Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 08:11 AM EST

PDB ID	:	6WRS
EMDB ID	:	EMD-21887
Title	:	Structure of the 50S subunit of the ribosome from Methicillin Resistant Staphylococcus aureus in complex with the antibiotic, tedizolid
Authors	:	Belousoff, M.J.
Deposited on	:	2020-04-30
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation 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:

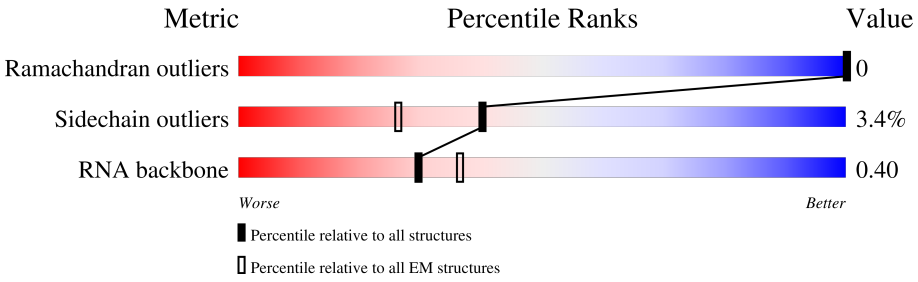
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=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	116	97%
2	B	277	95%
3	C	118	94%
4	D	105	91% 5%
5	E	117	91% 5%
6	F	91	85% 11%
7	G	105	95% 5%
8	H	107	78% 9% 13%

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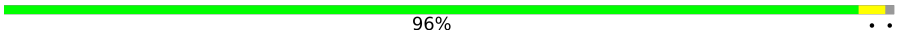
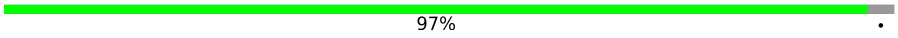
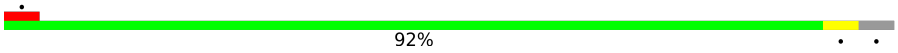
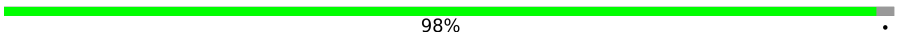
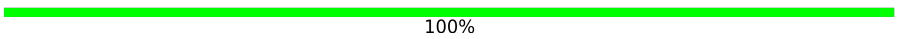
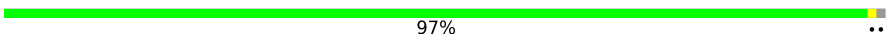
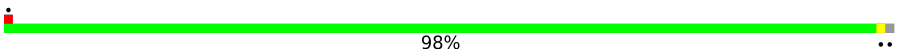
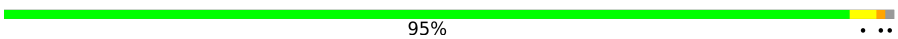
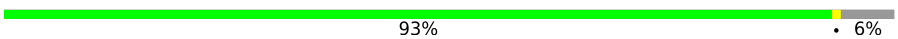
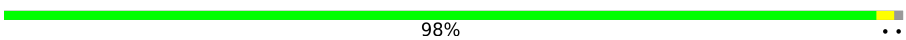
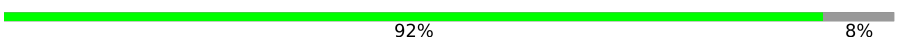
Mol	Chain	Length	Quality of chain
9	J	62	
10	K	72	
11	L	217	
12	M	58	
13	N	57	
14	O	49	
15	P	50	
16	Q	65	
17	R	37	
18	S	207	
19	V	145	
20	W	122	
21	X	146	
22	Y	144	
23	Z	122	
24	a	119	
25	1	2923	
26	2	115	
27	I	85	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 81130 atoms, of which 15 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 protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	113	Total	C	N	O	0	0
			915	576	184	155		

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 3 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 4 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			785	499	139	146	1		

- Molecule 5 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	110	ALA	GLY	variant	UNP A7X5F6

- Molecule 6 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			711	447	128	132	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	87	ASP	ILE	variant	UNP W8TUB4

- Molecule 7 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	100	Total	C	N	O	S	0	0
			770	486	141	142	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	54	SER	GLY	variant	UNP W8TRD5

- Molecule 8 is a protein called uL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			727	465	129	132	1		

- Molecule 9 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	62	ALA	-	insertion	UNP A0A077URJ8

- Molecule 10 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	58	Total	C	N	O	0	0
			481	296	92	93		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	215	Total	C	N	O	S	0	0
			1628	1018	299	306	5		

- Molecule 12 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	56	Total	C	N	O	0	0
			432	269	82	81		

- Molecule 13 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	50	Total	C	N	O	S	0	0
			397	241	83	68	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	54	ALA	VAL	variant	UNP A0A077UWR7

- Molecule 14 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	47	Total	C	N	O	S	0	0
			390	233	79	73	5		

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	44	Total	C	N	O	S	0	0
			372	228	90	53	1		

- Molecule 16 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 17 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 18 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	192	Total	C	N	O	S	0	0
			1472	924	271	275	2		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	143	Total	C	N	O	S	0	0
			1138	710	209	217	2		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	121	Total	C	N	O	S	0	0
			911	566	173	168	4		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	X	144	Total	C	N	O	0	0
			1082	669	213	200		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	121	Total	C	N	O	S	0	0
			955	586	183	185	1		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	a	110	Total	C	N	O	0	0
			857	536	165	156		

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	2698	Total	C	N	O	P	0	0
			57851	25835	10608	18715	2693		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1866	A	G	conflict	GB 1760383645

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	111	Total	C	N	O	P	0	0
			2358	1056	422	770	110		

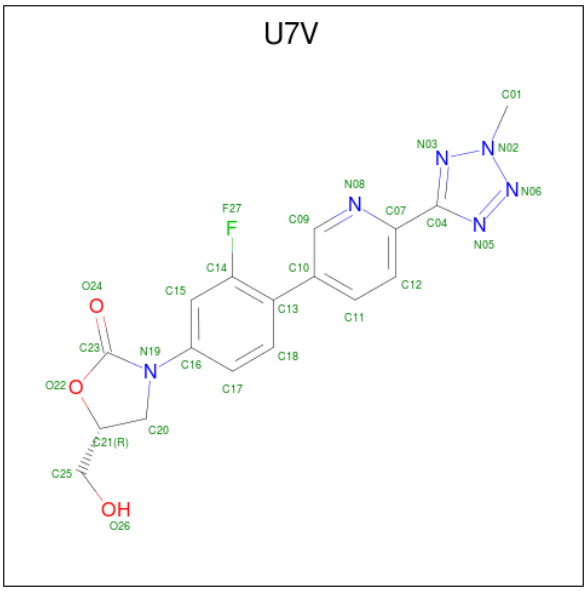
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	80	C	G	variant	GB 1750990749
2	109	C	G	variant	GB 1750990749
2	111	A	C	variant	GB 1750990749
2	112	G	A	variant	GB 1750990749

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	I	78	Total	C	N	O	0	0
			597	367	116	114		

- Molecule 28 is Tedizolid (three-letter code: U7V) (formula: $C_{17}H_{15}FN_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
28	1	1	Total	C	F	H	N	O	0
			42	17	1	15	6	3	

3 Residue-property plots (i)

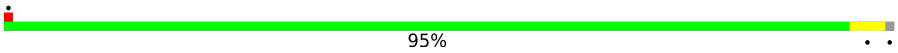
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 50S ribosomal protein L19

Chain A:

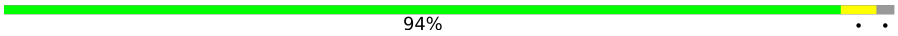
• Molecule 2: 50S ribosomal protein L2

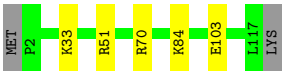
Chain B:



• Molecule 3: 50S ribosomal protein L20

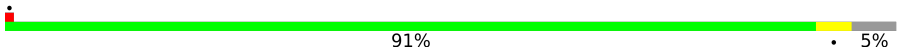
Chain C:

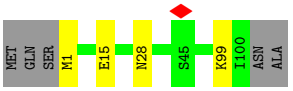




• Molecule 4: 50S ribosomal protein L21

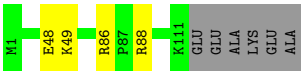
Chain D:





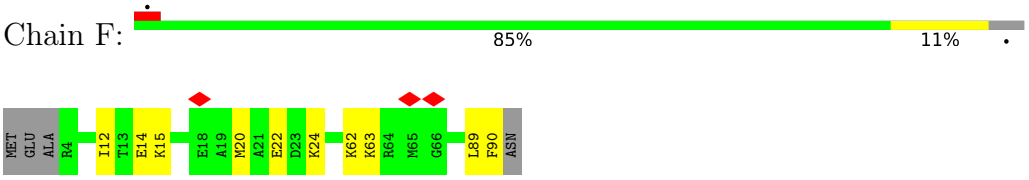
• Molecule 5: uL22

Chain E:



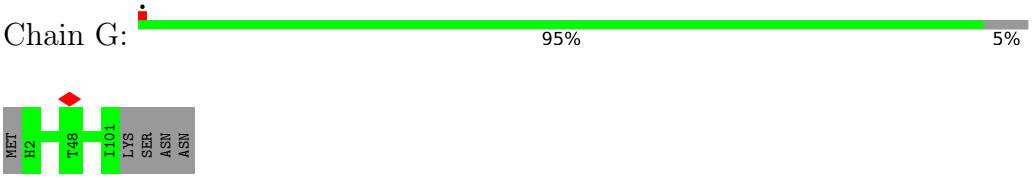
• Molecule 6: 50S ribosomal protein L23

Chain F:



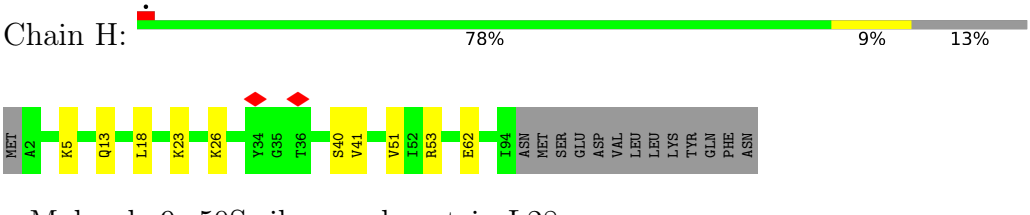
• Molecule 7: 50S ribosomal protein L24

Chain G:



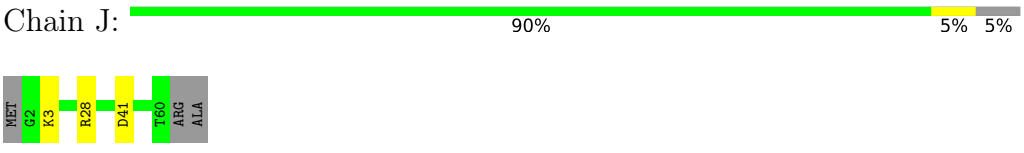
• Molecule 8: uL25

Chain H:



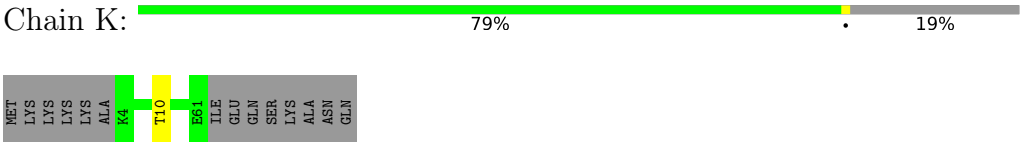
• Molecule 9: 50S ribosomal protein L28

Chain J:



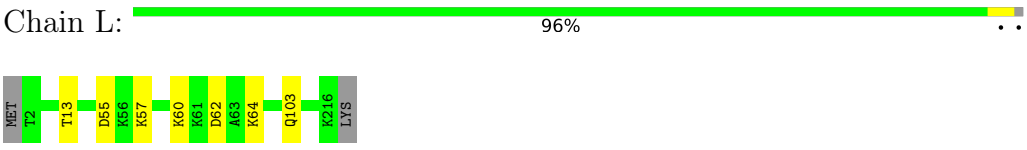
• Molecule 10: 50S ribosomal protein L29

Chain K:



