Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 10:36 AM EDT

PDB ID	:	7TTW / pdb_00007ttw
EMDB ID	:	EMD-26125
Title	:	50S ribosomal subunit from Staphylococcus aureus containing double mutation in uL3 imparting linezolid resistance
Authors	:	Belousoff, M.J.; Piper, S.; Johnson, R.
Deposited on	:	2022-02-02
Resolution	:	2.90 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:

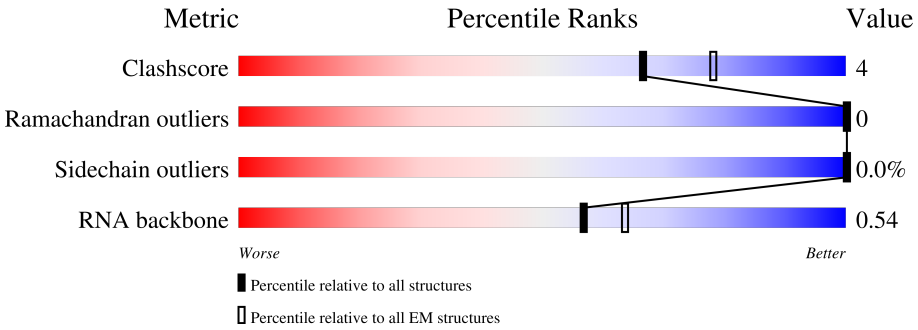
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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 <=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	83% 15% •
2	B	277	89% 10% •
3	C	118	92% 7% •
4	D	102	86% 11% • •
5	E	117	85% 9% 5%
6	F	87	87% 13%
7	G	105	71% 14% 14%

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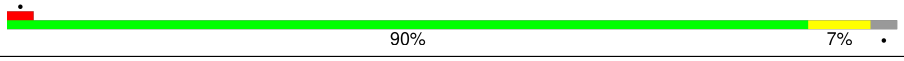
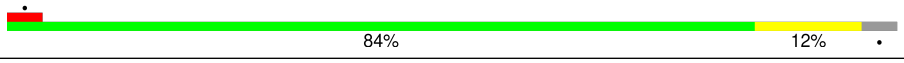
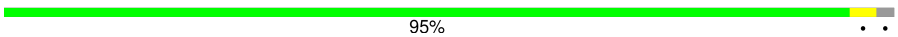
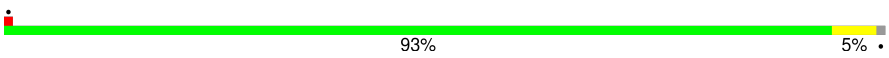
Mol	Chain	Length	Quality of chain
8	H	217	
9	I	94	
10	J	61	
11	K	73	
12	L	220	
13	M	59	
14	N	57	
15	O	49	
16	P	45	
17	Q	65	
18	R	37	
19	S	207	
20	V	145	
21	W	122	
22	X	146	
23	Y	144	
24	Z	122	
25	a	119	
26	1	2923	
27	2	115	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 80853 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 protein called 50S ribosomal protein L19.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	273	2085	1297	413	370	5	0	0

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

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L22.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	90	Total	C	N	O	S	0	0
			698	442	128	127	1		

- Molecule 8 is a protein called 50S ribosomal protein L25.

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 L27.

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

- Molecule 10 is a protein called 50S ribosomal protein L28.

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

- Molecule 11 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	61	Total	C	N	O	S	0	0
			503	310	95	97	1		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	215	Total	C	N	O	S	0	0
			1635	1023	302	306	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	155	ARG	GLY	conflict	UNP A0A0D1GR95
L	169	ILE	MET	conflict	UNP A0A0D1GR95

- Molecule 13 is a protein called 50S ribosomal protein L30.

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

- Molecule 14 is a protein called 50S ribosomal protein L32.

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

- Molecule 15 is a protein called 50S ribosomal protein L33.

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

- Molecule 16 is a protein called 50S ribosomal protein L34.

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

- Molecule 17 is a protein called 50S ribosomal protein L35.

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

- Molecule 18 is a protein called 50S ribosomal protein L36.

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

- Molecule 19 is a protein called 50S ribosomal protein L4.

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

- Molecule 20 is a protein called 50S ribosomal protein L13.

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

- Molecule 21 is a protein called 50S ribosomal protein L14.

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

- Molecule 22 is a protein called 50S ribosomal protein L15.

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

- Molecule 23 is a protein called 50S ribosomal protein L16.

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

- Molecule 24 is a protein called 50S ribosomal protein L17.

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

- Molecule 25 is a protein called 50S ribosomal protein L18.

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

- Molecule 26 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2690	Total 57665	C 25757	N 10573	O 18654	P 2681	0	0

- Molecule 27 is a RNA chain called 5S rRNA.

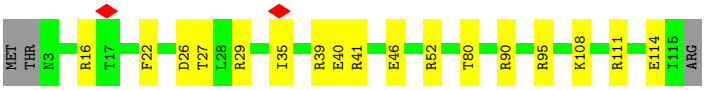
Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	111	Total 2361	C 1057	N 423	O 771	P 110	0	0

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.

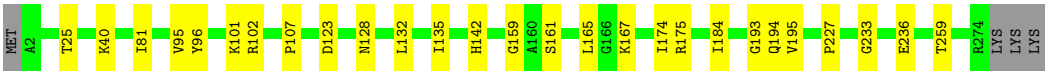
• Molecule 1: 50S ribosomal protein L19

Chain A:



• Molecule 2: 50S ribosomal protein L2

Chain B:

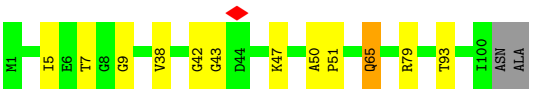


• Molecule 3: 50S ribosomal protein L20

Chain C:

• Molecule 4: 50S ribosomal protein L21

Chain D:

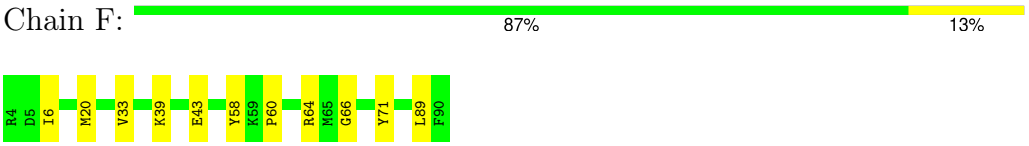


• Molecule 5: 50S ribosomal protein L22

Chain E:

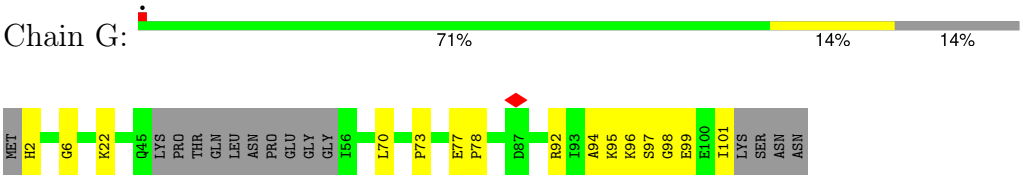
• Molecule 6: 50S ribosomal protein L23

Chain F:



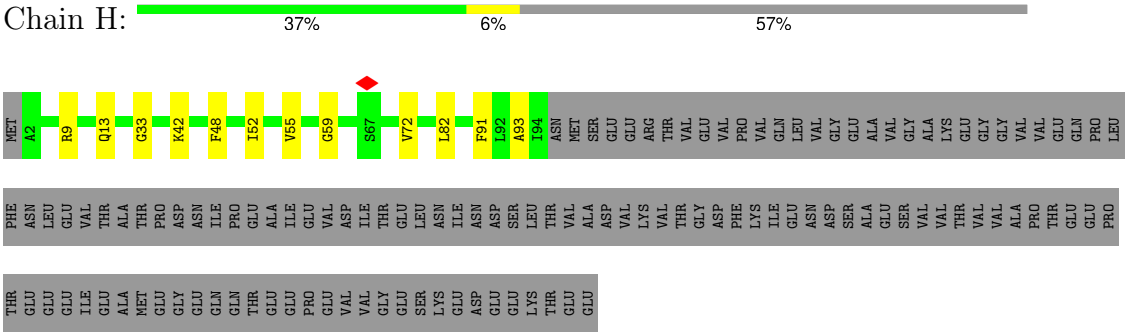
• Molecule 7: 50S ribosomal protein L24

Chain G:



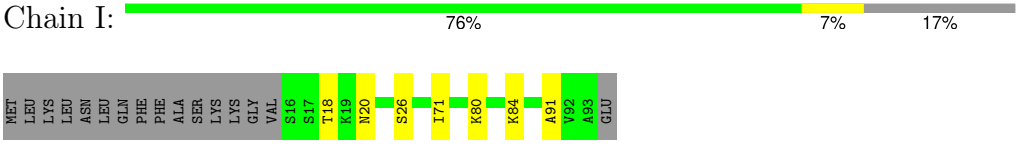
• Molecule 8: 50S ribosomal protein L25

Chain H:



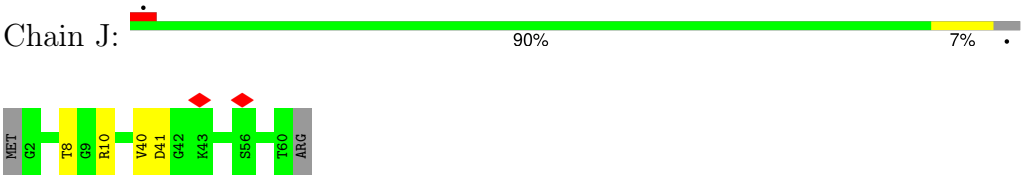
• Molecule 9: 50S ribosomal protein L27

Chain I:



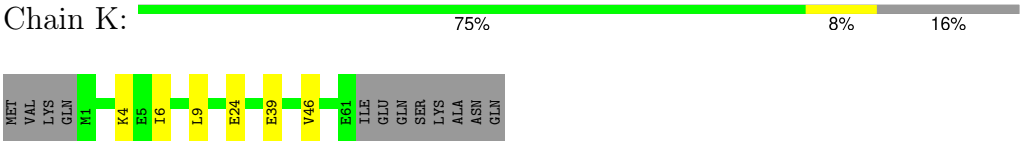
• Molecule 10: 50S ribosomal protein L28

Chain J:



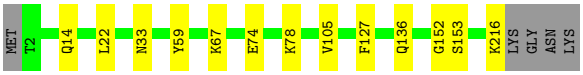
• Molecule 11: 50S ribosomal protein L29

Chain K:



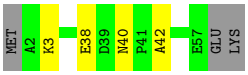
• Molecule 12: 50S ribosomal protein L3

Chain L:



• Molecule 13: 50S ribosomal protein L30

Chain M:

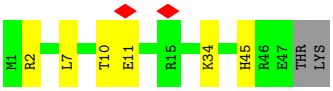


• Molecule 14: 50S ribosomal protein L32

Chain N:

• Molecule 15: 50S ribosomal protein L33

Chain O:

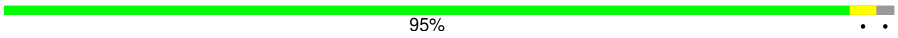


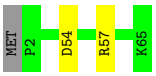
• Molecule 16: 50S ribosomal protein L34

Chain P:

• Molecule 17: 50S ribosomal protein L35

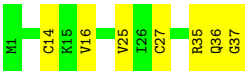
Chain Q:





• Molecule 18: 50S ribosomal protein L36

Chain R:

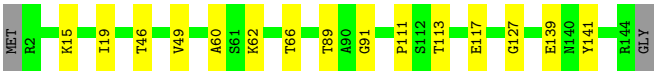


• Molecule 19: 50S ribosomal protein L4

Chain S:

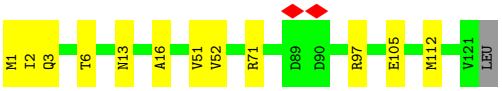
• Molecule 20: 50S ribosomal protein L13

Chain V:



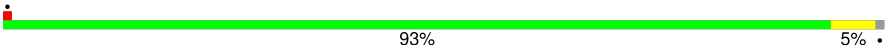
• Molecule 21: 50S ribosomal protein L14

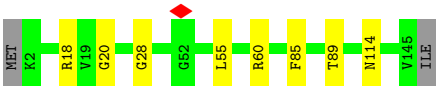
Chain W:



• Molecule 22: 50S ribosomal protein L15

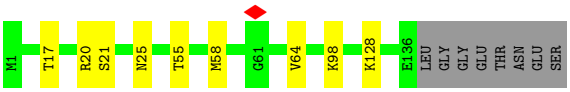
Chain X:





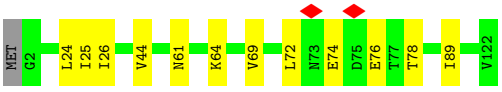
• Molecule 23: 50S ribosomal protein L16

Chain Y:



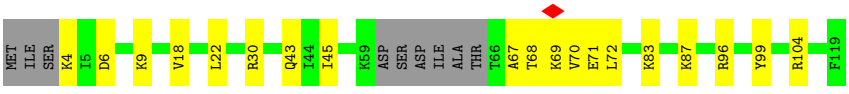
• Molecule 24: 50S ribosomal protein L17

Chain Z:



