



wwPDB EM Validation Summary Report ⓘ

Dec 4, 2024 – 04:38 am GMT

PDB ID : 9GUX
EMDB ID : EMD-51623
Title : 30S-TEC (TEC in expressome position) Inactive state 1
Authors : Rahil, H.; Weixlbaumer, A.; Webster, M.W.
Deposited on : 2024-09-20
Resolution : 3.30 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

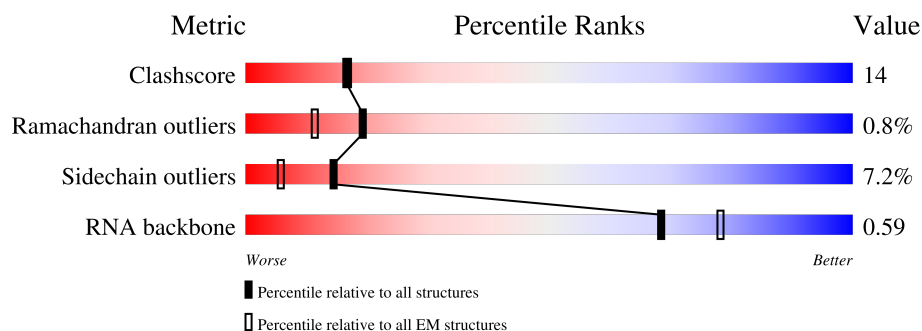
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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
















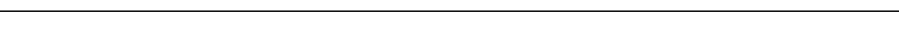


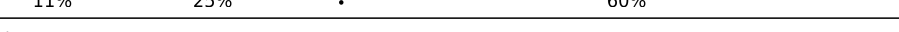
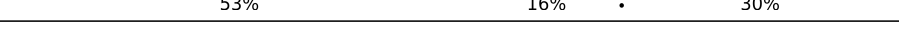





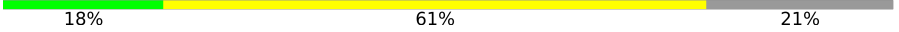
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1542	
2	B	557	
3	C	241	
4	D	233	
5	E	206	
6	F	157	
7	G	131	

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Mol	Chain	Length	Quality of chain
8	H	156	
9	I	130	
10	J	130	
11	K	103	
12	L	129	
13	M	124	
14	N	118	
15	O	101	
16	P	89	
17	Q	82	
18	R	84	
19	S	75	
20	T	92	
21	U	87	
22	V	71	
23	X	53	
24	1	329	
24	2	329	
25	3	1342	
26	4	1406	
27	5	91	
28	Z	180	
29	6	38	
30	7	39	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 81286 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
1	A	1512	Total	C	N	O	P	0	0
			32443	14476	5947	10508	1512		

- Molecule 2 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	260	Total	C	N	O	0	0
			1761	1092	318	351		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 7 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 9 is a protein called 30S ribosomal protein S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			808	504	155	148	1		

- Molecule 12 is a protein called 30S ribosomal protein S11.

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

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 17 is a protein called 30S ribosomal protein S16.

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

- Molecule 18 is a protein called 30S ribosomal protein S17.

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

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 21 is a protein called 30S ribosomal protein S20.

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

- Molecule 22 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	21	Total	C	N	O	P	0	0
			458	204	93	140	21		

- Molecule 24 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
24	2	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 25 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 26 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

- Molecule 27 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 28 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	153	Total	C	N	O	S	0	0
			1225	782	209	227	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	121	ALA	LYS	conflict	UNP P0AFG0

- Molecule 29 is a DNA chain called Non-Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	30	Total	C	N	O	P	0	0
			618	294	114	180	30		

- Molecule 30 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	A	131	Total	Mg	0
			131	131	
31	D	1	Total	Mg	0
			1	1	

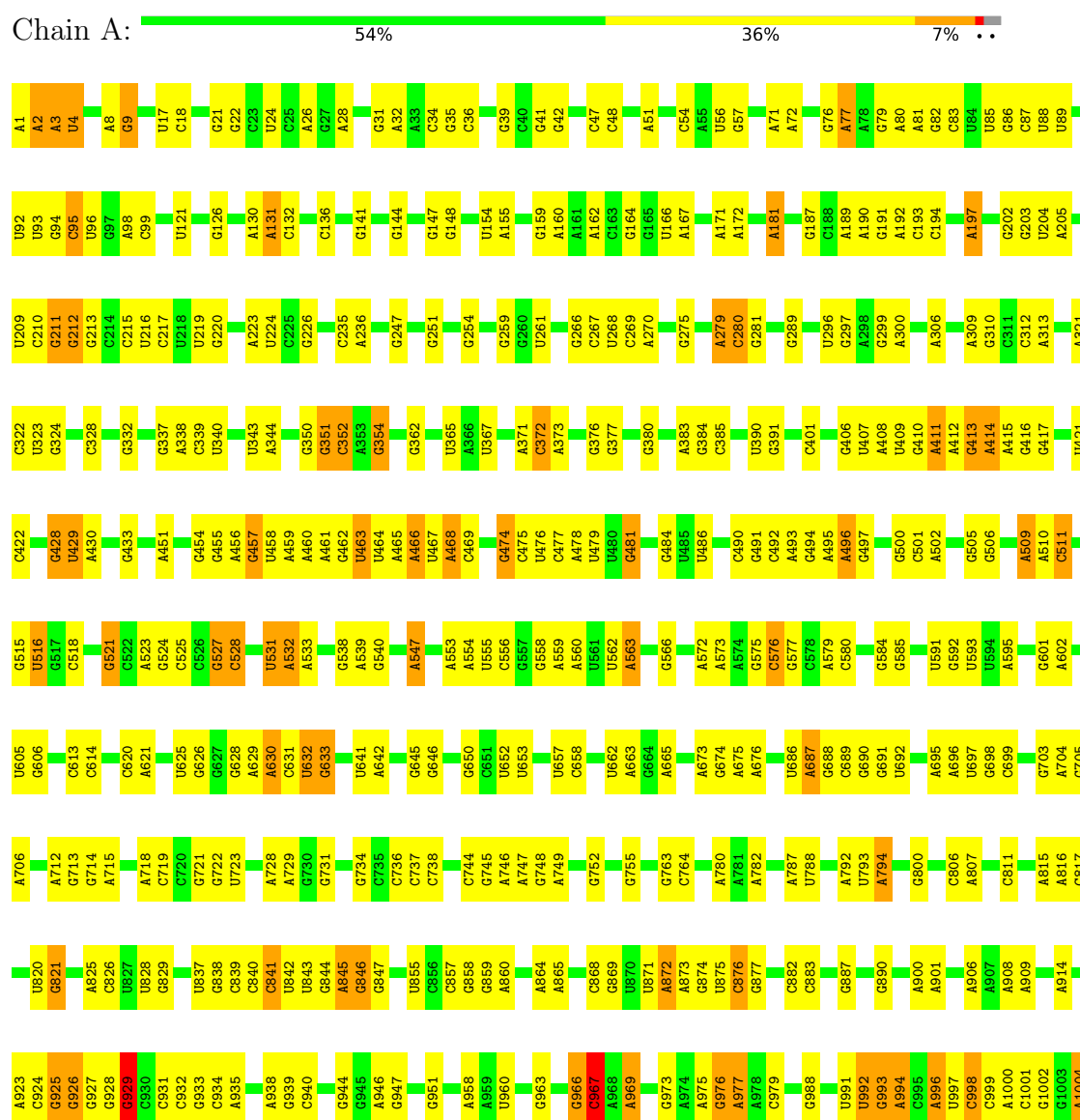
- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

