



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 07:38 AM EST

PDB ID : 6PPK
EMDB ID : EMD-20441
Title : RbgA+45SRbgA complex
Authors : Ortega, J.
Deposited on : 2019-07-07
Resolution : 4.40 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev43
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

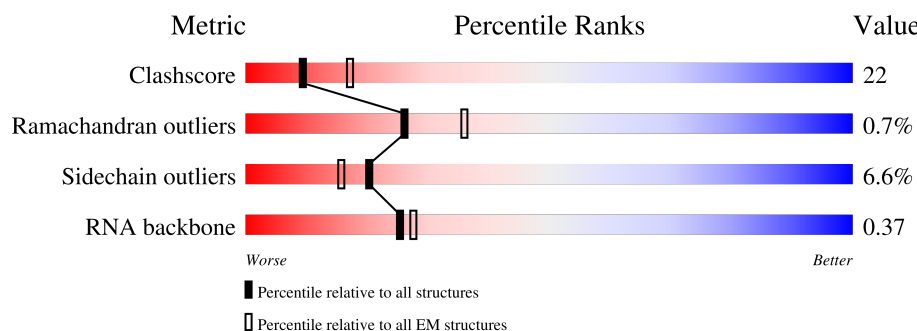
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





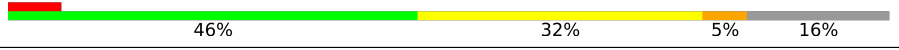

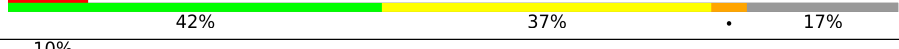
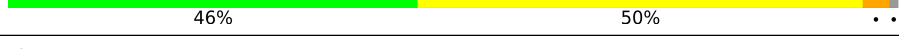

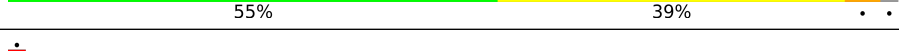
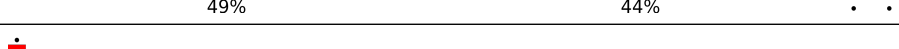
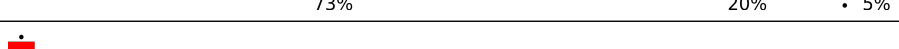




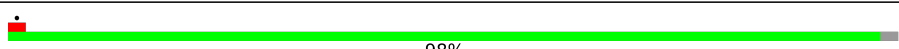


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2927	
2	B	119	
3	C	277	
4	D	209	
5	E	207	
6	F	179	
7	G	179	

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Mol	Chain	Length	Quality of chain
8	J	145	
9	K	122	
10	L	146	
11	N	120	
12	O	120	
13	P	115	
14	Q	118	
15	R	102	
16	S	113	
17	T	95	
18	U	103	
19	V	94	
20	Z	59	
21	b	59	
22	Y	66	
23	d	44	
24	W	282	

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
25	GNP	W	301	-	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 80451 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2658	Total	C	N	O	P	0	0
			57112	25477	10569	18408	2658		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2395	1068	435	780	112		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	260	Total	C	N	O	S	0	0
			2010	1253	392	359	6		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	197	Total	C	N	O	S	0	0
			1511	951	280	278	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	139	Total	C	N	O	S	0	0
			1090	694	190	199	7		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	109	Total	C	N	O	S	0	0
			829	518	153	157	1		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	141	Total	C	N	O	S	0	0
			1119	708	205	201	5		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	122	Total	C	N	O	S	0	0
			904	561	171	171	1		

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	118	Total	C	N	O	S	0	0
			947	580	185	178	4		

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	100	Total	C	N	O	0	0
			775	483	154	138		

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	114	Total	C	N	O	0	0
			936	595	184	157		

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	100	Total	C	N	O	S	0	0
			781	498	138	145			

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	90	Total	C	N	O	S	0	0
			724	452	133	136	3		

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	91	Total	C	N	O	S	0	0
			691	438	129	121	3		

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	78	Total	C	N	O	S	0	0
			604	375	118	111			

- Molecule 20 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 21 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

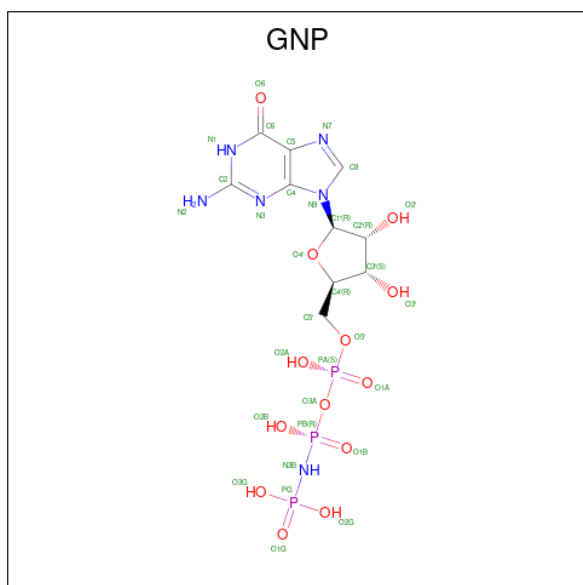
- Molecule 23 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	43	Total	C	N	O	S	0	0
			359	217	88	53	1		

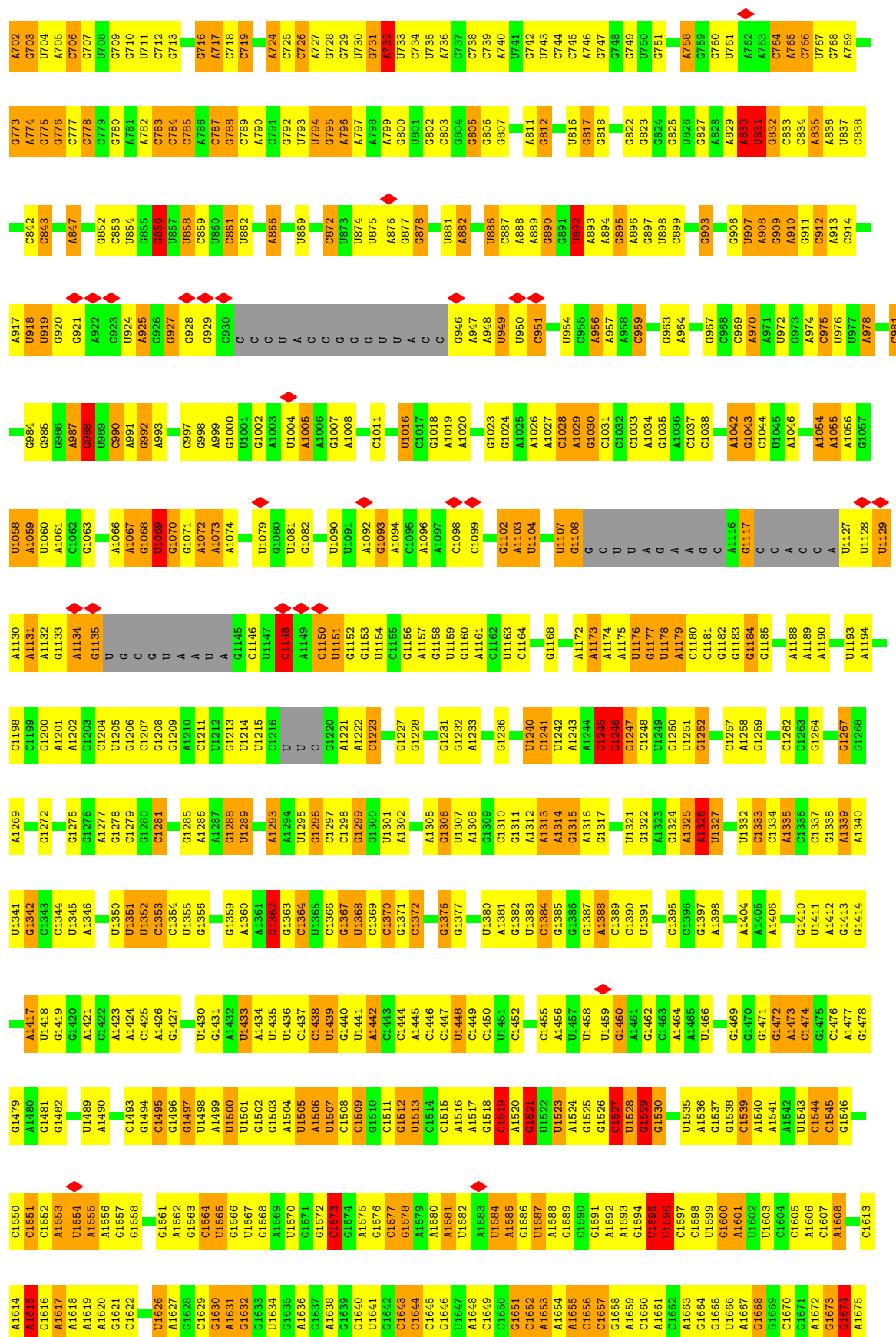
- Molecule 24 is a protein called Ribosome biogenesis GTPase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	252	Total	C	N	O	S	0	0
			1958	1250	343	359	6		