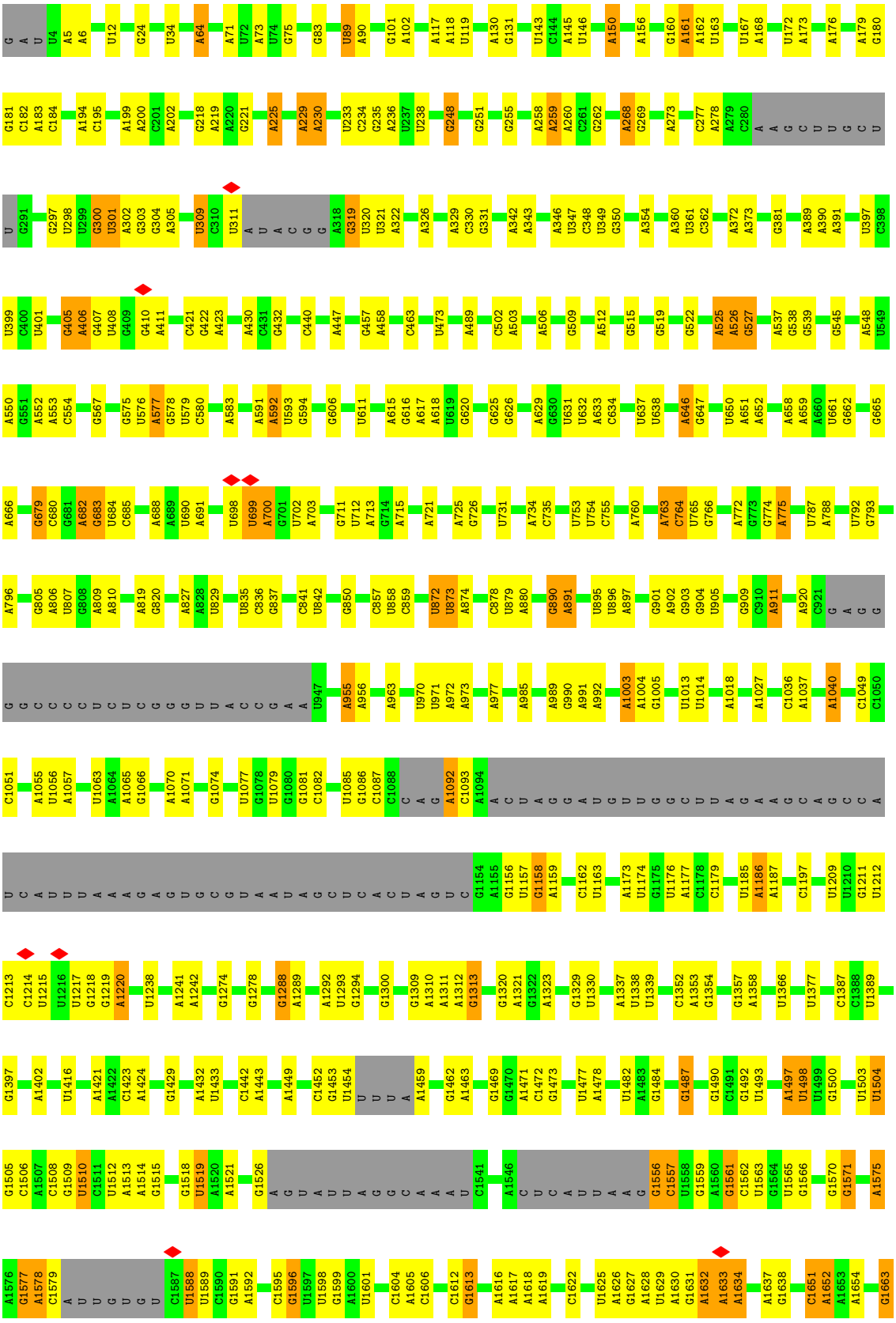
• Molecule 25: 50S ribosomal protein L18

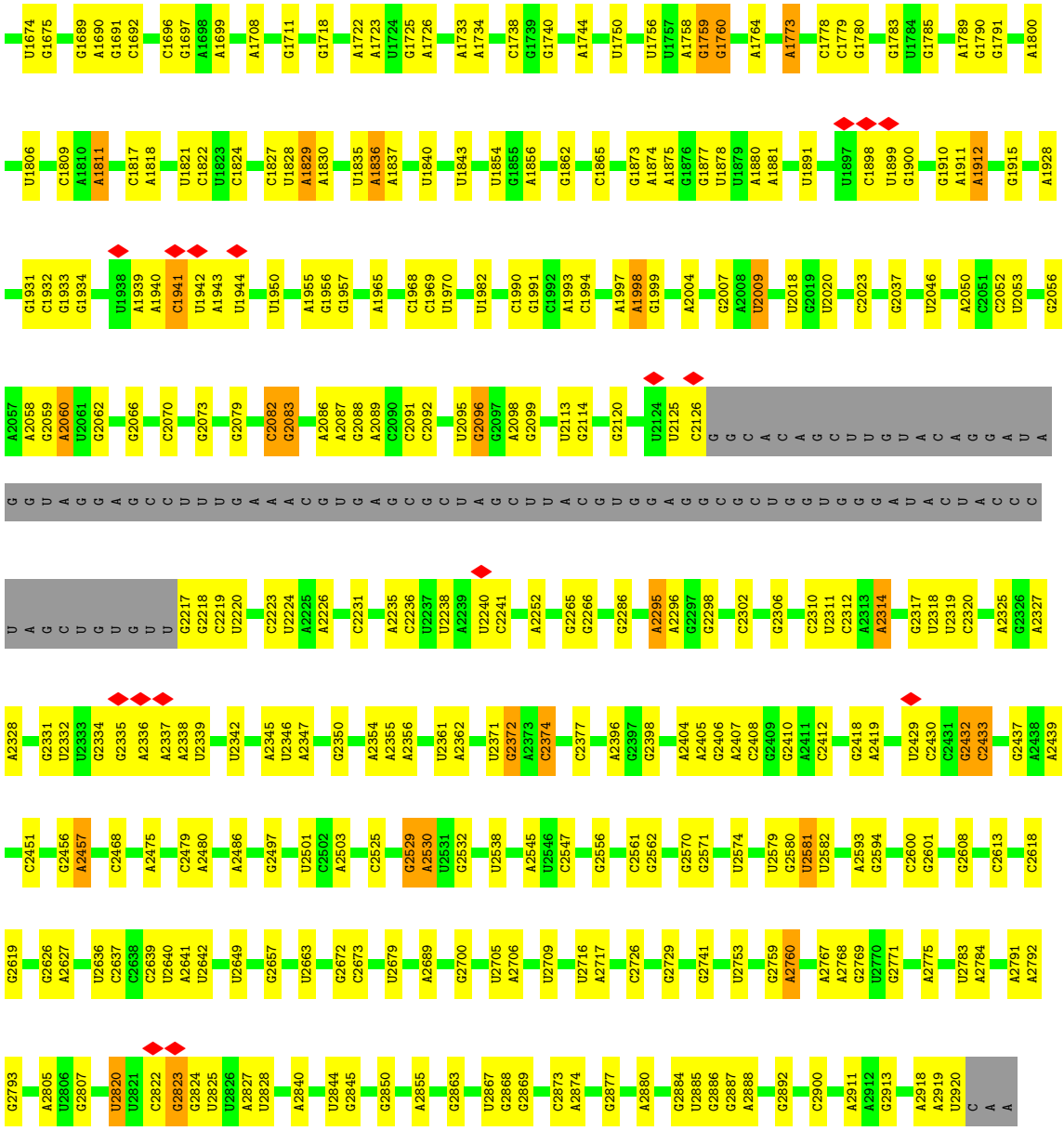
Chain a:



• Molecule 26: 23S rRNA

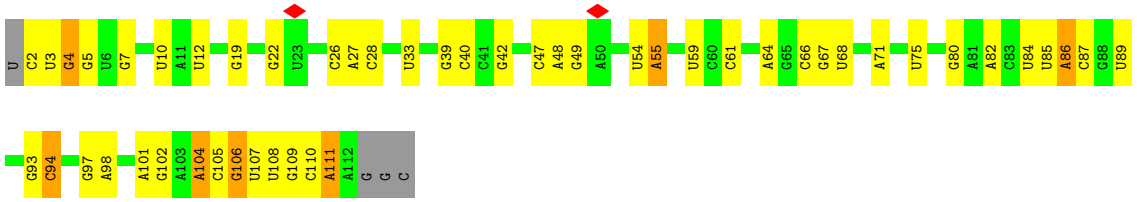
Chain 1:





• Molecule 27: 5S rRNA

Chain 2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	307600	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 ($e^-/Å^2$)	47.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.352	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	400.96, 400.96, 400.96	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.895, 0.895, 0.895	Depositor

5 Model quality

5.1 Standard geometry

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	0.13	0/927	0.29	0/1239
2	B	0.11	0/2120	0.30	0/2847
3	C	0.12	0/955	0.27	0/1265
4	D	0.12	0/795	0.33	0/1062
5	E	0.14	0/861	0.34	0/1159
6	F	0.12	0/719	0.31	0/959
7	G	0.12	0/704	0.30	0/938
8	H	0.30	0/735	0.43	0/986
9	I	0.14	0/603	0.33	0/801
10	J	0.13	0/469	0.31	0/625
11	K	0.11	0/504	0.33	0/670
12	L	0.13	0/1659	0.30	0/2226
13	M	0.12	0/434	0.28	0/585
14	N	0.13	0/404	0.37	0/537
15	O	0.09	0/393	0.27	0/523
16	P	0.12	0/376	0.32	0/491
17	Q	0.12	0/526	0.26	0/690
18	R	0.14	0/299	0.38	0/393
19	S	0.26	0/1494	0.44	0/2018
20	V	0.12	0/1160	0.30	0/1563
21	W	0.13	0/918	0.31	0/1232
22	X	0.12	0/1096	0.34	0/1461
23	Y	0.13	0/1113	0.33	0/1493
24	Z	0.13	0/959	0.30	0/1282
25	a	0.10	0/865	0.29	0/1154
26	1	0.14	0/64581	0.29	0/100711
27	2	0.11	0/2640	0.25	0/4112
All	All	0.14	0/88309	0.29	0/133022

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	915	0	987	11	0
2	B	2085	0	2192	17	0
3	C	943	0	1014	6	0
4	D	785	0	825	8	0
5	E	853	0	914	8	0
6	F	711	0	743	6	0
7	G	698	0	756	8	0
8	H	727	0	777	11	0
9	I	597	0	607	4	0
10	J	463	0	501	2	0
11	K	503	0	536	4	0
12	L	1635	0	1679	10	0
13	M	432	0	472	2	0
14	N	397	0	407	5	0
15	O	390	0	396	6	0
16	P	372	0	420	3	0
17	Q	521	0	586	2	0
18	R	296	0	340	4	0
19	S	1472	0	1520	13	0
20	V	1138	0	1130	9	0
21	W	911	0	970	7	0
22	X	1082	0	1119	6	0
23	Y	1089	0	1155	7	0
24	Z	955	0	1002	6	0
25	a	857	0	903	12	0
26	1	57665	0	29019	310	0
27	2	2361	0	1197	26	0
All	All	80853	0	52167	476	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 4.