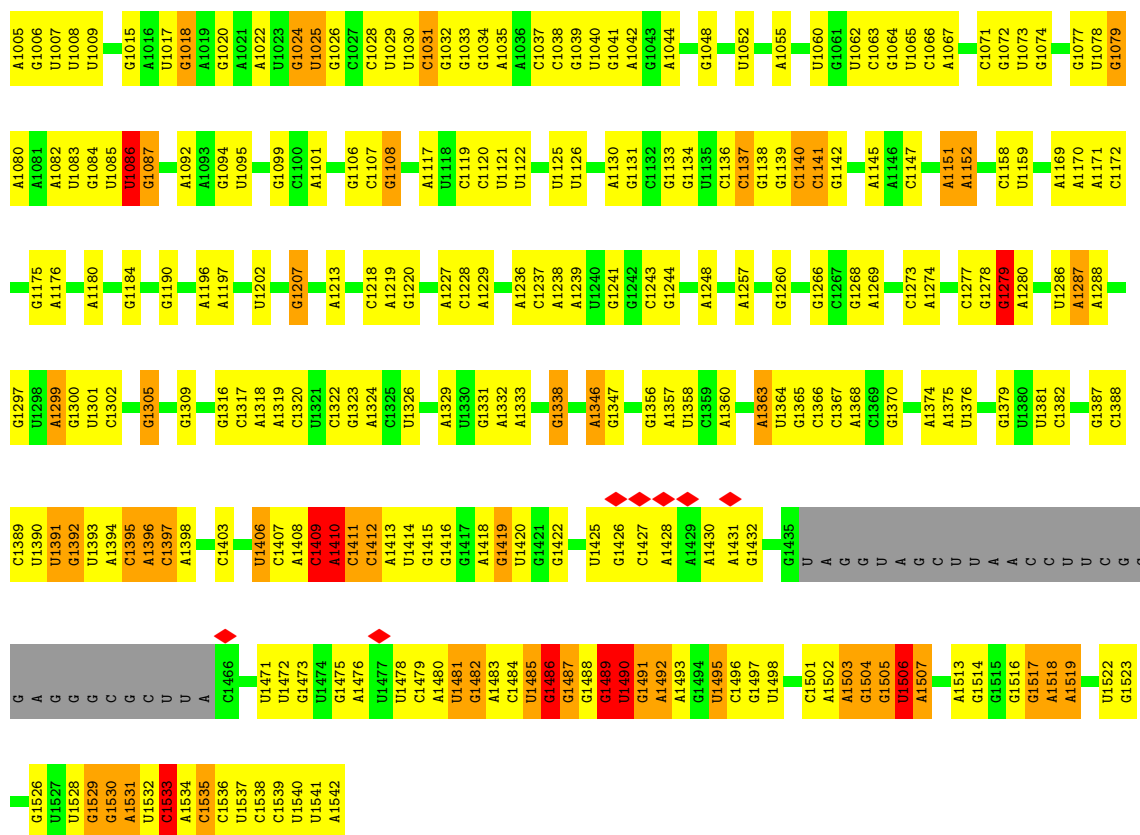
Mol	Chain	Residues	Atoms		AltConf
32	4	2	Total	Zn	0
			2	2	

3 Residue-property plots

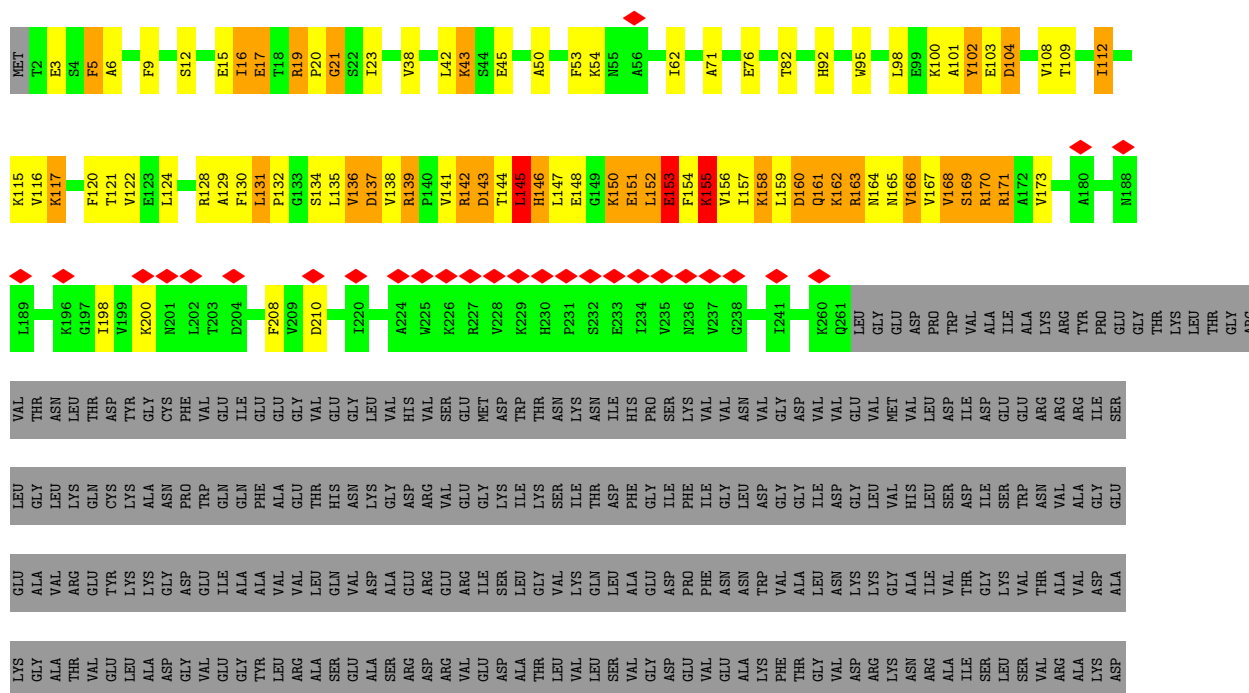
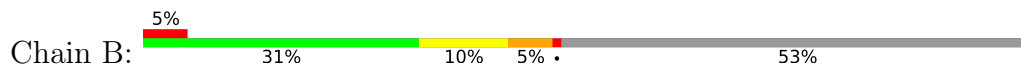
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 S1



GLU
ALA
ASP
GLU
LYS
ASP
ALA
ILE
ALA
THR
VAL
ASN
LYS
GLN
GLU
ASP
ALA
ASN
PHE
SER
ASN
ASN
ALA
MET
MET
ALA
GLU
ALA
PHE
LYS
ALA
LYS
GLY
GLU

• Molecule 3: 30S ribosomal protein S2

Chain C:  63% 27% 6%

MET A2 T20 T21 Y22 Y23 H39 L43 L44 K45 T46 V47 P48 M49 F50 L54 N58 K66 I67 L68 K73 S77 V80 D88 Q89 F91 T102 V107 I111 K112 R113 D116 L117 Q120 G124 T125 F126 D127 E133 A134 L135
T138 L141 K144 L145 L148 G149 I151 K152 D153 M154 D159 A160 L161 F162 V163 I164 D165 H168 F169 I173 K174 E175 V183 V187 D188 T189 N190 S191 V196 V199 N203 A206 I207 R208 A209 V210 Y213 L214 V217 T220 V221 R225 S226
Q227 ASP LEU ALA SER GLN ALA ALA GLU SER PHE VAL VAL GLU ALA GLU

• Molecule 4: Small ribosomal subunit protein uS3

Chain D:  59% 28% 9%

MET G2 G3 K4 V5 H6 P7 N8 P17 S20 T21 W22 T26 K27 D31 R32 L33 D34 S35 D36 F37 K38 Y39 R40 F46 L47 A50 R54 I55 E58 R59 P60 A61 K62 S63 T64 R65 T68 R72 I77 G78 K79 E82 D83 V84 E85 R86 L87
R88 R89 V90 D93 V97 P98 I103 R107 E110 L111 T121 S122 Q123 L124 E125 R126 S127 V128 M129 F130 M134 K135 R136 L144 K150 V151 G155 I162 A163 R169 R172 L175 L178 R179 A180 T191 Y193 V200 F203 K204 G205
E206 I207 M211 A212 VAL GLU PRO GLU LYS PRO ALA ALA GLN PRO LYS LYS GLN ARG GLY ARG LYS

• Molecule 5: Small ribosomal subunit protein uS4

Chain E:  60% 36%

MET A2 K8 L9 R14 E15 S23 A27 T28 D29 K31 T30 T34 A37 G42 A43 R44 D50 Y51 G52 V53 Q54 Q55 L55 R56 E57 K58 Q59 K60 V61 R62 E69 R70 Q71 N74 Y75 Y76 K77 E78 R81 L82 K83 G84 N85 E88 D89 N100 V101
V102 Y103 R104 M105 G106 F107 G108 A109 T110 A111 A112 A113 A114 R115 V125 I132 Y135 V143 S144 A145 R146 E147 K150 K151 V155 L159 L163 Q164 R165 E166 K167 L171 E172 V173 K177 M178 E179 G180 T181 F182 K183 D194 I195 N196 E197 H198 L199 V201
E202 L203 Y204 K206