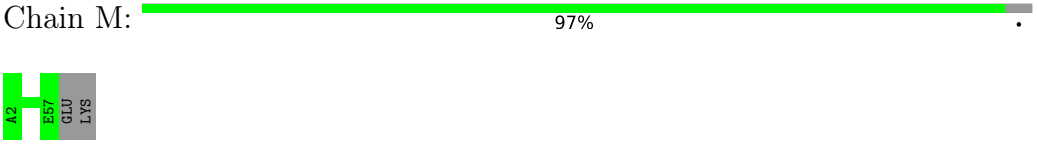
• Molecule 11: 50S ribosomal protein L3

Chain L:



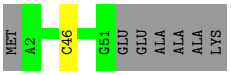
• Molecule 12: 50S ribosomal protein L30

Chain M:



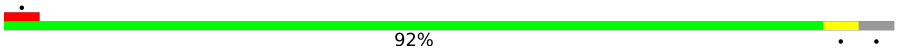
• Molecule 13: 50S ribosomal protein L32

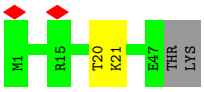
Chain N:



• Molecule 14: 50S ribosomal protein L33

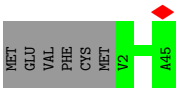
Chain O:





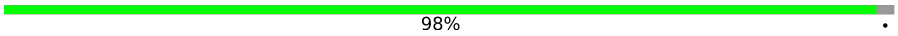
• Molecule 15: 50S ribosomal protein L34

Chain P:



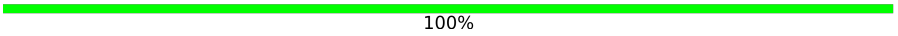
• Molecule 16: 50S ribosomal protein L35

Chain Q:



• Molecule 17: 50S ribosomal protein L36

Chain R:



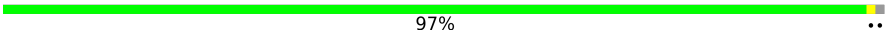
There are no outlier residues recorded for this chain.

• Molecule 18: 50S ribosomal protein L4

Chain S:

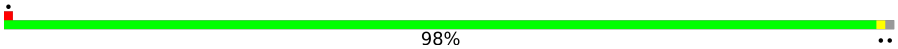
• Molecule 19: 50S ribosomal protein L13

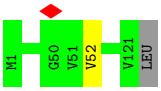
Chain V:



• Molecule 20: 50S ribosomal protein L14

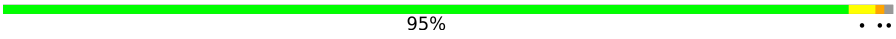
Chain W:

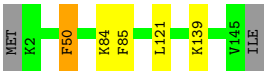




• Molecule 21: 50S ribosomal protein L15

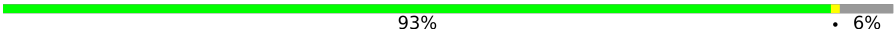
Chain X:





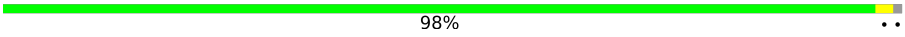
• Molecule 22: 50S ribosomal protein L16

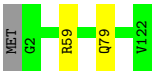
Chain Y:



• Molecule 23: 50S ribosomal protein L17

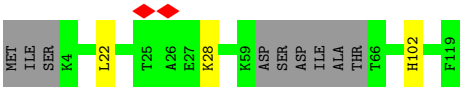
Chain Z:





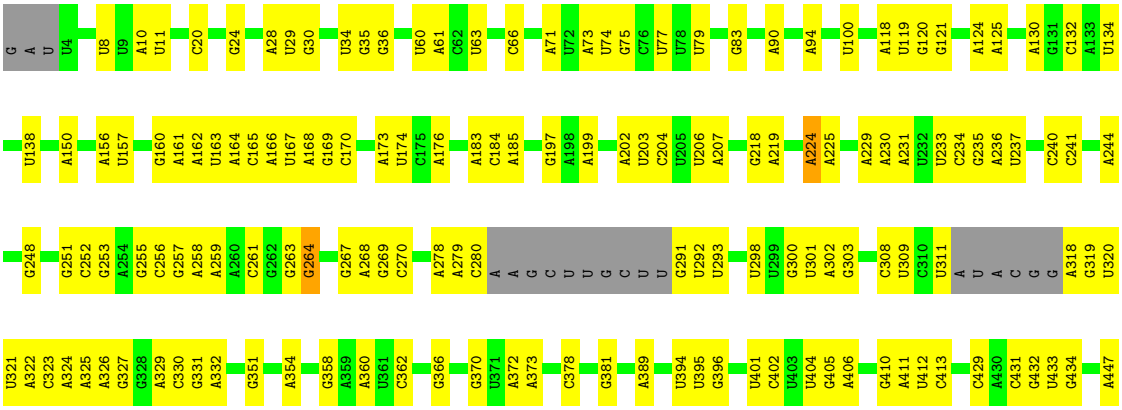
• Molecule 24: 50S ribosomal protein L18

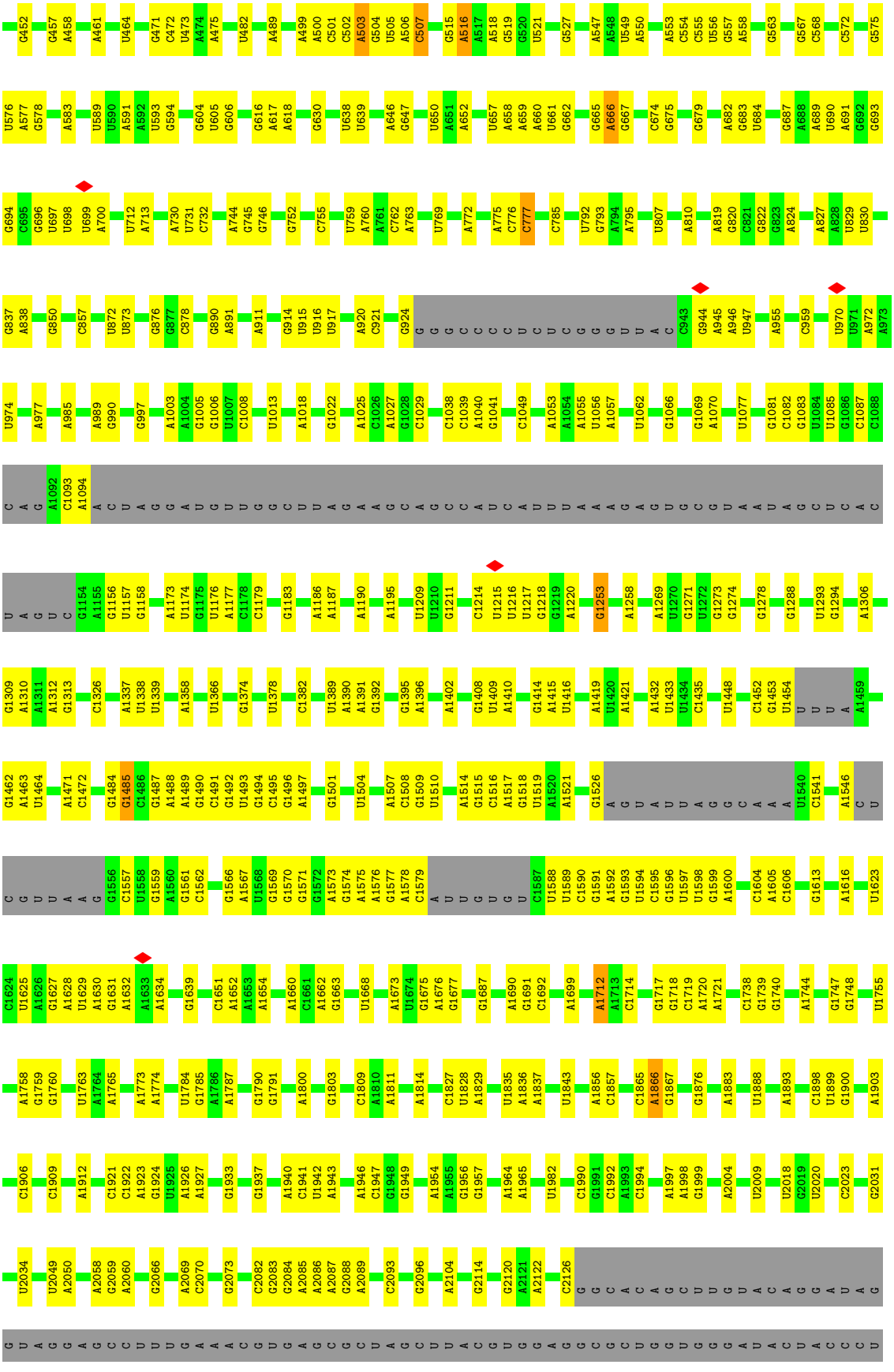
Chain a:

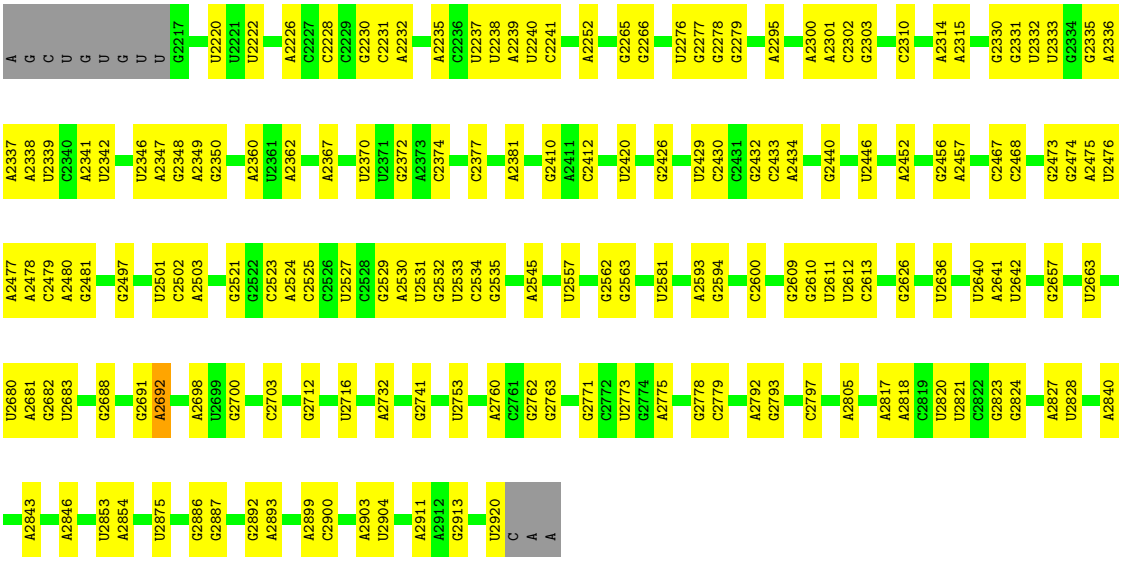


• Molecule 25: 23S rRNA

Chain 1:

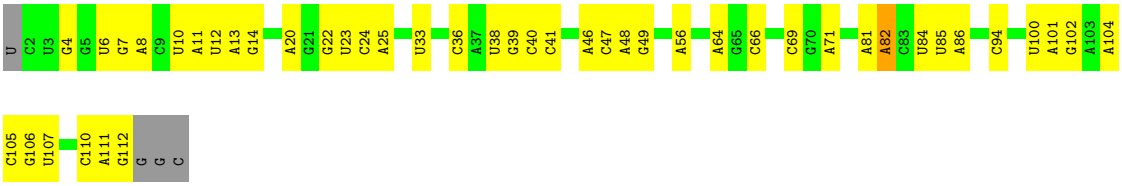






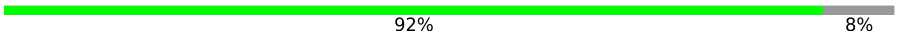
• Molecule 26: 5S rRNA

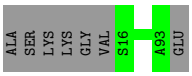
Chain 2:



• Molecule 27: 50S ribosomal protein L27

Chain I:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.432	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	410.4, 410.4, 410.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U7V