All (476) 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)
26:1:1484:G:H1	26:1:1599:G:H22	1.19	0.89
26:1:89:U:H3'	26:1:90:A:H2'	1.60	0.83
26:1:1515:G:H22	26:1:1565:U:H3	1.30	0.80
26:1:1577:G:H22	26:1:1589:U:H3	1.31	0.78
1:A:108:LYS:HA	1:A:111:ARG:HE	1.48	0.78
26:1:721:A:H8	26:1:2096:G:H21	1.33	0.77
26:1:1862:G:H1	26:1:1932:C:H5	1.31	0.76
16:P:2:VAL:N	26:1:1663:G:HO2'	1.83	0.75
27:2:67:G:O6	27:2:102:G:N2	2.19	0.75
26:1:1931:G:H21	26:1:1955:A:H8	1.35	0.75
26:1:1462:G:H8	26:1:1626:A:H62	1.34	0.74
24:Z:72:LEU:HD13	24:Z:78:THR:HG22	1.70	0.73
26:1:1806:U:OP2	26:1:1811:A:N6	2.21	0.73
26:1:2432:G:O2'	26:1:2433:C:OP2	2.07	0.73
2:B:161:SER:HB3	2:B:194:GLN:HG3	1.71	0.72
26:1:629:A:H62	26:1:1289:A:H2	1.39	0.71
26:1:615:A:H61	26:1:2056:G:H8	1.36	0.70
26:1:2007:G:O2'	26:1:2009:U:OP2	2.09	0.70
26:1:268:A:N6	26:1:473:U:O2'	2.24	0.70
26:1:221:G:H22	26:1:238:U:H4'	1.57	0.69
26:1:1497:A:N6	26:1:1500:G:OP2	2.21	0.69
26:1:89:U:OP2	26:1:90:A:O2'	2.10	0.69
26:1:1518:G:H1	26:1:1562:C:H42	1.39	0.69
5:E:42:ALA:HB2	26:1:2037:G:H5"	1.74	0.69
26:1:1492:G:H1	26:1:1506:C:H42	1.39	0.68
7:G:70:LEU:HD21	7:G:101:ILE:HG21	1.76	0.68
26:1:591:A:H4'	26:1:592:A:H5'	1.74	0.68
26:1:1484:G:H1	26:1:1599:G:N2	1.93	0.67
20:V:66:THR:HG21	26:1:1185:U:H2'	1.75	0.66
25:a:70:VAL:HG22	25:a:104:ARG:HG2	1.77	0.66
26:1:1487:G:H1	26:1:1596:G:H22	1.42	0.66
15:O:2:ARG:NH2	26:1:2312:C:OP2	2.29	0.66
26:1:350:G:OP2	26:1:350:G:N2	2.29	0.66
19:S:26:ILE:HG21	19:S:111:ARG:HH12	1.60	0.66
26:1:262:G:H21	26:1:666:A:H8	1.41	0.66
7:G:77:GLU:HG3	7:G:78:PRO:HD2	1.77	0.66
22:X:114:ASN:ND2	26:1:699:U:O4	2.30	0.65
24:Z:26:ILE:HD11	24:Z:69:VAL:HG21	1.79	0.65
26:1:2884:G:H2'	26:1:2885:U:C6	2.32	0.65
26:1:1939:A:O2'	26:1:1941:C:OP2	2.15	0.65
19:S:22:ALA:O	19:S:111:ARG:NH1	2.31	0.64
26:1:1493:U:H3	26:1:1505:G:H22	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:83:G:H21	26:1:102:A:H2	1.46	0.64
26:1:963:A:H62	26:1:2295:A:H2	1.46	0.64
26:1:1449:A:H8	26:1:1634:A:H62	1.44	0.64
27:2:4:G:H22	27:2:109:G:H22	1.44	0.64
16:P:25:THR:HG23	16:P:28:GLY:H	1.63	0.63
26:1:200:A:N6	26:1:2457:A:O2'	2.33	0.62
26:1:506:A:H61	26:1:515:G:H8	1.46	0.62
26:1:2083:G:H1	26:1:2639:C:H5	1.44	0.62
26:1:1598:U:H2'	26:1:1599:G:C8	2.34	0.62
2:B:107:PRO:HA	2:B:195:VAL:HA	1.81	0.62
26:1:646:A:N6	26:1:700:A:OP2	2.24	0.62
3:C:110:VAL:HG12	3:C:114:LYS:HE2	1.81	0.62
8:H:82:LEU:HD12	23:Y:20:ARG:HH12	1.64	0.61
26:1:2314:A:H62	26:1:2371:U:H3	1.47	0.61
26:1:1423:C:H2'	26:1:1424:A:C8	2.36	0.61
23:Y:128:LYS:NZ	26:1:1074:G:OP2	2.33	0.61
26:1:1631:G:O2'	26:1:1632:A:O5'	2.17	0.61
26:1:2820:U:O2	26:1:2822:C:O2'	2.17	0.61
26:1:1595:C:H2'	26:1:1596:G:C8	2.36	0.60
25:a:6:ASP:HB3	25:a:9:LYS:HB2	1.82	0.60
26:1:1881:A:H62	26:1:1915:G:H8	1.49	0.60
18:R:16:VAL:HG22	18:R:25:VAL:HG22	1.84	0.60
26:1:665:G:H4'	26:1:666:A:H5"	1.84	0.60
26:1:1459:A:H2	26:1:1631:G:H5'	1.67	0.59
26:1:2705:U:H2'	26:1:2706:A:H8	1.67	0.59
26:1:2355:A:H2'	26:1:2356:A:C8	2.38	0.59
2:B:135:ILE:O	2:B:167:LYS:NZ	2.27	0.59
17:Q:57:ARG:NH1	26:1:878:C:O2'	2.35	0.59
14:N:6:ARG:NH2	26:1:2046:U:OP2	2.35	0.59
15:O:34:LYS:NZ	26:1:2374:C:OP1	2.36	0.58
8:H:9:ARG:HD2	8:H:13:GLN:HE22	1.69	0.58
26:1:661:U:HO2'	26:1:662:G:H8	1.49	0.58
26:1:1185:U:H4'	26:1:1186:A:O4'	2.03	0.58
12:L:152:GLY:O	26:1:2538:U:O2'	2.18	0.58
26:1:1065:A:H61	26:1:1186:A:H61	1.50	0.58
8:H:55:VAL:HB	8:H:59:GLY:HA3	1.85	0.58
21:W:2:ILE:HG22	21:W:3:GLN:HG2	1.86	0.58
26:1:632:U:H2'	26:1:633:A:H8	1.69	0.58
26:1:1442:C:H2'	26:1:1443:A:H8	1.69	0.58
3:C:4:VAL:HG22	26:1:1238:U:H1'	1.85	0.58
12:L:216:LYS:HB2	26:1:2760:A:C2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1423:C:H2'	26:1:1424:A:H8	1.69	0.58
17:Q:54:ASP:OD1	17:Q:57:ARG:NH2	2.38	0.57
26:1:1915:G:OP2	26:1:1915:G:N2	2.33	0.57
25:a:68:THR:OG1	27:2:48:A:OP2	2.21	0.57
20:V:60:ALA:HB3	20:V:127:GLY:HA2	1.87	0.56
26:1:1512:U:H2'	26:1:1513:A:C8	2.40	0.56
26:1:2649:U:O2'	26:1:2845:G:N2	2.38	0.56
1:A:22:PHE:O	1:A:52:ARG:NH1	2.38	0.56
24:Z:24:LEU:HD23	24:Z:44:VAL:HG11	1.85	0.56
25:a:69:LYS:HD3	25:a:72:LEU:HD23	1.87	0.56
26:1:545:G:N1	26:1:548:A:OP2	2.37	0.56
26:1:1482:U:H3	26:1:1601:U:H5	1.51	0.56
3:C:92:ARG:NH2	26:1:1197:C:OP1	2.38	0.56
26:1:1497:A:H2'	26:1:1498:U:H2'	1.87	0.56
27:2:86:A:O2'	27:2:87:C:OP2	2.22	0.56
6:F:58:TYR:OH	26:1:1377:U:OP2	2.24	0.56
27:2:54:U:H4'	27:2:55:A:H5'	1.87	0.56
26:1:2125:U:H3	26:1:2218:G:H1	1.53	0.55
22:X:55:LEU:O	22:X:60:ARG:NH1	2.40	0.55
27:2:27:A:H2'	27:2:28:C:H6	1.71	0.55
2:B:236:GLU:HG3	26:1:2627:A:H2	1.70	0.55
8:H:9:ARG:HH11	8:H:13:GLN:HE21	1.54	0.55
18:R:36:GLN:HG2	18:R:37:GLY:H	1.71	0.55
26:1:991:A:H2'	26:1:992:A:C8	2.42	0.55
26:1:2705:U:H2'	26:1:2706:A:C8	2.41	0.55
26:1:702:U:H2'	26:1:703:A:C8	2.42	0.55
26:1:1353:A:H2'	26:1:1354:G:H8	1.72	0.55
19:S:117:LYS:NZ	19:S:189:ALA:O	2.40	0.55
26:1:273:A:OP2	26:1:297:G:N1	2.33	0.55
26:1:1462:G:OP2	26:1:1462:G:N2	2.37	0.55
27:2:2:C:H42	27:2:111:A:H61	1.53	0.55
1:A:90:ARG:NH2	1:A:114:GLU:OE1	2.41	0.54
26:1:2419:A:H2	26:1:2451:C:H42	1.55	0.54
26:1:1353:A:H2'	26:1:1354:G:C8	2.43	0.54
26:1:1780:G:N2	26:1:1783:G:OP2	2.26	0.54
26:1:793:G:N2	26:1:796:A:OP2	2.40	0.54
26:1:1423:C:O2'	26:1:1512:U:O2	2.25	0.54
26:1:1081:G:H1	26:1:1162:C:H42	1.55	0.54
10:J:40:VAL:HG22	10:J:41:ASP:H	1.73	0.54
26:1:405:G:H2'	26:1:406:A:C8	2.42	0.54
26:1:1865:C:H5	26:1:1928:A:H62	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2418:G:O2'	26:1:2451:C:N4	2.39	0.53
26:1:422:G:H2'	26:1:423:A:C8	2.43	0.53
26:1:1632:A:H4'	26:1:1633:A:C8	2.42	0.53
15:O:2:ARG:HH21	26:1:2311:U:H3'	1.72	0.53
19:S:155:VAL:HB	19:S:194:ILE:HG22	1.89	0.53
25:a:43:GLN:HG3	25:a:45:ILE:HD11	1.90	0.53
26:1:2327:A:H2'	26:1:2328:A:C8	2.43	0.53
26:1:896:U:H2'	26:1:897:A:H8	1.74	0.53
5:E:25:ARG:NH2	5:E:74:ALA:O	2.32	0.52
9:I:18:THR:HG22	9:I:20:ASN:H	1.75	0.52
26:1:406:A:H2'	26:1:407:G:C8	2.44	0.52
27:2:5:G:H22	27:2:108:U:H3	1.56	0.52
26:1:632:U:H2'	26:1:633:A:C8	2.44	0.52
15:O:10:THR:HG22	15:O:11:GLU:HG3	1.91	0.52
27:2:12:U:OP2	27:2:68:U:O2'	2.28	0.52
8:H:9:ARG:HD2	8:H:13:GLN:NE2	2.25	0.51
8:H:48:PHE:O	8:H:52:ILE:HG12	2.10	0.51
26:1:1514:A:H2	26:1:1566:G:H22	1.58	0.51
19:S:24:PHE:HB3	19:S:118:VAL:HG21	1.92	0.51
20:V:46:THR:HB	20:V:49:VAL:HG12	1.91	0.51
27:2:4:G:H22	27:2:109:G:N2	2.08	0.51
20:V:89:THR:HG22	20:V:91:GLY:H	1.75	0.51
21:W:13:ASN:HB2	21:W:97:ARG:HB2	1.93	0.51
4:D:5:ILE:HG22	4:D:38:VAL:HG22	1.92	0.51
26:1:2235:A:H2'	26:1:2236:C:C6	2.46	0.51
4:D:50:ALA:HB1	4:D:51:PRO:HA	1.92	0.51
8:H:33:GLY:HA3	8:H:93:ALA:HB3	1.92	0.51
26:1:901:G:H2'	26:1:902:A:C8	2.46	0.51
3:C:83:LEU:HD22	3:C:88:ILE:HG13	1.91	0.51
26:1:909:G:H21	26:1:911:A:H61	1.59	0.51
21:W:71:ARG:NH1	21:W:105:GLU:OE2	2.44	0.51
26:1:2052:C:H2'	26:1:2053:U:C6	2.46	0.51
8:H:82:LEU:HD12	23:Y:20:ARG:NH1	2.25	0.50
19:S:157:GLU:HG2	19:S:158:ASN:N	2.26	0.50
2:B:227:PRO:HA	2:B:233:GLY:HA2	1.91	0.50
9:I:26:SER:OG	26:1:2298:G:OP1	2.28	0.50
4:D:7:THR:O	4:D:7:THR:HG22	2.11	0.50
26:1:64:A:H61	26:1:90:A:H61	1.58	0.50
26:1:64:A:H61	26:1:90:A:N6	2.10	0.50
22:X:55:LEU:HD23	22:X:60:ARG:HB3	1.94	0.50
26:1:878:C:H2'	26:1:879:U:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1241:A:H2'	26:1:1242:A:C8	2.47	0.50
27:2:107:U:H2'	27:2:108:U:C6	2.47	0.50
26:1:1941:C:O2'	26:1:1943:A:N6	2.42	0.50
26:1:2608:G:N2	26:1:2608:G:OP2	2.40	0.50
4:D:9:GLY:O	26:1:1040:A:H1'	2.11	0.49
12:L:127:PHE:HE2	26:1:1699:A:H1'	1.77	0.49
5:E:13:ALA:HB3	5:E:16:LYS:HD2	1.93	0.49
26:1:1806:U:H5	26:1:1811:A:N7	2.11	0.49
7:G:94:ALA:HB2	7:G:101:ILE:HD11	1.95	0.49
25:a:30:ARG:HH21	25:a:45:ILE:HD13	1.76	0.49
26:1:631:U:H2'	26:1:632:U:C6	2.48	0.49
26:1:890:G:O2'	26:1:891:A:O5'	2.30	0.49
26:1:1756:U:H3	26:1:1773:A:N6	2.10	0.49
26:1:682:A:H4'	26:1:683:G:H5'	1.95	0.49
26:1:1442:C:H2'	26:1:1443:A:C8	2.47	0.49
11:K:4:LYS:HG2	11:K:6:ILE:HD12	1.95	0.49
21:W:16:ALA:HB2	21:W:52:VAL:HG11	1.95	0.49
21:W:112:MET:HE3	21:W:112:MET:HA	1.94	0.49
26:1:422:G:H2'	26:1:423:A:H8	1.77	0.49
1:A:29:ARG:NH1	1:A:46:GLU:OE1	2.45	0.49
2:B:95:VAL:HG22	2:B:101:LYS:HG2	1.95	0.49
16:P:38:LYS:NZ	26:1:515:G:H1	2.11	0.49
21:W:51:VAL:HG23	21:W:52:VAL:HG23	1.95	0.49
26:1:1829:A:H2'	26:1:1830:A:C8	2.48	0.49
2:B:142:HIS:ND1	2:B:193:GLY:O	2.40	0.49
2:B:159:GLY:H	2:B:195:VAL:HG23	1.78	0.49
2:B:259:THR:HG1	26:1:1824:C:HO2'	1.57	0.49
5:E:92:ARG:HG3	5:E:92:ARG:HH11	1.77	0.49
26:1:309:U:H3	26:1:407:G:H22	1.61	0.49
26:1:1505:G:HO2'	26:1:2729:G:HO2'	1.60	0.49
27:2:4:G:H1	27:2:109:G:H1	1.61	0.48
26:1:2885:U:OP2	26:1:2886:G:O2'	2.22	0.48
12:L:127:PHE:CE2	26:1:1699:A:H1'	2.48	0.48
26:1:579:U:H2'	26:1:580:C:C6	2.49	0.48
26:1:2844:U:H2'	26:1:2845:G:O4'	2.13	0.48
2:B:174:ILE:HD12	2:B:184:ILE:HD12	1.95	0.48
26:1:259:A:H2'	26:1:260:A:C8	2.48	0.48
26:1:1726:A:H61	26:1:1750:U:H3	1.61	0.48
26:1:2404:A:H2'	26:1:2405:A:C8	2.48	0.48
26:1:229:A:O2'	26:1:230:A:OP1	2.29	0.48
26:1:2618:C:H2'	26:1:2619:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:342:A:N3	26:1:362:C:O2'	2.43	0.48
20:V:19:ILE:HG12	20:V:141:TYR:HB3	1.96	0.48
26:1:879:U:C2	26:1:880:A:C8	3.02	0.48
27:2:101:A:H3'	27:2:102:G:H8	1.78	0.48
27:2:108:U:H2'	27:2:109:G:C8	2.48	0.48
26:1:277:C:H2'	26:1:278:A:H8	1.79	0.48
26:1:509:G:N2	26:1:512:A:OP2	2.44	0.48
26:1:725:A:H2'	26:1:726:G:C8	2.49	0.48
26:1:1512:U:H2'	26:1:1513:A:H8	1.79	0.48
12:L:67:LYS:HE3	26:1:2850:G:H5'	1.95	0.48
26:1:527:G:O2'	26:1:552:A:N6	2.46	0.48
26:1:679:G:H2'	26:1:680:C:C6	2.49	0.48
26:1:793:G:N3	26:1:793:G:H2'	2.29	0.48
26:1:1993:A:N3	26:1:2619:G:O2'	2.36	0.48
26:1:2618:C:H2'	26:1:2619:G:C8	2.49	0.47
27:2:104:A:H2'	27:2:105:C:C6	2.49	0.47
8:H:33:GLY:HA3	8:H:93:ALA:H	1.79	0.47
26:1:262:G:N2	26:1:666:A:H8	2.11	0.47
26:1:421:C:H2'	26:1:422:G:H8	1.78	0.47
26:1:1854:U:OP1	26:1:1998:A:O2'	2.28	0.47
19:S:17:ILE:HG12	19:S:196:GLU:HG2	1.96	0.47
26:1:343:A:O2'	26:1:361:U:O2	2.31	0.47
26:1:1219:G:H8	26:1:1219:G:OP2	1.96	0.47
26:1:1725:G:H21	26:1:1789:A:H3'	1.80	0.47
26:1:1836:A:H2'	26:1:1837:A:C8	2.49	0.47
26:1:2918:A:H2'	26:1:2919:A:C8	2.49	0.47
12:L:78:LYS:HB2	12:L:78:LYS:HE3	1.74	0.47
26:1:1313:G:OP2	26:1:1689:G:O2'	2.28	0.47
26:1:841:C:H2'	26:1:842:U:C6	2.50	0.47
1:A:35:ILE:HG13	1:A:40:GLU:HG3	1.97	0.47
12:L:14:GLN:HB2	12:L:22:LEU:HD11	1.95	0.47
26:1:181:G:H2'	26:1:182:C:O4'	2.15	0.47
26:1:754:U:H2'	26:1:755:C:C6	2.50	0.47
26:1:774:G:H5'	26:1:775:A:H5"	1.96	0.47
26:1:903:G:O2'	26:1:2296:A:H5"	2.14	0.47
26:1:1003:A:H2'	26:1:1004:A:C8	2.50	0.47
26:1:1877:G:H2'	26:1:1878:U:C6	2.50	0.47
26:1:1880:A:H2'	26:1:1881:A:C8	2.50	0.47
26:1:2318:U:H2'	26:1:2319:U:C6	2.50	0.47
27:2:80:G:H1	27:2:89:U:H3	1.61	0.47
19:S:118:VAL:HG22	19:S:123:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:80:LYS:HB3	9:I:84:LYS:HB3	1.97	0.47
26:1:1449:A:N6	26:1:1632:A:N7	2.63	0.47
27:2:27:A:H2'	27:2:28:C:C6	2.49	0.47
7:G:97:SER:OG	7:G:98:GLY:N	2.48	0.47
22:X:18:ARG:NH2	26:1:1288:G:N7	2.62	0.47
26:1:194:A:H2'	26:1:195:C:C6	2.50	0.47
26:1:787:U:H2'	26:1:788:A:C8	2.50	0.47
26:1:1477:U:H2'	26:1:1478:A:C8	2.49	0.47
26:1:765:U:H2'	26:1:766:G:C8	2.50	0.46
26:1:1637:A:H2'	26:1:1638:G:C8	2.50	0.46
26:1:1708:A:H61	26:1:2023:C:H42	1.62	0.46
27:2:4:G:N2	27:2:109:G:H22	2.12	0.46
26:1:390:A:H2'	26:1:391:A:C8	2.50	0.46
26:1:577:A:H4'	26:1:578:G:C8	2.50	0.46
26:1:793:G:H22	26:1:796:A:H5'	1.81	0.46
26:1:1508:C:H3'	26:1:1509:G:C8	2.50	0.46
15:O:7:LEU:HB3	15:O:45:HIS:HB3	1.97	0.46
26:1:300:G:H5"	26:1:301:U:H5	1.80	0.46
26:1:2217:G:H2'	26:1:2218:G:C8	2.50	0.46
26:1:2319:U:H2'	26:1:2320:C:H6	1.80	0.46
26:1:1329:G:H2'	26:1:1330:U:C6	2.50	0.46
26:1:1778:C:H2'	26:1:1779:C:C6	2.50	0.46
4:D:43:GLY:O	4:D:47:LYS:NZ	2.48	0.46
26:1:1562:C:H2'	26:1:1563:U:H6	1.79	0.46
27:2:75:U:H3	27:2:94:C:H5	1.63	0.46