• Molecule 6: 30S ribosomal protein S5

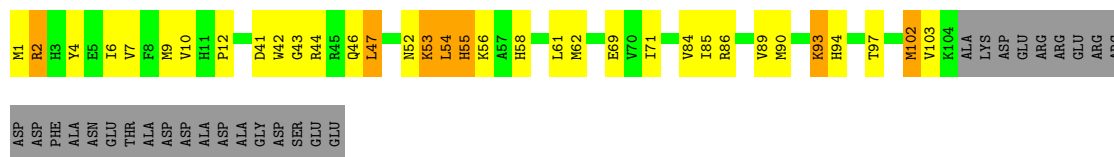
Chain F:  64% 30% 5%

E10 L11 Q12 E13 K14 L15 K23 T24 R29 T34 A35 N43 G44 R45 V46 G47 P48 G49 Y50 R54 I60 K66 A67 I72 L76 N77 T80 L81 Q82 K86 H89 T90 G91 A99 T103 G104 I105 G108 M111 R112 A113 V114 L115 E116

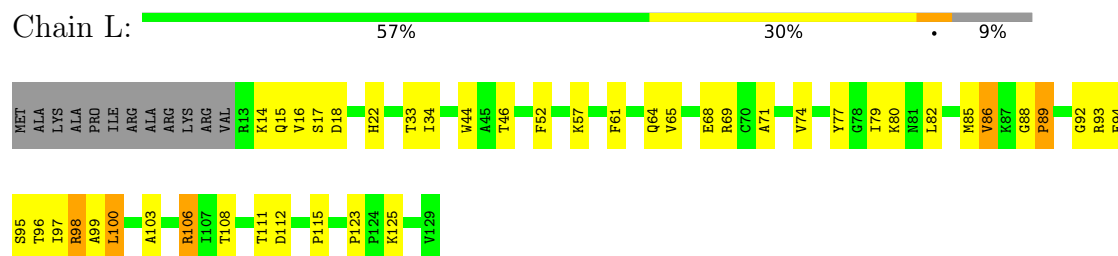


- Molecule 7: Small ribosomal subunit protein bS6

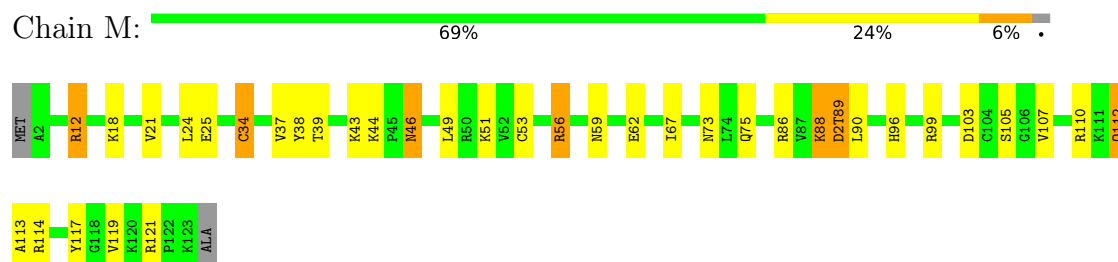
Chain G: 53% 21% 5% 21%



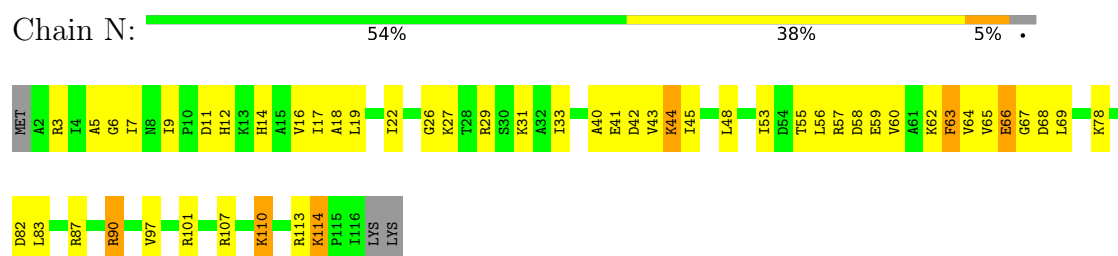
- Molecule 12: 30S ribosomal protein S11



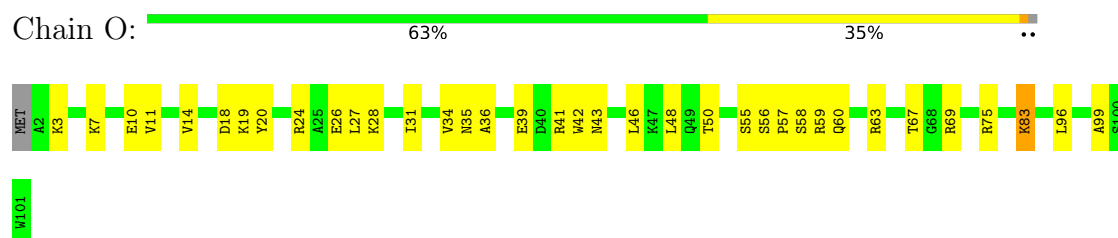
- Molecule 13: 30S ribosomal protein S12



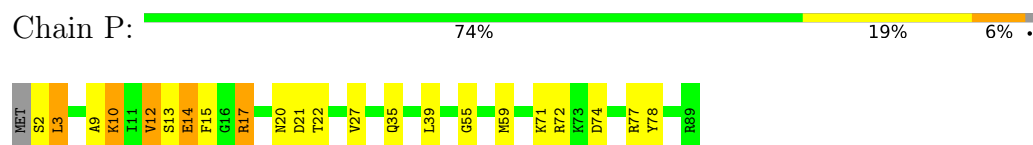
- Molecule 14: 30S ribosomal protein S13



- Molecule 15: 30S ribosomal protein S14



- Molecule 16: Small ribosomal subunit protein uS15



- Molecule 17: 30S ribosomal protein S16

- Molecule 18: 30S ribosomal protein S17

- Molecule 19: 30S ribosomal protein S18

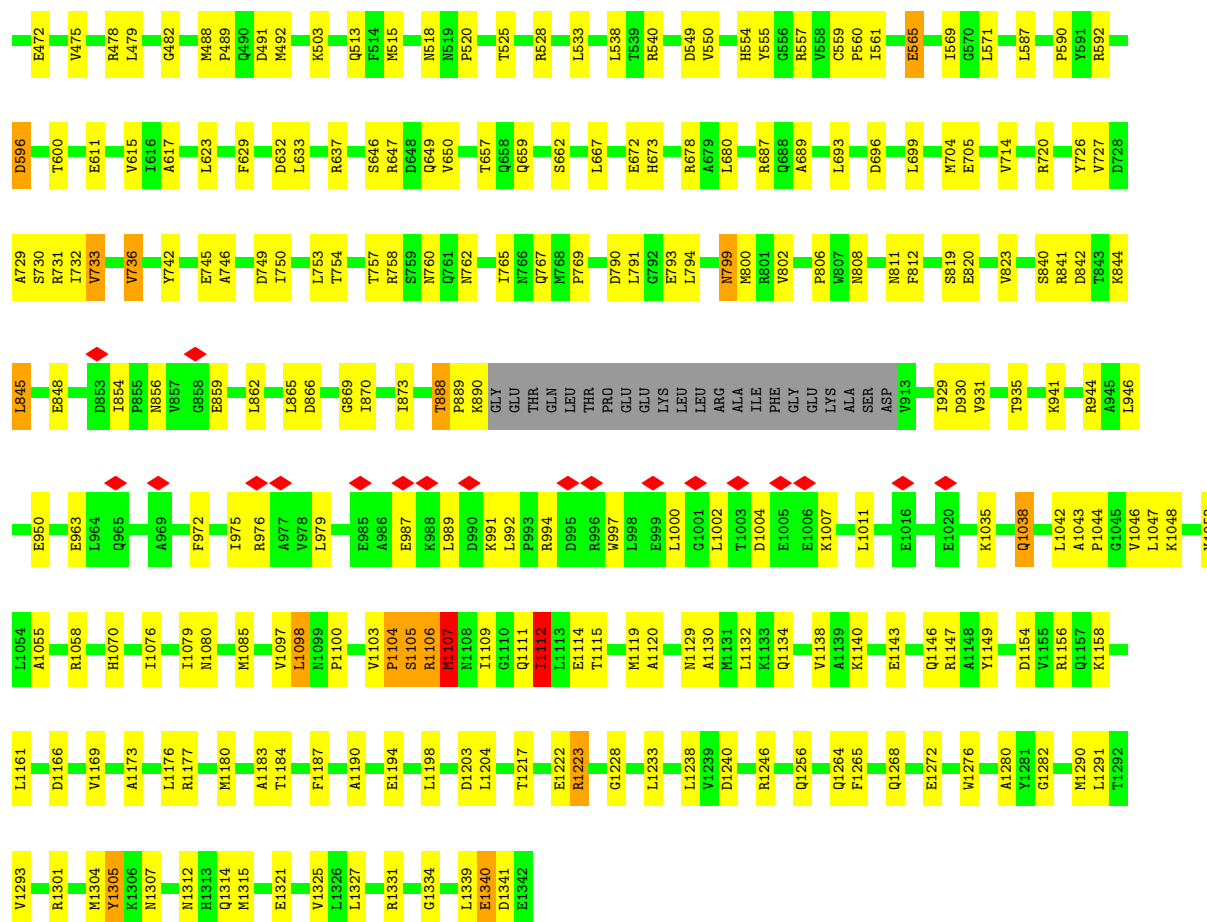
- Molecule 20: 30S ribosomal protein S19