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	0.38	0/927	0.50	0/1239
2	B	0.48	0/2129	0.54	0/2858
3	C	0.44	0/955	0.47	0/1265
4	D	0.40	0/795	0.52	0/1062
5	E	0.36	0/861	0.49	0/1159
6	F	0.40	0/719	0.51	0/959
7	G	0.34	0/779	0.51	0/1042
8	H	0.33	0/735	0.52	0/986
9	J	0.36	0/469	0.56	0/625
10	K	0.40	0/482	0.53	0/642
11	L	0.41	0/1652	0.59	0/2216
12	M	0.42	0/434	0.56	0/585
13	N	0.41	0/404	0.52	0/537
14	O	0.36	0/393	0.56	0/523
15	P	0.47	0/376	0.51	0/491
16	Q	0.44	0/526	0.52	0/690
17	R	0.36	0/299	0.48	0/393
18	S	0.42	0/1494	0.55	0/2018
19	V	0.47	0/1160	0.56	0/1563
20	W	0.38	0/918	0.53	0/1232
21	X	0.42	0/1096	0.58	1/1461 (0.1%)
22	Y	0.42	0/1113	0.51	0/1493
23	Z	0.42	0/959	0.56	0/1282
24	a	0.35	0/865	0.50	0/1154
25	1	0.86	0/64789	0.89	30/101033 (0.0%)
26	2	0.54	0/2636	0.94	3/4105 (0.1%)
27	I	0.45	0/603	0.51	0/801
All	All	0.77	0/88568	0.83	34/133414 (0.0%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	2235	A	C4'-C3'-O3'	5.96	124.93	113.00
25	1	777	C	C4'-C3'-O3'	5.95	124.89	113.00
25	1	257	G	N9-C1'-C2'	-5.91	105.50	112.00
25	1	516	A	N9-C1'-C2'	-5.88	105.54	112.00
26	2	82	A	C4'-C3'-O3'	5.72	124.44	113.00
25	1	674	C	C4'-C3'-O3'	5.69	124.38	113.00
25	1	1866	A	C4'-C3'-O3'	5.65	124.30	113.00
25	1	878	C	C4'-C3'-O3'	5.64	124.29	113.00
25	1	1597	U	C4'-C3'-O3'	5.58	124.16	113.00
25	1	1485	G	C4'-C3'-O3'	5.56	124.12	113.00
25	1	1577	G	N9-C1'-C2'	-5.54	105.91	112.00
25	1	2692	A	N9-C1'-C2'	-5.54	105.91	112.00
25	1	1253	G	N9-C1'-C2'	-5.53	105.92	112.00
25	1	1013	U	N1-C1'-C2'	-5.53	105.92	112.00
25	1	224	A	C2'-C3'-O3'	-5.51	97.37	109.50
25	1	1714	C	N1-C1'-C2'	-5.51	105.94	112.00
25	1	1866	A	N9-C1'-C2'	-5.49	105.97	112.00
21	X	50	PHE	CB-CA-C	5.45	121.30	110.40
26	2	69	C	C4'-C3'-O3'	5.42	123.83	113.00
26	2	102	G	N9-C1'-C2'	-5.39	106.08	112.00
25	1	1253	G	C4'-C3'-O3'	5.36	123.72	113.00
25	1	1391	A	N9-C1'-C2'	-5.34	106.12	112.00
25	1	503	A	C2'-C3'-O3'	-5.31	97.81	109.50
25	1	1013	U	C4'-C3'-O3'	5.27	123.54	113.00
25	1	503	A	C4'-C3'-O3'	-5.24	98.39	109.40
25	1	507	C	C4'-C3'-O3'	5.23	123.45	113.00
25	1	224	A	P-O3'-C3'	5.22	125.97	119.70
25	1	674	C	C1'-C2'-O2'	-5.20	95.01	110.60
25	1	878	C	N1-C1'-C2'	-5.12	106.36	112.00
25	1	666	A	N9-C1'-C2'	-5.10	106.39	112.00
25	1	264	G	N9-C1'-C2'	-5.09	106.40	112.00
25	1	604	G	N9-C1'-C2'	-5.08	106.42	112.00
25	1	1712	A	P-O3'-C3'	5.07	125.79	119.70
25	1	1712	A	C2'-C3'-O3'	-5.07	98.35	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
1	A	111/116 (96%)	103 (93%)	8 (7%)	0	100	100
2	B	272/277 (98%)	248 (91%)	24 (9%)	0	100	100
3	C	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
4	D	98/105 (93%)	90 (92%)	8 (8%)	0	100	100
5	E	109/117 (93%)	103 (94%)	6 (6%)	0	100	100
6	F	85/91 (93%)	73 (86%)	12 (14%)	0	100	100
7	G	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
8	H	91/107 (85%)	86 (94%)	5 (6%)	0	100	100
9	J	57/62 (92%)	52 (91%)	5 (9%)	0	100	100
10	K	56/72 (78%)	55 (98%)	1 (2%)	0	100	100
11	L	213/217 (98%)	194 (91%)	19 (9%)	0	100	100
12	M	54/58 (93%)	50 (93%)	4 (7%)	0	100	100
13	N	48/57 (84%)	44 (92%)	4 (8%)	0	100	100
14	O	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
15	P	42/50 (84%)	42 (100%)	0	0	100	100
16	Q	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
17	R	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
18	S	190/207 (92%)	174 (92%)	16 (8%)	0	100	100
19	V	141/145 (97%)	133 (94%)	8 (6%)	0	100	100
20	W	119/122 (98%)	109 (92%)	10 (8%)	0	100	100
21	X	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
22	Y	134/144 (93%)	122 (91%)	12 (9%)	0	100	100
23	Z	119/122 (98%)	108 (91%)	11 (9%)	0	100	100
24	a	106/119 (89%)	97 (92%)	9 (8%)	0	100	100
27	I	76/85 (89%)	70 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2617/2793 (94%)	2424 (93%)	193 (7%)	0	100 100

There are no Ramachandran outliers to report.

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
1	A	99/102 (97%)	98 (99%)	1 (1%)	76 90
2	B	221/224 (99%)	210 (95%)	11 (5%)	24 60
3	C	96/98 (98%)	91 (95%)	5 (5%)	23 59
4	D	85/89 (96%)	81 (95%)	4 (5%)	26 62
5	E	90/94 (96%)	86 (96%)	4 (4%)	28 64
6	F	79/82 (96%)	69 (87%)	10 (13%)	4 20
7	G	85/91 (93%)	85 (100%)	0	100 100
8	H	81/95 (85%)	71 (88%)	10 (12%)	4 21
9	J	49/51 (96%)	46 (94%)	3 (6%)	18 54
10	K	53/65 (82%)	52 (98%)	1 (2%)	57 81
11	L	173/175 (99%)	166 (96%)	7 (4%)	31 66
12	M	50/52 (96%)	50 (100%)	0	100 100
13	N	45/49 (92%)	44 (98%)	1 (2%)	52 79
14	O	45/47 (96%)	43 (96%)	2 (4%)	28 64
15	P	39/45 (87%)	39 (100%)	0	100 100
16	Q	55/56 (98%)	55 (100%)	0	100 100
17	R	35/35 (100%)	35 (100%)	0	100 100
18	S	158/170 (93%)	156 (99%)	2 (1%)	69 87
19	V	122/123 (99%)	120 (98%)	2 (2%)	62 84
20	W	99/100 (99%)	98 (99%)	1 (1%)	76 90
21	X	110/112 (98%)	105 (96%)	5 (4%)	27 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	Y	113/119 (95%)	111 (98%)	2 (2%)	59 82
23	Z	101/102 (99%)	99 (98%)	2 (2%)	55 80
24	a	87/95 (92%)	84 (97%)	3 (3%)	37 70
27	I	61/66 (92%)	61 (100%)	0	100 100
All	All	2231/2337 (96%)	2155 (97%)	76 (3%)	40 70

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
2	B	17	THR
2	B	72	ASP
2	B	115	ILE
2	B	117	GLU
2	B	123	ASP
2	B	124	ILE
2	B	167	LYS
2	B	168	GLU
2	B	172	VAL
2	B	180	GLU
2	B	184	ILE
3	C	33	LYS
3	C	51	ARG
3	C	70	ARG
3	C	84	LYS
3	C	103	GLU
4	D	1	MET
4	D	15	GLU
4	D	28	ASN
4	D	99	LYS
5	E	48	GLU
5	E	49	LYS
5	E	86	ARG
5	E	88	ARG
6	F	12	ILE
6	F	14	GLU
6	F	15	LYS
6	F	20	MET
6	F	22	GLU
6	F	24	LYS
6	F	62	LYS

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Mol	Chain	Res	Type
6	F	63	LYS
6	F	89	LEU
6	F	90	PHE
8	H	5	LYS
8	H	13	GLN
8	H	18	LEU
8	H	23	LYS
8	H	26	LYS
8	H	40	SER
8	H	41	VAL
8	H	51	VAL
8	H	53	ARG
8	H	62	GLU
9	J	3	LYS
9	J	28	ARG
9	J	41	ASP
10	K	10	THR
11	L	13	THR
11	L	55	ASP
11	L	57	LYS
11	L	60	LYS
11	L	62	ASP
11	L	64	LYS
11	L	103	GLN
13	N	46	CYS
14	O	20	THR
14	O	21	LYS
18	S	23	VAL
18	S	26	ILE
19	V	48	HIS
19	V	65	PHE
20	W	52	VAL
21	X	50	PHE
21	X	84	LYS
21	X	85	PHE
21	X	121	LEU
21	X	139	LYS
22	Y	14	ARG
22	Y	136	GLU
23	Z	59	ARG
23	Z	79	GLN
24	a	22	LEU

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Mol	Chain	Res	Type
24	a	28	LYS
24	a	102	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
2	B	53	HIS
2	B	54	HIS
4	D	90	GLN
6	F	54	ASN
6	F	69	GLN
7	G	44	HIS
7	G	67	ASN
8	H	38	ASN
9	J	30	ASN
9	J	34	GLN
11	L	143	HIS
13	N	50	ASN
16	Q	35	ASN
17	R	36	GLN
18	S	67	GLN
18	S	121	ASN
18	S	158	ASN
19	V	48	HIS
19	V	59	ASN
19	V	78	HIS
19	V	81	HIS
21	X	54	GLN
22	Y	25	ASN
23	Z	79	GLN
24	a	15	HIS
24	a	43	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	1	2689/2923 (91%)	742 (27%)	137 (5%)
26	2	110/115 (95%)	41 (37%)	10 (9%)
All	All	2799/3038 (92%)	783 (27%)	147 (5%)

All (783) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	1	8	U
25	1	11	U
25	1	20	C
25	1	24	G
25	1	28	A
25	1	29	U
25	1	30	G
25	1	34	U
25	1	35	G
25	1	36	G
25	1	60	U
25	1	61	A
25	1	63	U
25	1	66	C
25	1	71	A
25	1	73	A
25	1	74	U
25	1	75	G
25	1	77	U
25	1	79	U
25	1	83	G
25	1	90	A
25	1	94	A
25	1	100	U
25	1	118	A
25	1	119	U
25	1	120	G
25	1	121	G
25	1	124	A
25	1	125	A
25	1	130	A
25	1	132	C
25	1	134	U
25	1	138	U
25	1	150	A
25	1	156	A
25	1	157	U
25	1	160	G
25	1	161	A
25	1	162	A
25	1	163	U
25	1	164	A

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Mol	Chain	Res	Type
25	1	165	C
25	1	166	A
25	1	167	U
25	1	168	A
25	1	169	G
25	1	170	C
25	1	173	A
25	1	174	U
25	1	176	A
25	1	183	A
25	1	184	C
25	1	185	A
25	1	197	G
25	1	199	A
25	1	202	A
25	1	203	U
25	1	204	C
25	1	206	U
25	1	207	A
25	1	218	G
25	1	219	A
25	1	224	A
25	1	225	A
25	1	230	A
25	1	231	A
25	1	233	U
25	1	234	C
25	1	235	G
25	1	236	A
25	1	237	U
25	1	241	C
25	1	244	A
25	1	248	G
25	1	251	G
25	1	252	C
25	1	253	G
25	1	255	G
25	1	256	C
25	1	258	A
25	1	259	A
25	1	261	C
25	1	263	G