26:1:1891:U:OP1	26:1:2437:G:O2'	2.31	0.46
5:E:21:LEU:HD22	5:E:74:ALA:HB1	1.98	0.46
26:1:858:U:H2'	26:1:859:C:H6	1.81	0.46
26:1:1063:U:OP1	26:1:1079:U:O2'	2.22	0.46
26:1:1484:G:H22	26:1:1599:G:N2	2.13	0.46
27:2:107:U:H2'	27:2:108:U:H6	1.80	0.46
5:E:64:MET:SD	5:E:109:ASP:HB2	2.56	0.46
6:F:64:ARG:NH1	6:F:66:GLY:O	2.49	0.46
26:1:2824:G:H2'	26:1:2825:U:O2	2.16	0.46
26:1:661:U:O2'	26:1:662:G:H8	1.99	0.46
26:1:1510:U:H3	26:1:1571:G:H1	1.63	0.46
5:E:78:GLU:O	26:1:24:G:O2'	2.33	0.45
26:1:873:U:H2'	26:1:874:A:C8	2.51	0.45
10:J:8:THR:HG21	10:J:10:ARG:NH1	2.31	0.45
20:V:15:LYS:NZ	20:V:139:GLU:OE1	2.44	0.45
26:1:83:G:N2	26:1:101:G:H1'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1157:U:H2'	26:1:1158:G:H5"	1.97	0.45
22:X:20:GLY:HA2	22:X:28:GLY:O	2.16	0.45
26:1:895:U:H5	26:1:973:A:N1	2.14	0.45
26:1:1013:U:H2'	26:1:1014:U:C6	2.50	0.45
26:1:1352:C:O2'	26:1:1429:G:N3	2.49	0.45
26:1:2091:C:H2'	26:1:2092:C:C6	2.51	0.45
26:1:734:A:H2'	26:1:735:C:C6	2.52	0.45
26:1:2457:A:N3	26:1:2457:A:H2'	2.31	0.45
1:A:16:ARG:NH1	1:A:80:THR:O	2.49	0.45
3:C:13:ARG:HH21	26:1:1289:A:H5"	1.81	0.45
26:1:1158:G:H2'	26:1:1159:A:C8	2.51	0.45
26:1:1575:A:H2	26:1:1591:G:H22	1.63	0.45
26:1:161:A:H2	26:1:167:U:H3	1.63	0.45
20:V:113:THR:O	20:V:117:GLU:HG2	2.16	0.45
26:1:1462:G:H8	26:1:1626:A:N6	2.10	0.45
26:1:1588:U:H2'	26:1:1589:U:C6	2.52	0.45
27:2:101:A:H3'	27:2:102:G:C8	2.52	0.45
26:1:346:A:H2'	26:1:347:U:C6	2.52	0.45
26:1:754:U:H2'	26:1:755:C:H6	1.80	0.45
26:1:2570:G:H2'	26:1:2571:G:C8	2.52	0.45
23:Y:21:SER:OG	23:Y:25:ASN:OD1	2.33	0.44
26:1:1092:A:H2	26:1:1157:U:H1'	1.82	0.44
26:1:1733:A:H2'	26:1:1734:A:C8	2.52	0.44
6:F:39:LYS:O	6:F:43:GLU:HG3	2.17	0.44
26:1:390:A:H2'	26:1:391:A:H8	1.82	0.44
26:1:2354:A:H2'	26:1:2355:A:C8	2.52	0.44
26:1:2867:U:H2'	26:1:2868:G:O4'	2.17	0.44
27:2:26:C:H2'	27:2:27:A:O4'	2.17	0.44
26:1:5:A:H2'	26:1:6:A:C8	2.53	0.44
26:1:878:C:H2'	26:1:879:U:H6	1.81	0.44
26:1:2319:U:H2'	26:1:2320:C:C6	2.52	0.44
26:1:259:A:H2'	26:1:260:A:H8	1.82	0.44
26:1:1521:A:N6	26:1:1559:G:H22	2.14	0.44
26:1:1632:A:H5'	26:1:1633:A:H5'	1.99	0.44
22:X:85:PHE:HB3	22:X:89:THR:HG21	2.00	0.44
26:1:348:C:H2'	26:1:349:U:C6	2.52	0.44
26:1:711:G:H2'	26:1:712:U:C6	2.53	0.44
26:1:763:A:H2'	26:1:764:C:C6	2.53	0.44
26:1:2672:G:H4'	26:1:2759:G:O2'	2.17	0.44
27:2:7:G:H1	27:2:106:G:H21	1.65	0.44
12:L:33:ASN:HB3	12:L:105:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:3:LYS:NZ	13:M:38:GLU:OE2	2.42	0.44
26:1:522:G:N1	26:1:525:A:OP2	2.43	0.44
24:Z:25:ILE:HG23	24:Z:89:ILE:HD12	2.00	0.44
26:1:2479:C:H2'	26:1:2480:A:C8	2.53	0.44
5:E:58:ALA:HB1	5:E:64:MET:HE3	1.99	0.44
19:S:80:ALA:HB3	19:S:83:TRP:CD1	2.52	0.44
26:1:2223:C:H2'	26:1:2224:U:C6	2.53	0.44
26:1:2886:G:C2	26:1:2888:A:H1'	2.53	0.44
2:B:165:LEU:HD21	2:B:175:ARG:HH21	1.83	0.43
26:1:633:A:H2'	26:1:634:C:C6	2.53	0.43
26:1:1911:A:O2'	26:1:1912:A:H8	2.01	0.43
23:Y:55:THR:HG22	23:Y:64:VAL:HG21	2.00	0.43
26:1:637:U:H2'	26:1:638:U:C6	2.53	0.43
7:G:2:HIS:O	7:G:92:ARG:NH1	2.51	0.43
19:S:148:GLN:HB3	19:S:152:VAL:HG11	2.00	0.43
26:1:346:A:H2'	26:1:347:U:H6	1.83	0.43
26:1:753:U:H2'	26:1:754:U:H6	1.83	0.43
26:1:1219:G:O2'	26:1:1220:A:H8	2.01	0.43
26:1:1969:C:OP2	26:1:1970:U:O2'	2.30	0.43
1:A:27:THR:HB	1:A:90:ARG:HG2	2.00	0.43
26:1:304:G:C2	26:1:305:A:C8	3.07	0.43
26:1:625:G:H2'	26:1:626:G:C8	2.53	0.43
26:1:1722:A:C4	26:1:1723:A:C8	3.07	0.43
26:1:2113:U:H2'	26:1:2114:G:C8	2.53	0.43
24:Z:61:ASN:HA	24:Z:64:LYS:HE2	2.00	0.43
26:1:319:G:H1'	26:1:401:U:H3	1.84	0.43
26:1:991:A:H2'	26:1:992:A:H8	1.83	0.43
13:M:40:ASN:HD21	13:M:42:ALA:HB3	1.83	0.43
26:1:1651:C:H4'	26:1:1652:A:H5'	2.00	0.43
2:B:40:LYS:HD3	26:1:1840:U:H5"	2.00	0.43
2:B:123:ASP:OD1	2:B:128:ASN:ND2	2.52	0.43
9:I:71:ILE:HD12	9:I:91:ALA:HB2	1.99	0.43
14:N:42:VAL:HG12	14:N:49:TYR:HB2	2.00	0.43
19:S:182:ASN:HB2	19:S:185:ASP:HB2	1.99	0.43
26:1:2217:G:H2'	26:1:2218:G:H8	1.84	0.43
4:D:65:GLN:OE1	4:D:93:THR:OG1	2.34	0.43
26:1:651:A:H2'	26:1:652:A:H8	1.84	0.43
2:B:236:GLU:HG3	26:1:2627:A:C2	2.52	0.43
6:F:60:PRO:HB2	6:F:71:TYR:HD1	1.84	0.43
26:1:702:U:H2'	26:1:703:A:H8	1.82	0.43
26:1:1081:G:H2'	26:1:1082:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1588:U:H2'	26:1:1589:U:H6	1.83	0.43
26:1:2581:U:H2'	26:1:2582:U:C6	2.54	0.43
26:1:1632:A:H4'	26:1:1633:A:H8	1.83	0.43
26:1:2060:A:O2'	26:1:2062:G:OP2	2.31	0.43
8:H:9:ARG:HG2	8:H:42:LYS:HE3	2.01	0.42
26:1:525:A:H1'	26:1:526:A:H5"	2.00	0.42
26:1:872:U:O2'	26:1:2095:U:N3	2.52	0.42
26:1:2098:A:H2'	26:1:2099:G:C8	2.54	0.42
15:O:2:ARG:NH2	26:1:2311:U:H3'	2.34	0.42
26:1:225:A:N6	26:1:235:G:H1'	2.35	0.42
26:1:651:A:H2'	26:1:652:A:C8	2.54	0.42
26:1:684:U:H2'	26:1:685:C:C6	2.54	0.42
26:1:2873:C:H2'	26:1:2874:A:H8	1.84	0.42
27:2:97:G:H2'	27:2:98:A:C8	2.54	0.42
11:K:24:GLU:HB3	11:K:46:VAL:HG21	2.01	0.42
19:S:157:GLU:HG2	19:S:158:ASN:H	1.84	0.42
26:1:248:G:O2'	26:1:430:A:N1	2.43	0.42
26:1:1211:G:H2'	26:1:1212:U:C6	2.54	0.42
26:1:2919:A:H2'	26:1:2920:U:C6	2.55	0.42
26:1:1617:A:H2'	26:1:1618:A:C8	2.54	0.42
26:1:1725:G:HO2'	26:1:1789:A:HO2'	1.61	0.42
26:1:2372:G:N3	26:1:2408:C:H2'	2.33	0.42
2:B:25:THR:HG22	2:B:81:ILE:H	1.84	0.42
12:L:136:GLN:OE1	12:L:153:SER:HB2	2.19	0.42
19:S:151:LYS:HB2	19:S:151:LYS:HE3	1.82	0.42
20:V:111:PRO:HD3	26:1:1051:C:H4'	2.02	0.42
26:1:787:U:H2'	26:1:788:A:H8	1.83	0.42
26:1:2318:U:H2'	26:1:2319:U:H6	1.84	0.42
26:1:1618:A:H2'	26:1:1619:A:C8	2.53	0.42
7:G:95:LYS:O	7:G:96:LYS:HG2	2.19	0.42
12:L:59:TYR:HB2	12:L:74:GLU:OE2	2.20	0.42
26:1:688:A:N1	26:1:2396:A:O2'	2.50	0.42
26:1:2823:G:N2	26:1:2823:G:OP1	2.53	0.42
1:A:95:ARG:HA	1:A:95:ARG:HD2	1.84	0.42
25:a:104:ARG:HG3	27:2:47:C:OP1	2.19	0.42
26:1:1696:C:H2'	26:1:1697:G:O4'	2.19	0.42
1:A:35:ILE:O	1:A:35:ILE:HG22	2.20	0.42
14:N:7:ARG:HD2	26:1:1300:G:H21	1.85	0.42
14:N:29:GLU:OE1	14:N:29:GLU:N	2.50	0.42
23:Y:58:MET:HE1	23:Y:64:VAL:HG22	2.02	0.42
25:a:83:LYS:O	25:a:87:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:96:ARG:NH2	25:a:99:TYR:O	2.48	0.42
27:2:82:A:H61	27:2:87:C:H42	1.67	0.42
8:H:72:VAL:HG11	8:H:91:PHE:HB3	2.02	0.41
21:W:1:MET:H2	21:W:6:THR:HB	1.85	0.41
26:1:538:G:H2'	26:1:539:G:O4'	2.20	0.41
26:1:1674:U:H2'	26:1:1675:G:O4'	2.20	0.41
26:1:2767:A:H2'	26:1:2768:A:C8	2.55	0.41
26:1:1821:U:H2'	26:1:1822:C:C6	2.55	0.41
18:R:35:ARG:NE	26:1:2769:G:OP1	2.52	0.41
26:1:805:G:H2'	26:1:806:A:O4'	2.19	0.41
26:1:2355:A:H2'	26:1:2356:A:H8	1.84	0.41
26:1:955:A:H2'	26:1:956:A:C8	2.55	0.41
7:G:6:GLY:HA2	7:G:22:LYS:NZ	2.35	0.41
26:1:1357:G:OP2	26:1:1357:G:N2	2.25	0.41
26:1:2082:C:H5'	26:1:2083:G:H5"	2.02	0.41
26:1:2579:U:O2'	26:1:2580:G:N2	2.54	0.41
6:F:6:ILE:HD12	6:F:33:VAL:HG11	2.02	0.41
26:1:145:A:H2'	26:1:146:U:C6	2.56	0.41
26:1:2406:G:H2'	26:1:2407:A:C8	2.55	0.41
4:D:42:GLY:HA2	4:D:47:LYS:HD2	2.03	0.41
6:F:20:MET:HE1	6:F:89:LEU:HD21	2.02	0.41
23:Y:17:THR:HA	23:Y:98:LYS:HE2	2.03	0.41
24:Z:74:GLU:HG3	24:Z:76:GLU:HG2	2.03	0.41
25:a:18:VAL:HG22	25:a:22:LEU:HD12	2.02	0.41
26:1:2317:G:H2'	26:1:2318:U:C6	2.55	0.41
26:1:2877:G:N2	26:1:2880:A:OP2	2.52	0.41
1:A:39:ARG:NH1	1:A:41:ARG:HB3	2.35	0.41
2:B:96:TYR:HE2	2:B:102:ARG:HG3	1.85	0.41
26:1:268:A:H2'	26:1:269:G:H4'	2.03	0.41
26:1:2529:G:H5"	26:1:2530:A:H5'	2.03	0.41
1:A:26:ASP:OD1	1:A:26:ASP:N	2.51	0.41
14:N:35:GLU:OE2	14:N:45:ASN:HB2	2.20	0.41
20:V:62:LYS:HB3	20:V:62:LYS:HE2	1.88	0.41
25:a:4:LYS:HE2	25:a:4:LYS:HB2	1.82	0.41
26:1:150:A:H61	26:1:179:A:H2	1.69	0.41
26:1:229:A:H2'	26:1:230:A:C8	2.56	0.41
26:1:713:A:H2'	26:1:715:A:H62	1.85	0.41
26:1:904:G:O2'	26:1:905:U:OP2	2.39	0.41
26:1:1213:C:H2'	26:1:1215:U:OP2	2.21	0.41
26:1:1487:G:H1	26:1:1596:G:N2	2.15	0.41
26:1:1577:G:C5	26:1:1578:A:H1'	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1817:C:H2'	26:1:1818:A:C8	2.55	0.41
26:1:1821:U:H2'	26:1:1822:C:H6	1.86	0.41
26:1:2325:A:H61	26:1:2345:A:H1'	1.86	0.41
26:1:2873:C:H2'	26:1:2874:A:C8	2.56	0.41
25:a:67:ALA:HB3	25:a:71:GLU:H	1.86	0.41
26:1:1320:G:N2	26:1:1323:A:OP2	2.54	0.41
26:1:1504:U:H2'	26:1:1505:G:C8	2.56	0.41
26:1:1759:G:H3'	26:1:1760:G:H5"	2.03	0.41
26:1:1556:G:H4'	26:1:1557:C:OP1	2.20	0.40
7:G:73:PRO:HG2	7:G:99:GLU:HG2	2.02	0.40
11:K:39:GLU:O	11:K:39:GLU:HG2	2.21	0.40
18:R:14:CYS:HB2	18:R:27:CYS:HA	2.02	0.40
26:1:130:A:H2'	26:1:131:G:H8	1.86	0.40
3:C:106:PHE:O	3:C:110:VAL:HG23	2.21	0.40
11:K:9:LEU:HD23	11:K:9:LEU:H	1.86	0.40
26:1:858:U:H2'	26:1:859:C:C6	2.55	0.40
26:1:1036:C:H2'	26:1:1037:A:H8	1.87	0.40
2:B:132:LEU:HD23	2:B:135:ILE:HD12	2.02	0.40
26:1:172:U:H2'	26:1:173:A:H8	1.86	0.40
26:1:620:G:O2'	26:1:1292:A:OP1	2.39	0.40
26:1:1519:U:O2'	26:1:1561:G:O6	2.33	0.40
26:1:1873:G:H2'	26:1:1874:A:C8	2.56	0.40
4:D:79:ARG:NH2	26:1:615:A:OP2	2.42	0.40
26:1:1612:C:O2'	26:1:1613:G:H5"	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	111/116 (96%)	105 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	271/277 (98%)	260 (96%)	11 (4%)	0	100	100
3	C	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
4	D	98/102 (96%)	93 (95%)	5 (5%)	0	100	100
5	E	109/117 (93%)	105 (96%)	4 (4%)	0	100	100
6	F	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
7	G	86/105 (82%)	79 (92%)	7 (8%)	0	100	100
8	H	91/217 (42%)	89 (98%)	2 (2%)	0	100	100
9	I	76/94 (81%)	73 (96%)	3 (4%)	0	100	100
10	J	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
11	K	59/73 (81%)	55 (93%)	4 (7%)	0	100	100
12	L	213/220 (97%)	207 (97%)	6 (3%)	0	100	100
13	M	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
14	N	48/57 (84%)	44 (92%)	4 (8%)	0	100	100
15	O	45/49 (92%)	45 (100%)	0	0	100	100
16	P	42/45 (93%)	41 (98%)	1 (2%)	0	100	100
17	Q	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
18	R	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
19	S	190/207 (92%)	181 (95%)	9 (5%)	0	100	100
20	V	141/145 (97%)	137 (97%)	4 (3%)	0	100	100
21	W	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
22	X	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
23	Y	134/144 (93%)	130 (97%)	4 (3%)	0	100	100
24	Z	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
25	a	106/119 (89%)	99 (93%)	7 (7%)	0	100	100
All	All	2607/2904 (90%)	2495 (96%)	112 (4%)	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%)	99 (100%)	0	100	100
2	B	220/224 (98%)	220 (100%)	0	100	100
3	C	96/98 (98%)	96 (100%)	0	100	100
4	D	85/86 (99%)	84 (99%)	1 (1%)	67	89
5	E	90/94 (96%)	90 (100%)	0	100	100
6	F	79/79 (100%)	79 (100%)	0	100	100
7	G	77/90 (86%)	77 (100%)	0	100	100
8	H	81/190 (43%)	81 (100%)	0	100	100
9	I	61/75 (81%)	61 (100%)	0	100	100
10	J	49/51 (96%)	49 (100%)	0	100	100
11	K	55/66 (83%)	55 (100%)	0	100	100
12	L	174/178 (98%)	174 (100%)	0	100	100
13	M	50/53 (94%)	50 (100%)	0	100	100
14	N	45/50 (90%)	45 (100%)	0	100	100
15	O	45/47 (96%)	45 (100%)	0	100	100
16	P	39/40 (98%)	39 (100%)	0	100	100
17	Q	55/56 (98%)	55 (100%)	0	100	100
18	R	35/35 (100%)	35 (100%)	0	100	100
19	S	158/170 (93%)	158 (100%)	0	100	100
20	V	122/123 (99%)	122 (100%)	0	100	100
21	W	99/100 (99%)	99 (100%)	0	100	100
22	X	110/112 (98%)	110 (100%)	0	100	100
23	Y	113/119 (95%)	113 (100%)	0	100	100
24	Z	101/102 (99%)	101 (100%)	0	100	100
25	a	87/95 (92%)	87 (100%)	0	100	100
All	All	2225/2435 (91%)	2224 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	65	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	79	HIS
2	B	134	ASN
3	C	108	GLN
5	E	28	ASN
5	E	97	ASN
7	G	8	ASN
8	H	13	GLN
8	H	58	ASN
8	H	85	GLN
9	I	58	ASN
11	K	17	GLN
12	L	47	ASN
12	L	148	HIS
19	S	130	ASN
19	S	162	ASN
20	V	11	ASN
20	V	41	ASN
22	X	70	ASN
23	Y	13	HIS
23	Y	25	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2681/2923 (91%)	416 (15%)	9 (0%)
27	2	110/115 (95%)	25 (22%)	0
All	All	2791/3038 (91%)	441 (15%)	9 (0%)

