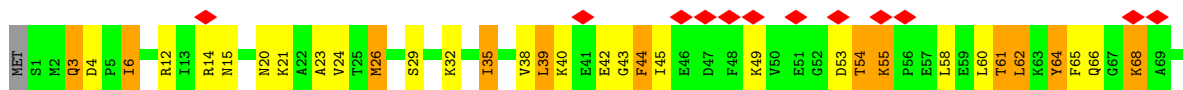
• Molecule 5: 30S ribosomal protein S6



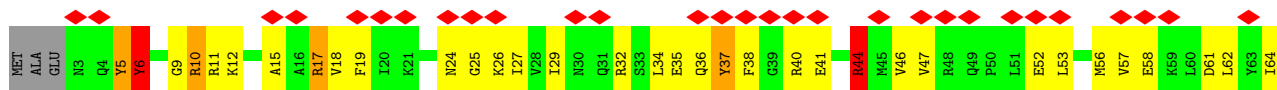
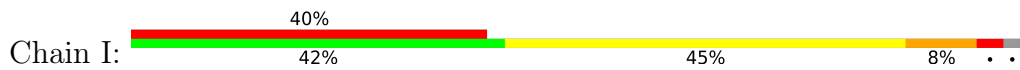
• Molecule 6: 30S ribosomal protein S7

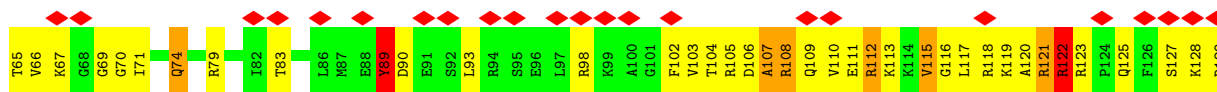


• Molecule 7: 30S ribosomal protein S8

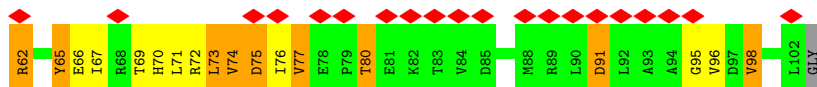
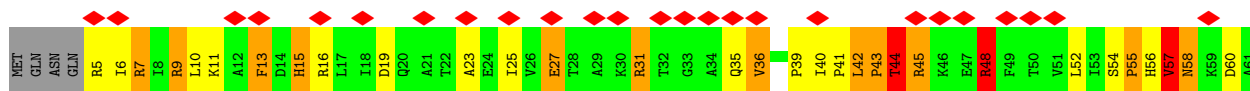
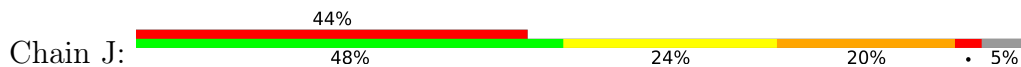


• Molecule 8: 30S ribosomal protein S9

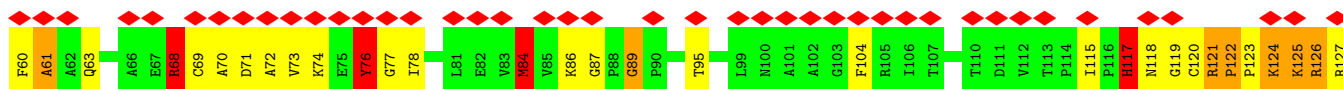
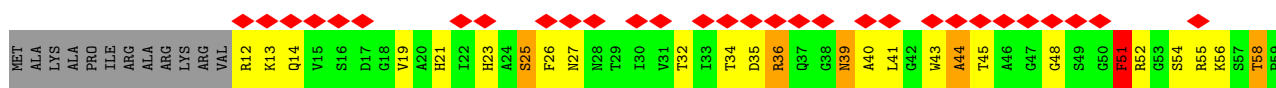




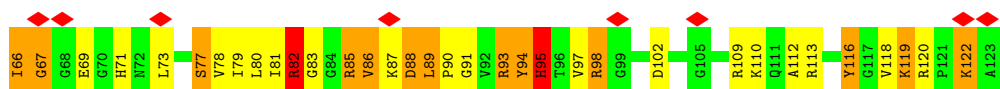
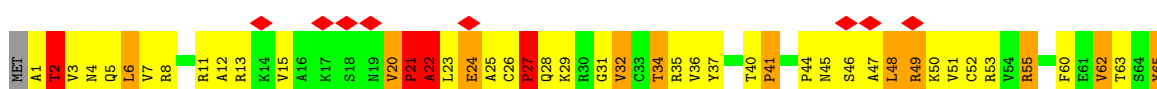
• Molecule 9: 30S ribosomal protein S10



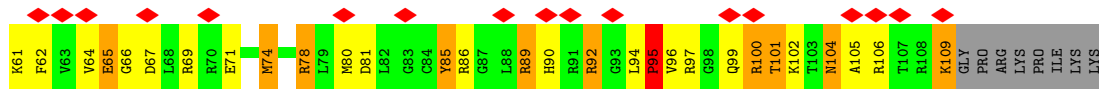
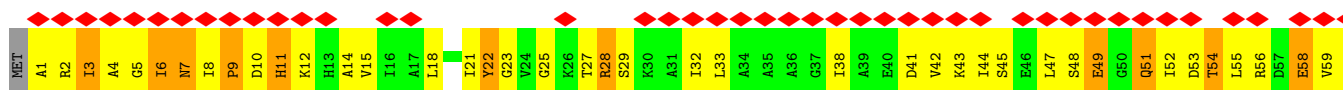
• Molecule 10: 30S ribosomal protein S11



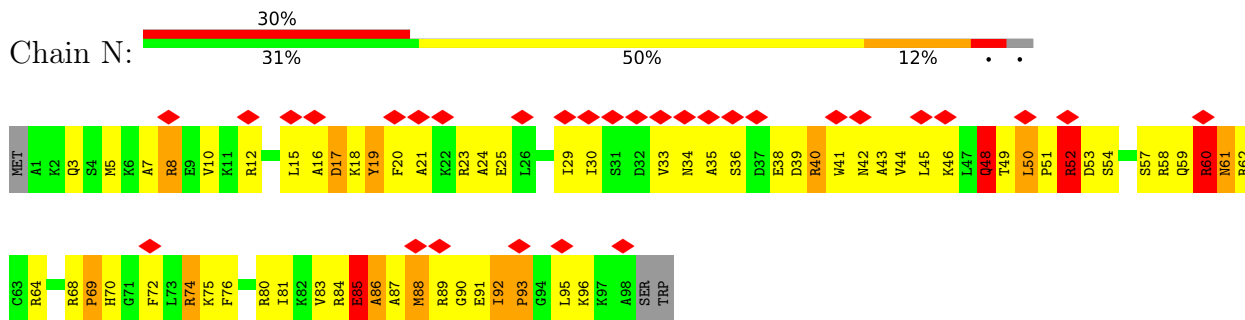
• Molecule 11: 30S ribosomal protein S12



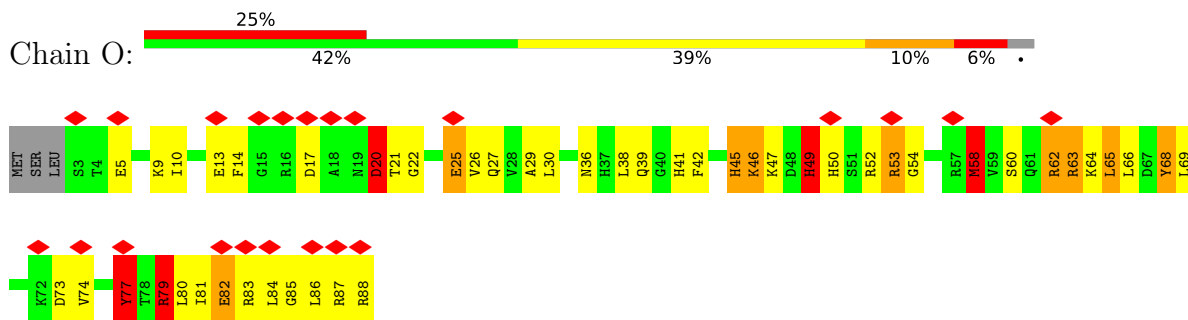
• Molecule 12: 30S ribosomal protein S13