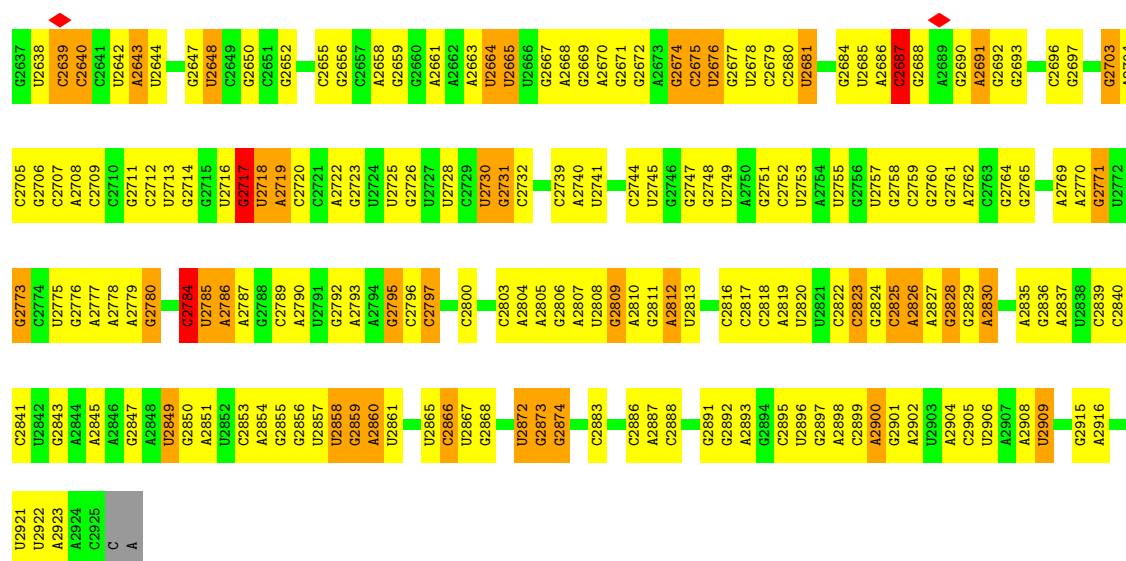
- Molecule 25 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



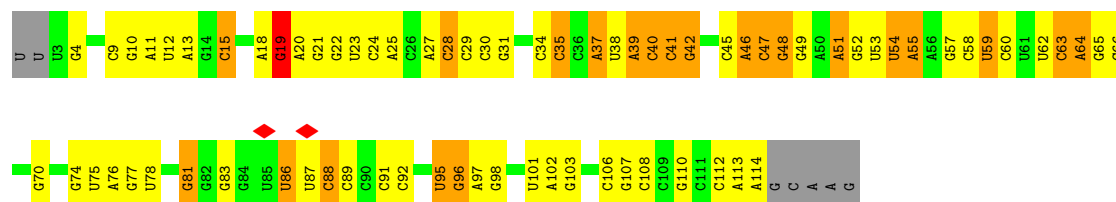
Mol	Chain	Residues	Atoms					AltConf
25	W	1	Total	C	N	O	P	0
			32	10	6	13	3	