All (441) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	12	U
26	1	34	U
26	1	64	A
26	1	71	A
26	1	73	A
26	1	75	G
26	1	89	U
26	1	117	A

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Mol	Chain	Res	Type
26	1	118	A
26	1	119	U
26	1	143	U
26	1	150	A
26	1	156	A
26	1	160	G
26	1	161	A
26	1	162	A
26	1	163	U
26	1	168	A
26	1	176	A
26	1	180	G
26	1	183	A
26	1	184	C
26	1	199	A
26	1	202	A
26	1	218	G
26	1	219	A
26	1	225	A
26	1	230	A
26	1	233	U
26	1	234	C
26	1	236	A
26	1	248	G
26	1	251	G
26	1	255	G
26	1	258	A
26	1	259	A
26	1	268	A
26	1	298	U
26	1	300	G
26	1	301	U
26	1	302	A
26	1	303	G
26	1	309	U
26	1	311	U
26	1	319	G
26	1	320	U
26	1	321	U
26	1	322	A
26	1	326	A
26	1	329	A

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Mol	Chain	Res	Type
26	1	330	C
26	1	331	G
26	1	354	A
26	1	360	A
26	1	372	A
26	1	373	A
26	1	381	G
26	1	389	A
26	1	397	U
26	1	399	U
26	1	405	G
26	1	406	A
26	1	408	U
26	1	410	G
26	1	411	A
26	1	432	G
26	1	440	C
26	1	447	A
26	1	457	G
26	1	458	A
26	1	463	C
26	1	489	A
26	1	502	C
26	1	503	A
26	1	519	G
26	1	526	A
26	1	527	G
26	1	537	A
26	1	550	A
26	1	553	A
26	1	554	C
26	1	567	G
26	1	575	G
26	1	576	U
26	1	577	A
26	1	583	A
26	1	592	A
26	1	593	U
26	1	594	G
26	1	606	G
26	1	611	U
26	1	616	G