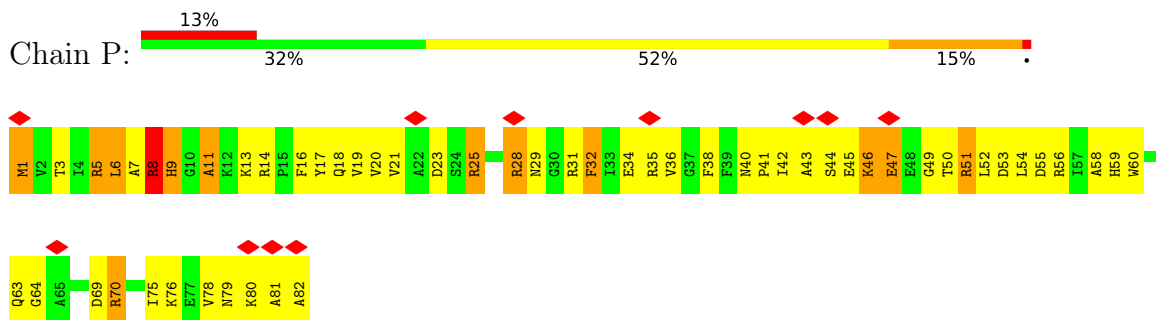
• Molecule 13: 30S ribosomal protein S14



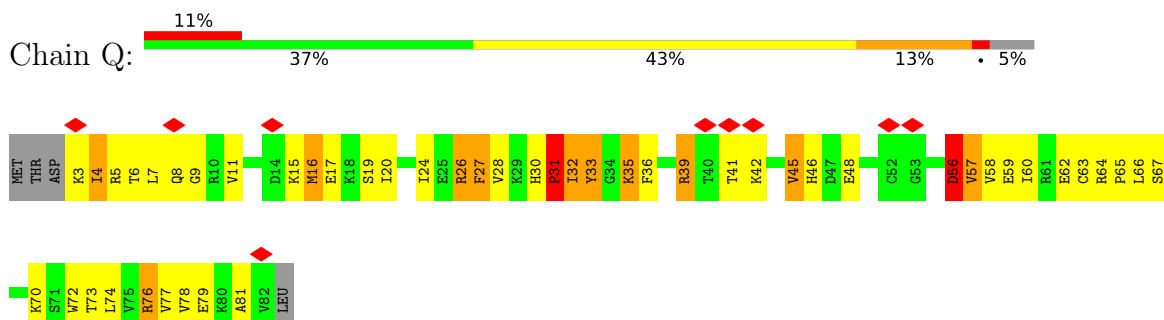
• Molecule 14: 30S ribosomal protein S15



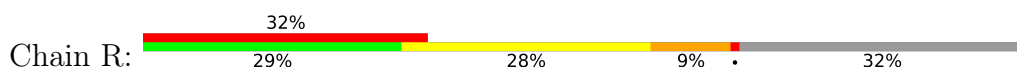
• Molecule 15: 30S ribosomal protein S16

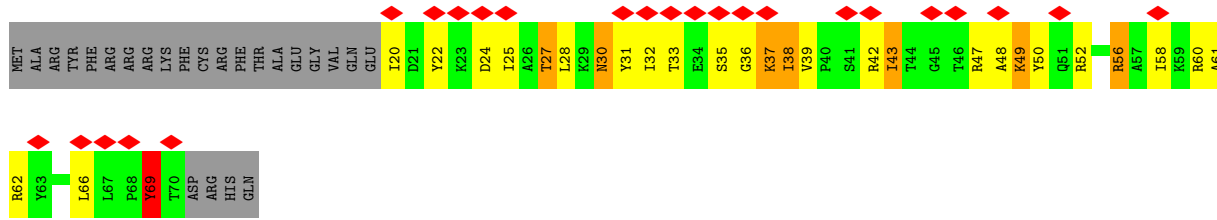


• Molecule 16: 30S ribosomal protein S17

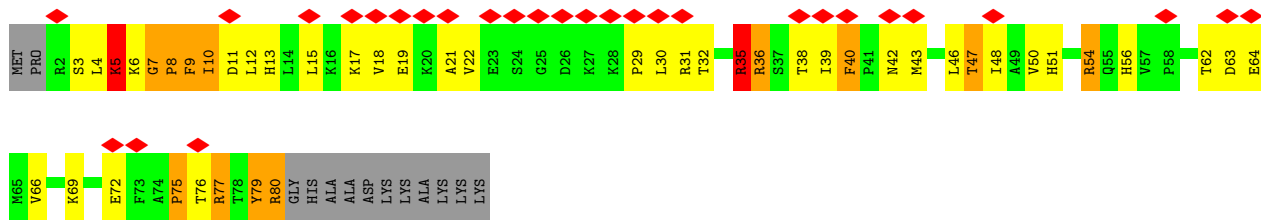


• Molecule 17: 30S ribosomal protein S18

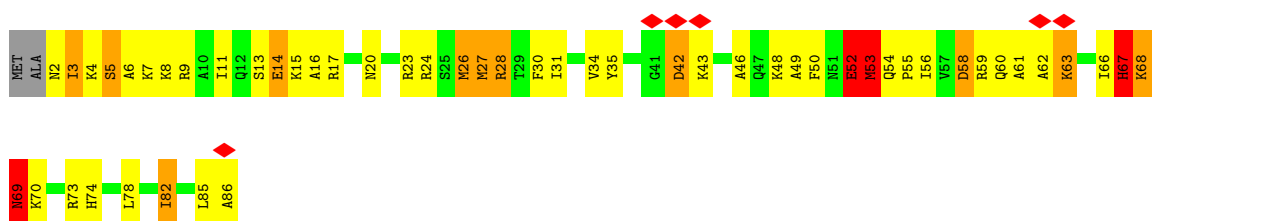




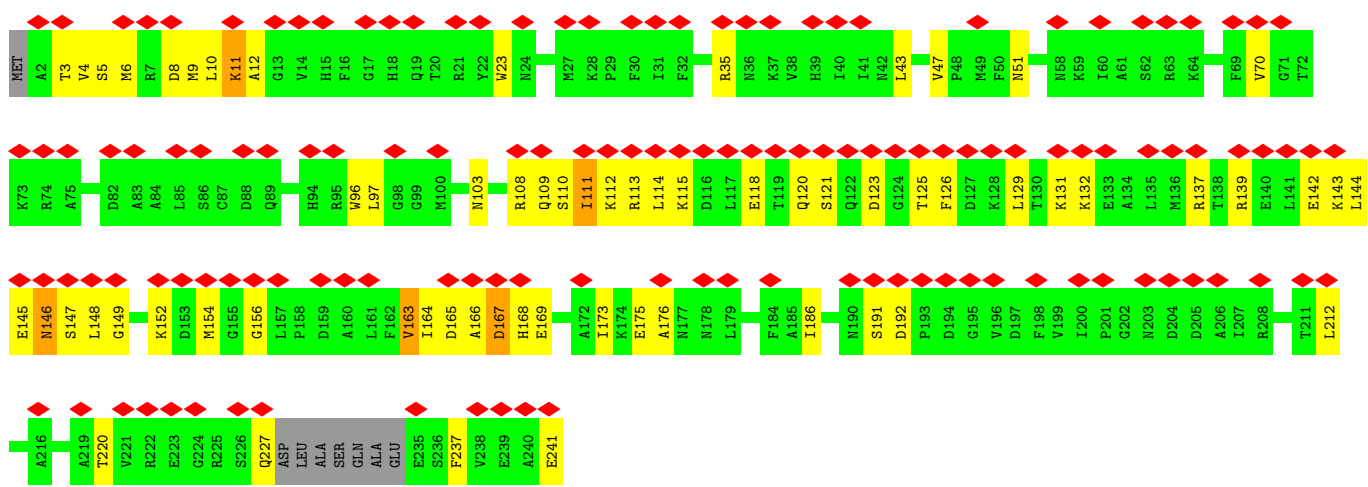
• Molecule 18: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S2