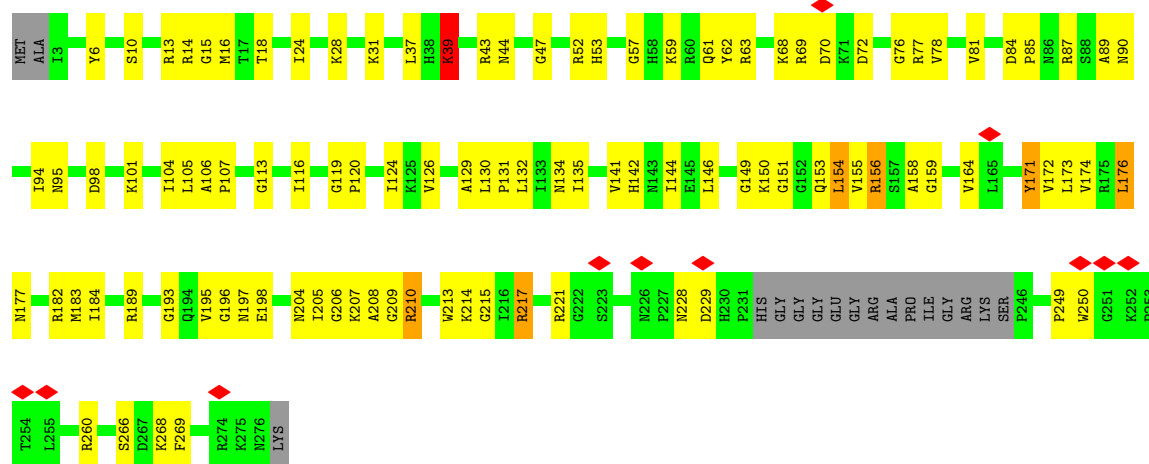




- Molecule 2: 5S rRNA

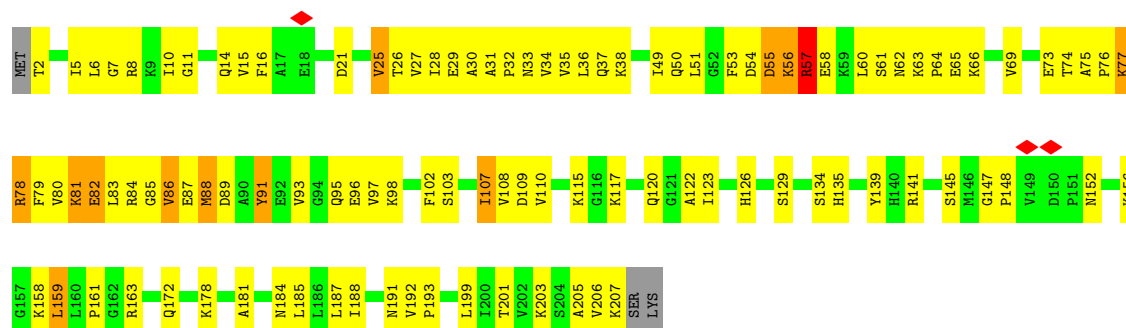


- Molecule 3: 50S ribosomal protein L2

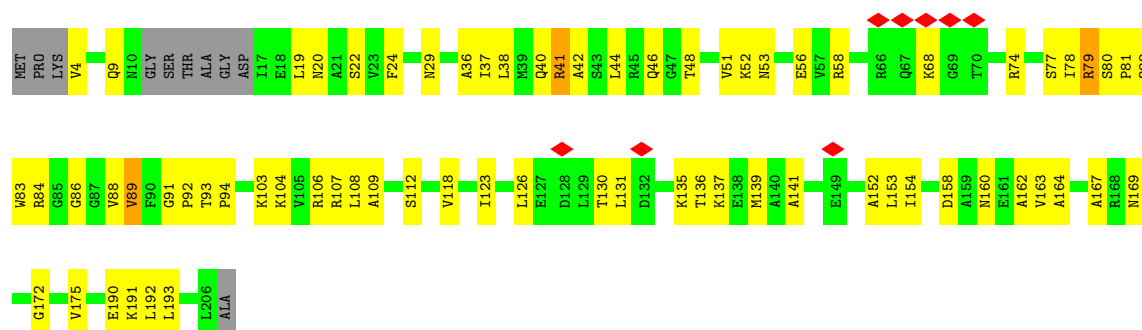


- Molecule 4: 50S ribosomal protein L3

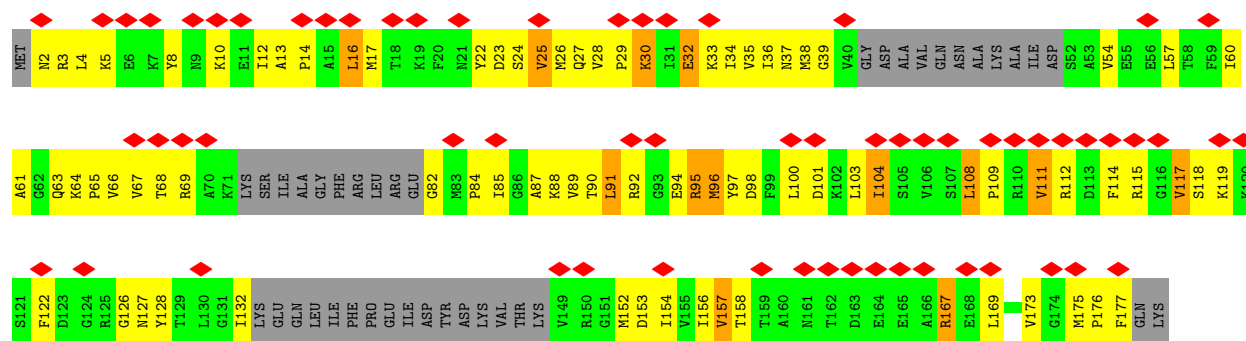




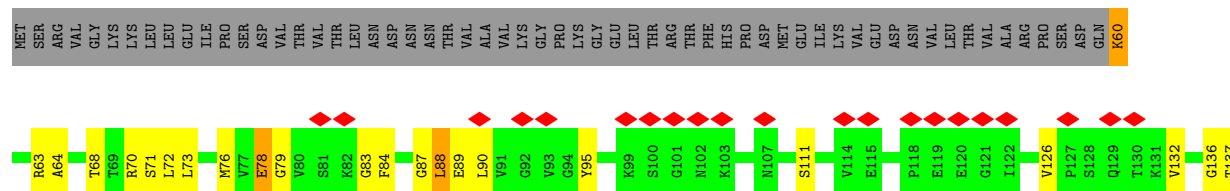
• Molecule 5: 50S ribosomal protein L4

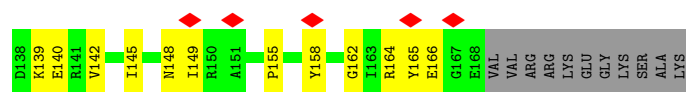


• Molecule 6: 50S ribosomal protein L5

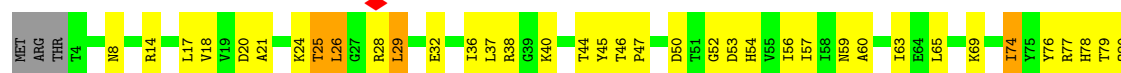


• Molecule 7: 50S ribosomal protein L6

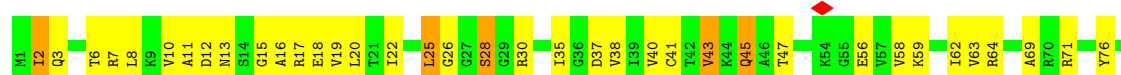




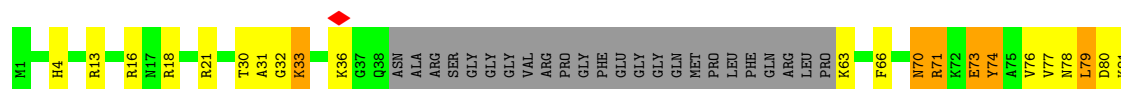
- Molecule 8: 50S ribosomal protein L13



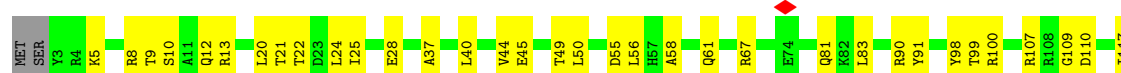
- Molecule 9: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L15

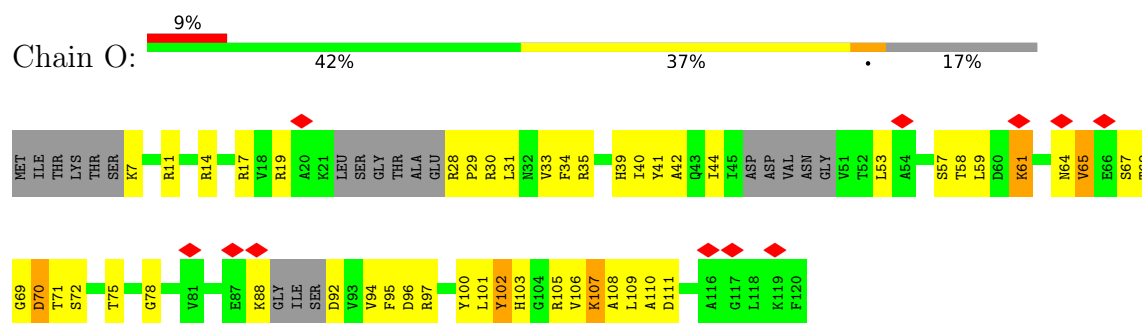


- Molecule 11: 50S ribosomal protein L17

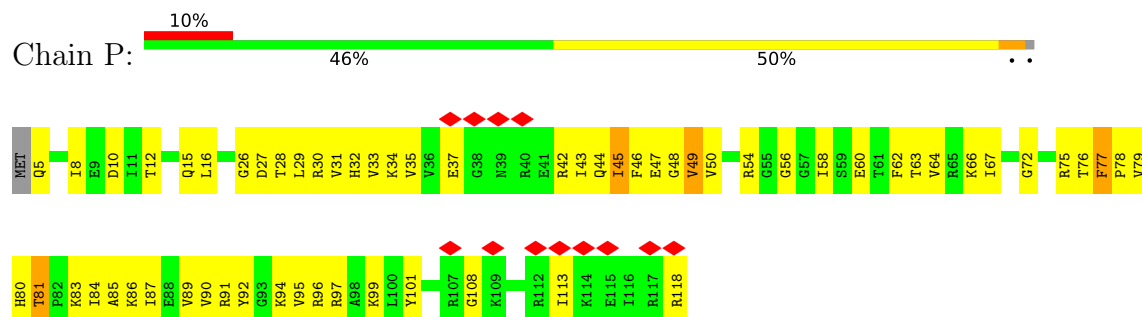


- Molecule 12: 50S ribosomal protein L18

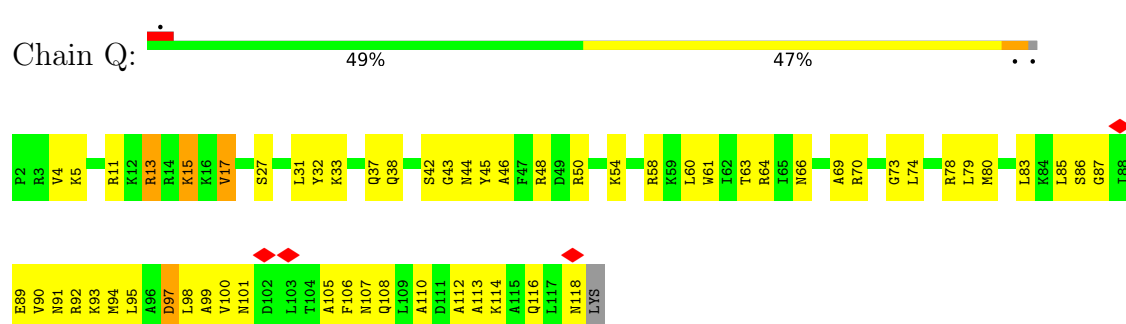




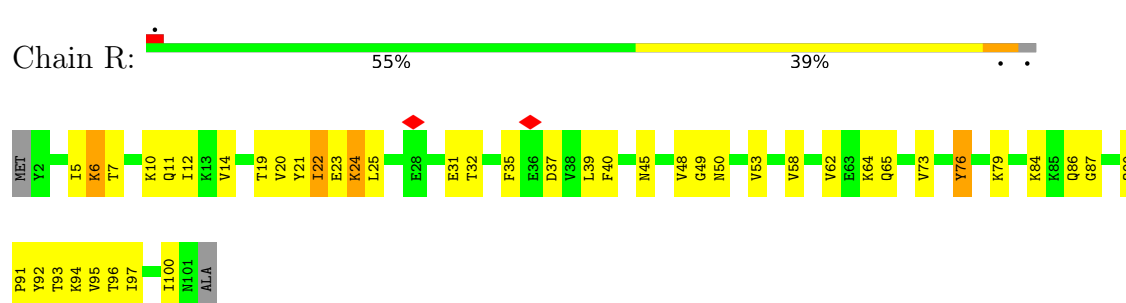
• Molecule 13: 50S ribosomal protein L19



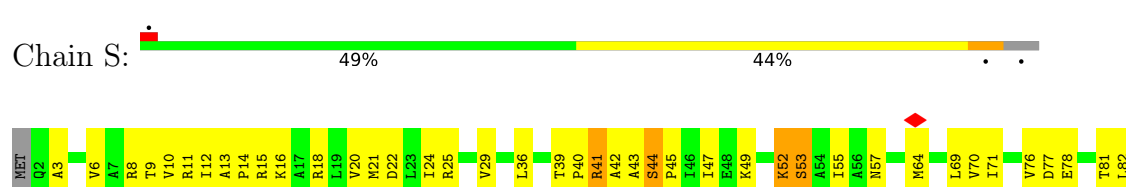
• Molecule 14: 50S ribosomal protein L20



• Molecule 15: 50S ribosomal protein L21



• Molecule 16: 50S ribosomal protein L22

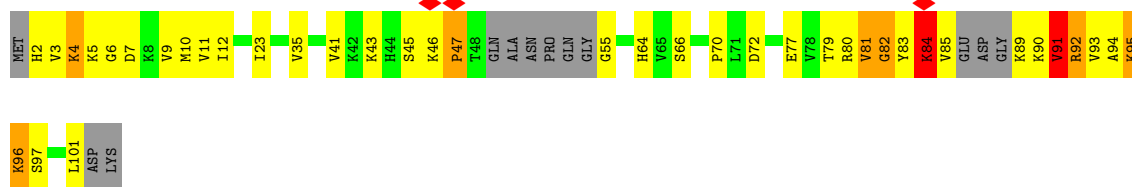




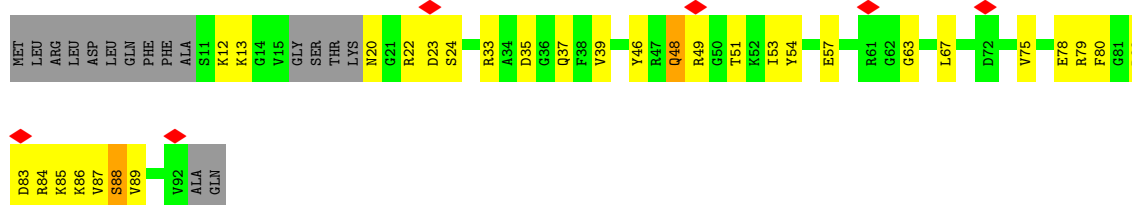
- Molecule 17: 50S ribosomal protein L23



- Molecule 18: 50S ribosomal protein L24



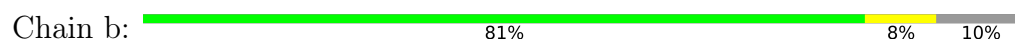
- Molecule 19: 50S ribosomal protein L27