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Mol	Chain	Res	Type
25	1	264	G
25	1	267	G
25	1	268	A
25	1	269	G
25	1	270	C
25	1	278	A
25	1	279	A
25	1	280	C
25	1	292	U
25	1	293	U
25	1	298	U
25	1	300	G
25	1	301	U
25	1	302	A
25	1	303	G
25	1	308	C
25	1	309	U
25	1	311	U
25	1	319	G
25	1	320	U
25	1	321	U
25	1	322	A
25	1	323	C
25	1	324	A
25	1	325	A
25	1	326	A
25	1	327	G
25	1	329	A
25	1	330	C
25	1	331	G
25	1	332	A
25	1	351	G
25	1	354	A
25	1	358	G
25	1	360	A
25	1	362	C
25	1	366	G
25	1	370	G
25	1	372	A
25	1	373	A
25	1	378	C
25	1	381	G

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Mol	Chain	Res	Type
25	1	389	A
25	1	395	U
25	1	396	G
25	1	402	C
25	1	404	U
25	1	405	G
25	1	406	A
25	1	410	G
25	1	411	A
25	1	412	U
25	1	413	C
25	1	429	C
25	1	431	C
25	1	432	G
25	1	433	U
25	1	434	G
25	1	447	A
25	1	452	G
25	1	457	G
25	1	458	A
25	1	461	A
25	1	464	U
25	1	472	C
25	1	473	U
25	1	475	A
25	1	482	U
25	1	489	A
25	1	499	A
25	1	500	A
25	1	501	C
25	1	502	C
25	1	503	A
25	1	504	G
25	1	505	U
25	1	506	A
25	1	507	C
25	1	515	G
25	1	516	A
25	1	518	A
25	1	519	G
25	1	521	U
25	1	527	G

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Mol	Chain	Res	Type
25	1	547	A
25	1	549	U
25	1	550	A
25	1	553	A
25	1	554	C
25	1	555	C
25	1	556	U
25	1	557	G
25	1	558	A
25	1	563	G
25	1	567	G
25	1	568	C
25	1	572	C
25	1	575	G
25	1	576	U
25	1	577	A
25	1	578	G
25	1	583	A
25	1	589	U
25	1	591	A
25	1	593	U
25	1	594	G
25	1	605	U
25	1	606	G
25	1	616	G
25	1	617	A
25	1	618	A
25	1	630	G
25	1	638	U
25	1	639	U
25	1	646	A
25	1	647	G
25	1	650	U
25	1	652	A
25	1	657	U
25	1	658	A
25	1	659	A
25	1	660	A
25	1	661	U
25	1	662	G
25	1	665	G
25	1	666	A

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Mol	Chain	Res	Type
25	1	667	G
25	1	675	G
25	1	679	G
25	1	683	G
25	1	684	U
25	1	687	G
25	1	689	A
25	1	690	U
25	1	691	A
25	1	693	G
25	1	694	G
25	1	696	G
25	1	697	U
25	1	698	U
25	1	699	U
25	1	700	A
25	1	712	U
25	1	713	A
25	1	730	A
25	1	731	U
25	1	732	C
25	1	744	A
25	1	745	G
25	1	746	G
25	1	752	G
25	1	755	C
25	1	759	U
25	1	760	A
25	1	762	C
25	1	763	A
25	1	769	U
25	1	772	A
25	1	775	A
25	1	776	C
25	1	777	C
25	1	785	C
25	1	792	U
25	1	793	G
25	1	795	A
25	1	807	U
25	1	810	A
25	1	819	A

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Mol	Chain	Res	Type
25	1	820	G
25	1	822	G
25	1	824	A
25	1	827	A
25	1	829	U
25	1	830	U
25	1	837	G
25	1	838	A
25	1	850	G
25	1	857	C
25	1	872	U
25	1	873	U
25	1	876	G
25	1	890	G
25	1	891	A
25	1	911	A
25	1	915	U
25	1	916	U
25	1	917	U
25	1	920	A
25	1	921	C
25	1	924	G
25	1	944	G
25	1	945	A
25	1	946	A
25	1	947	U
25	1	955	A
25	1	959	C
25	1	970	U
25	1	972	A
25	1	974	U
25	1	977	A
25	1	985	A
25	1	989	A
25	1	990	G
25	1	997	G
25	1	1003	A
25	1	1005	G
25	1	1006	G
25	1	1008	C
25	1	1018	A
25	1	1022	G

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Mol	Chain	Res	Type
25	1	1025	A
25	1	1027	A
25	1	1029	C
25	1	1039	C
25	1	1040	A
25	1	1041	G
25	1	1049	C
25	1	1053	A
25	1	1055	A
25	1	1056	U
25	1	1057	A
25	1	1062	U
25	1	1066	G
25	1	1069	G
25	1	1070	A
25	1	1077	U
25	1	1081	G
25	1	1082	C
25	1	1083	G
25	1	1085	U
25	1	1087	C
25	1	1093	C
25	1	1094	A
25	1	1156	G
25	1	1157	U
25	1	1158	G
25	1	1173	A
25	1	1174	U
25	1	1176	U
25	1	1177	A
25	1	1179	C
25	1	1183	G
25	1	1186	A
25	1	1187	A
25	1	1190	A
25	1	1195	A
25	1	1209	U
25	1	1211	G
25	1	1214	C
25	1	1215	U
25	1	1216	U
25	1	1217	U

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Mol	Chain	Res	Type
25	1	1218	G
25	1	1220	A
25	1	1253	G
25	1	1258	A
25	1	1269	A
25	1	1271	G
25	1	1273	G
25	1	1274	G
25	1	1278	G
25	1	1288	G
25	1	1293	U
25	1	1294	G
25	1	1306	A
25	1	1309	G
25	1	1310	A
25	1	1312	A
25	1	1313	G
25	1	1326	C
25	1	1337	A
25	1	1338	U
25	1	1339	U
25	1	1358	A
25	1	1366	U
25	1	1374	G
25	1	1378	U
25	1	1382	C
25	1	1389	U
25	1	1390	A
25	1	1392	G
25	1	1396	A
25	1	1402	A
25	1	1409	U
25	1	1410	A
25	1	1414	G
25	1	1415	A
25	1	1416	U
25	1	1419	A
25	1	1421	A
25	1	1432	A
25	1	1433	U
25	1	1435	C
25	1	1448	U

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Mol	Chain	Res	Type
25	1	1452	C
25	1	1453	G
25	1	1454	U
25	1	1462	G
25	1	1463	A
25	1	1464	U
25	1	1471	A
25	1	1472	C
25	1	1484	G
25	1	1485	G
25	1	1487	G
25	1	1488	A
25	1	1489	A
25	1	1490	G
25	1	1491	C
25	1	1492	G
25	1	1493	U
25	1	1494	G
25	1	1495	C
25	1	1496	G
25	1	1497	A
25	1	1501	G
25	1	1504	U
25	1	1508	C
25	1	1509	G
25	1	1510	U
25	1	1514	A
25	1	1515	G
25	1	1516	C
25	1	1517	A
25	1	1518	G
25	1	1519	U
25	1	1521	A
25	1	1526	G
25	1	1541	C
25	1	1546	A
25	1	1557	C
25	1	1559	G
25	1	1561	G
25	1	1562	C
25	1	1566	G
25	1	1567	A

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Mol	Chain	Res	Type
25	1	1569	G
25	1	1570	G
25	1	1571	G
25	1	1573	A
25	1	1574	G
25	1	1575	A
25	1	1576	A
25	1	1578	A
25	1	1579	C
25	1	1588	U
25	1	1589	U
25	1	1590	C
25	1	1591	G
25	1	1592	A
25	1	1593	G
25	1	1594	U
25	1	1595	C
25	1	1596	G
25	1	1598	U
25	1	1599	G
25	1	1600	A
25	1	1604	C
25	1	1605	A
25	1	1606	C
25	1	1613	G
25	1	1616	A
25	1	1623	U
25	1	1625	U
25	1	1627	G
25	1	1628	A
25	1	1629	U
25	1	1630	A
25	1	1631	G
25	1	1632	A
25	1	1634	A
25	1	1639	G
25	1	1651	C
25	1	1652	A
25	1	1654	A
25	1	1660	A
25	1	1662	A
25	1	1663	G

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Mol	Chain	Res	Type
25	1	1668	U
25	1	1673	A
25	1	1675	G
25	1	1676	A
25	1	1677	G
25	1	1687	G
25	1	1690	A
25	1	1691	G
25	1	1692	C
25	1	1699	A
25	1	1718	G
25	1	1719	C
25	1	1720	A
25	1	1721	A
25	1	1738	C
25	1	1739	G
25	1	1740	G
25	1	1744	A
25	1	1747	G
25	1	1748	G
25	1	1755	U
25	1	1758	A
25	1	1759	G
25	1	1760	G
25	1	1763	U
25	1	1765	A
25	1	1773	A
25	1	1774	A
25	1	1784	U
25	1	1785	G
25	1	1787	A
25	1	1790	G
25	1	1791	G
25	1	1800	A
25	1	1803	G
25	1	1809	C
25	1	1811	A
25	1	1814	A
25	1	1827	C
25	1	1828	U
25	1	1829	A
25	1	1835	U

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Mol	Chain	Res	Type
25	1	1836	A
25	1	1837	A
25	1	1843	U
25	1	1856	A
25	1	1857	C
25	1	1865	C
25	1	1866	A
25	1	1867	G
25	1	1876	G
25	1	1883	A
25	1	1888	U
25	1	1893	A
25	1	1898	C
25	1	1899	U
25	1	1900	G
25	1	1903	A
25	1	1906	C
25	1	1909	C
25	1	1912	A
25	1	1921	C
25	1	1922	C
25	1	1923	A
25	1	1924	G
25	1	1926	A
25	1	1927	A
25	1	1933	G
25	1	1937	G
25	1	1940	A
25	1	1941	C
25	1	1942	U
25	1	1943	A
25	1	1946	A
25	1	1947	C
25	1	1949	G
25	1	1954	A
25	1	1956	G
25	1	1957	G
25	1	1964	A
25	1	1965	A
25	1	1982	U
25	1	1990	C
25	1	1992	C

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Mol	Chain	Res	Type
25	1	1994	C
25	1	1997	A
25	1	1998	A
25	1	1999	G
25	1	2004	A
25	1	2009	U
25	1	2018	U
25	1	2020	U
25	1	2023	C
25	1	2031	G
25	1	2034	U
25	1	2049	U
25	1	2050	A
25	1	2058	A
25	1	2059	G
25	1	2060	A
25	1	2066	G
25	1	2069	A
25	1	2070	C
25	1	2073	G
25	1	2082	C
25	1	2083	G
25	1	2084	G
25	1	2085	A
25	1	2086	A
25	1	2087	A
25	1	2088	G
25	1	2089	A
25	1	2093	C
25	1	2096	G
25	1	2104	A
25	1	2114	G
25	1	2120	G
25	1	2122	A
25	1	2126	C
25	1	2220	U
25	1	2222	U
25	1	2226	A
25	1	2228	C
25	1	2230	G
25	1	2231	C
25	1	2232	A

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Mol	Chain	Res	Type
25	1	2237	U
25	1	2238	U
25	1	2239	A
25	1	2240	U
25	1	2241	C
25	1	2252	A
25	1	2265	G
25	1	2266	G
25	1	2276	U
25	1	2277	G
25	1	2278	G
25	1	2279	G
25	1	2295	A
25	1	2300	A
25	1	2301	A
25	1	2302	C
25	1	2303	G
25	1	2310	C
25	1	2314	A
25	1	2315	A
25	1	2331	G
25	1	2332	U
25	1	2333	U
25	1	2335	G
25	1	2336	A
25	1	2337	A
25	1	2338	A
25	1	2339	U
25	1	2341	A
25	1	2342	U
25	1	2346	U
25	1	2347	A
25	1	2348	G
25	1	2349	A
25	1	2350	G
25	1	2360	A
25	1	2362	A
25	1	2367	A
25	1	2370	U
25	1	2372	G
25	1	2374	C
25	1	2377	C

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Mol	Chain	Res	Type
25	1	2381	A
25	1	2410	G
25	1	2412	C
25	1	2420	U
25	1	2426	G
25	1	2429	U
25	1	2430	C
25	1	2433	C
25	1	2434	A
25	1	2440	G
25	1	2446	U
25	1	2452	A
25	1	2456	G
25	1	2457	A
25	1	2467	C
25	1	2468	C
25	1	2473	G
25	1	2474	G
25	1	2475	A
25	1	2476	U
25	1	2478	A
25	1	2479	C
25	1	2480	A
25	1	2481	G
25	1	2497	G
25	1	2501	U
25	1	2502	C
25	1	2503	A
25	1	2521	G
25	1	2523	C
25	1	2524	A
25	1	2525	C
25	1	2527	U
25	1	2529	G
25	1	2530	A
25	1	2531	U
25	1	2532	G
25	1	2533	U
25	1	2534	C
25	1	2535	G
25	1	2545	A
25	1	2557	U