- Molecule 21: 30S ribosomal protein S20

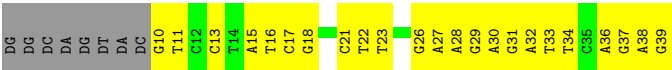
- Molecule 22: 30S ribosomal protein S21

- Molecule 23: mRNA

- Molecule 24: DNA-directed RNA polymerase subunit alpha



Chain 6: 18% 61% 21%



● Molecule 30: Template DNA strand

Chain 7: 28% 46% . 23%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.95	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	4.625	Depositor
Minimum map value	-1.259	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.148	Depositor
Recommended contour level	0.303	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 5MC, PSU, D2T, MA6, ZN, 2MG, MG

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	0.81	0/36116	0.88	31/56333 (0.1%)
2	B	0.39	0/1776	0.62	0/2413
3	C	0.34	0/1796	0.57	0/2420
4	D	0.42	0/1680	0.57	0/2263
5	E	0.40	0/1665	0.58	2/2227 (0.1%)
6	F	0.38	0/1165	0.57	0/1568
7	G	0.36	0/867	0.56	0/1171
8	H	0.35	0/1219	0.53	0/1635
9	I	0.39	0/989	0.53	0/1326
10	J	0.43	0/1043	0.61	0/1387
11	K	0.41	0/818	0.68	1/1105 (0.1%)
12	L	0.36	0/893	0.55	0/1205
13	M	0.43	0/954	0.56	0/1279
14	N	0.39	0/900	0.58	0/1204
15	O	0.41	0/817	0.55	0/1088
16	P	0.34	0/722	0.48	0/964
17	Q	0.49	0/659	0.63	0/884
18	R	0.37	0/657	0.57	0/881
19	S	0.39	0/553	0.50	0/742
20	T	0.46	0/680	0.60	0/915
21	U	0.34	0/676	0.49	0/895
22	V	0.39	0/597	0.54	0/792
23	X	0.48	0/513	0.79	0/797
24	1	0.38	0/1797	0.52	0/2436
24	2	0.35	0/1703	0.53	0/2308
25	3	0.37	0/10581	0.50	0/14275
26	4	0.37	0/10532	0.52	0/14219
27	5	0.30	0/711	0.46	0/956
28	Z	0.39	0/1251	0.57	1/1686 (0.1%)
29	6	0.65	0/693	0.96	0/1068
30	7	0.64	0/676	0.97	1/1039 (0.1%)
All	All	0.61	0/85699	0.73	36/123481 (0.0%)

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
20	T	0	1
25	3	0	1
26	4	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1087	G	C4-N9-C1'	9.67	139.07	126.50
1	A	1087	G	C8-N9-C1'	-9.06	115.23	127.00
30	7	19	DG	O4'-C4'-C3'	-8.81	100.72	106.00
1	A	1489	G	C8-N9-C4	-7.87	103.25	106.40
1	A	1087	G	C6-C5-N7	-7.73	125.76	130.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	3	1112	ILE	Peptide
26	4	426	ALA	Peptide
20	T	32	ARG	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	32443	0	16346	551	0
2	B	1761	0	1537	143	0
3	C	1765	0	1792	46	0
4	D	1653	0	1727	41	0
5	E	1643	0	1707	61	0
6	F	1152	0	1196	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	848	0	846	21	0
8	H	1203	0	1254	36	0
9	I	979	0	1031	19	0
10	J	1031	0	1076	42	0
11	K	808	0	845	40	0
12	L	877	0	887	41	0
13	M	951	0	1012	29	0
14	N	891	0	952	41	0
15	O	805	0	844	26	0
16	P	714	0	734	13	0
17	Q	649	0	666	27	0
18	R	648	0	691	12	0
19	S	544	0	565	10	0
20	T	663	0	688	15	0
21	U	670	0	719	15	0
22	V	589	0	629	21	0
23	X	458	0	233	17	0
24	1	1775	0	1800	35	0
24	2	1684	0	1713	45	0
25	3	10415	0	10432	279	0
26	4	10375	0	10599	385	0
27	5	709	0	719	18	0
28	Z	1225	0	1203	49	0
29	6	618	0	339	22	0
30	7	606	0	338	25	0
31	A	131	0	0	0	0
31	D	1	0	0	0	0
32	4	2	0	0	0	0
All	All	81286	0	65120	1982	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 14.

The worst 5 of 1982 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)
25:3:845:LEU:HB2	25:3:890:LYS:HD2	1.18	1.15
26:4:271:ARG:HB3	26:4:275:ARG:HH12	1.00	1.11
25:3:845:LEU:CB	25:3:890:LYS:HD2	1.83	1.08
26:4:271:ARG:HB3	26:4:275:ARG:NH1	1.69	1.05
2:B:158:LYS:HB3	2:B:167:VAL:HB	1.07	1.02

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	258/557 (46%)	223 (86%)	25 (10%)	10 (4%)	2	16
3	C	224/241 (93%)	207 (92%)	16 (7%)	1 (0%)	30	61
4	D	209/233 (90%)	193 (92%)	14 (7%)	2 (1%)	13	42
5	E	203/206 (98%)	199 (98%)	3 (2%)	1 (0%)	25	56
6	F	154/157 (98%)	138 (90%)	15 (10%)	1 (1%)	22	53
7	G	102/131 (78%)	96 (94%)	6 (6%)	0	100	100
8	H	151/156 (97%)	137 (91%)	12 (8%)	2 (1%)	10	36
9	I	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
10	J	126/130 (97%)	109 (86%)	16 (13%)	1 (1%)	16	46
11	K	99/103 (96%)	90 (91%)	8 (8%)	1 (1%)	13	42
12	L	115/129 (89%)	102 (89%)	12 (10%)	1 (1%)	14	44
13	M	119/124 (96%)	106 (89%)	12 (10%)	1 (1%)	16	46
14	N	113/118 (96%)	102 (90%)	8 (7%)	3 (3%)	4	22
15	O	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	13	42
16	P	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
17	Q	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
18	R	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
19	S	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
20	T	81/92 (88%)	70 (86%)	9 (11%)	2 (2%)	4	24
21	U	84/87 (97%)	84 (100%)	0	0	100	100
22	V	68/71 (96%)	58 (85%)	10 (15%)	0	100	100
24	1	227/329 (69%)	223 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	2	215/329 (65%)	206 (96%)	6 (3%)	3 (1%)	9	34
25	3	1316/1342 (98%)	1235 (94%)	76 (6%)	5 (0%)	30	61
26	4	1327/1406 (94%)	1240 (93%)	75 (6%)	12 (1%)	14	44
27	5	88/91 (97%)	83 (94%)	5 (6%)	0	100	100
28	Z	147/180 (82%)	136 (92%)	10 (7%)	1 (1%)	19	50
All	All	5959/6773 (88%)	5539 (93%)	372 (6%)	48 (1%)	19	46