- Molecule 20: 50S ribosomal protein L30

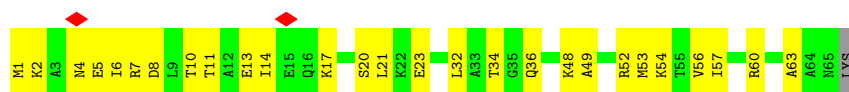


- Molecule 21: 50S ribosomal protein L32



- Molecule 22: 50S ribosomal protein L29

Chain Y:  58% 41%




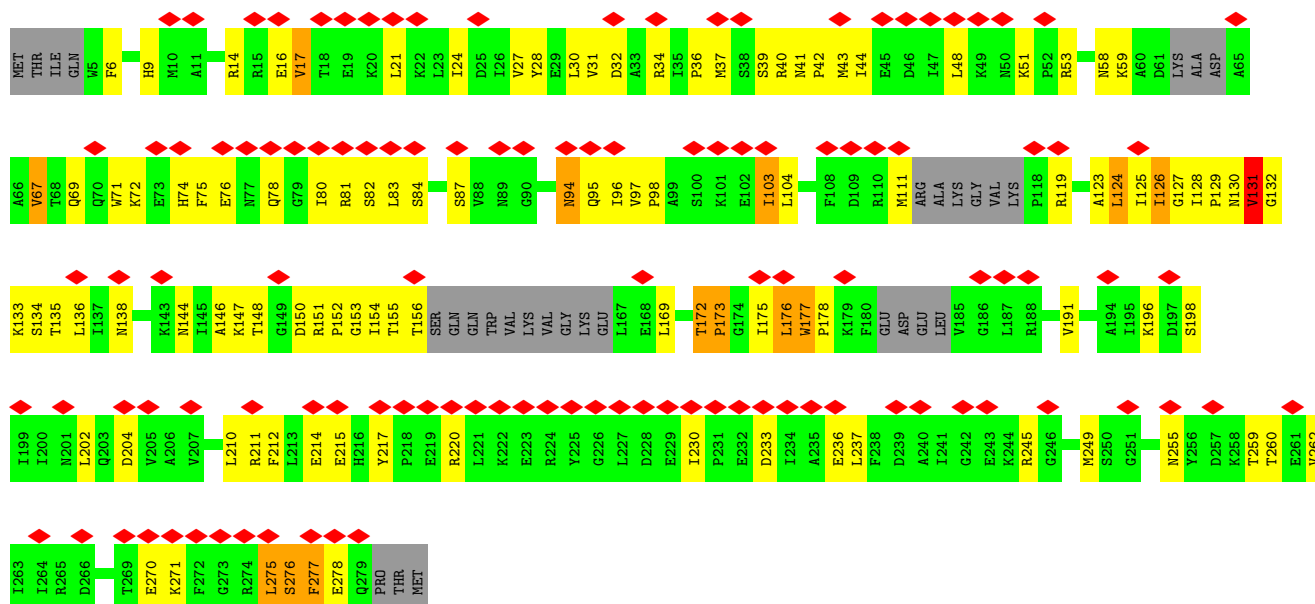
- Molecule 23: 50S ribosomal protein L34

Chain d:  98%



- Molecule 24: Ribosome biogenesis GTPase A

Chain W:  41% 50% 34% 5% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81392	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP

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	1.04	14/63968 (0.0%)	1.25	497/99771 (0.5%)
2	B	0.62	0/2678	1.18	21/4174 (0.5%)
3	C	0.41	0/2044	0.59	1/2741 (0.0%)
4	D	0.38	0/1591	0.59	2/2132 (0.1%)
5	E	0.43	0/1528	0.59	0/2061
6	F	0.21	0/1102	0.37	0/1476
7	G	0.30	0/841	0.54	1/1130 (0.1%)
8	J	0.36	0/1142	0.52	0/1537
9	K	0.38	0/927	0.81	7/1245 (0.6%)
10	L	0.33	0/910	0.47	0/1210
11	N	0.44	0/954	0.61	0/1276
12	O	0.26	0/781	0.48	0/1042
13	P	0.37	0/949	0.62	1/1269 (0.1%)
14	Q	0.51	0/952	0.56	0/1266
15	R	0.48	1/792 (0.1%)	0.56	0/1063
16	S	0.43	0/851	0.54	0/1146
17	T	0.46	0/730	0.60	0/974
18	U	0.34	0/698	0.60	2/929 (0.2%)
19	V	0.40	0/611	0.77	3/810 (0.4%)
20	Z	0.33	0/457	0.50	0/613
21	b	0.40	0/425	0.59	0/563
22	Y	0.35	0/531	0.51	0/707
23	d	0.54	0/362	0.56	0/473
24	W	0.29	0/1987	0.51	0/2680
All	All	0.91	15/87811 (0.0%)	1.14	535/132288 (0.4%)

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
5	E	0	1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	A	N9-C4	-6.73	1.33	1.37
1	A	830	A	N9-C4	-6.22	1.34	1.37
1	A	630	A	N9-C4	-6.14	1.34	1.37
1	A	2860	A	N9-C4	-5.97	1.34	1.37
1	A	1679	A	N9-C4	-5.71	1.34	1.37

The worst 5 of 535 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	2	ILE	CB-CA-C	12.98	137.56	111.60
19	V	82	ARG	CB-CA-C	11.91	134.21	110.40
1	A	1352	U	C2-N1-C1'	11.62	131.65	117.70
1	A	2825	C	C2-N1-C1'	11.49	131.44	118.80
1	A	2825	C	N1-C2-O2	11.39	125.73	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	41	ARG	Peptide

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	57112	0	28735	1143	0
2	B	2395	0	1212	66	0
3	C	2010	0	2100	138	0
4	D	1569	0	1635	190	0
5	E	1511	0	1598	59	0
6	F	1090	0	1136	203	0
7	G	829	0	851	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	1119	0	1159	94	0
9	K	920	0	977	75	0
10	L	904	0	957	77	0
11	N	947	0	978	33	0
12	O	775	0	807	79	0
13	P	936	0	1008	92	0
14	Q	940	0	1005	76	0
15	R	781	0	820	66	0
16	S	842	0	899	71	0
17	T	724	0	768	15	0
18	U	691	0	755	87	0
19	V	604	0	614	59	0
20	Z	455	0	491	19	0
21	b	418	0	439	0	0
22	Y	530	0	568	34	0
23	d	359	0	398	0	0
24	W	1958	0	1979	203	0
25	W	32	0	13	10	0
All	All	80451	0	51902	2529	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 22.

The worst 5 of 2529 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)
10:L:117:LEU:CD2	10:L:136:VAL:HA	1.29	1.58
6:F:122:PHE:CE2	6:F:167:ARG:NH2	1.69	1.57
8:J:26:LEU:HA	8:J:29:LEU:CD1	1.40	1.50
13:P:33:VAL:HG21	13:P:77:PHE:CZ	1.48	1.47
24:W:81:ARG:NH1	24:W:103:ILE:CG1	1.79	1.45

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	256/277 (92%)	230 (90%)	24 (9%)	2 (1%)	19	60
4	D	204/209 (98%)	176 (86%)	27 (13%)	1 (0%)	29	68
5	E	193/207 (93%)	167 (86%)	26 (14%)	0	100	100
6	F	131/179 (73%)	114 (87%)	14 (11%)	3 (2%)	6	37
7	G	107/179 (60%)	93 (87%)	14 (13%)	0	100	100
8	J	139/145 (96%)	122 (88%)	17 (12%)	0	100	100
9	K	120/122 (98%)	100 (83%)	20 (17%)	0	100	100
10	L	118/146 (81%)	101 (86%)	16 (14%)	1 (1%)	19	60
11	N	116/120 (97%)	108 (93%)	8 (7%)	0	100	100
12	O	92/120 (77%)	84 (91%)	8 (9%)	0	100	100
13	P	112/115 (97%)	98 (88%)	13 (12%)	1 (1%)	17	56
14	Q	115/118 (98%)	105 (91%)	10 (9%)	0	100	100
15	R	98/102 (96%)	82 (84%)	15 (15%)	1 (1%)	15	54
16	S	107/113 (95%)	97 (91%)	9 (8%)	1 (1%)	17	56
17	T	88/95 (93%)	77 (88%)	11 (12%)	0	100	100
18	U	85/103 (82%)	62 (73%)	19 (22%)	4 (5%)	2	24
19	V	74/94 (79%)	67 (90%)	7 (10%)	0	100	100
20	Z	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
21	b	51/59 (86%)	42 (82%)	9 (18%)	0	100	100
22	Y	63/66 (96%)	55 (87%)	8 (13%)	0	100	100
23	d	41/44 (93%)	38 (93%)	3 (7%)	0	100	100
24	W	242/282 (86%)	213 (88%)	26 (11%)	3 (1%)	13	50
All	All	2608/2954 (88%)	2283 (88%)	308 (12%)	17 (1%)	26	62