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Mol	Chain	Res	Type
25	1	2562	G
25	1	2563	G
25	1	2581	U
25	1	2593	A
25	1	2594	G
25	1	2600	C
25	1	2609	G
25	1	2610	G
25	1	2611	U
25	1	2612	U
25	1	2613	C
25	1	2626	G
25	1	2636	U
25	1	2640	U
25	1	2641	A
25	1	2642	U
25	1	2657	G
25	1	2663	U
25	1	2680	U
25	1	2681	A
25	1	2682	G
25	1	2683	U
25	1	2688	G
25	1	2691	G
25	1	2692	A
25	1	2698	A
25	1	2700	G
25	1	2703	C
25	1	2712	G
25	1	2716	U
25	1	2732	A
25	1	2741	G
25	1	2753	U
25	1	2760	A
25	1	2762	G
25	1	2763	G
25	1	2771	G
25	1	2773	U
25	1	2775	A
25	1	2778	G
25	1	2779	C
25	1	2792	A

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Mol	Chain	Res	Type
25	1	2793	G
25	1	2797	C
25	1	2805	A
25	1	2817	A
25	1	2818	A
25	1	2820	U
25	1	2821	U
25	1	2823	G
25	1	2824	G
25	1	2827	A
25	1	2828	U
25	1	2840	A
25	1	2843	A
25	1	2846	A
25	1	2853	U
25	1	2854	A
25	1	2875	U
25	1	2886	G
25	1	2887	G
25	1	2892	G
25	1	2893	A
25	1	2899	A
25	1	2900	C
25	1	2903	A
25	1	2904	U
25	1	2911	A
25	1	2913	G
25	1	2920	U
26	2	4	G
26	2	7	G
26	2	8	A
26	2	10	U
26	2	11	A
26	2	12	U
26	2	13	A
26	2	14	G
26	2	20	A
26	2	22	G
26	2	23	U
26	2	24	C
26	2	25	A
26	2	33	U

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Mol	Chain	Res	Type
26	2	36	C
26	2	38	U
26	2	39	G
26	2	40	C
26	2	41	C
26	2	46	A
26	2	47	C
26	2	48	A
26	2	49	G
26	2	56	A
26	2	64	A
26	2	66	C
26	2	71	A
26	2	82	A
26	2	84	U
26	2	85	U
26	2	86	A
26	2	94	C
26	2	100	U
26	2	101	A
26	2	104	A
26	2	105	C
26	2	106	G
26	2	107	U
26	2	110	C
26	2	111	A
26	2	112	G

All (147) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	1	10	A
25	1	28	A
25	1	34	U
25	1	60	U
25	1	73	A
25	1	74	U
25	1	160	G
25	1	161	A
25	1	166	A
25	1	167	U
25	1	199	A

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Mol	Chain	Res	Type
25	1	224	A
25	1	229	A
25	1	240	C
25	1	251	G
25	1	252	C
25	1	253	G
25	1	263	G
25	1	267	G
25	1	268	A
25	1	278	A
25	1	279	A
25	1	291	G
25	1	292	U
25	1	301	U
25	1	318	A
25	1	320	U
25	1	321	U
25	1	322	A
25	1	323	C
25	1	324	A
25	1	325	A
25	1	326	A
25	1	327	G
25	1	330	C
25	1	331	G
25	1	394	U
25	1	395	U
25	1	401	U
25	1	431	C
25	1	432	G
25	1	433	U
25	1	471	G
25	1	472	C
25	1	473	U
25	1	499	A
25	1	500	A
25	1	501	C
25	1	502	C
25	1	503	A
25	1	504	G
25	1	554	C
25	1	556	U

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Mol	Chain	Res	Type
25	1	557	G
25	1	577	A
25	1	660	A
25	1	665	G
25	1	682	A
25	1	689	A
25	1	690	U
25	1	696	G
25	1	745	G
25	1	890	G
25	1	914	G
25	1	916	U
25	1	1005	G
25	1	1038	C
25	1	1039	C
25	1	1273	G
25	1	1274	G
25	1	1389	U
25	1	1395	G
25	1	1408	G
25	1	1414	G
25	1	1415	A
25	1	1484	G
25	1	1487	G
25	1	1488	A
25	1	1489	A
25	1	1490	G
25	1	1491	C
25	1	1493	U
25	1	1507	A
25	1	1508	C
25	1	1509	G
25	1	1514	A
25	1	1515	G
25	1	1566	G
25	1	1573	A
25	1	1574	G
25	1	1575	A
25	1	1576	A
25	1	1590	C
25	1	1591	G
25	1	1593	G

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Mol	Chain	Res	Type
25	1	1594	U
25	1	1595	C
25	1	1596	G
25	1	1599	G
25	1	1675	G
25	1	1712	A
25	1	1717	G
25	1	1718	G
25	1	1865	C
25	1	1926	A
25	1	2084	G
25	1	2085	A
25	1	2087	A
25	1	2088	G
25	1	2089	A
25	1	2237	U
25	1	2238	U
25	1	2239	A
25	1	2240	U
25	1	2276	U
25	1	2277	G
25	1	2278	G
25	1	2300	A
25	1	2301	A
25	1	2302	C
25	1	2330	G
25	1	2432	G
25	1	2474	G
25	1	2475	A
25	1	2477	A
25	1	2524	A
25	1	2530	A
25	1	2531	U
25	1	2532	G
25	1	2533	U
25	1	2610	G
25	1	2612	U
25	1	2680	U
25	1	2681	A
25	1	2682	G
25	1	2691	G
25	1	2827	A

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Mol	Chain	Res	Type
26	2	6	U
26	2	10	U
26	2	11	A
26	2	12	U
26	2	13	A
26	2	46	A
26	2	47	C
26	2	81	A
26	2	105	C
26	2	106	G

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	$\#\|Z\| > 2$
28	U7V	1	3001	-	28,30,30	2.52	4 (14%)	35,43,43	3.56	21 (60%)

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
28	U7V	1	3001	-	-	6/14/26/26	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	3001	U7V	C23-N19	9.68	1.46	1.36
28	1	3001	U7V	O22-C23	6.37	1.43	1.35
28	1	3001	U7V	C20-N19	-3.70	1.40	1.47
28	1	3001	U7V	O22-C21	-3.51	1.41	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	3001	U7V	C20-N19-C23	-8.50	106.36	111.28
28	1	3001	U7V	C21-O22-C23	-8.25	103.64	110.15
28	1	3001	U7V	O22-C23-N19	-6.72	105.20	109.83
28	1	3001	U7V	C20-N19-C16	5.99	131.59	121.45
28	1	3001	U7V	C04-C07-N08	5.67	123.23	116.75
28	1	3001	U7V	N03-C04-N05	-4.89	108.10	111.85
28	1	3001	U7V	O22-C23-O24	4.69	127.57	122.37
28	1	3001	U7V	O22-C21-C20	4.14	108.75	104.57
28	1	3001	U7V	C01-N02-N06	3.91	127.56	122.66
28	1	3001	U7V	C16-N19-C23	-3.61	122.05	125.91
28	1	3001	U7V	C18-C13-C14	3.38	120.98	116.10
28	1	3001	U7V	C12-C07-C04	-3.23	116.17	120.19
28	1	3001	U7V	C11-C10-C13	-3.23	115.67	120.91
28	1	3001	U7V	C09-N08-C07	2.86	121.66	117.90
28	1	3001	U7V	C17-C16-N19	-2.79	116.11	120.18
28	1	3001	U7V	C10-C09-N08	-2.51	120.18	124.32
28	1	3001	U7V	C21-C20-N19	2.51	104.33	101.81
28	1	3001	U7V	C15-C14-C13	-2.45	119.78	123.64
28	1	3001	U7V	C04-N05-N06	2.44	107.36	105.47
28	1	3001	U7V	O24-C23-N19	-2.12	127.23	128.91
28	1	3001	U7V	C15-C16-N19	2.03	122.76	119.85

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	1	3001	U7V	N05-C04-C07-N08
28	1	3001	U7V	C15-C16-N19-C23
28	1	3001	U7V	C17-C16-N19-C23

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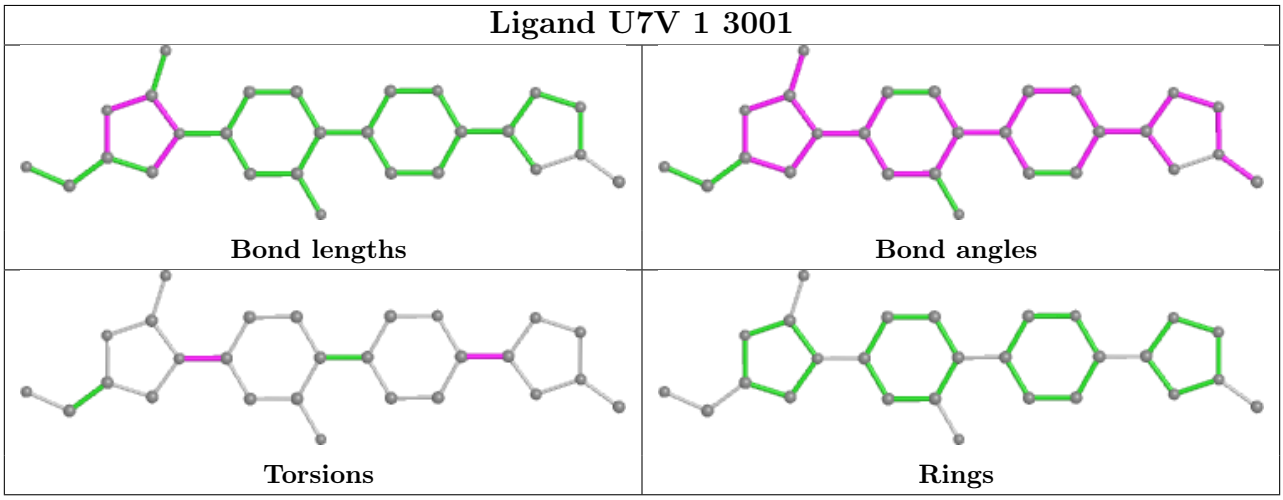
Mol	Chain	Res	Type	Atoms
28	1	3001	U7V	N03-C04-C07-N08
28	1	3001	U7V	N05-C04-C07-C12
28	1	3001	U7V	N03-C04-C07-C12

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

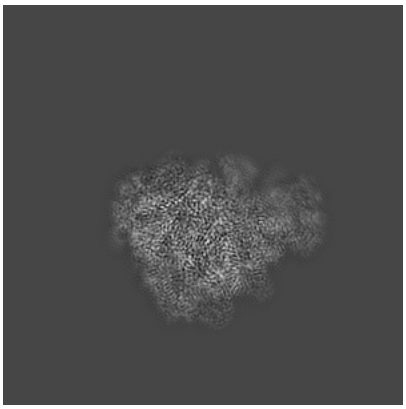
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21887. These allow visual inspection of the internal detail of the map and identification of artifacts.