• Molecule 21: Small ribosomal subunit biogenesis GTPase RsgA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130462	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	34482	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0309	Depositor
Map size (Å)	319.0, 319.0, 319.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	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: GGM, 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	A	2.66	229/36645 (0.6%)	1.59	597/57061 (1.0%)
2	C	1.47	1/1651 (0.1%)	1.59	23/2225 (1.0%)
3	D	1.67	6/1661 (0.4%)	1.66	27/2223 (1.2%)
4	E	1.78	5/1118 (0.4%)	1.72	21/1504 (1.4%)
5	F	1.33	0/835	1.61	10/1128 (0.9%)
6	G	1.30	1/1173 (0.1%)	1.58	13/1573 (0.8%)
7	H	1.65	3/985 (0.3%)	1.71	15/1322 (1.1%)
8	I	1.44	0/1034	1.65	12/1375 (0.9%)
9	J	1.41	1/796 (0.1%)	1.66	19/1077 (1.8%)
10	K	1.32	0/885	1.53	15/1195 (1.3%)
11	L	1.76	6/965 (0.6%)	1.79	23/1296 (1.8%)
12	M	1.31	0/851	1.44	9/1136 (0.8%)
13	N	1.67	2/769 (0.3%)	1.36	5/1026 (0.5%)
14	O	1.51	0/708	1.55	11/946 (1.2%)
15	P	1.68	0/659	1.72	12/884 (1.4%)
16	Q	1.57	0/657	1.70	10/881 (1.1%)
17	R	1.16	0/420	1.27	4/565 (0.7%)
18	S	1.15	0/633	1.35	6/853 (0.7%)
19	T	1.60	0/671	1.60	7/888 (0.8%)
20	B	0.54	2/1864 (0.1%)	0.92	6/2511 (0.2%)
21	Z	0.79	16/2388 (0.7%)	1.28	60/3259 (1.8%)
All	All	2.28	272/57368 (0.5%)	1.57	905/84928 (1.1%)

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
1	A	1	7
2	C	0	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	17
4	E	0	9
5	F	0	6
6	G	0	6
7	H	0	5
8	I	0	10
9	J	0	7
10	K	0	2
11	L	0	7
12	M	0	2
13	N	0	3
14	O	0	6
15	P	0	5
16	Q	0	2
17	R	0	2
18	S	0	4
19	T	0	4
21	Z	0	11
All	All	1	135

The worst 5 of 272 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	801	U	O3'-P	-90.89	0.52	1.61
1	A	1012	A	O3'-P	-90.78	0.52	1.61
1	A	901	A	O3'-P	-87.79	0.55	1.61
1	A	1310	G	O3'-P	-83.62	0.60	1.61
1	A	354	G	O3'-P	-82.82	0.61	1.61

The worst 5 of 905 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	801	U	P-O3'-C3'	-77.19	27.07	119.70
1	A	639	G	OP2-P-O3'	-41.14	14.70	105.20
1	A	944	G	P-O3'-C3'	40.49	168.28	119.70
1	A	804	U	P-O3'-C3'	37.59	164.81	119.70
1	A	1508	A	P-O3'-C3'	35.20	161.94	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1243	C	C3'

5 of 135 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	437	U	Sidechain
1	A	438	U	Sidechain
1	A	496	A	Sidechain
1	A	521	G	Sidechain

## 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	32767	0	16531	9892	0
2	C	1624	0	1699	134	0
3	D	1639	0	1699	141	0
4	E	1105	0	1148	92	0
5	F	817	0	808	114	0
6	G	1160	0	1207	89	0
7	H	975	0	1023	77	0
8	I	1022	0	1070	103	0
9	J	786	0	828	62	0
10	K	869	0	877	116	0
11	L	951	0	1007	125	0
12	M	845	0	900	135	0
13	N	759	0	789	179	0
14	O	700	0	723	68	0
15	P	649	0	665	50	0
16	Q	648	0	690	79	0
17	R	414	0	439	85	0
18	S	619	0	628	155	0
19	T	665	0	710	54	0
20	B	1830	0	1839	147	0
21	Z	2348	0	2103	553	0
22	Z	1	0	0	0	0
23	Z	32	0	12	32	0
All	All	53225	0	37395	11485	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 128.

The worst 5 of 11485 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:1088:G:C2	1:A:1098:C:N3	1.67	1.59
1:A:714:G:H2'	1:A:715:A:C8	1.08	1.58
1:A:510:A:O3'	1:A:511:C:P	1.16	1.54
1:A:317:U:C4	1:A:337:G:C2	1.98	1.51
1:A:253:A:N6	1:A:274:A:C6	1.79	1.51

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	C	204/233 (88%)	149 (73%)	40 (20%)	15 (7%)	1	13
3	D	203/206 (98%)	162 (80%)	25 (12%)	16 (8%)	1	12
4	E	148/167 (89%)	119 (80%)	23 (16%)	6 (4%)	3	22
5	F	98/131 (75%)	76 (78%)	10 (10%)	12 (12%)	0	5
6	G	147/179 (82%)	115 (78%)	25 (17%)	7 (5%)	2	20
7	H	127/130 (98%)	104 (82%)	18 (14%)	5 (4%)	3	23
8	I	125/130 (96%)	93 (74%)	22 (18%)	10 (8%)	1	12
9	J	96/103 (93%)	70 (73%)	16 (17%)	10 (10%)	0	8
10	K	114/129 (88%)	86 (75%)	19 (17%)	9 (8%)	1	12
11	L	121/124 (98%)	81 (67%)	26 (22%)	14 (12%)	0	6
12	M	105/118 (89%)	78 (74%)	18 (17%)	9 (9%)	1	11
13	N	96/101 (95%)	61 (64%)	24 (25%)	11 (12%)	0	6
14	O	84/89 (94%)	68 (81%)	13 (16%)	3 (4%)	3	25
15	P	80/82 (98%)	64 (80%)	9 (11%)	7 (9%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	78/84 (93%)	50 (64%)	22 (28%)	6 (8%)	1	12
17	R	49/75 (65%)	35 (71%)	12 (24%)	2 (4%)	3	22
18	S	77/92 (84%)	55 (71%)	15 (20%)	7 (9%)	1	10
19	T	83/87 (95%)	72 (87%)	4 (5%)	7 (8%)	1	11
20	B	231/241 (96%)	218 (94%)	11 (5%)	2 (1%)	17	56
21	Z	319/334 (96%)	259 (81%)	41 (13%)	19 (6%)	1	16
All	All	2585/2835 (91%)	2015 (78%)	393 (15%)	177 (7%)	2	14

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	62	SER
2	C	158	GLY
2	C	174	LEU
2	C	178	ARG
2	C	195	ILE