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	R	24	LYS
16	S	90	MET
18	U	82	GLY
24	W	172	THR
3	C	215	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	215/225 (96%)	209 (97%)	6 (3%)	43 65
4	D	167/170 (98%)	150 (90%)	17 (10%)	7 27
5	E	164/170 (96%)	162 (99%)	2 (1%)	71 84
6	F	120/154 (78%)	106 (88%)	14 (12%)	5 23
7	G	88/151 (58%)	82 (93%)	6 (7%)	16 43
8	J	120/123 (98%)	112 (93%)	8 (7%)	16 43
9	K	101/101 (100%)	98 (97%)	3 (3%)	41 63
10	L	93/110 (84%)	75 (81%)	18 (19%)	1 9
11	N	98/100 (98%)	98 (100%)	0	100 100
12	O	77/93 (83%)	68 (88%)	9 (12%)	5 23
13	P	99/100 (99%)	94 (95%)	5 (5%)	24 50
14	Q	96/97 (99%)	89 (93%)	7 (7%)	14 41
15	R	83/84 (99%)	80 (96%)	3 (4%)	35 60
16	S	90/93 (97%)	85 (94%)	5 (6%)	21 48
17	T	81/85 (95%)	78 (96%)	3 (4%)	34 59
18	U	78/87 (90%)	65 (83%)	13 (17%)	2 14
19	V	61/74 (82%)	59 (97%)	2 (3%)	38 61
20	Z	52/53 (98%)	50 (96%)	2 (4%)	33 58
21	b	47/53 (89%)	42 (89%)	5 (11%)	6 26
22	Y	56/57 (98%)	54 (96%)	2 (4%)	35 60
23	d	38/39 (97%)	38 (100%)	0	100 100
24	W	205/244 (84%)	188 (92%)	17 (8%)	11 37
All	All	2229/2463 (90%)	2082 (93%)	147 (7%)	20 43

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	U	92	ARG
24	W	177	TRP
19	V	48	GLN
24	W	17	VAL
8	J	54	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
13	P	80	HIS
24	W	9	HIS
14	Q	107	ASN
24	W	216	HIS
22	Y	36	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2643/2927 (90%)	955 (36%)	55 (2%)
2	B	111/119 (93%)	38 (34%)	3 (2%)
All	All	2754/3046 (90%)	993 (36%)	58 (2%)

5 of 993 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	U
1	A	11	G
1	A	13	A
1	A	23	G

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1245	G
2	B	47	C
1	A	1438	C
1	A	2858	U
1	A	2454	A

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](#)

1 ligand 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	$\# Z > 2$
25	GNP	W	301	-	29,34,34	1.78	4 (13%)	33,54,54	2.04	8 (24%)

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
25	GNP	W	301	-	-	3/14/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	301	GNP	PG-N3B	4.63	1.75	1.63
25	W	301	GNP	PB-N3B	4.60	1.75	1.63
25	W	301	GNP	C5-C6	4.21	1.48	1.41
25	W	301	GNP	C5-C4	2.47	1.47	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	W	301	GNP	C2-N3-C4	4.95	121.02	115.36
25	W	301	GNP	C2-N1-C6	4.02	122.32	115.93
25	W	301	GNP	C5-C6-N1	-3.98	117.99	123.43
25	W	301	GNP	C4-C5-C6	-3.75	117.21	120.80
25	W	301	GNP	PB-O3A-PA	-3.47	120.41	132.62

There are no chirality outliers.

All (3) torsion outliers are listed below:

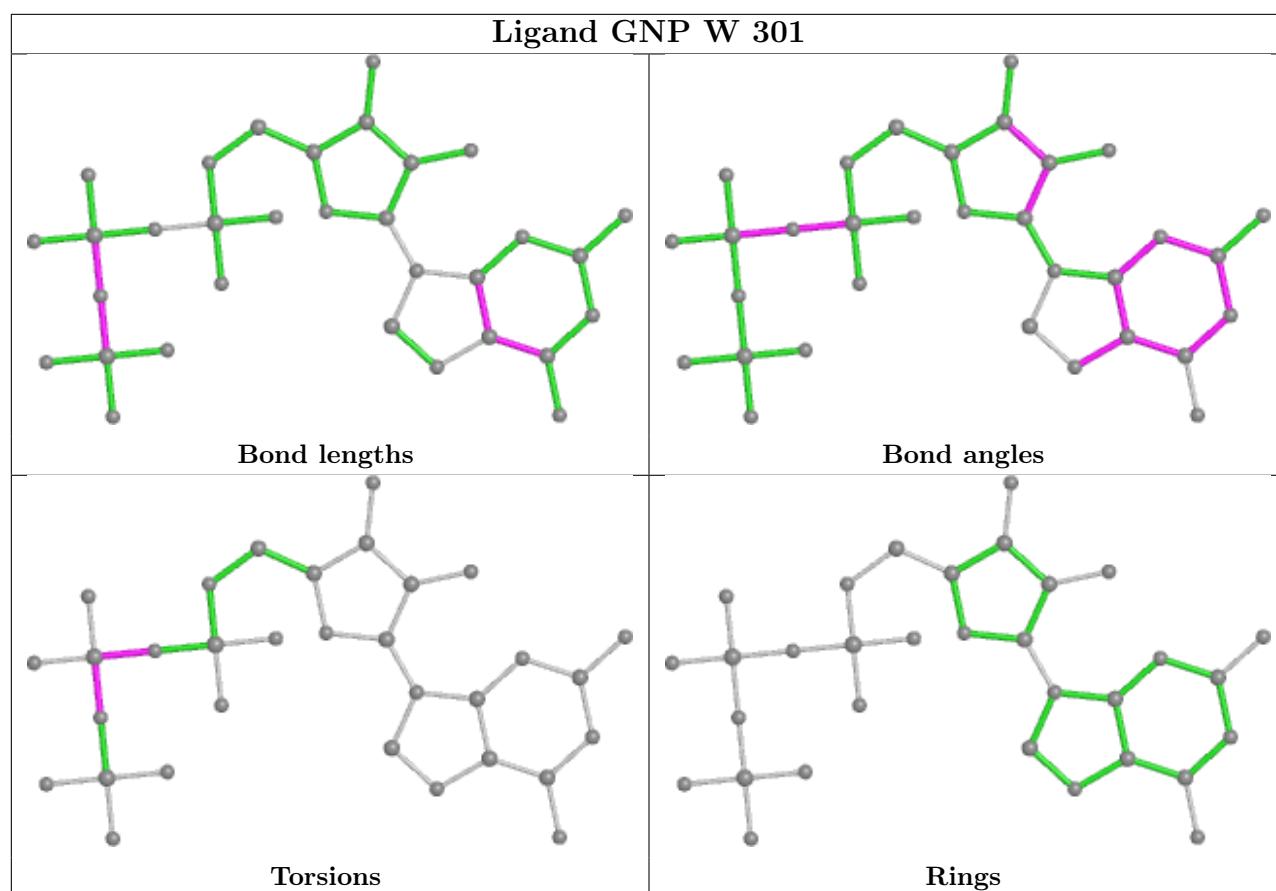
Mol	Chain	Res	Type	Atoms
25	W	301	GNP	PG-N3B-PB-O1B
25	W	301	GNP	PA-O3A-PB-O1B
25	W	301	GNP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	W	301	GNP	10	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](#)

There are no chain breaks in this entry.

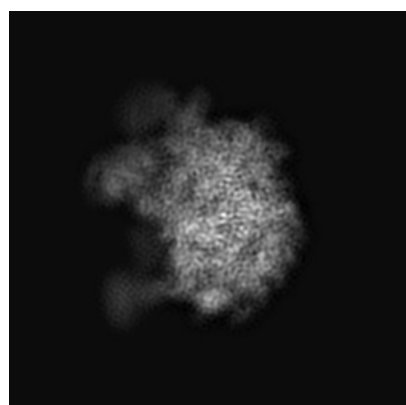
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20441. These allow visual inspection of the internal detail of the map and identification of artifacts.

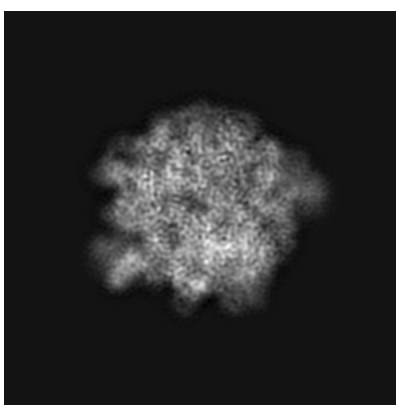
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

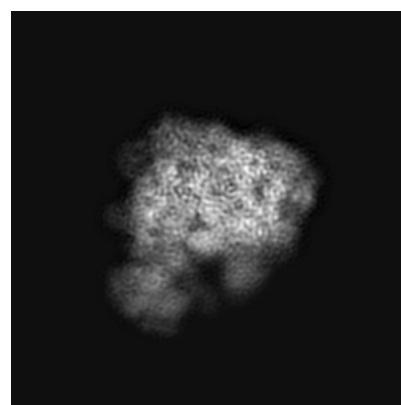
6.1.1 Primary map



X



Y

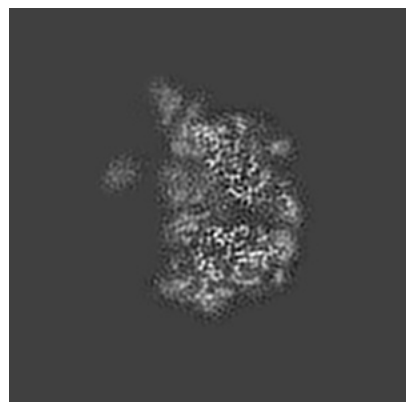


Z

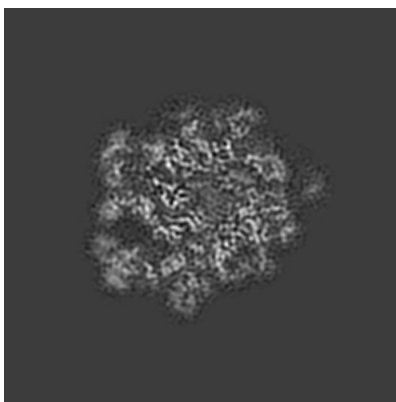
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