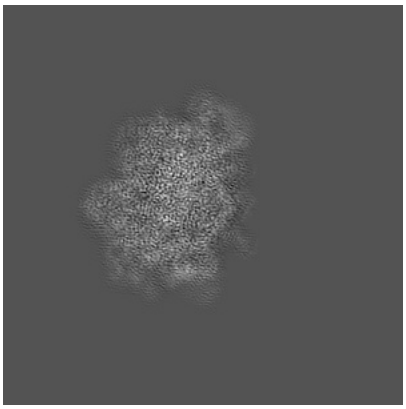
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

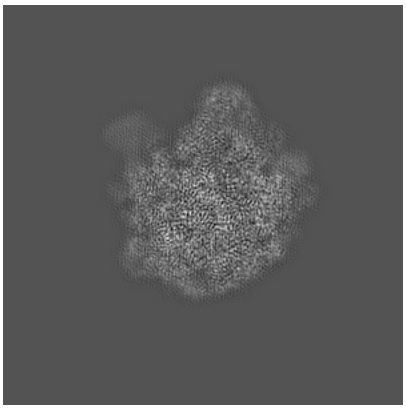
6.1.1 Primary map



X

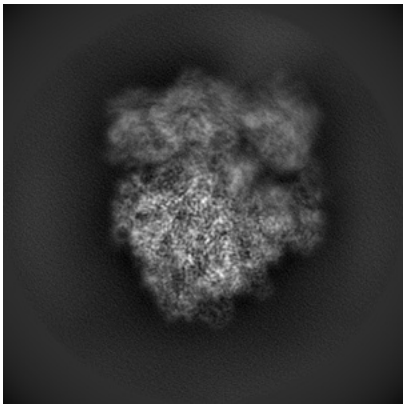


Y

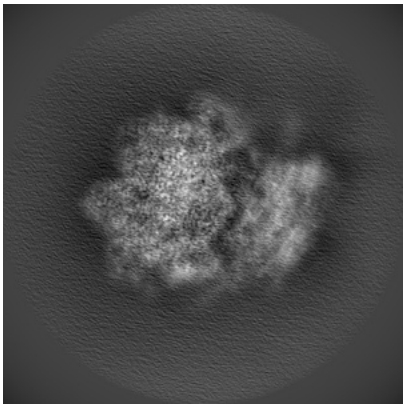


Z

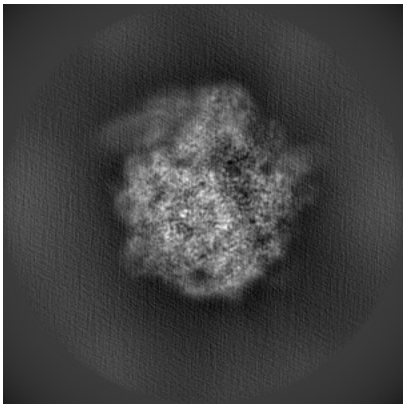
6.1.2 Raw map



X



Y

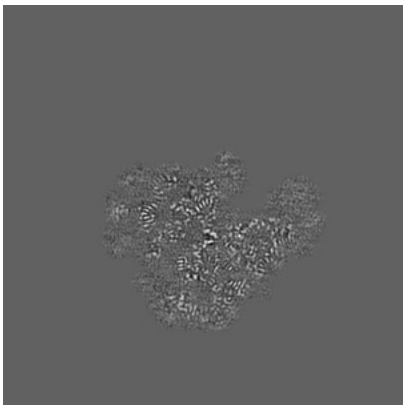


Z

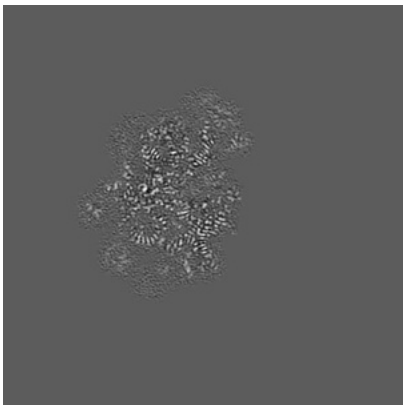
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

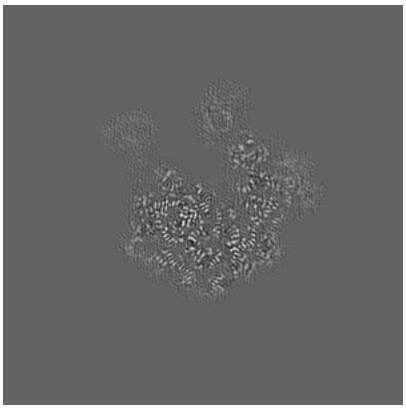
6.2.1 Primary map



X Index: 180

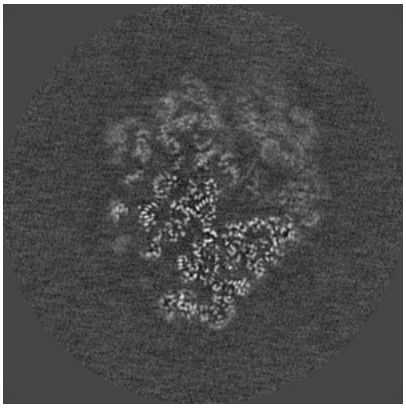


Y Index: 180

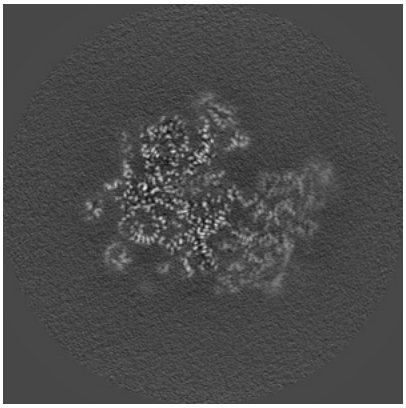


Z Index: 180

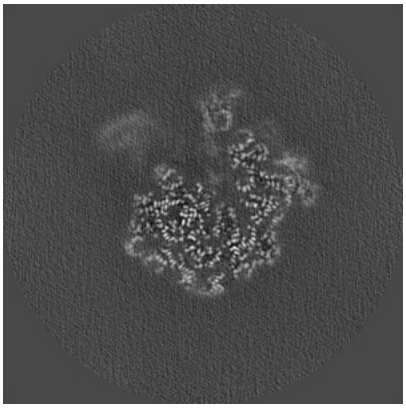
6.2.2 Raw map



X Index: 180



Y Index: 180

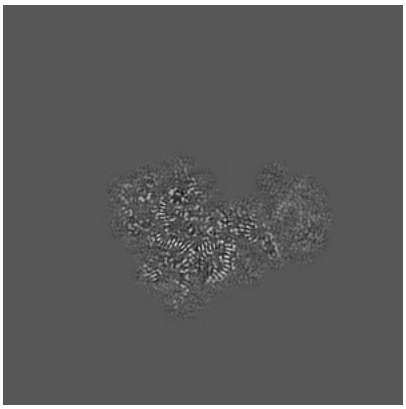


Z Index: 180

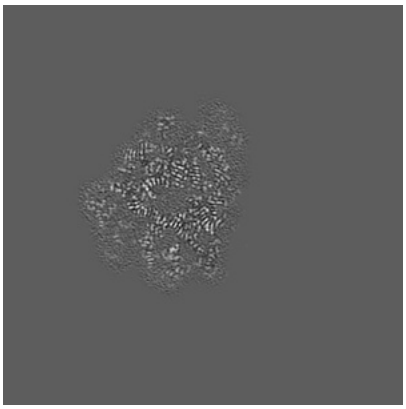
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

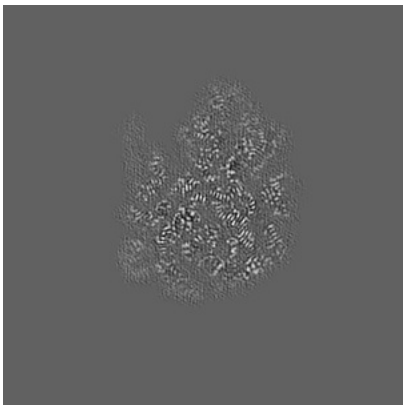
6.3.1 Primary map



X Index: 202

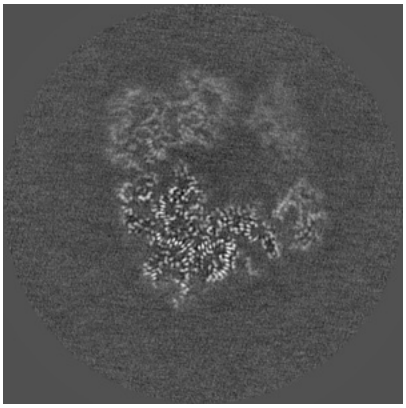


Y Index: 168

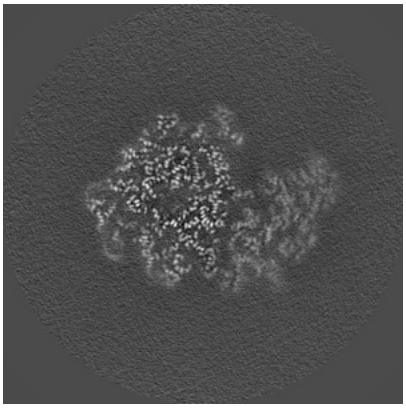


Z Index: 157

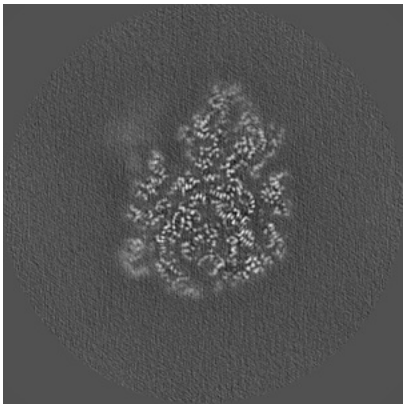
6.3.2 Raw map



X Index: 202



Y Index: 169

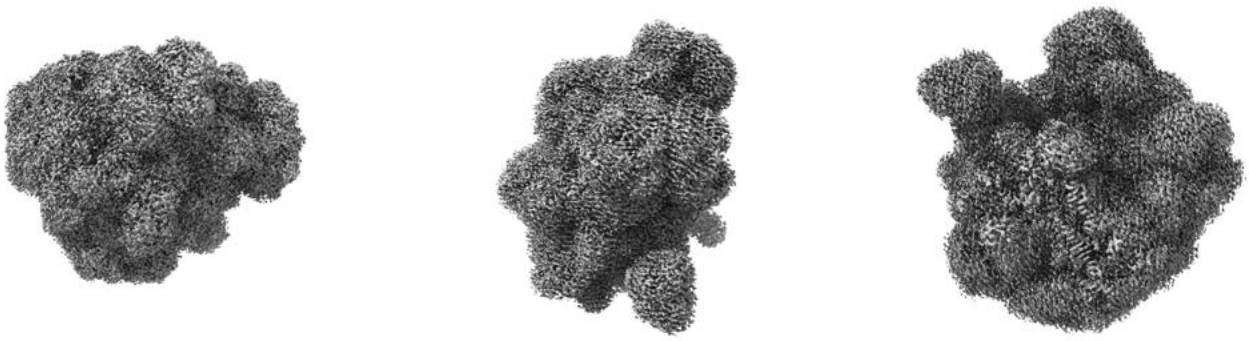


Z Index: 157

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

6.4 Orthogonal surface views (i)

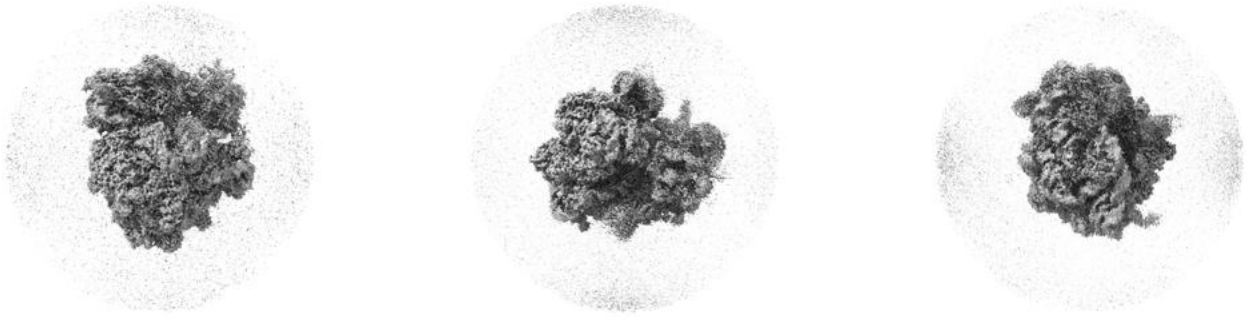
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