### 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	C	170/190 (90%)	156 (92%)	14 (8%)	11	34
3	D	171/173 (99%)	141 (82%)	30 (18%)	2	11
4	E	113/126 (90%)	100 (88%)	13 (12%)	5	21
5	F	87/112 (78%)	81 (93%)	6 (7%)	15	40
6	G	121/147 (82%)	109 (90%)	12 (10%)	8	26
7	H	103/105 (98%)	92 (89%)	11 (11%)	6	23
8	I	105/107 (98%)	94 (90%)	11 (10%)	7	24
9	J	86/90 (96%)	75 (87%)	11 (13%)	4	18
10	K	89/99 (90%)	77 (86%)	12 (14%)	4	17
11	L	102/104 (98%)	92 (90%)	10 (10%)	8	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	88/96 (92%)	77 (88%)	11 (12%)	4	19
13	N	74/84 (88%)	67 (90%)	7 (10%)	8	28
14	O	74/77 (96%)	68 (92%)	6 (8%)	11	35
15	P	65/65 (100%)	54 (83%)	11 (17%)	2	12
16	Q	74/78 (95%)	68 (92%)	6 (8%)	11	35
17	R	43/65 (66%)	37 (86%)	6 (14%)	3	17
18	S	66/79 (84%)	62 (94%)	4 (6%)	18	44
19	T	65/66 (98%)	55 (85%)	10 (15%)	2	14
20	B	194/199 (98%)	189 (97%)	5 (3%)	46	66
21	Z	234/286 (82%)	204 (87%)	30 (13%)	4	18
All	All	2124/2348 (90%)	1898 (89%)	226 (11%)	10	24

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	84	MET
21	Z	302	CYS
13	N	49	THR
21	Z	289	GLU
21	Z	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
12	M	90	HIS
19	T	60	GLN
13	N	48	GLN
15	P	29	ASN
20	B	168	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1486/1527 (97%)	735 (49%)	92 (6%)

5 of 735 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	8	A
1	A	9	G
1	A	10	A
1	A	14	U

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	882	C
1	A	1243	C
1	A	910	C
1	A	1065	U
1	A	1313	U

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
23	GGM	Z	402	21	29,34,45	2.12	7 (24%)	32,54,69	3.48	12 (37%)

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
23	GGM	Z	402	21	-	3/14/38/48	0/3/3/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	402	GGM	O4'-C1'	5.40	1.48	1.41
23	Z	402	GGM	C2'-C1'	-4.33	1.47	1.53
23	Z	402	GGM	C5-C6	-3.99	1.39	1.47
23	Z	402	GGM	C3'-C2'	-2.95	1.45	1.53
23	Z	402	GGM	C6-N1	2.47	1.41	1.37

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	402	GGM	C3'-C2'-C1'	14.74	123.17	100.98
23	Z	402	GGM	O4'-C1'-C2'	-6.88	96.87	106.93
23	Z	402	GGM	O1G-PG-N3B	-4.54	105.09	111.77
23	Z	402	GGM	C2'-C3'-C4'	-4.47	93.95	102.64
23	Z	402	GGM	O1B-PB-O2B	3.45	117.15	109.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Z	402	GGM	PG-N3B-PB-O2B
23	Z	402	GGM	PB-N3B-PG-O1G
23	Z	402	GGM	PG-N3B-PB-O3A

There are no ring outliers.

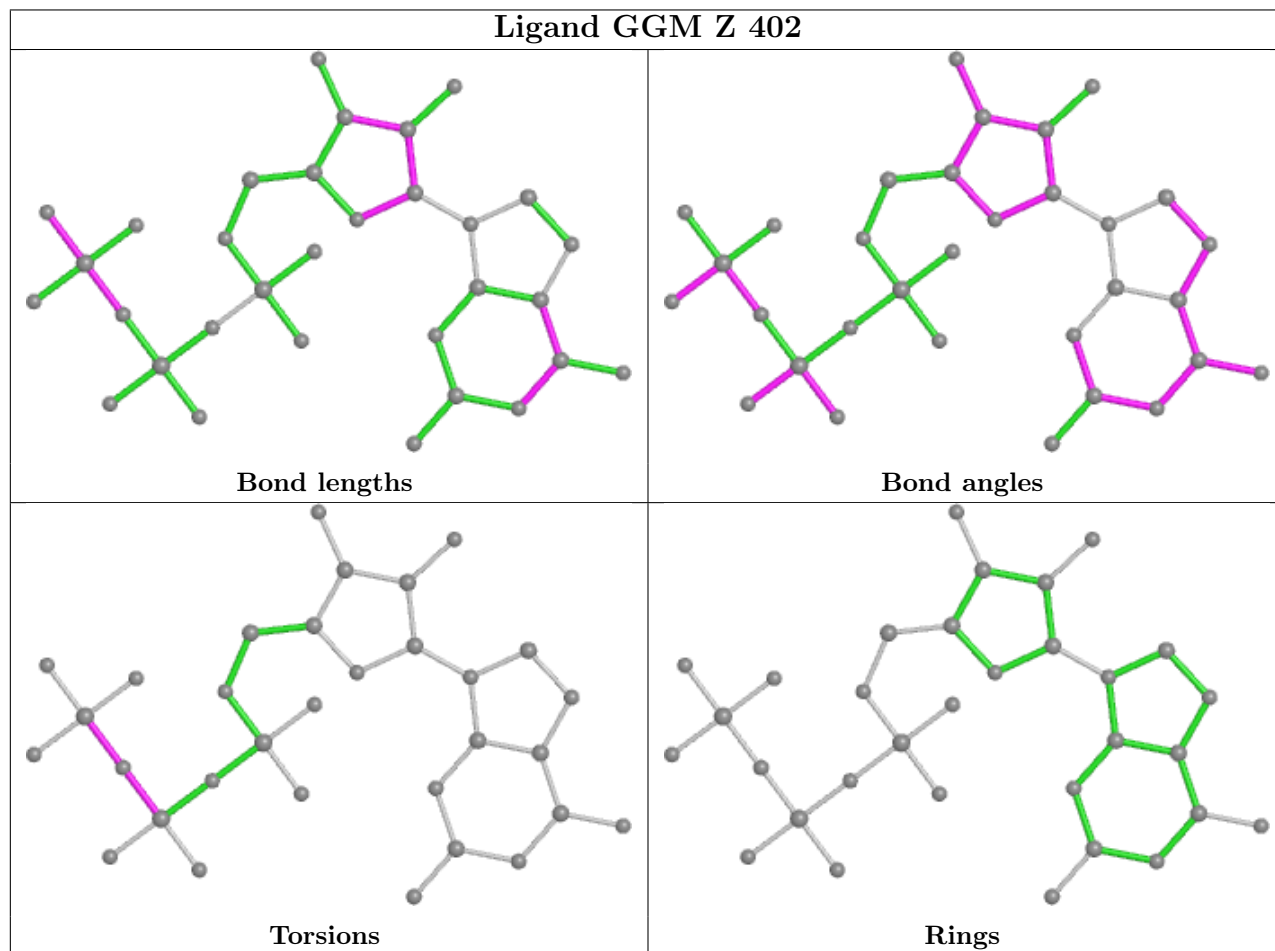
1 monomer is involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Z	402	GGM	32	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be



highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	195
21	Z	4
12	M	1

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Mol	Chain	Number of breaks
13	N	1
20	B	1

The worst 5 of 202 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1249:C	O3'	1250:A	P	3.76
1	A	646:G	O3'	647:C	P	3.66
1	A	886:G	O3'	887:G	P	3.56
1	A	1309:G	O3'	1310:G	P	3.30
1	A	317:U	O3'	318:G	P	3.28

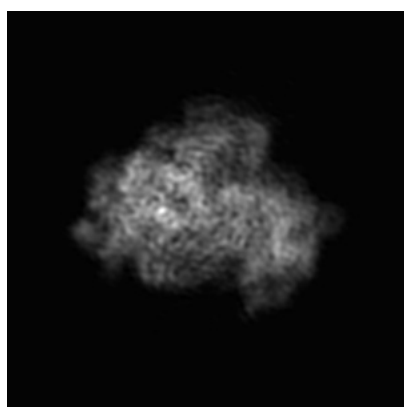
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8621. These allow visual inspection of the internal detail of the map and identification of artifacts.