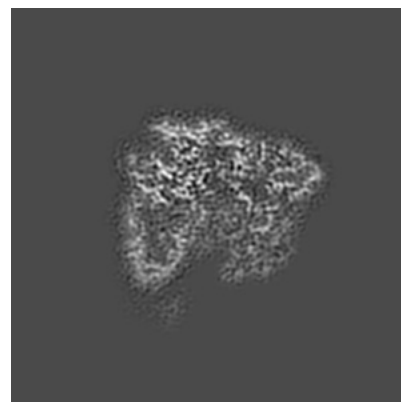
6.2.1 Primary map



X Index: 120



Y Index: 120

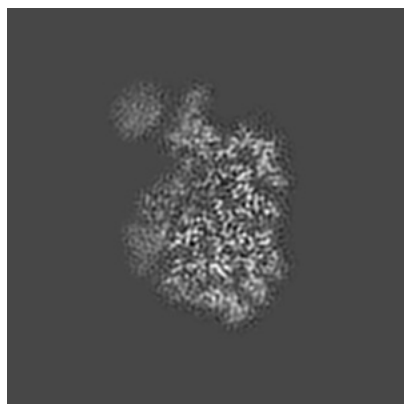


Z Index: 120

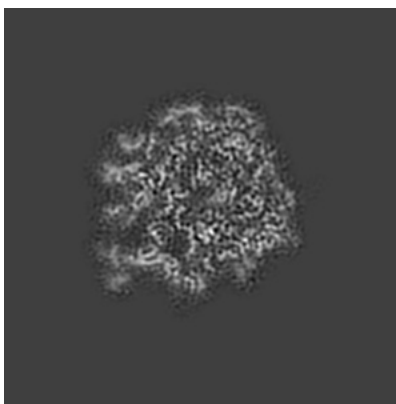
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

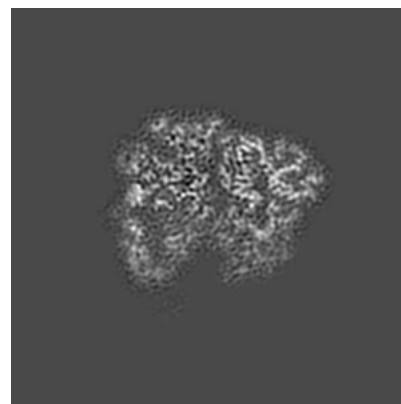
6.3.1 Primary map



X Index: 140



Y Index: 127



Z Index: 117

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

6.4 Orthogonal surface views [i](#)

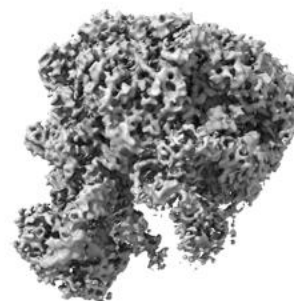
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

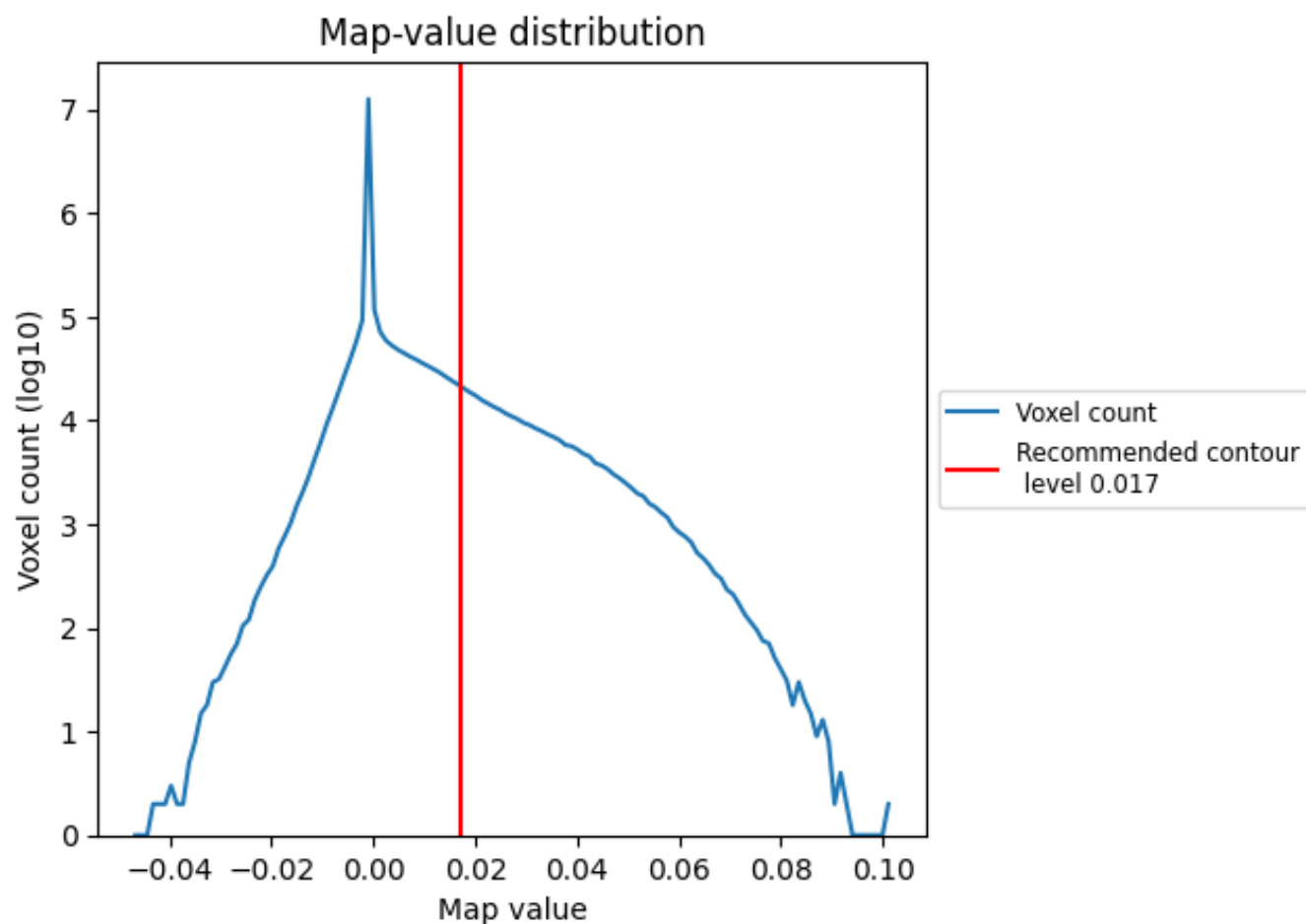
6.5 Mask visualisation

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

7 Map analysis [i](#)

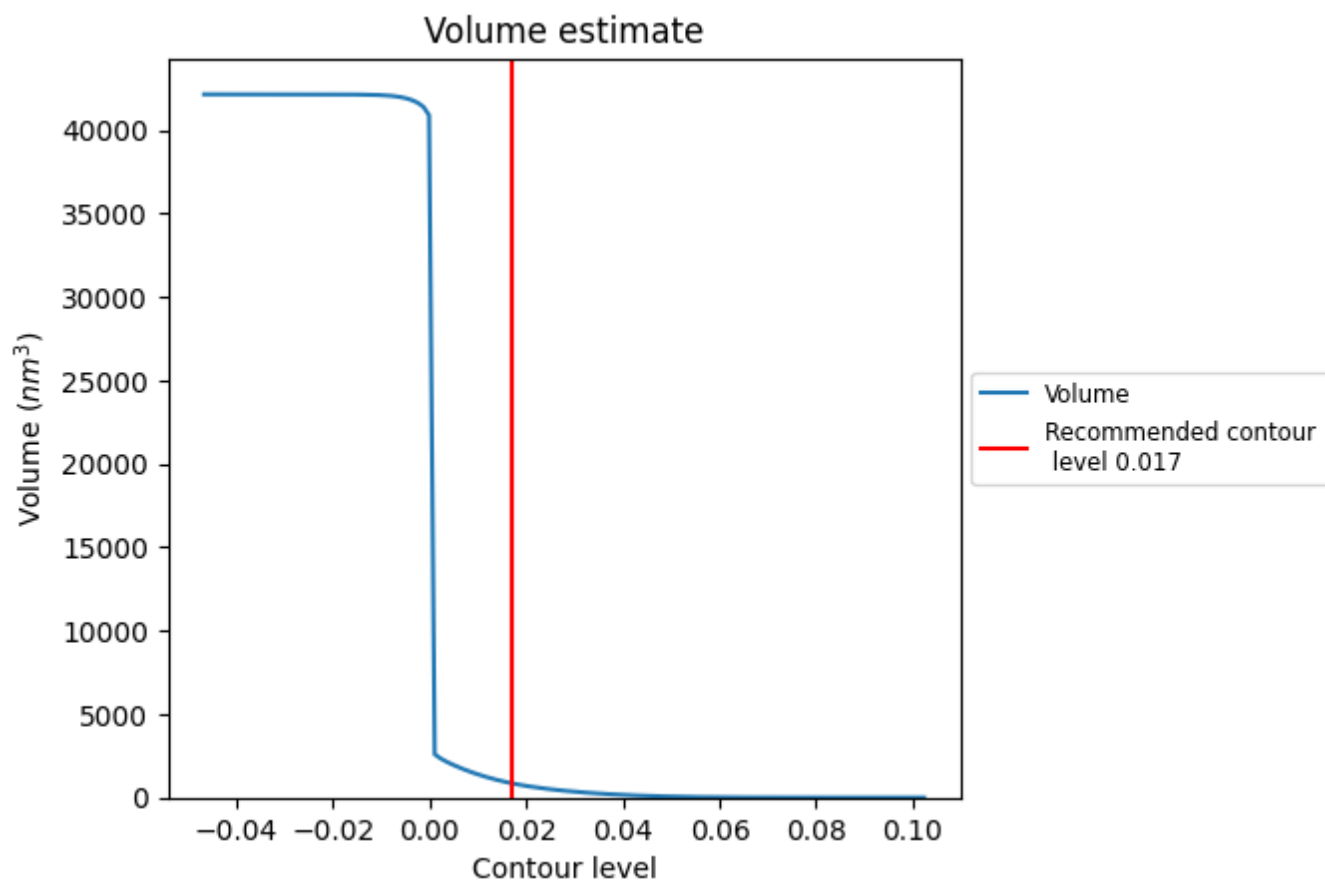
This section contains the results of statistical analysis of the map.