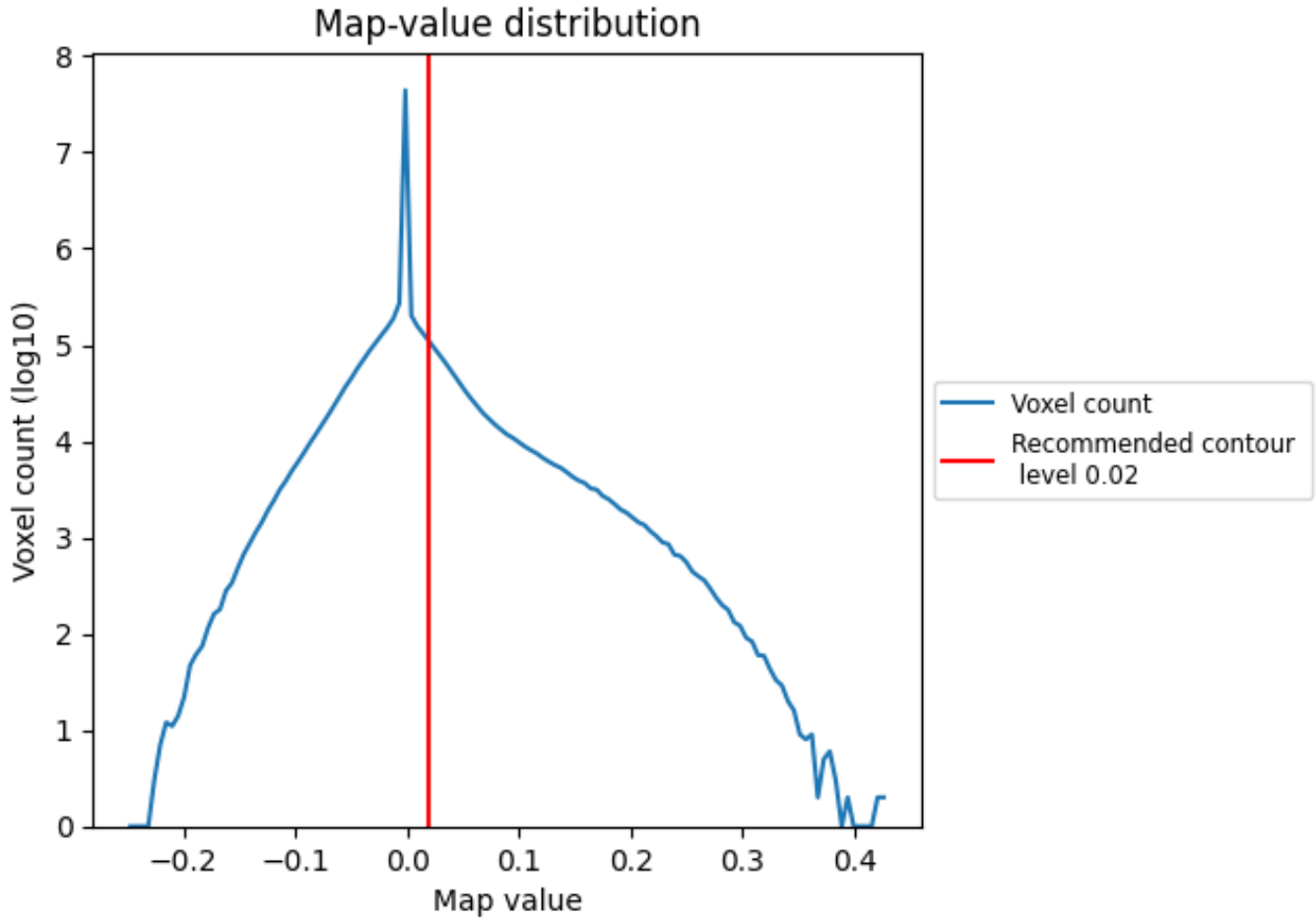
6.5 Mask visualisation (i)

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

7 Map analysis

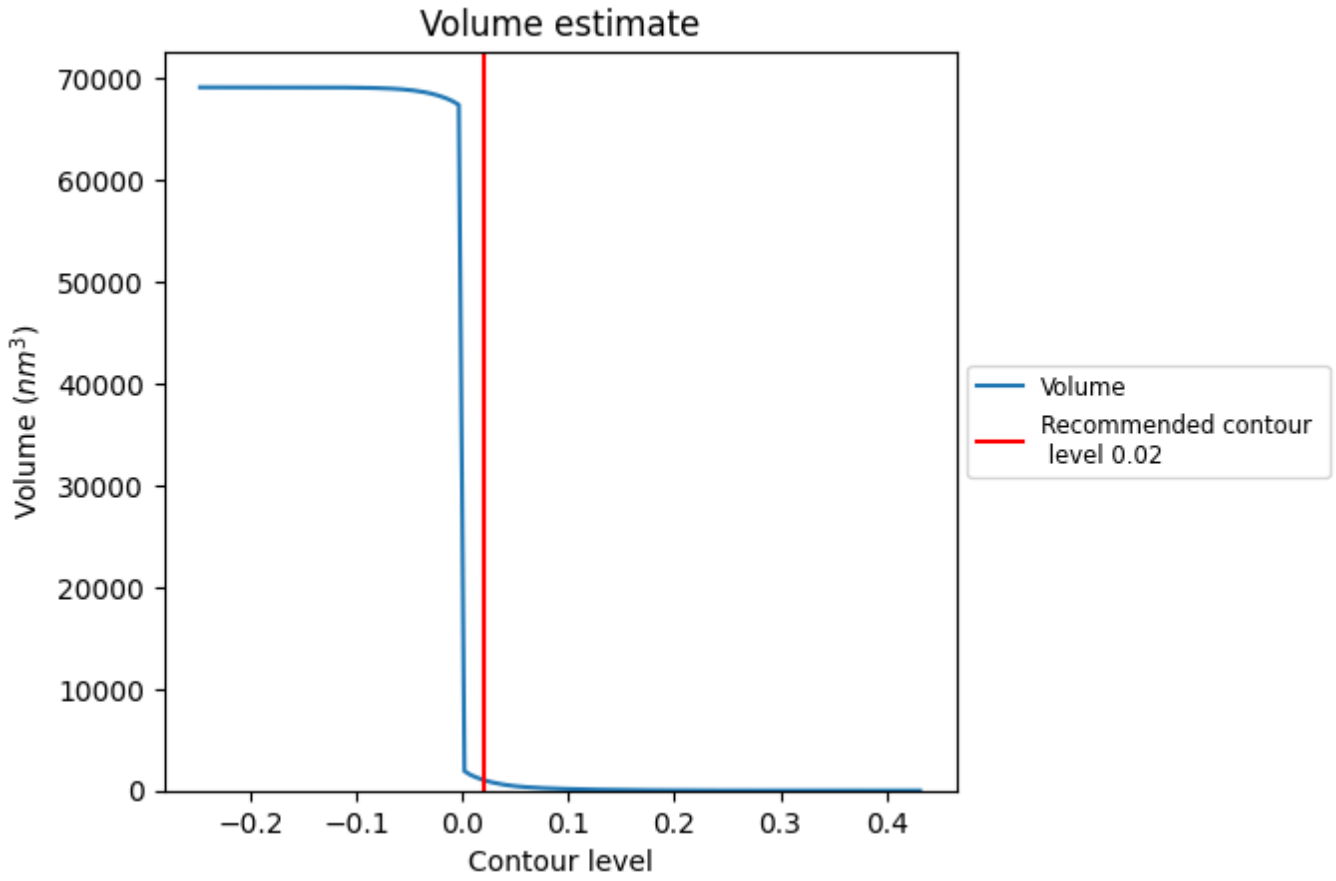
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

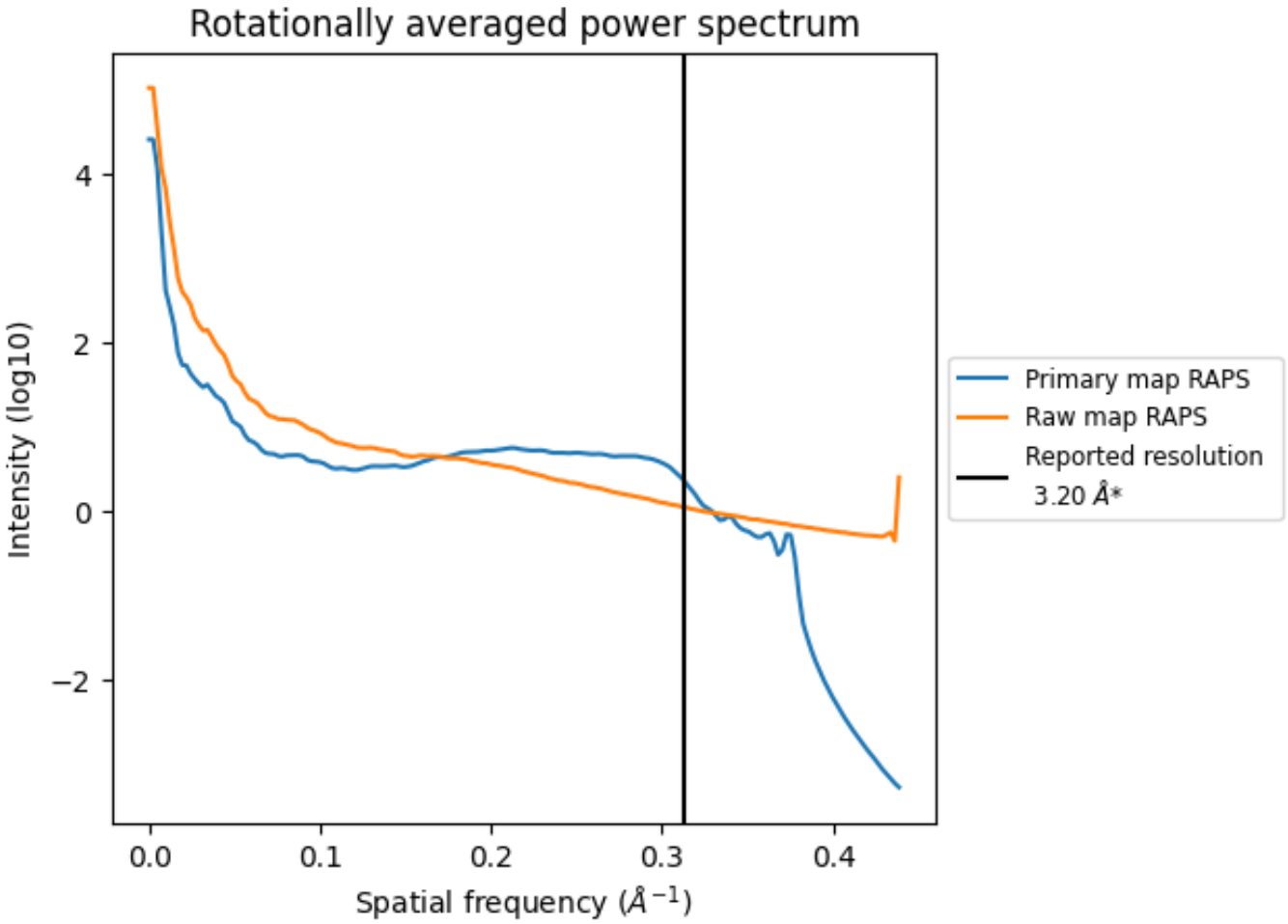
7.2 Volume estimate



The volume at the recommended contour level is 1046 nm^3; this corresponds to an approximate mass of 945 kDa.