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	61	ALA
5	E	107	PHE
6	F	90	THR
13	M	88	LYS
24	2	16	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	143/461 (31%)	114 (80%)	29 (20%)	1	4
3	C	187/199 (94%)	171 (91%)	16 (9%)	8	30
4	D	172/190 (90%)	153 (89%)	19 (11%)	5	20
5	E	172/173 (99%)	159 (92%)	13 (8%)	11	34
6	F	119/119 (100%)	105 (88%)	14 (12%)	4	17
7	G	91/112 (81%)	76 (84%)	15 (16%)	2	9
8	H	126/129 (98%)	116 (92%)	10 (8%)	10	32
9	I	104/105 (99%)	97 (93%)	7 (7%)	13	39
10	J	106/107 (99%)	95 (90%)	11 (10%)	5	22
11	K	88/90 (98%)	79 (90%)	9 (10%)	6	23
12	L	90/99 (91%)	84 (93%)	6 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	102/103 (99%)	92 (90%)	10 (10%)	6	24
14	N	93/96 (97%)	88 (95%)	5 (5%)	18	46
15	O	83/84 (99%)	81 (98%)	2 (2%)	44	68
16	P	76/77 (99%)	70 (92%)	6 (8%)	10	32
17	Q	65/65 (100%)	60 (92%)	5 (8%)	10	33
18	R	74/78 (95%)	73 (99%)	1 (1%)	62	78
19	S	57/65 (88%)	57 (100%)	0	100	100
20	T	72/79 (91%)	64 (89%)	8 (11%)	5	19
21	U	65/66 (98%)	62 (95%)	3 (5%)	23	52
22	V	60/61 (98%)	58 (97%)	2 (3%)	33	60
24	1	197/286 (69%)	192 (98%)	5 (2%)	42	67
24	2	187/286 (65%)	175 (94%)	12 (6%)	14	40
25	3	1139/1157 (98%)	1085 (95%)	54 (5%)	22	51
26	4	1118/1167 (96%)	1036 (93%)	82 (7%)	11	35
27	5	74/75 (99%)	74 (100%)	0	100	100
28	Z	135/157 (86%)	119 (88%)	16 (12%)	4	17
All	All	4995/5686 (88%)	4635 (93%)	360 (7%)	14	36

5 of 360 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	3	623	LEU
26	4	428	THR
25	3	799	ASN
25	3	1305	TYR
26	4	800	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
26	4	341	ASN
26	4	1252	HIS
26	4	424	ASN
26	4	817	HIS
27	5	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1542 (97%)	234 (15%)	17 (1%)
23	X	19/53 (35%)	3 (15%)	0
All	All	1527/1595 (95%)	237 (15%)	17 (1%)

5 of 237 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	3	A
1	A	4	U
1	A	9	G
1	A	31	G

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1506	U
1	A	1533	C
1	A	1485	U
1	A	1486	G
1	A	1489	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	967	1	18,22,23	3.92	7 (38%)	26,32,35	1.07	1 (3%)
13	D2T	M	89	13	7,9,10	1.02	0	6,11,13	2.22	2 (33%)
1	PSU	A	516	1	18,21,22	1.07	3 (16%)	22,30,33	1.75	5 (22%)
1	2MG	A	1516	1	18,26,27	1.02	1 (5%)	16,38,41	1.29	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	966	1	18,26,27	2.33	7 (38%)	16,38,41	1.40	3 (18%)
1	MA6	A	1519	1	18,26,27	1.09	1 (5%)	19,38,41	1.94	7 (36%)
1	MA6	A	1518	1	18,26,27	1.38	3 (16%)	19,38,41	4.28	2 (10%)
1	2MG	A	1207	1,31	18,26,27	2.25	7 (38%)	16,38,41	1.46	4 (25%)
1	G7M	A	527	1	20,26,27	1.12	2 (10%)	17,39,42	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	967	1	-	3/7/25/26	0/2/2/2
13	D2T	M	89	13	-	2/7/12/14	-
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
1	2MG	A	966	1	-	2/5/27/28	0/3/3/3
1	MA6	A	1519	1	-	7/7/29/30	0/3/3/3
1	MA6	A	1518	1	-	3/7/29/30	0/3/3/3
1	2MG	A	1207	1,31	-	2/5/27/28	0/3/3/3
1	G7M	A	527	1	-	2/3/25/26	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C6-C5	10.05	1.51	1.34
1	A	967	5MC	C4-N3	7.08	1.46	1.34
1	A	967	5MC	C2-N3	6.56	1.49	1.36
1	A	967	5MC	C4-N4	5.31	1.47	1.34
1	A	967	5MC	C6-N1	4.89	1.46	1.38

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	MA6	N1-C6-N6	-17.86	98.26	117.06
1	A	1518	MA6	N3-C2-N1	-4.70	121.33	128.68
1	A	516	PSU	N1-C2-N3	4.42	120.14	115.13
1	A	516	PSU	C4-N3-C2	-4.39	120.02	126.34
13	M	89	D2T	CB1-SB-CB	3.68	109.10	102.44

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	967	5MC	1	0
13	M	89	D2T	2	0
1	A	516	PSU	1	0
1	A	1519	MA6	3	0
1	A	1518	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 134 ligands modelled in this entry, 134 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

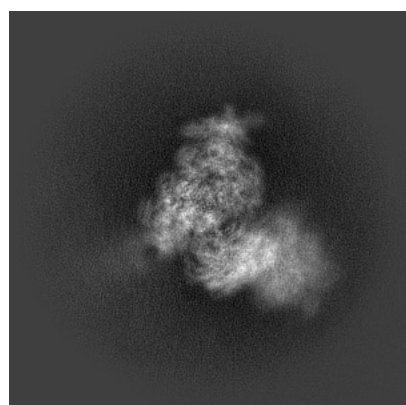
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51623. These allow visual inspection of the internal detail of the map and identification of artifacts.

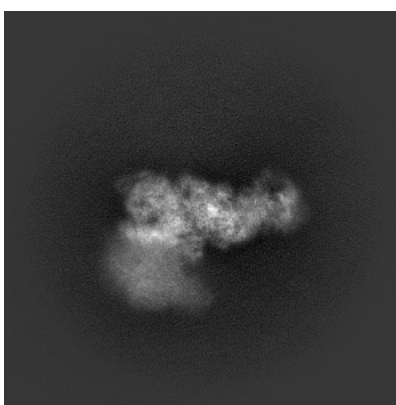
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

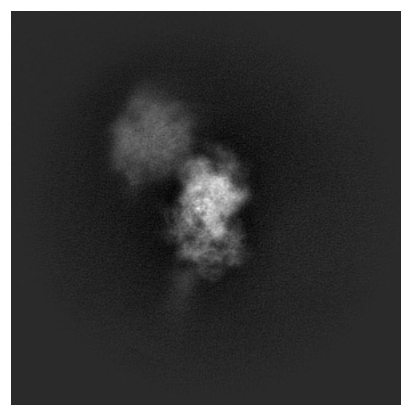
6.1.1 Primary map



X



Y

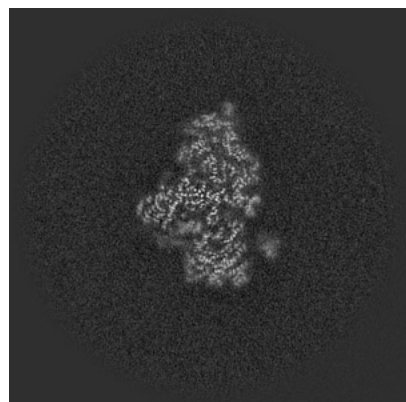


Z

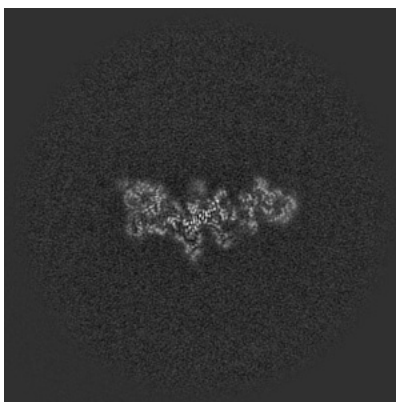
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

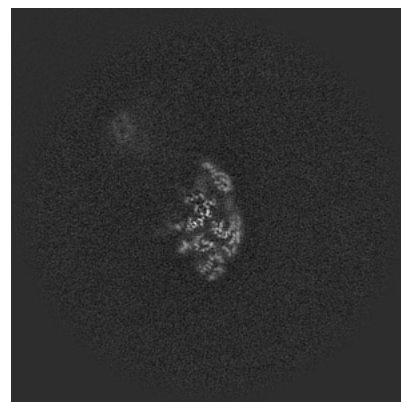
6.2.1 Primary map



X Index: 300



Y Index: 300

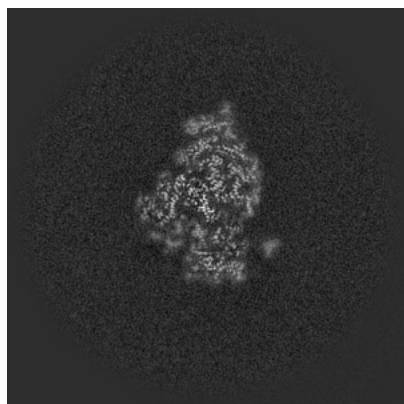


Z Index: 300

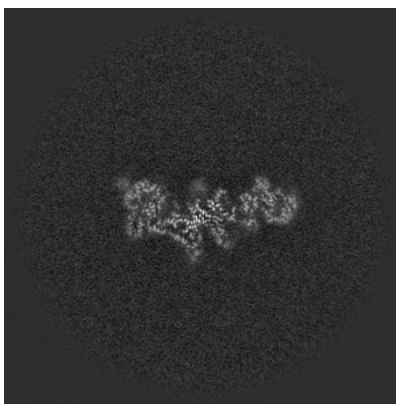
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