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.

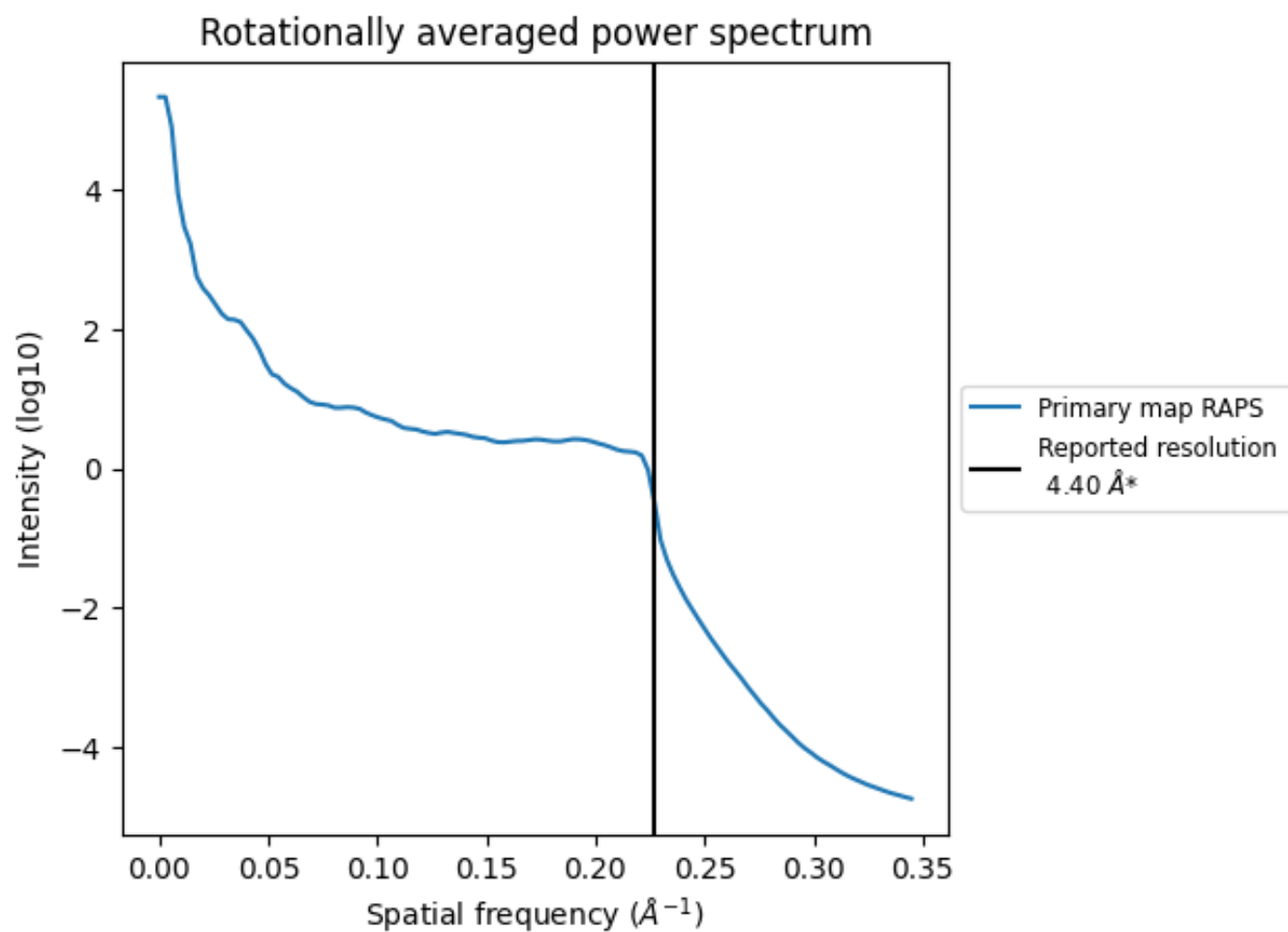
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 855 nm³; this corresponds to an approximate mass of 772 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

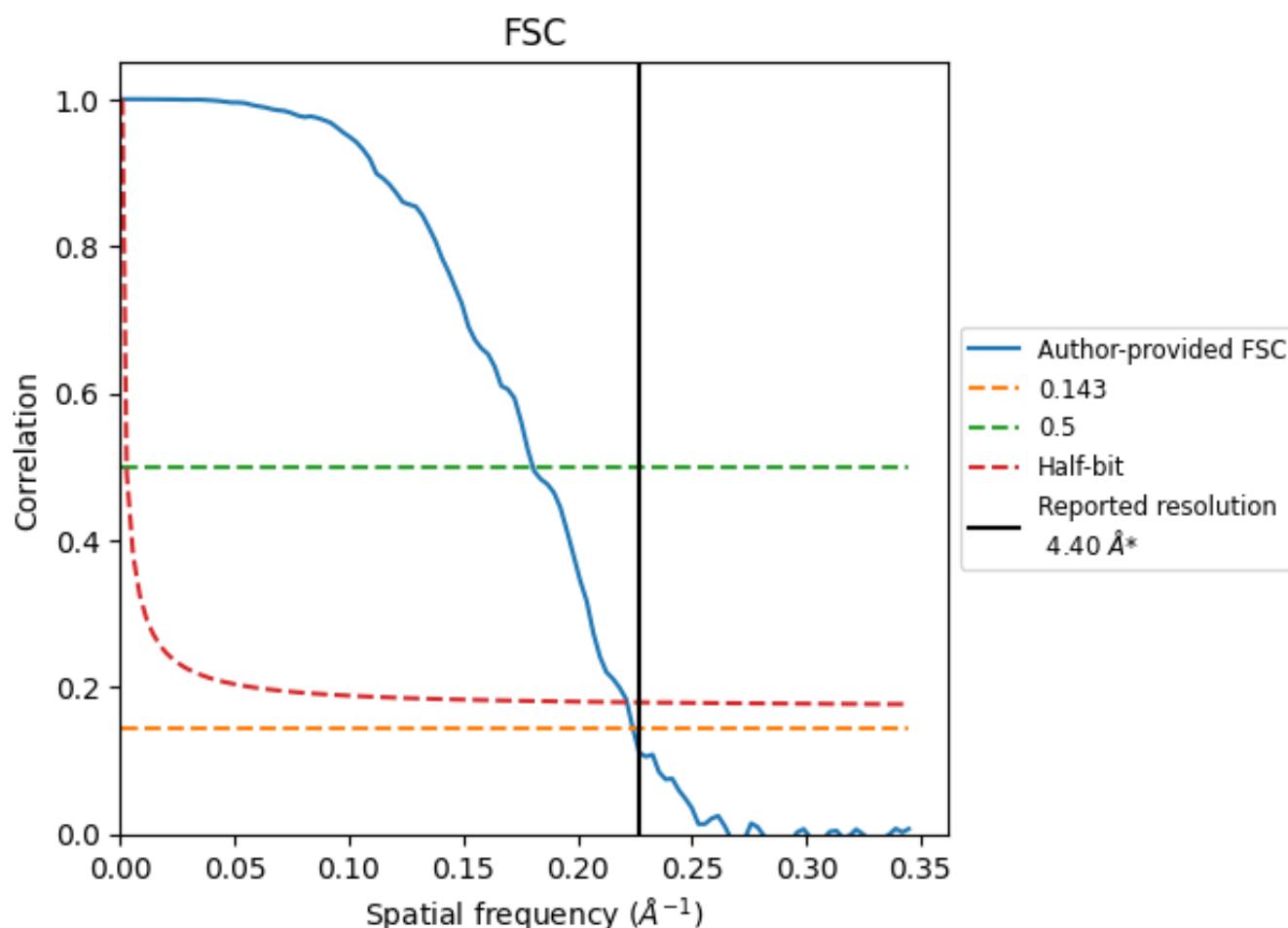


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

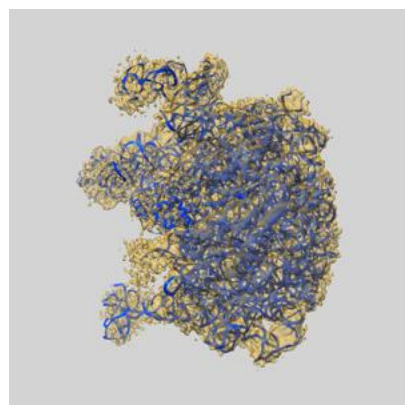
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.46	5.54	4.51
Unmasked-calculated*	-	-	-

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

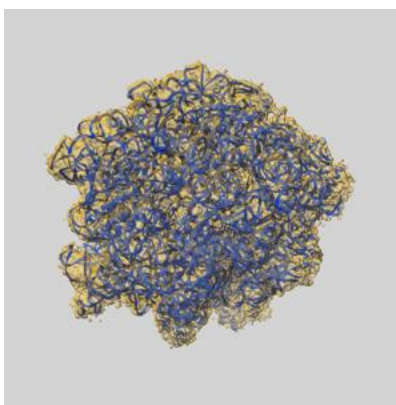
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20441 and PDB model 6PPK. Per-residue inclusion information can be found in section [3](#) on page [8](#).