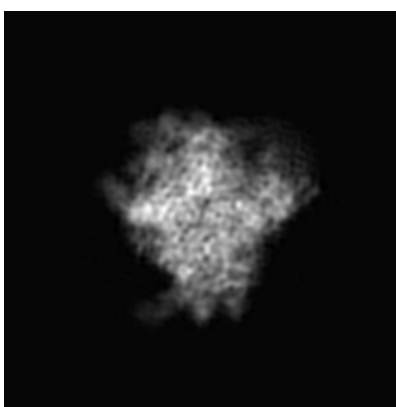
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

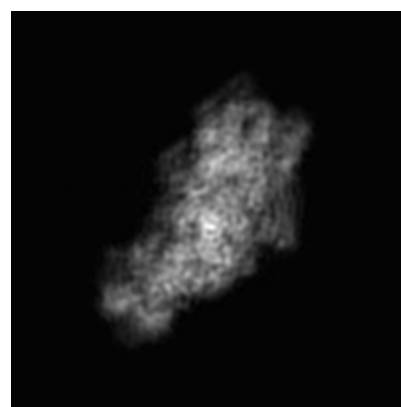
#### 6.1.1 Primary map



X



Y

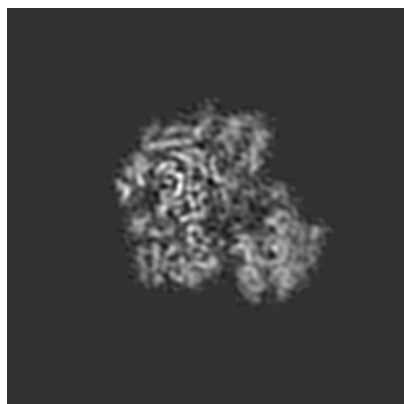


Z

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

### 6.2 Central slices [i](#)

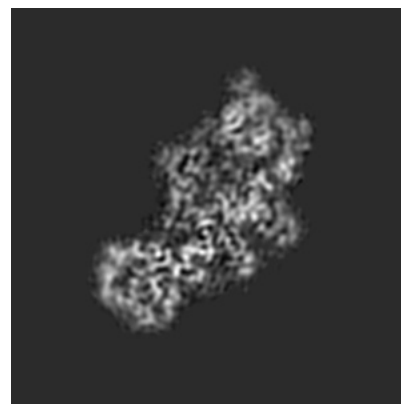
#### 6.2.1 Primary map



X Index: 110



Y Index: 110

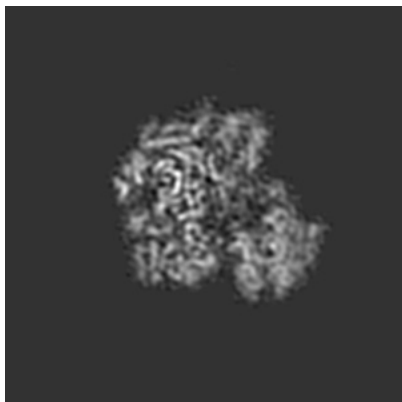


Z Index: 110

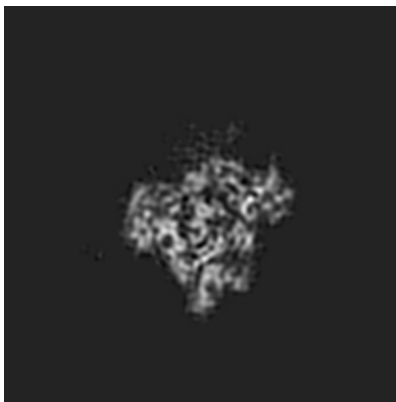
The images above show central slices of the map in three orthogonal directions.

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

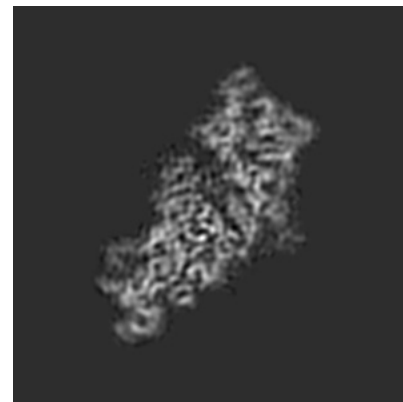
### 6.3.1 Primary map



X Index: 110



Y Index: 84

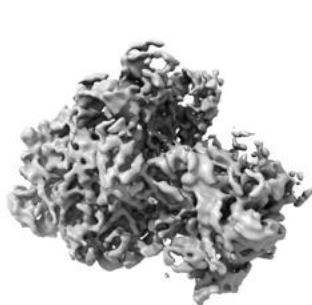


Z Index: 103

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

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

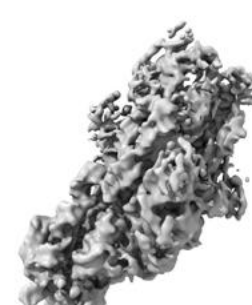
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0309. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

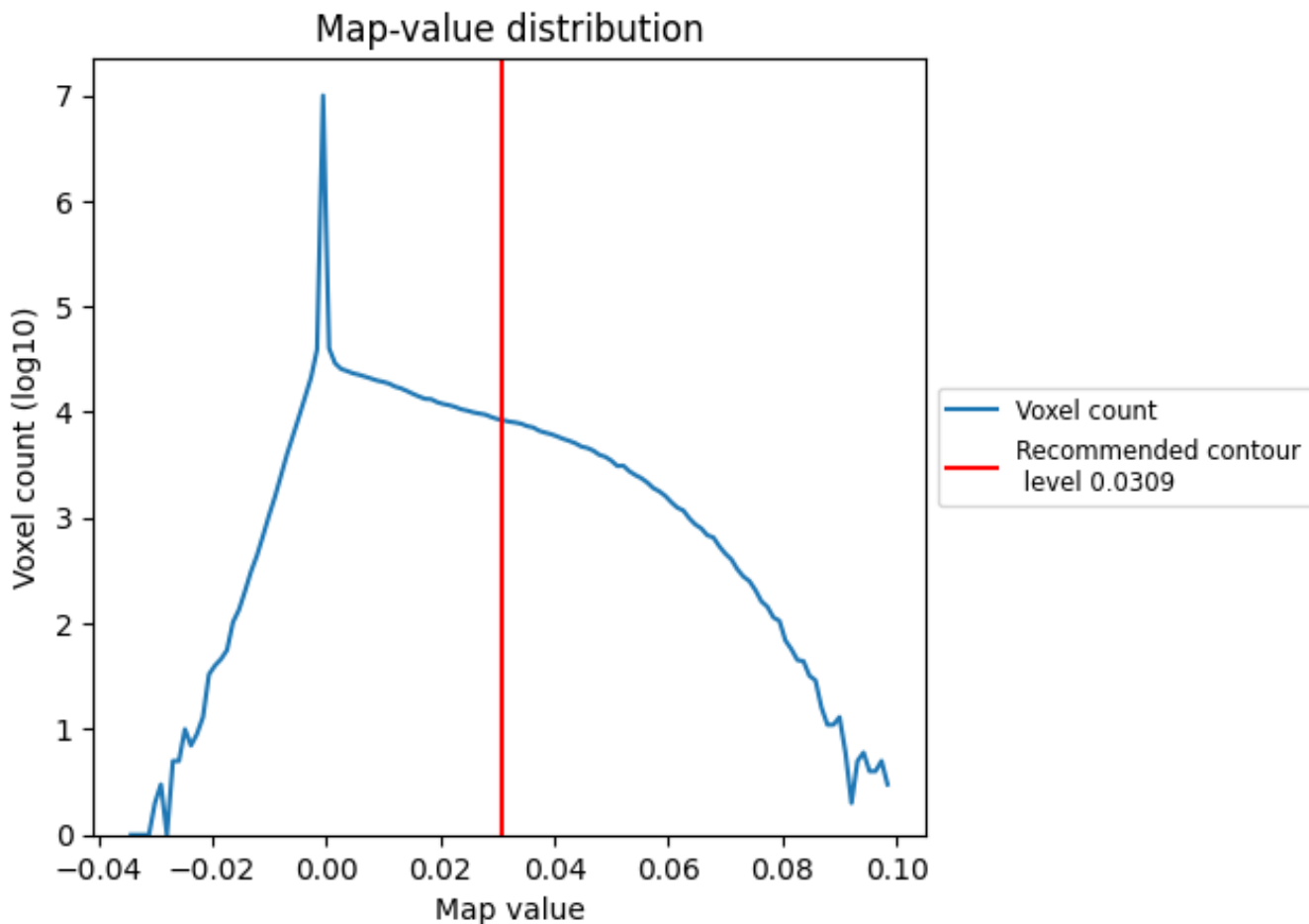
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