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

7.3 Rotationally averaged power spectrum (i)

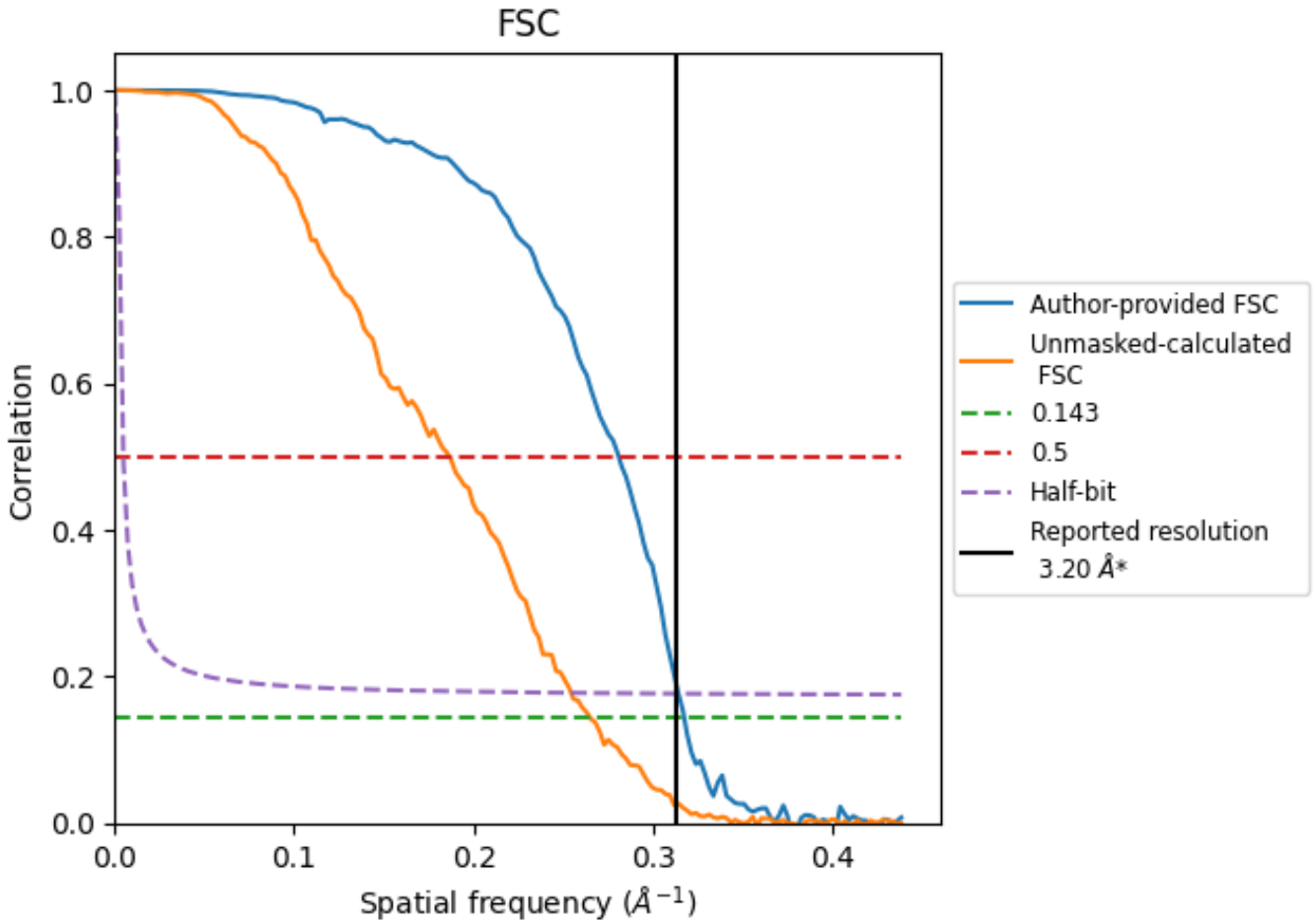


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

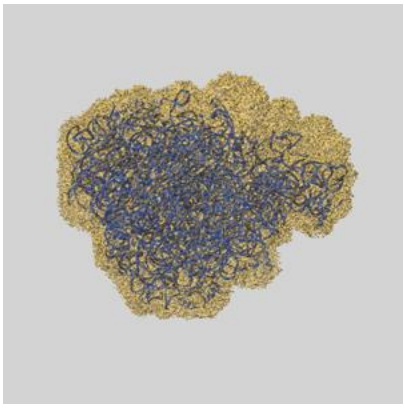
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.56	3.18
Unmasked-calculated*	3.77	5.36	3.93

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.77 differs from the reported value 3.2 by more than 10 %

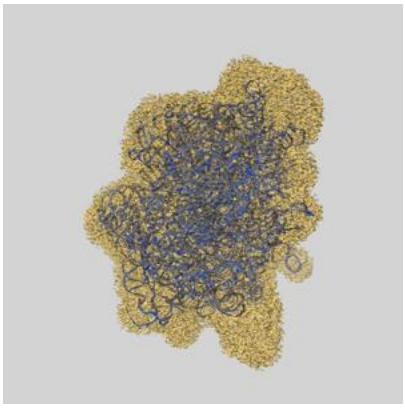
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21887 and PDB model 6WRS. Per-residue inclusion information can be found in section 3 on page 10.

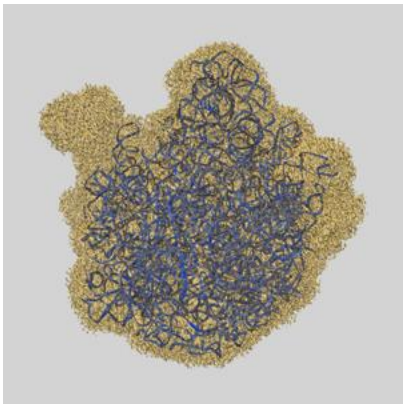
9.1 Map-model overlay



X



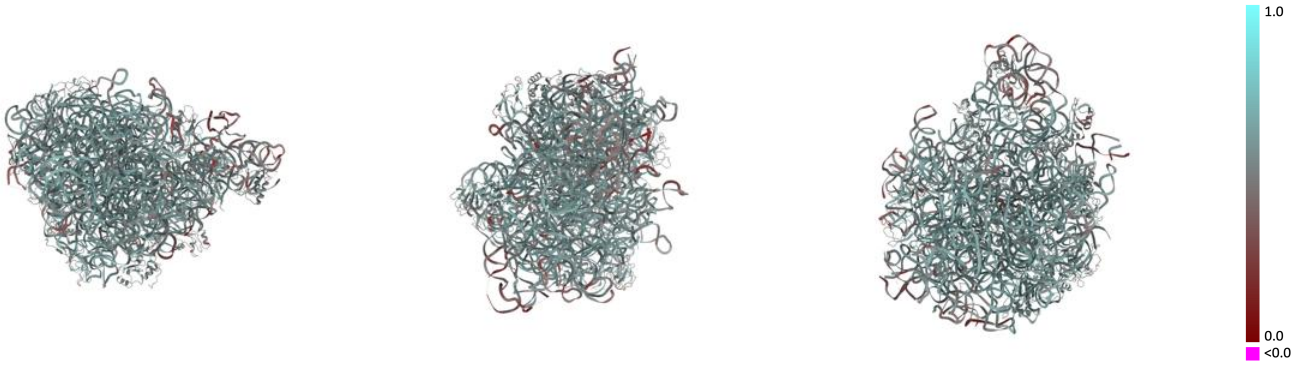
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

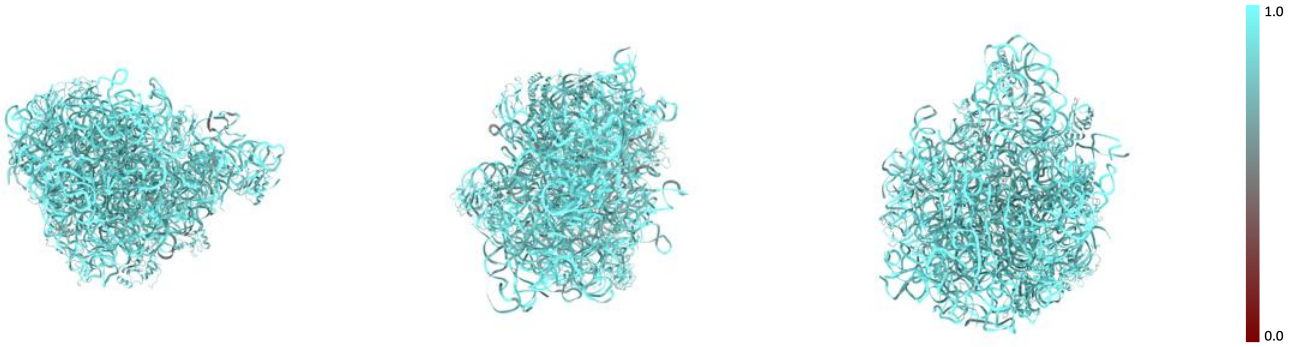
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

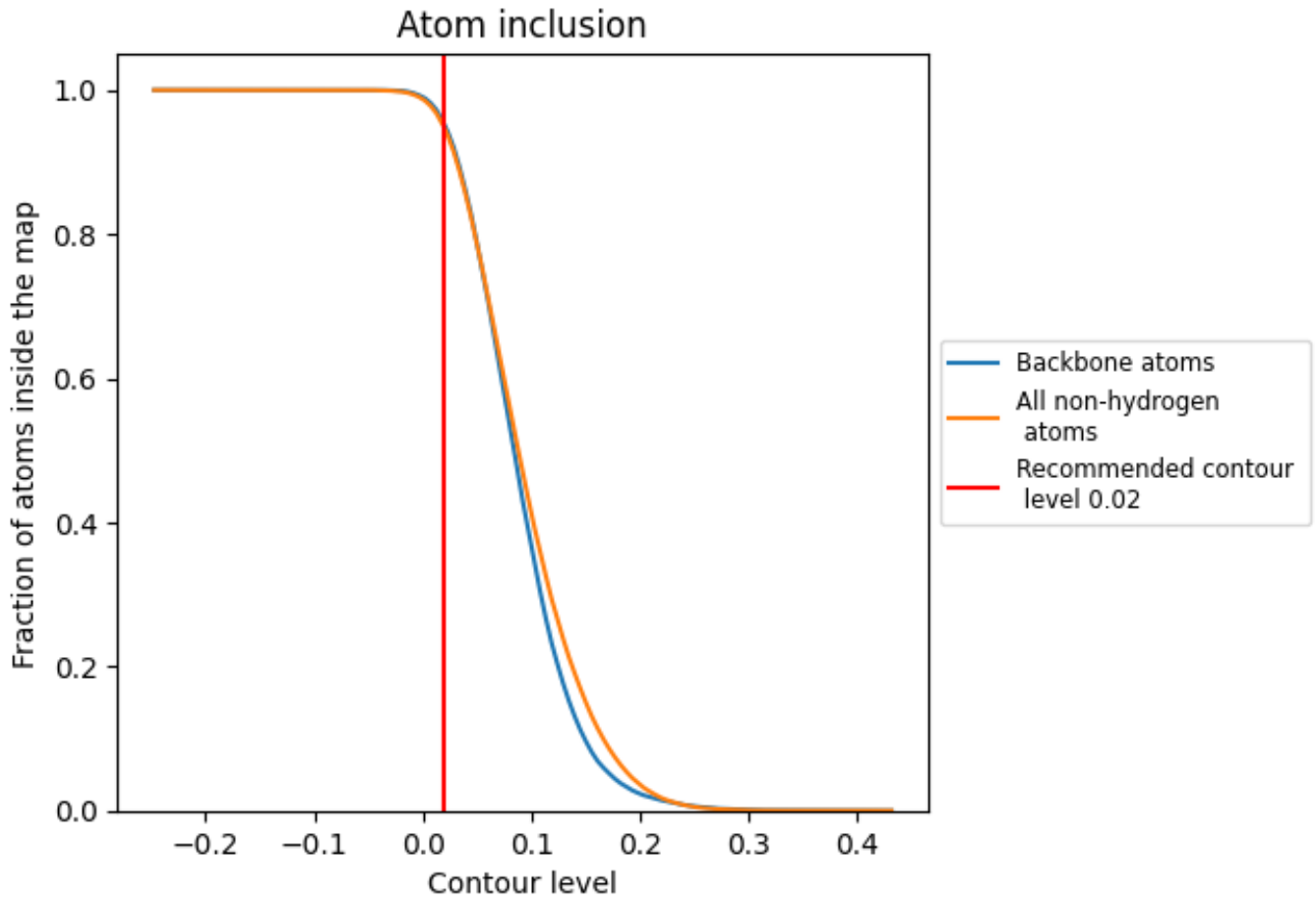
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9474	0.5610
1	0.9585	0.5690
2	0.9122	0.4700
A	0.9317	0.5620
B	0.9308	0.5720
C	0.9253	0.5680
D	0.9224	0.5480
E	0.9543	0.5810
F	0.8918	0.5220
G	0.8938	0.5010
H	0.8109	0.4400
I	0.9550	0.5820
J	0.8949	0.5260
K	0.8710	0.4890
L	0.9171	0.5520
M	0.9363	0.5660
N	0.9426	0.5680
O	0.8727	0.5130
P	0.9715	0.6180
Q	0.9741	0.6060
R	0.9379	0.5630
S	0.9223	0.5600
V	0.9459	0.5610
W	0.9088	0.5440
X	0.9169	0.5430
Y	0.9298	0.5540
Z	0.9241	0.5620
a	0.8970	0.4970