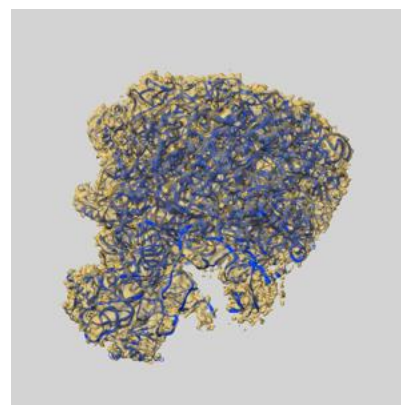
9.1 Map-model overlay [i](#)



X



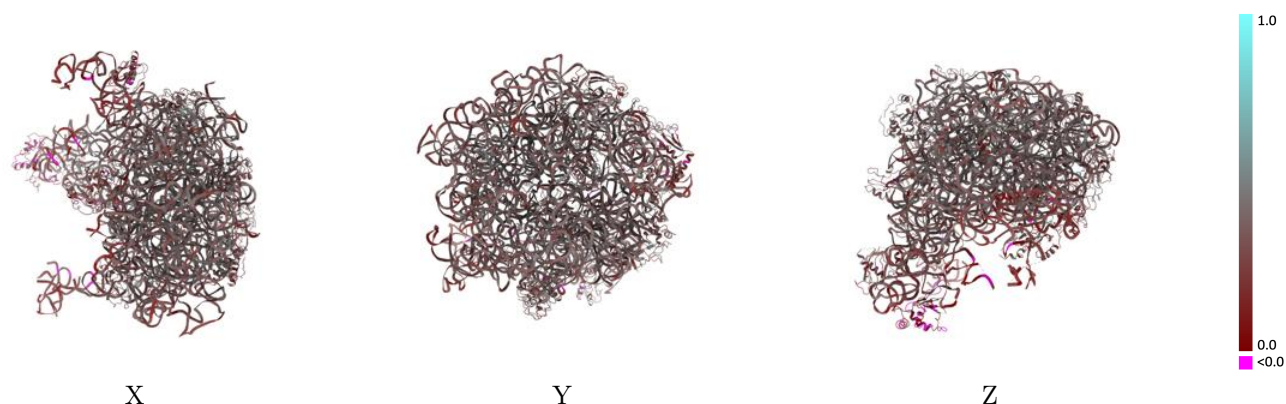
Y



Z

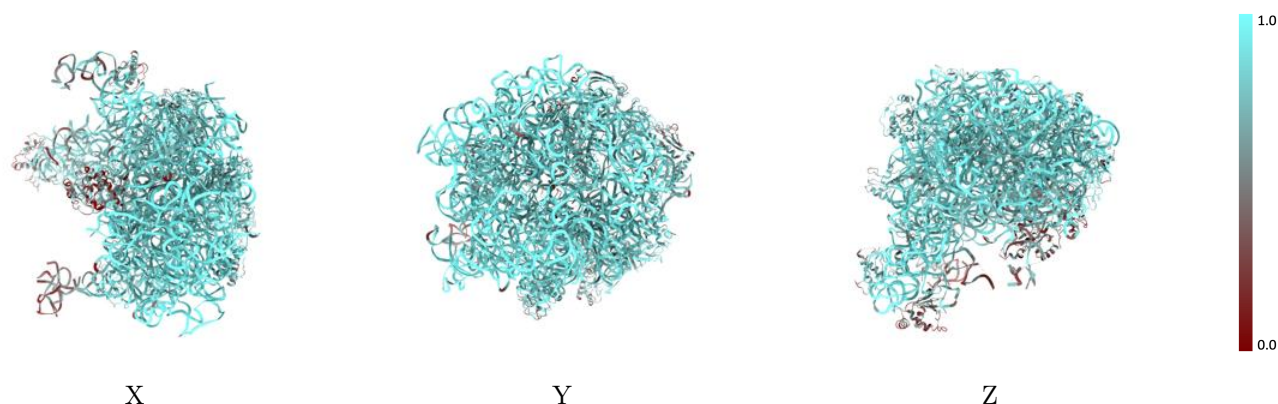
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



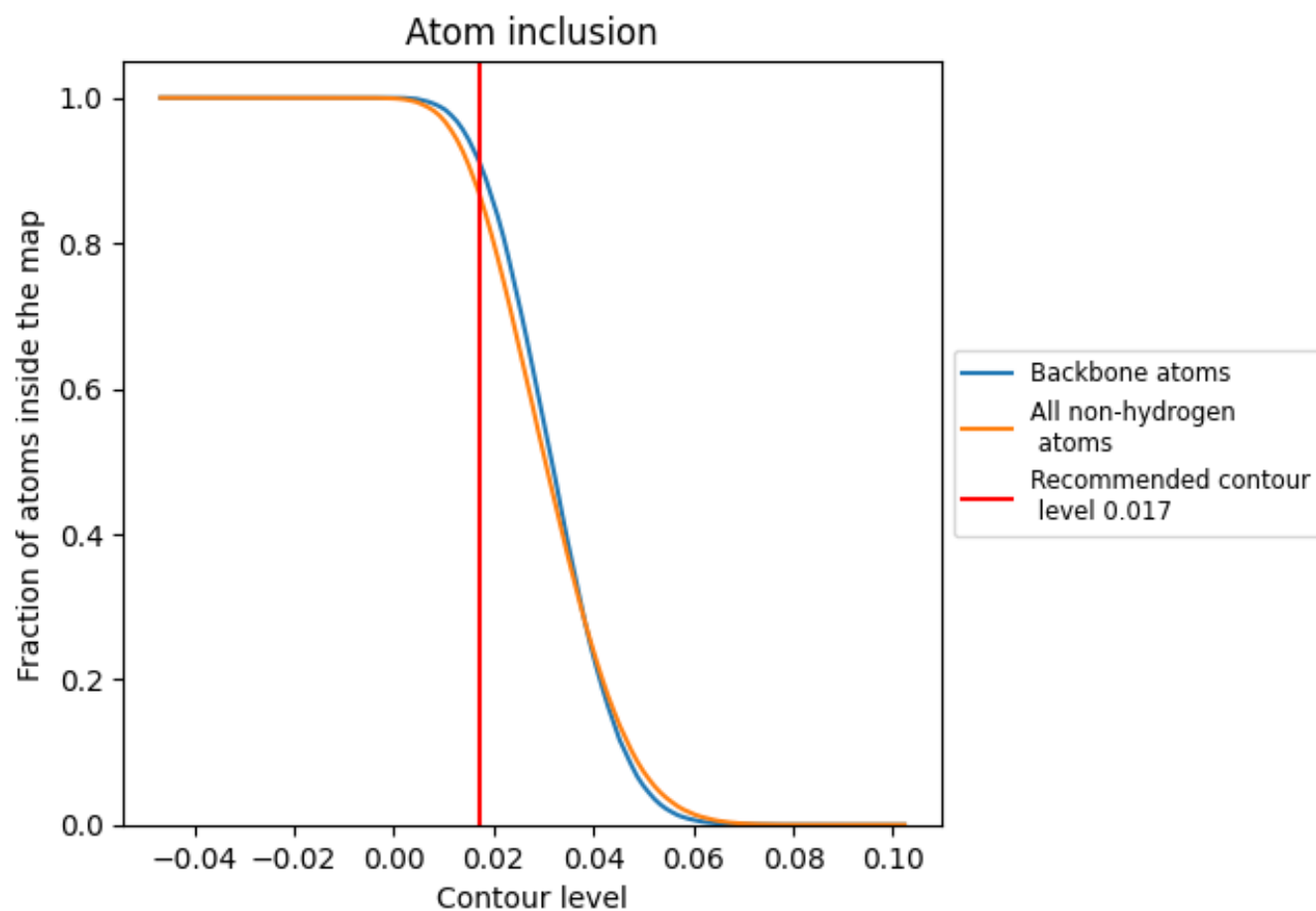
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8707	 0.3540
A	 0.9208	 0.3570
B	 0.8965	 0.3060
C	 0.7983	 0.3770
D	 0.7782	 0.3900
E	 0.7889	 0.3850
F	 0.4268	 0.1090
G	 0.5909	 0.2660
J	 0.7925	 0.3700
K	 0.8027	 0.3930
L	 0.7508	 0.3500
N	 0.8211	 0.3890
O	 0.6907	 0.2740
P	 0.7439	 0.3450
Q	 0.8493	 0.3740
R	 0.8301	 0.4010
S	 0.8059	 0.3960
T	 0.8393	 0.4080
U	 0.7822	 0.3500
V	 0.6981	 0.3630
W	 0.4275	 0.3160
Y	 0.7996	 0.3440
Z	 0.7326	 0.3500
b	 0.8198	 0.3980
d	 0.8754	 0.4290