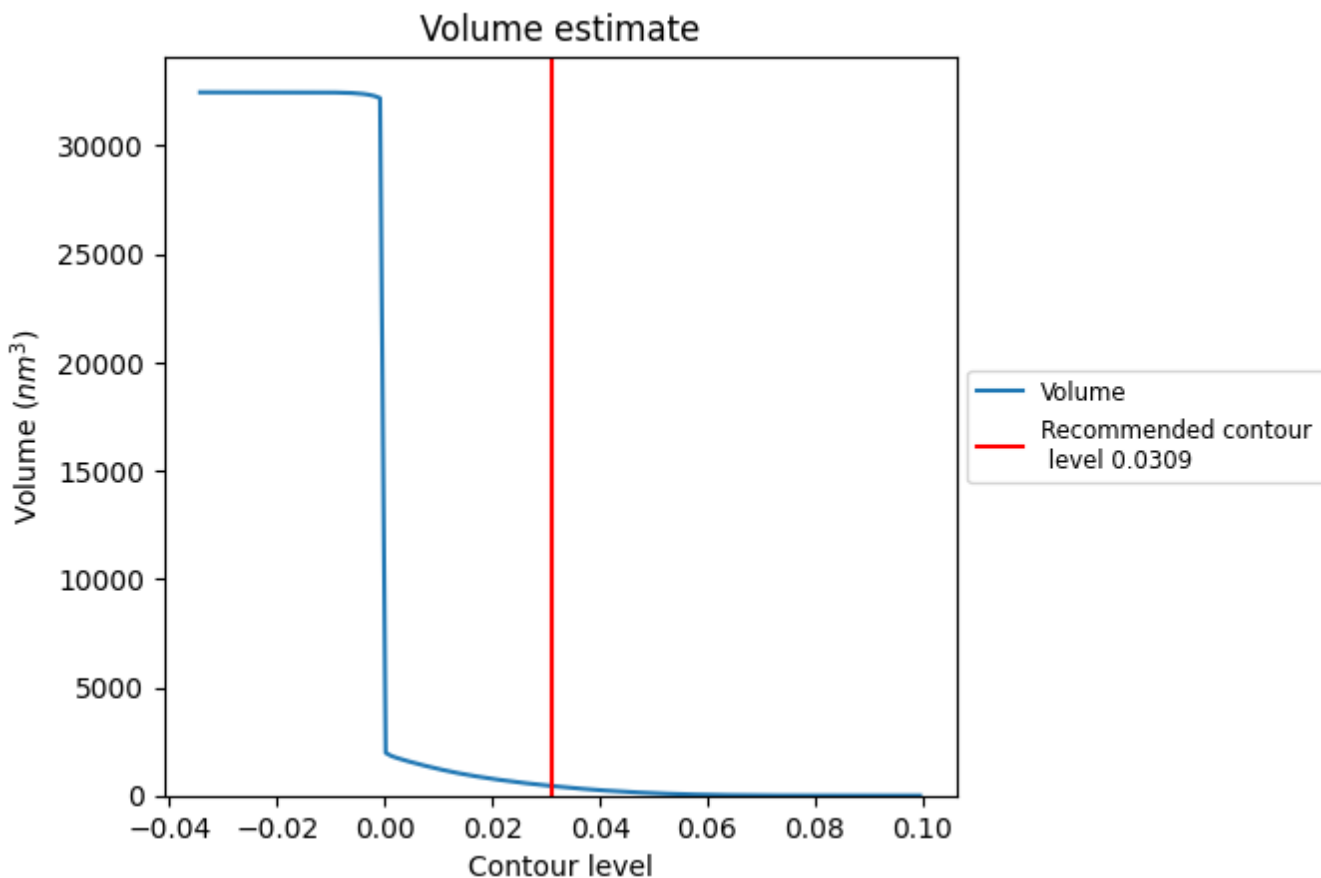
This section contains the results of statistical analysis of the map.

### 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.

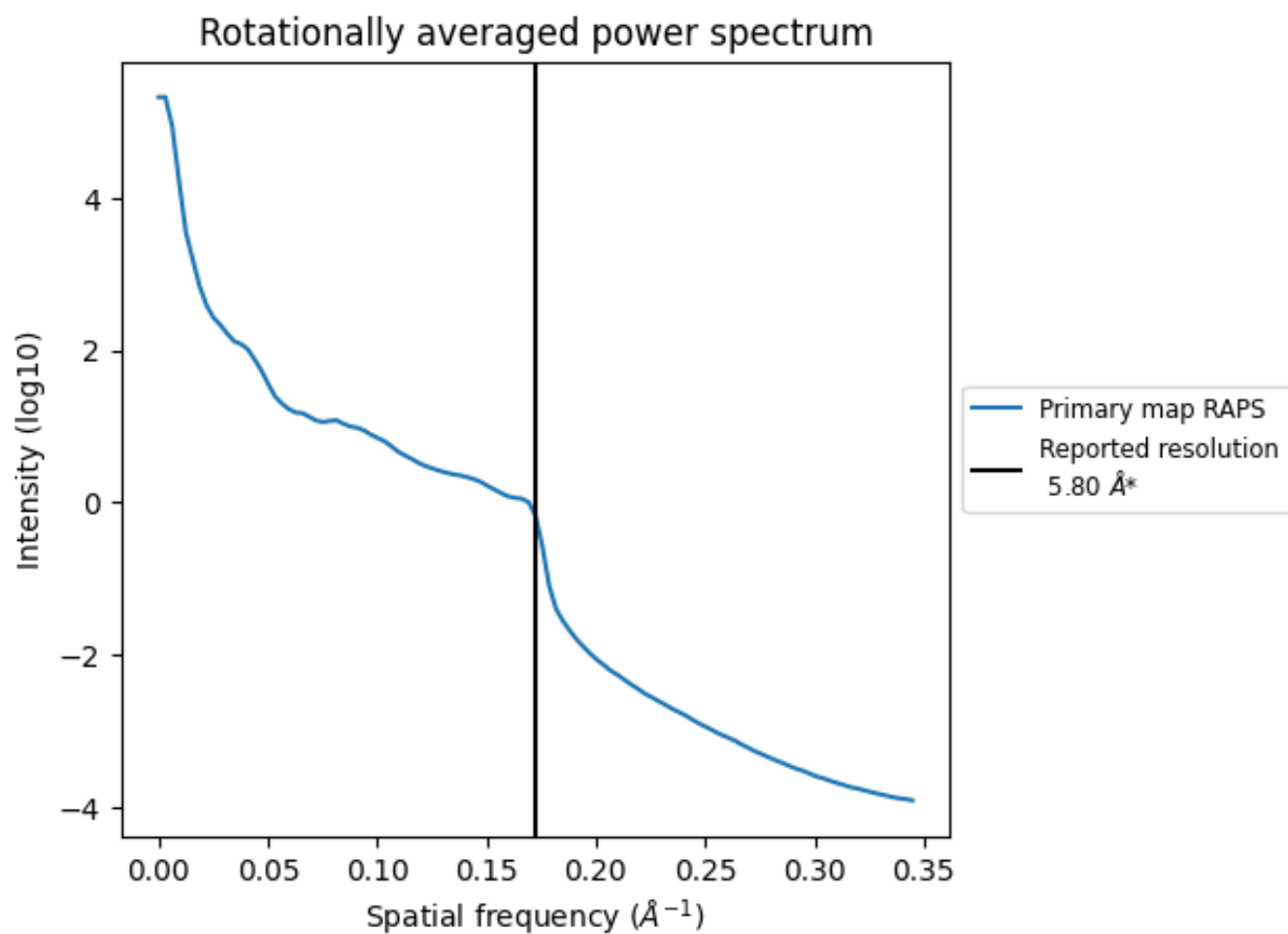
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 446 nm<sup>3</sup>; this corresponds to an approximate mass of 403 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](#)