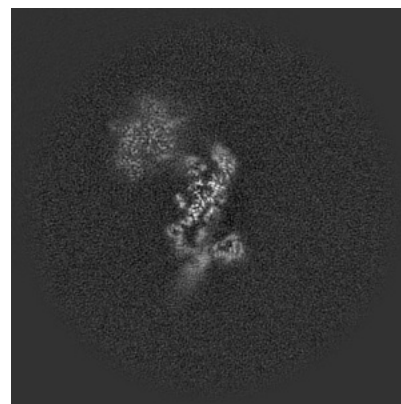
6.3.1 Primary map



X Index: 295



Y Index: 302

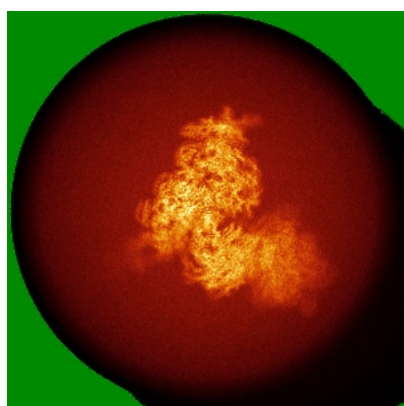


Z Index: 257

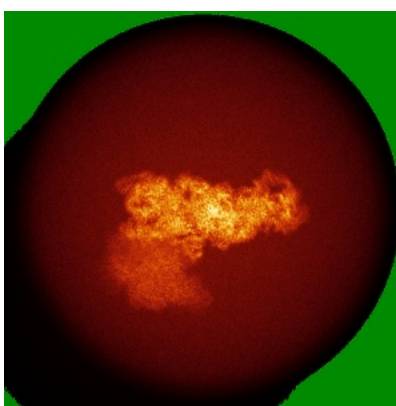
The images above show the largest variance slices of the map in three orthogonal directions.

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

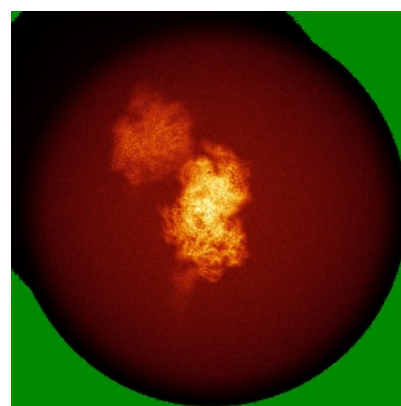
6.4.1 Primary map



X



Y



Z

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](#)

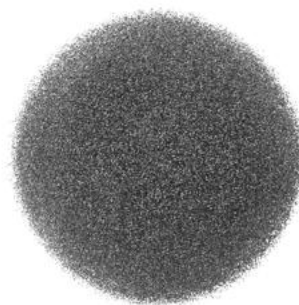
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.303. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

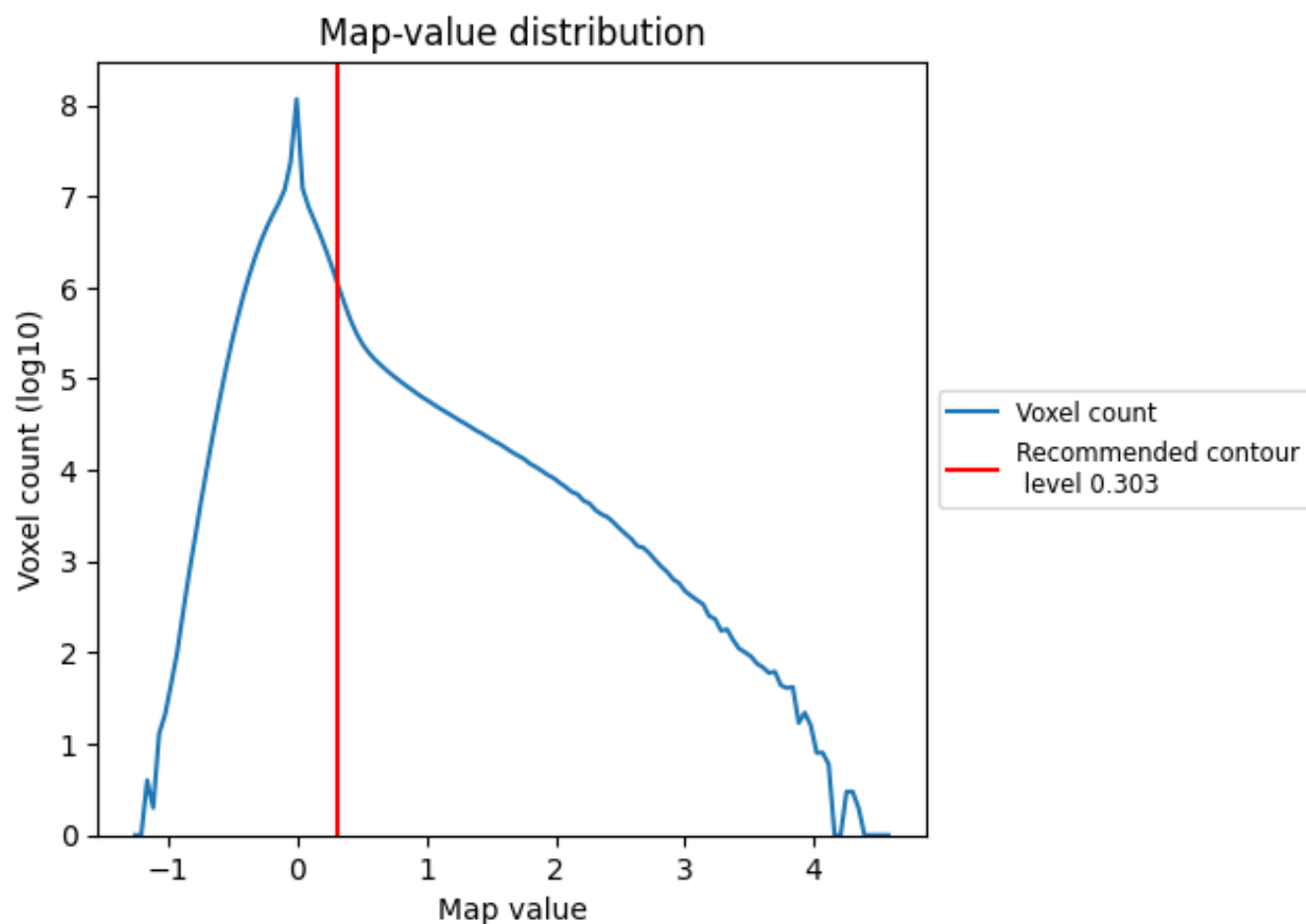
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