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Mol	Chain	Res	Type
26	1	617	A
26	1	618	A
26	1	646	A
26	1	647	G
26	1	650	U
26	1	658	A
26	1	659	A
26	1	679	G
26	1	682	A
26	1	683	G
26	1	690	U
26	1	691	A
26	1	698	U
26	1	699	U
26	1	700	A
26	1	731	U
26	1	760	A
26	1	763	A
26	1	764	C
26	1	772	A
26	1	775	A
26	1	792	U
26	1	807	U
26	1	809	A
26	1	810	A
26	1	819	A
26	1	820	G
26	1	827	A
26	1	829	U
26	1	835	U
26	1	836	C
26	1	837	G
26	1	850	G
26	1	857	C
26	1	872	U
26	1	873	U
26	1	891	A
26	1	911	A
26	1	920	A
26	1	955	A
26	1	970	U
26	1	971	U

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Mol	Chain	Res	Type
26	1	972	A
26	1	977	A
26	1	985	A
26	1	989	A
26	1	990	G
26	1	1003	A
26	1	1005	G
26	1	1018	A
26	1	1027	A
26	1	1040	A
26	1	1049	C
26	1	1055	A
26	1	1056	U
26	1	1057	A
26	1	1066	G
26	1	1070	A
26	1	1071	A
26	1	1077	U
26	1	1085	U
26	1	1086	G
26	1	1087	C
26	1	1093	C
26	1	1156	G
26	1	1158	G
26	1	1163	U
26	1	1173	A
26	1	1174	U
26	1	1176	U
26	1	1177	A
26	1	1179	C
26	1	1186	A
26	1	1187	A
26	1	1209	U
26	1	1214	C
26	1	1217	U
26	1	1218	G
26	1	1220	A
26	1	1274	G
26	1	1278	G
26	1	1288	G
26	1	1293	U
26	1	1294	G

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Mol	Chain	Res	Type
26	1	1309	G
26	1	1310	A
26	1	1311	A
26	1	1312	A
26	1	1313	G
26	1	1321	A
26	1	1337	A
26	1	1338	U
26	1	1339	U
26	1	1358	A
26	1	1366	U
26	1	1387	C
26	1	1389	U
26	1	1397	G
26	1	1402	A
26	1	1416	U
26	1	1421	A
26	1	1432	A
26	1	1433	U
26	1	1452	C
26	1	1453	G
26	1	1454	U
26	1	1463	A
26	1	1469	G
26	1	1471	A
26	1	1472	C
26	1	1473	G
26	1	1487	G
26	1	1490	G
26	1	1497	A
26	1	1498	U
26	1	1503	U
26	1	1504	U
26	1	1510	U
26	1	1519	U
26	1	1526	G
26	1	1557	C
26	1	1561	G
26	1	1570	G
26	1	1571	G
26	1	1575	A
26	1	1577	G

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Mol	Chain	Res	Type
26	1	1578	A
26	1	1579	C
26	1	1588	U
26	1	1592	A
26	1	1596	G
26	1	1604	C
26	1	1605	A
26	1	1606	C
26	1	1613	G
26	1	1616	A
26	1	1622	C
26	1	1625	U
26	1	1627	G
26	1	1628	A
26	1	1629	U
26	1	1630	A
26	1	1632	A
26	1	1633	A
26	1	1634	A
26	1	1651	C
26	1	1652	A
26	1	1654	A
26	1	1663	G
26	1	1690	A
26	1	1691	G
26	1	1692	C
26	1	1711	G
26	1	1718	G
26	1	1738	C
26	1	1740	G
26	1	1744	A
26	1	1758	A
26	1	1759	G
26	1	1760	G
26	1	1764	A
26	1	1773	A
26	1	1785	G
26	1	1790	G
26	1	1791	G
26	1	1800	A
26	1	1809	C
26	1	1811	A

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Mol	Chain	Res	Type
26	1	1827	C
26	1	1828	U
26	1	1829	A
26	1	1835	U
26	1	1836	A
26	1	1843	U
26	1	1856	A
26	1	1875	A
26	1	1898	C
26	1	1899	U
26	1	1900	G
26	1	1910	G
26	1	1912	A
26	1	1933	G
26	1	1934	G
26	1	1940	A
26	1	1941	C
26	1	1942	U
26	1	1944	U
26	1	1950	U
26	1	1956	G
26	1	1957	G
26	1	1965	A
26	1	1968	C
26	1	1982	U
26	1	1990	C
26	1	1991	G
26	1	1994	C
26	1	1997	A
26	1	1998	A
26	1	1999	G
26	1	2004	A
26	1	2009	U
26	1	2018	U
26	1	2020	U
26	1	2050	A
26	1	2058	A
26	1	2059	G
26	1	2060	A
26	1	2066	G
26	1	2070	C
26	1	2073	G

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Mol	Chain	Res	Type
26	1	2079	G
26	1	2082	C
26	1	2083	G
26	1	2086	A
26	1	2087	A
26	1	2088	G
26	1	2089	A
26	1	2096	G
26	1	2120	G
26	1	2126	C
26	1	2219	C
26	1	2220	U
26	1	2226	A
26	1	2231	C
26	1	2238	U
26	1	2240	U
26	1	2241	C
26	1	2252	A
26	1	2265	G
26	1	2266	G
26	1	2286	G
26	1	2295	A
26	1	2302	C
26	1	2306	G
26	1	2310	C
26	1	2314	A
26	1	2331	G
26	1	2332	U
26	1	2334	G
26	1	2335	G
26	1	2336	A
26	1	2337	A
26	1	2338	A
26	1	2339	U
26	1	2342	U
26	1	2346	U
26	1	2347	A
26	1	2350	G
26	1	2361	U
26	1	2362	A
26	1	2372	G
26	1	2374	C

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Mol	Chain	Res	Type
26	1	2377	C
26	1	2398	G
26	1	2410	G
26	1	2412	C
26	1	2429	U
26	1	2430	C
26	1	2433	C
26	1	2439	A
26	1	2456	G
26	1	2457	A
26	1	2468	C
26	1	2475	A
26	1	2486	A
26	1	2497	G
26	1	2501	U
26	1	2503	A
26	1	2525	C
26	1	2529	G
26	1	2530	A
26	1	2532	G
26	1	2545	A
26	1	2547	C
26	1	2556	G
26	1	2561	C
26	1	2562	G
26	1	2574	U
26	1	2581	U
26	1	2593	A
26	1	2594	G
26	1	2600	C
26	1	2601	G
26	1	2613	C
26	1	2626	G
26	1	2636	U
26	1	2637	C
26	1	2640	U
26	1	2641	A
26	1	2642	U
26	1	2657	G
26	1	2663	U
26	1	2673	C
26	1	2679	U

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Mol	Chain	Res	Type
26	1	2689	A
26	1	2700	G
26	1	2709	U
26	1	2716	U
26	1	2717	A
26	1	2726	C
26	1	2741	G
26	1	2753	U
26	1	2760	A
26	1	2771	G
26	1	2775	A
26	1	2784	A
26	1	2791	A
26	1	2792	A
26	1	2793	G
26	1	2805	A
26	1	2807	G
26	1	2820	U
26	1	2823	G
26	1	2827	A
26	1	2828	U
26	1	2840	A
26	1	2855	A
26	1	2863	G
26	1	2869	G
26	1	2887	G
26	1	2892	G
26	1	2900	C
26	1	2911	A
26	1	2913	G
27	2	3	U
27	2	4	G
27	2	10	U
27	2	19	G
27	2	22	G
27	2	33	U
27	2	39	G
27	2	40	C
27	2	42	G
27	2	49	G
27	2	55	A
27	2	59	U

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Mol	Chain	Res	Type
27	2	61	C
27	2	64	A
27	2	66	C
27	2	71	A
27	2	84	U
27	2	85	U
27	2	86	A
27	2	93	G
27	2	94	C
27	2	104	A
27	2	106	G
27	2	110	C
27	2	111	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1	229	A
26	1	405	G
26	1	525	A
26	1	890	G
26	1	1092	A
26	1	1556	G
26	1	2432	G
26	1	2783	U
26	1	2827	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

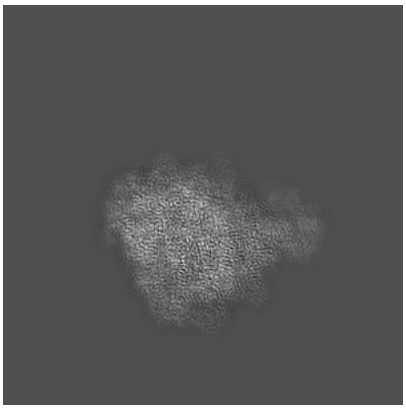
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26125. These allow visual inspection of the internal detail of the map and identification of artifacts.

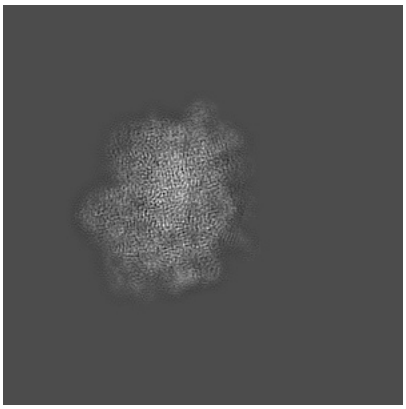
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

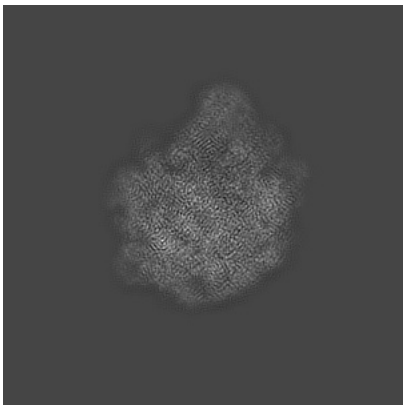
6.1.1 Primary map



X

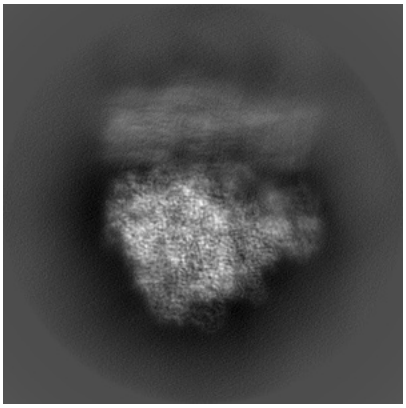


Y

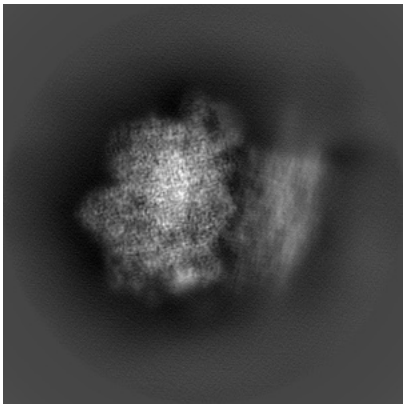


Z

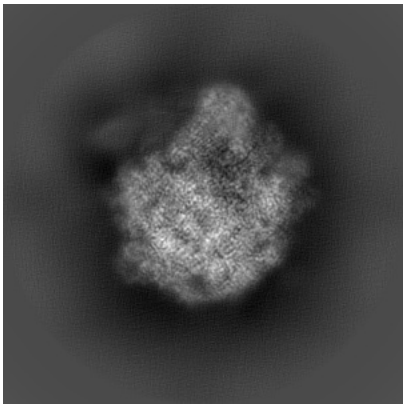
6.1.2 Raw map



X



Y

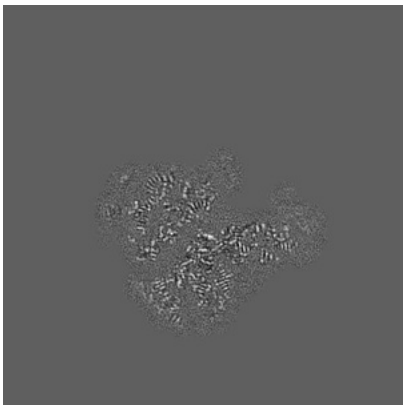


Z

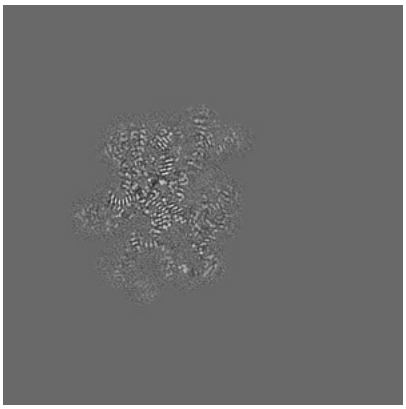
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