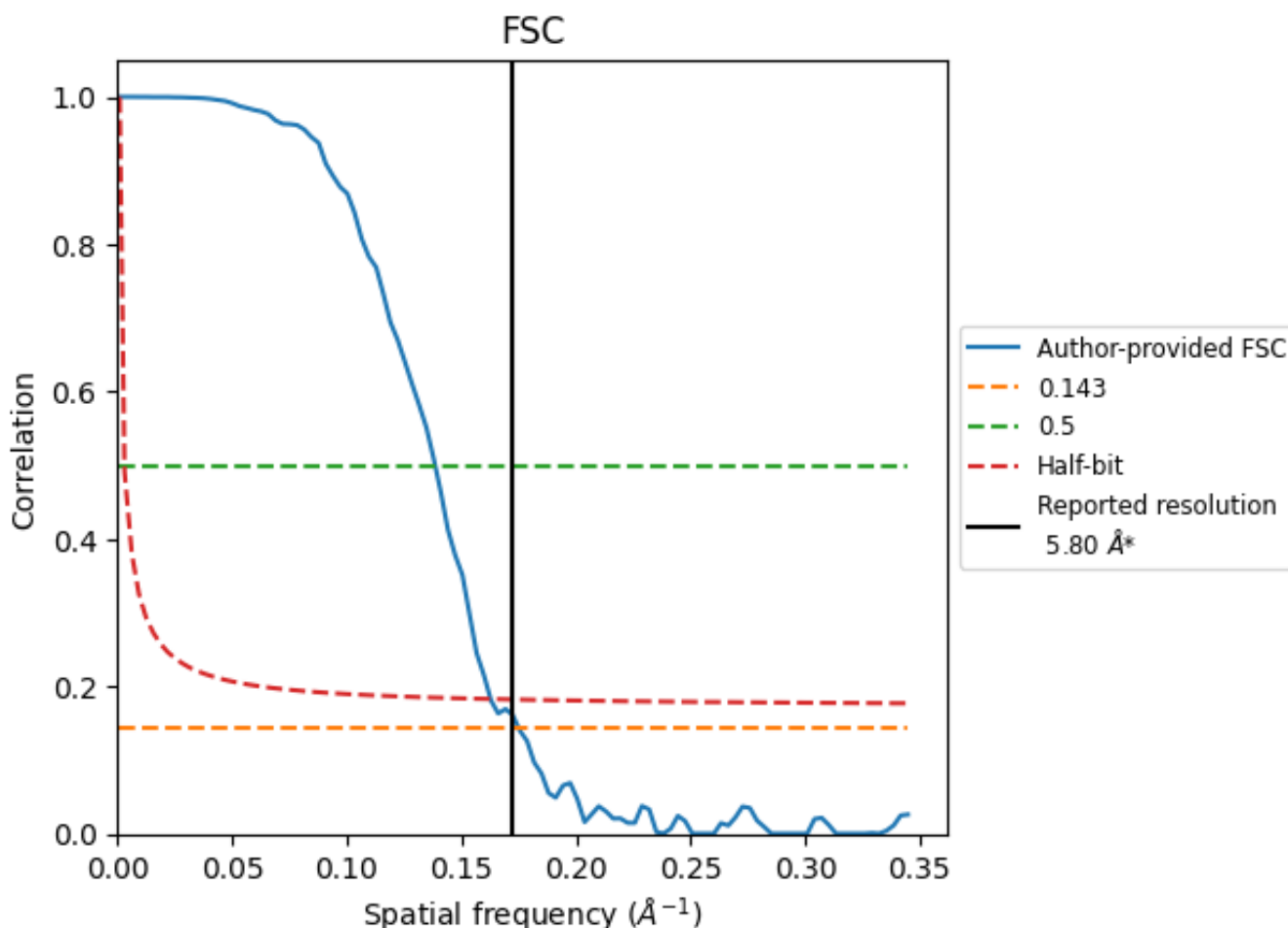
\*Reported resolution corresponds to spatial frequency of  $0.172 \text{\AA}^{-1}$



## 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 0.172 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

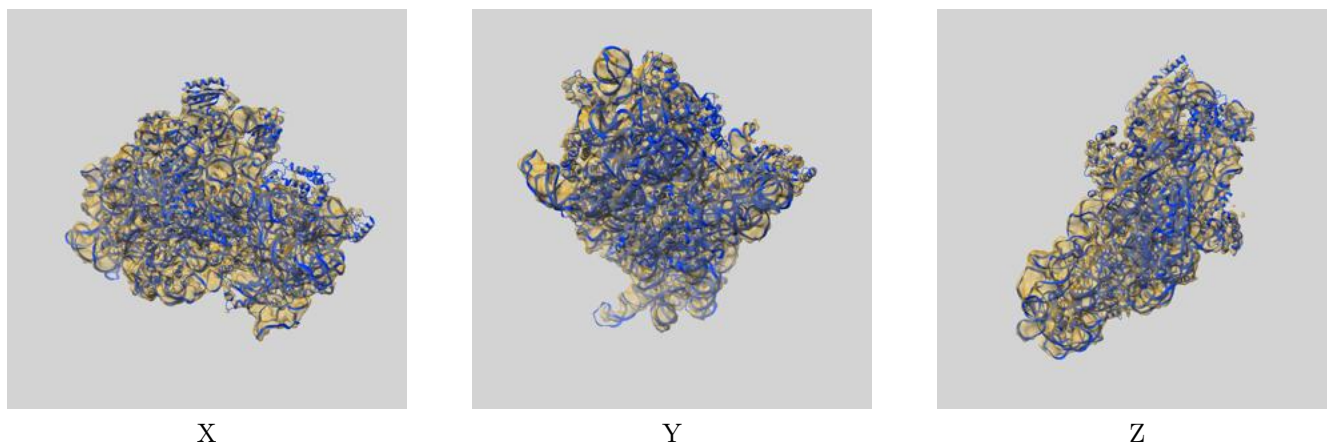
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	5.71	7.22	6.14
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