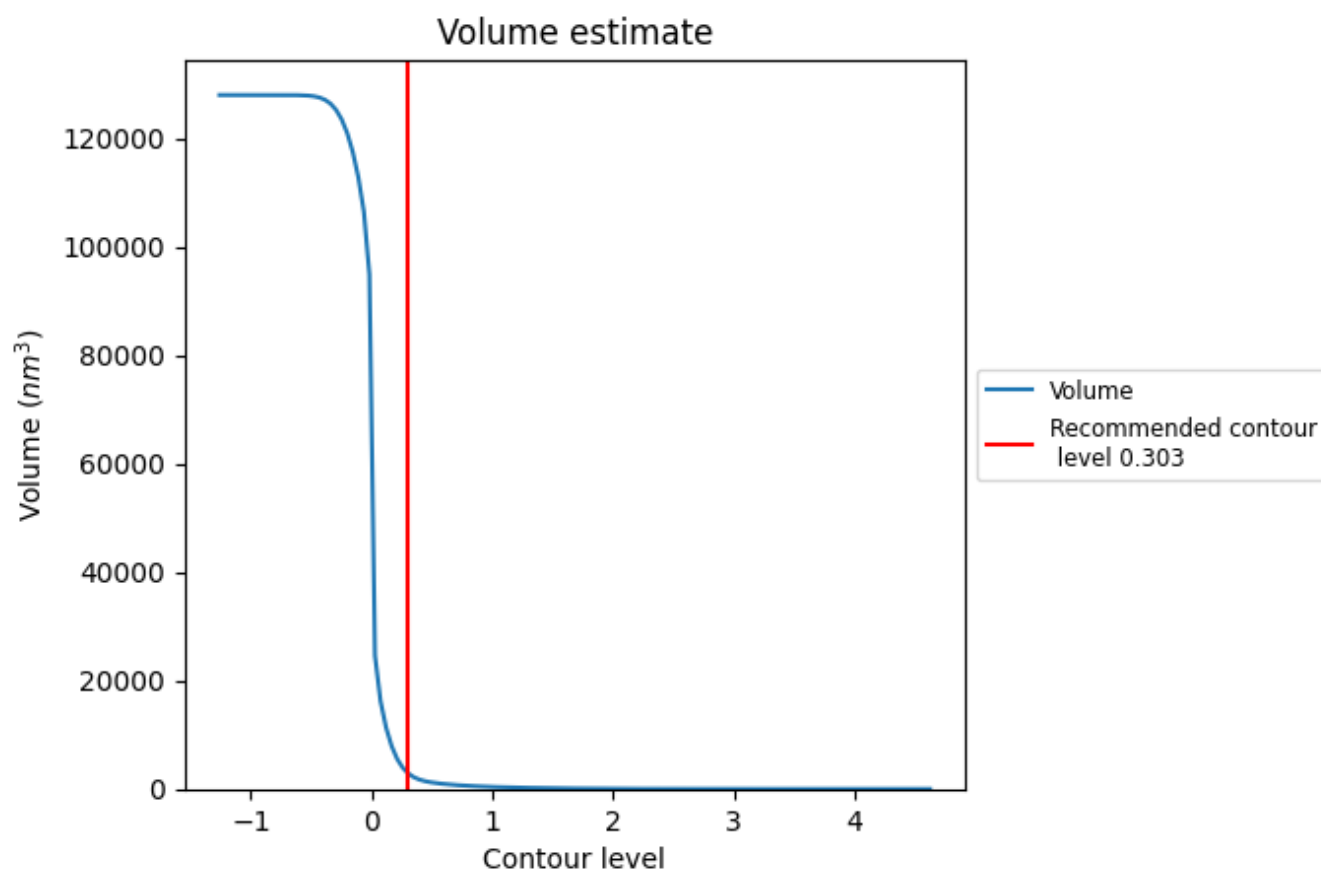
This section contains the results of statistical analysis of the map.

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.

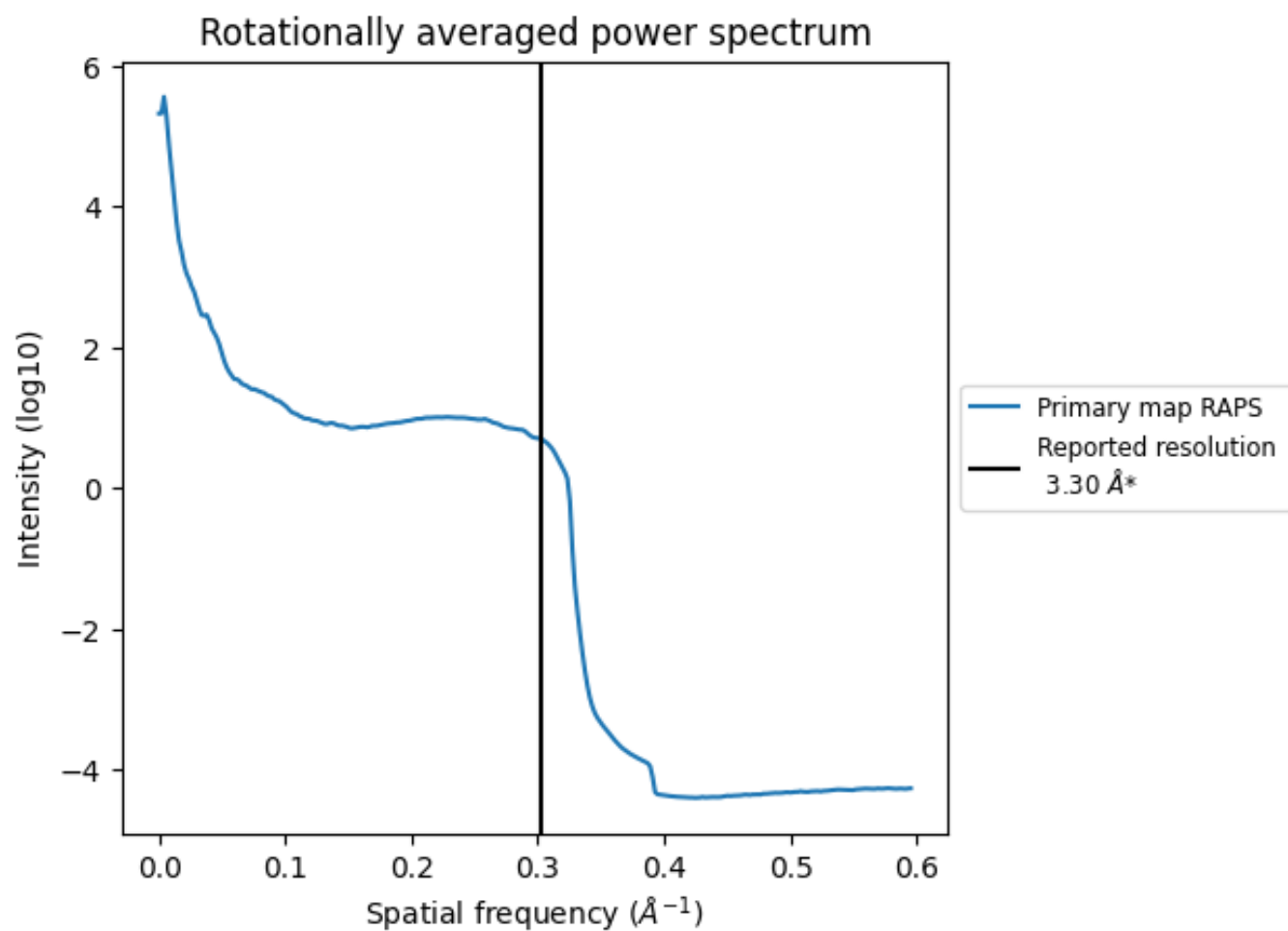
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2883 nm^3 ; this corresponds to an approximate mass of 2604 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 0.303 Å⁻¹

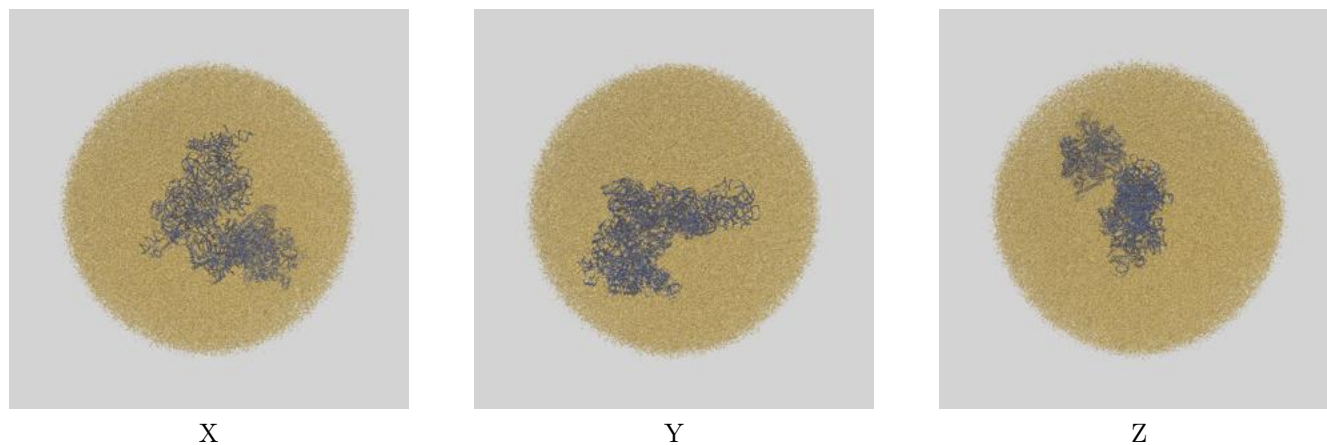
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