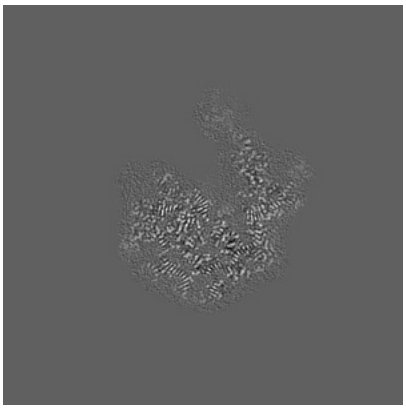
6.2.1 Primary map



X Index: 224

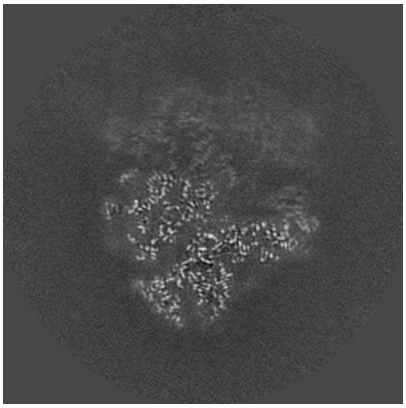


Y Index: 224

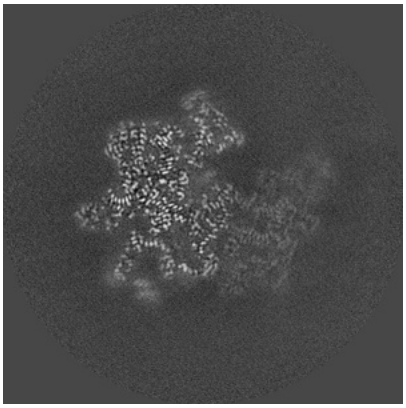


Z Index: 224

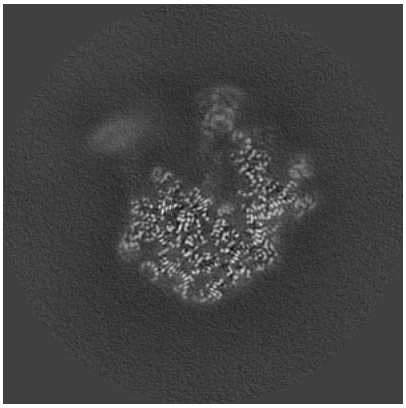
6.2.2 Raw map



X Index: 224



Y Index: 224

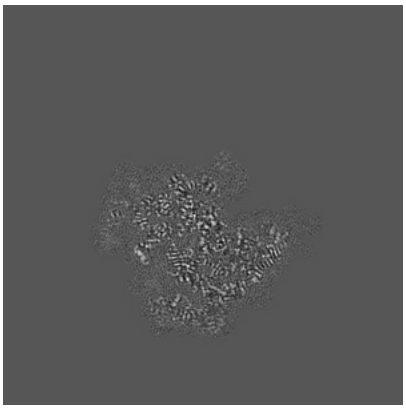


Z Index: 224

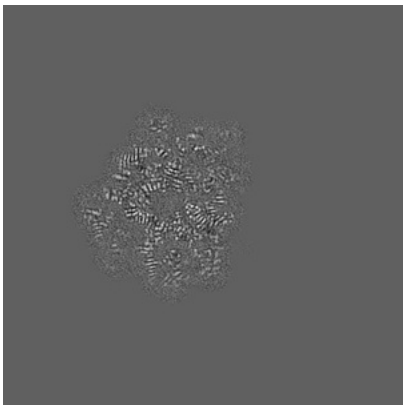
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

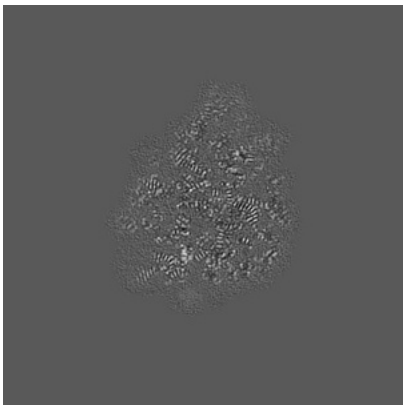
6.3.1 Primary map



X Index: 211

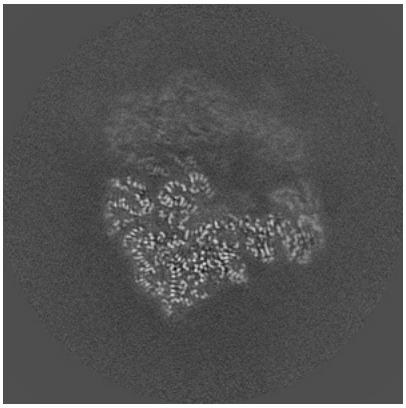


Y Index: 201

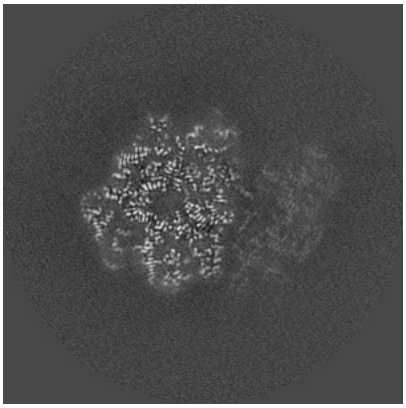


Z Index: 183

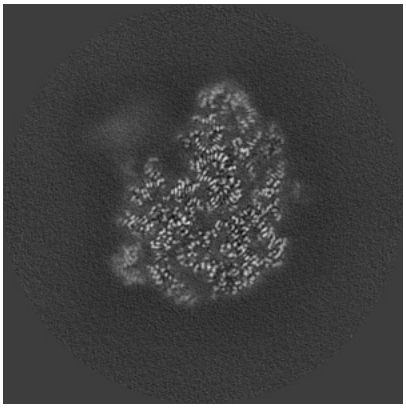
6.3.2 Raw map



X Index: 239



Y Index: 201

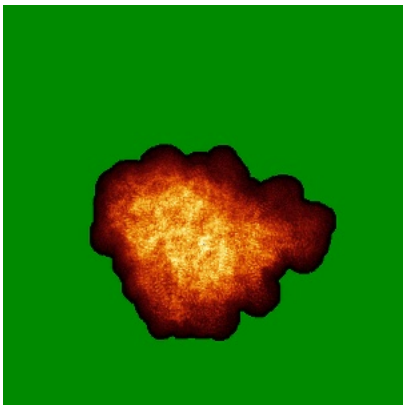


Z Index: 197

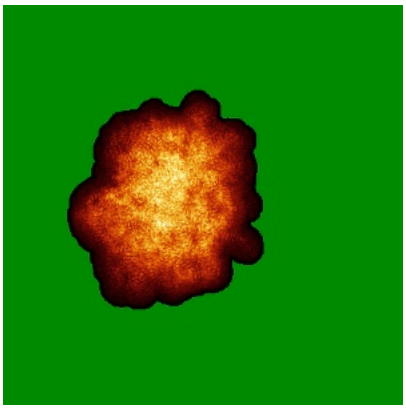
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

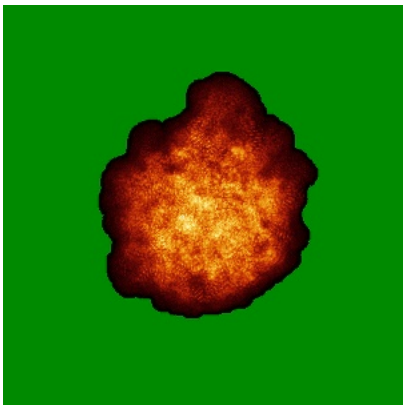
6.4.1 Primary map



X

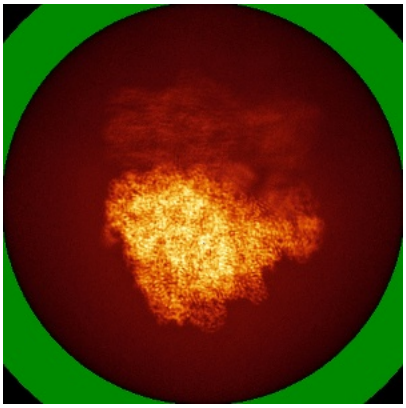


Y

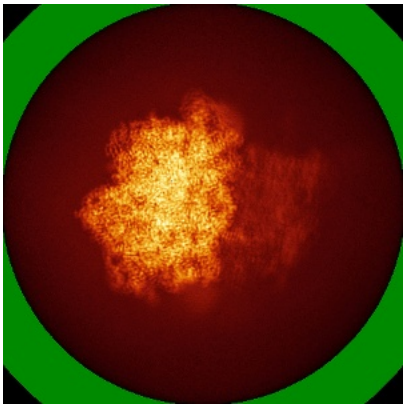


Z

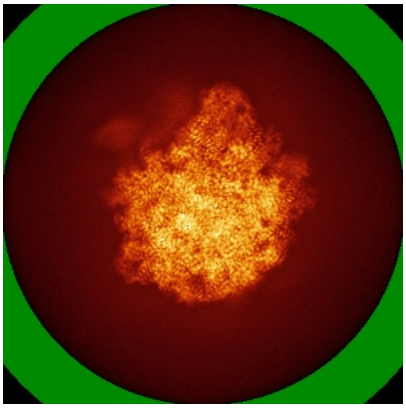
6.4.2 Raw map



X



Y

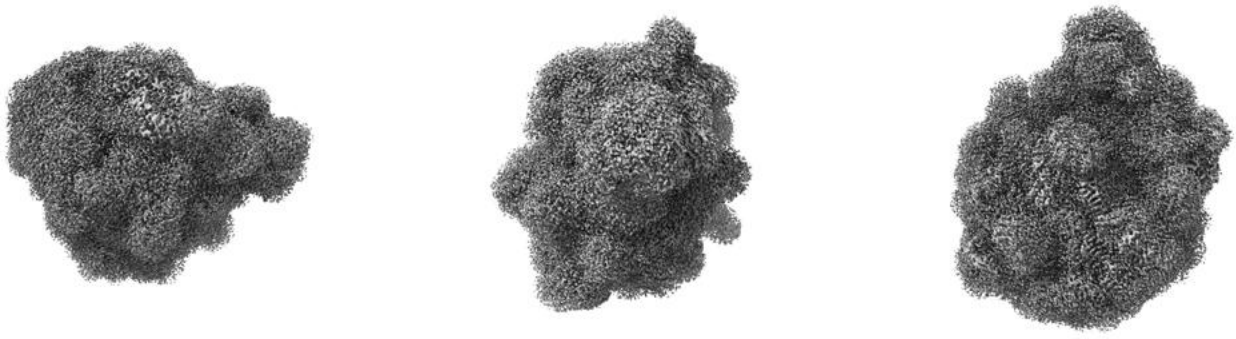


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



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.

6.5.2 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.

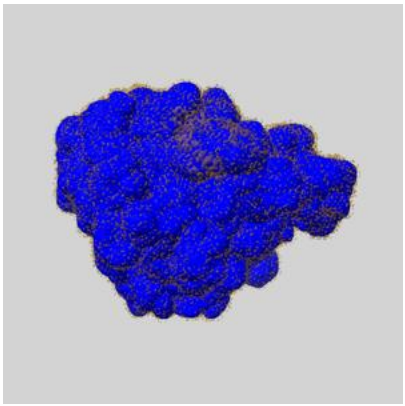
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

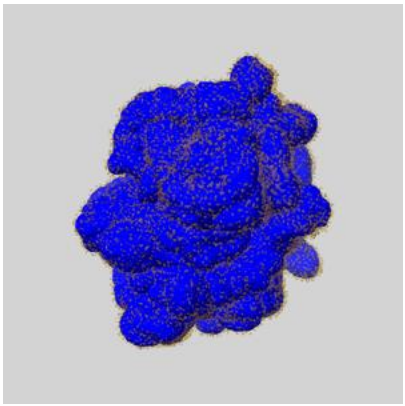
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

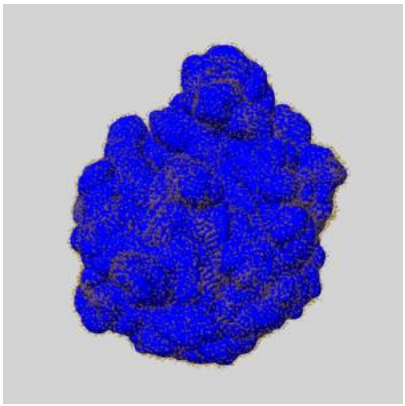
6.6.1 emd_26125_msk_1.map (i)