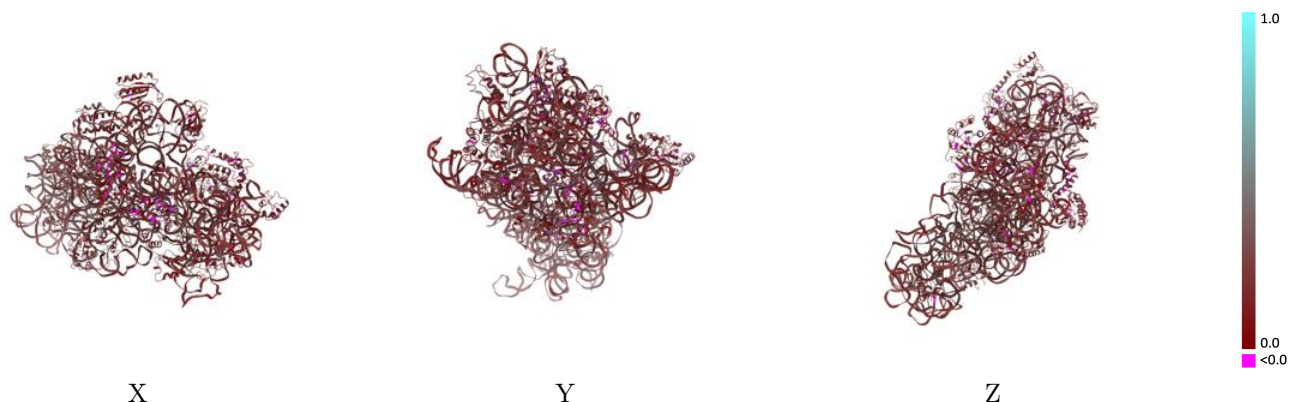
This section contains information regarding the fit between EMDB map EMD-8621 and PDB model 5UZ4. Per-residue inclusion information can be found in section 3 on page 8.

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



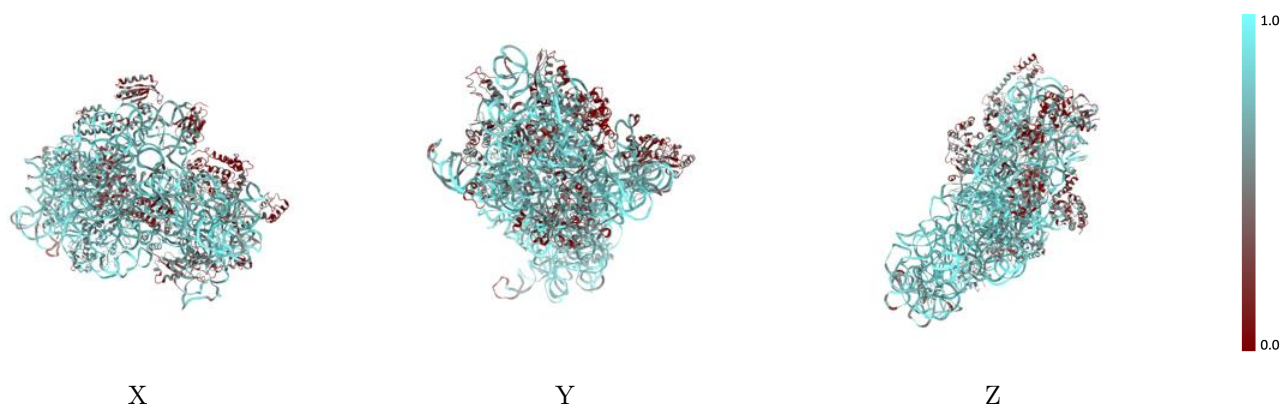
The images above show the 3D surface view of the map at the recommended contour level 0.0309 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



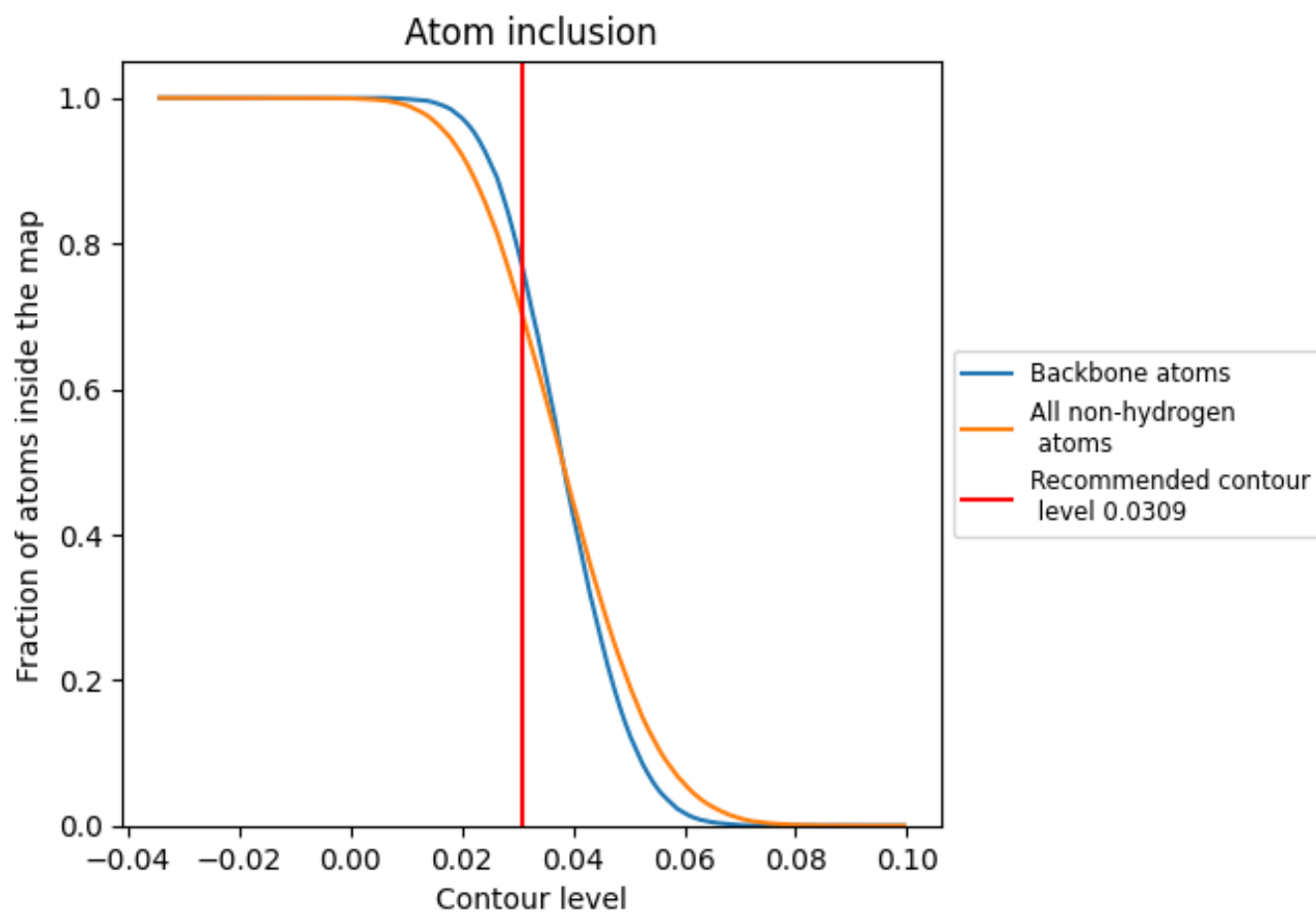
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0309).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.0309) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7025	 0.2320
A	 0.8417	 0.2390
B	 0.3459	 0.1380
C	 0.5475	 0.2460
D	 0.6274	 0.2430
E	 0.6630	 0.2670
F	 0.3204	 0.2100
G	 0.1600	 0.2100
H	 0.6412	 0.2650
I	 0.4556	 0.2130
J	 0.4074	 0.2360
K	 0.3231	 0.2140
L	 0.6848	 0.2930
M	 0.3644	 0.2070
N	 0.5185	 0.1930
O	 0.5519	 0.2220
P	 0.6683	 0.2600
Q	 0.6361	 0.2610
R	 0.4156	 0.1950
S	 0.4926	 0.2000
T	 0.6308	 0.2190
Z	 0.3285	 0.1930