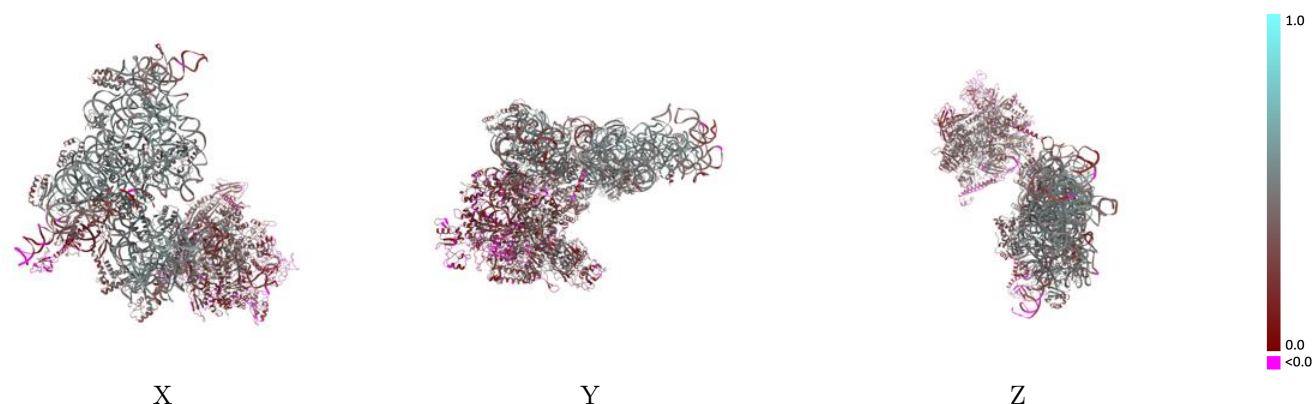
This section contains information regarding the fit between EMDB map EMD-51623 and PDB model 9GUX. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



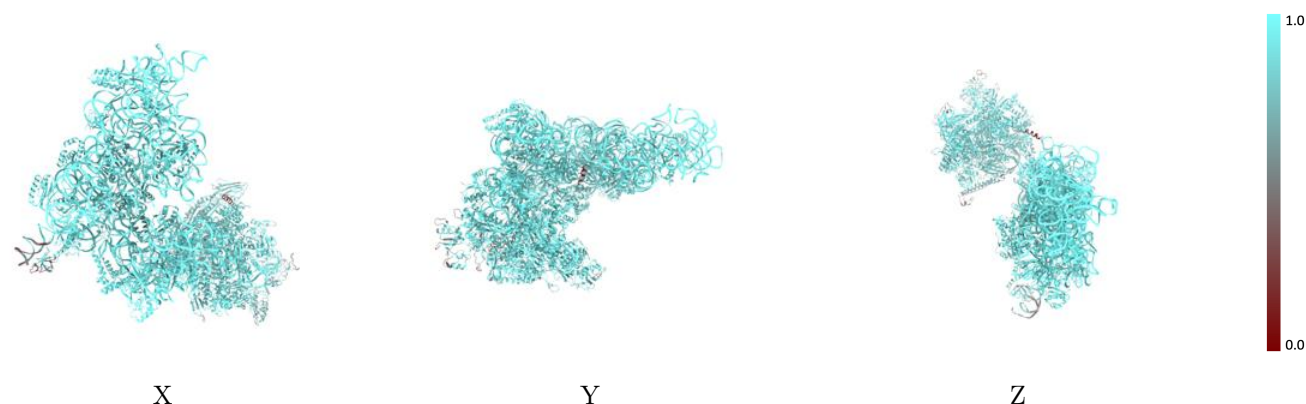
The images above show the 3D surface view of the map at the recommended contour level 0.303 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



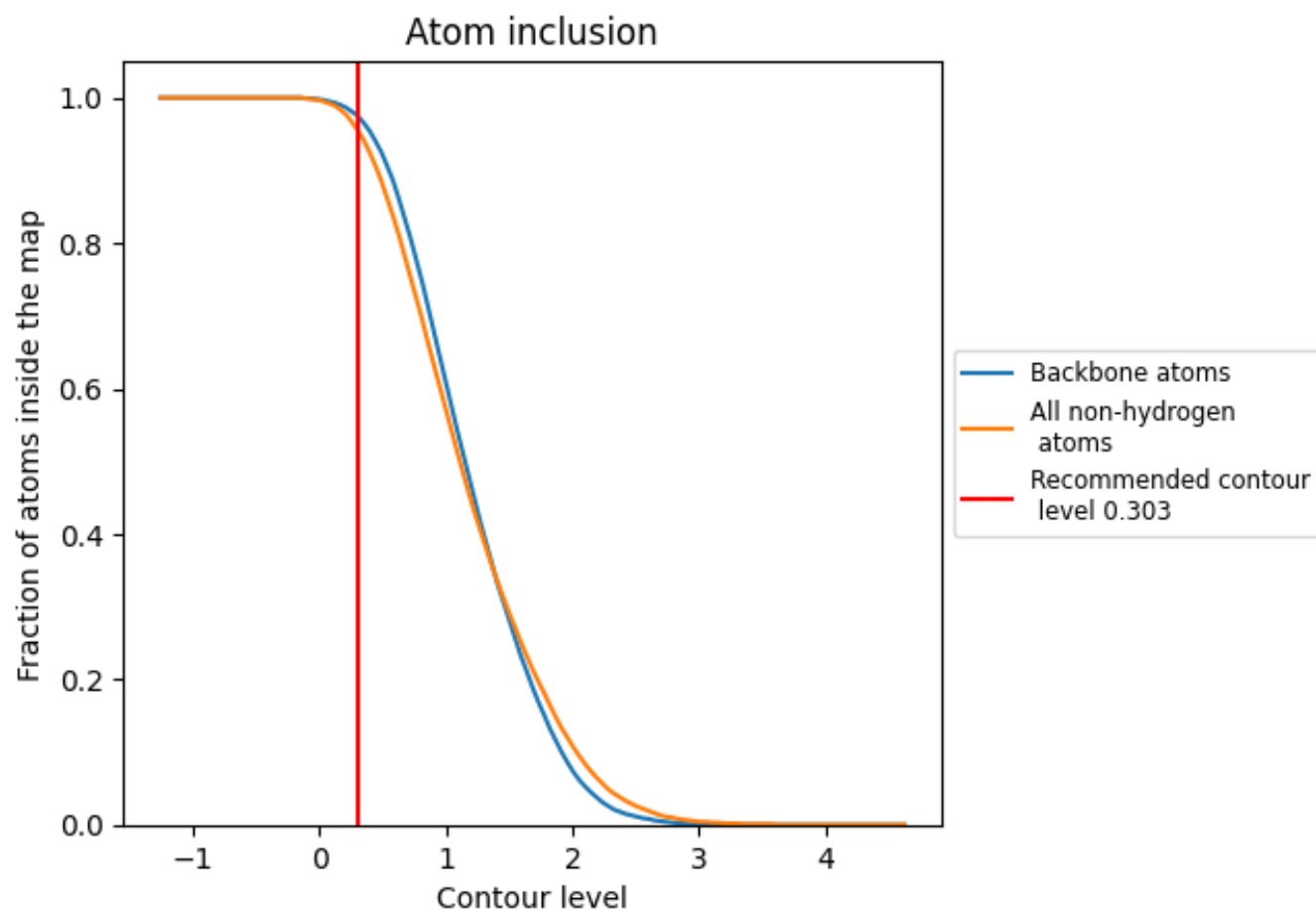
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.303).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.303) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.3740
1	 0.8880	 0.3020
2	 0.8630	 0.2520
3	 0.9020	 0.2700
4	 0.9240	 0.2640
5	 0.8270	 0.2340
6	 0.9140	 0.1200
7	 0.9690	 0.2350
A	 0.9910	 0.4550
B	 0.8650	 0.1640
C	 0.9640	 0.4160
D	 0.9710	 0.4500
E	 0.9680	 0.4250
F	 0.9650	 0.4510
G	 0.9650	 0.4050
H	 0.9620	 0.3470
I	 0.9660	 0.4860
J	 0.9770	 0.4390
K	 0.9580	 0.3980
L	 0.9670	 0.3480
M	 0.9780	 0.4710
N	 0.9720	 0.3980
O	 0.9780	 0.4610
P	 0.9650	 0.4300
Q	 0.9710	 0.4670
R	 0.9700	 0.4280
S	 0.9750	 0.4600
T	 0.9820	 0.4590
U	 0.9760	 0.4110
V	 0.9550	 0.3820
X	 0.9410	 0.1920
Z	 0.9230	 0.1710