X



Y

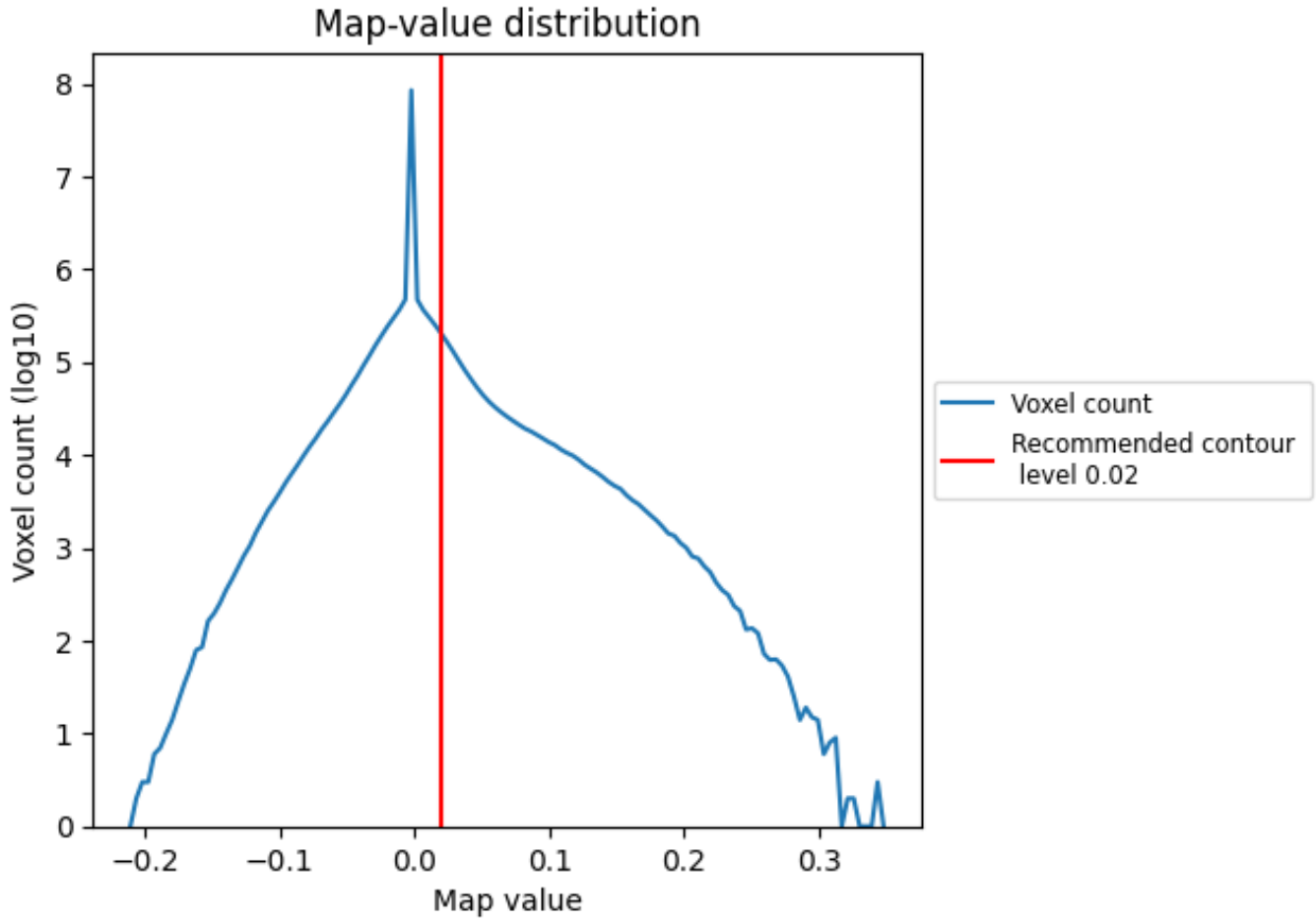


Z

7 Map analysis

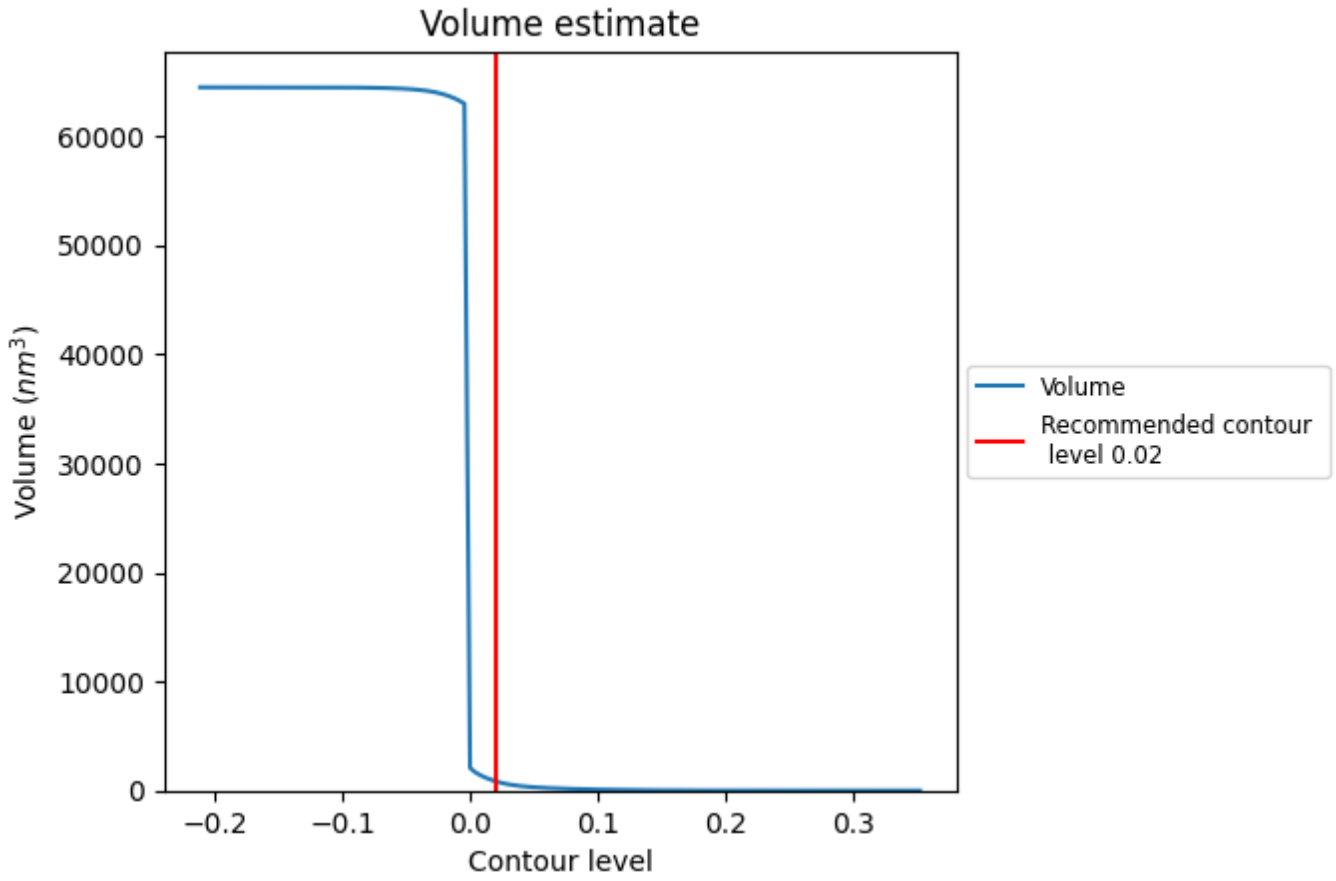
This section contains the results of statistical analysis of the map.

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.

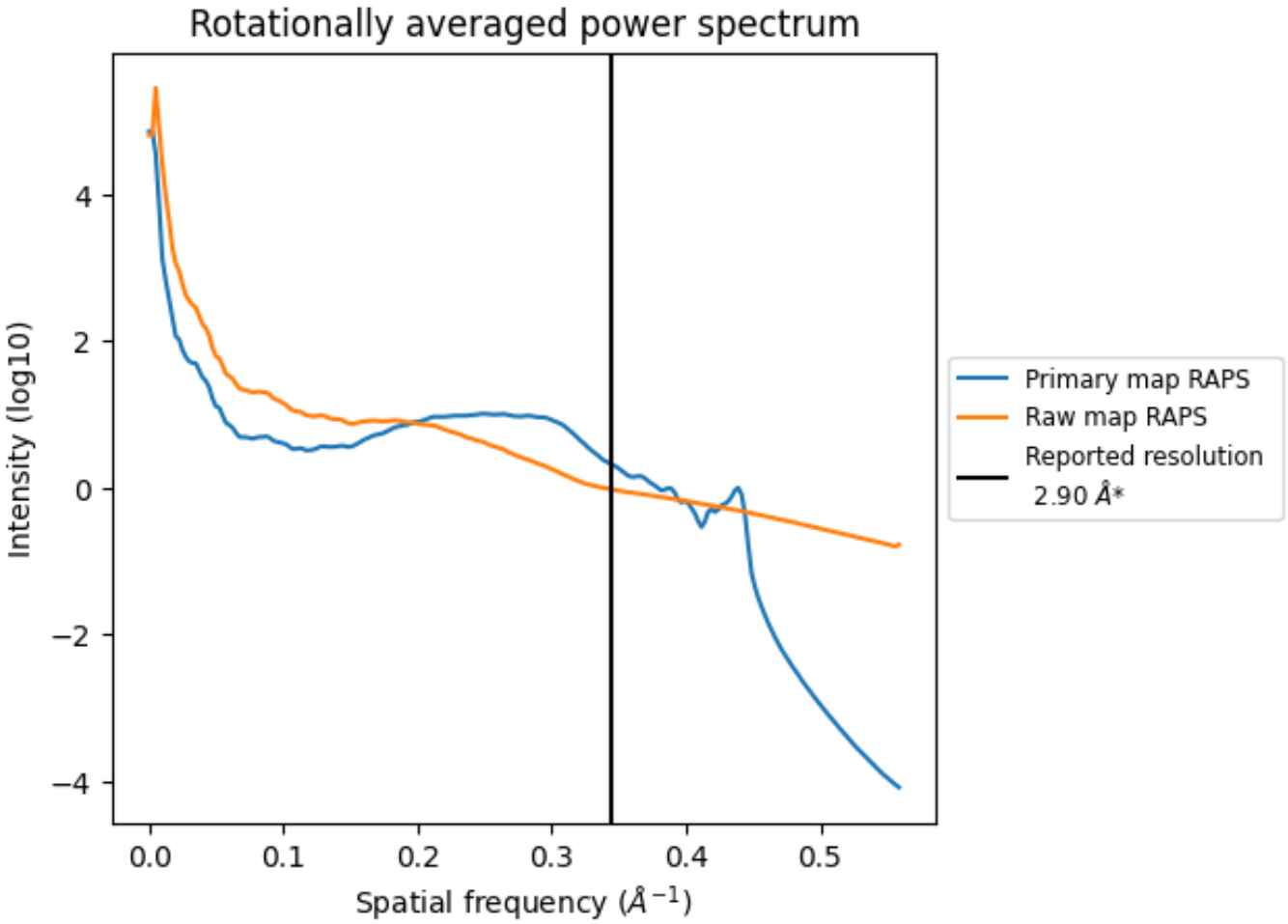
7.2 Volume estimate



The volume at the recommended contour level is 864 nm^3; this corresponds to an approximate mass of 781 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)

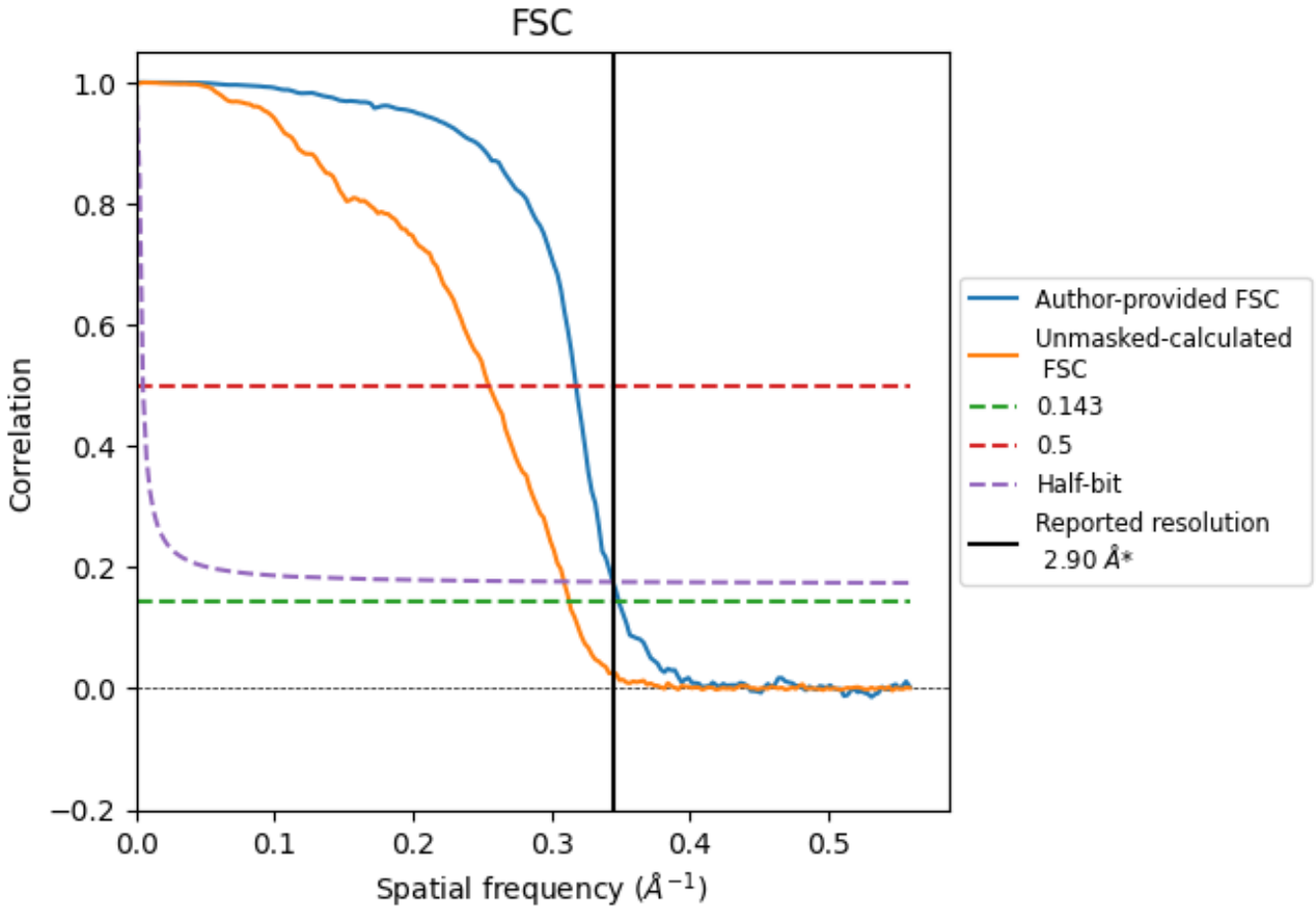


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

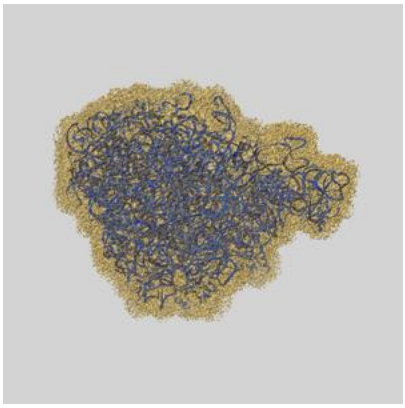
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.87	3.15	2.90
Unmasked-calculated*	3.20	3.93	3.24

*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 3.20 differs from the reported value 2.9 by more than 10 %

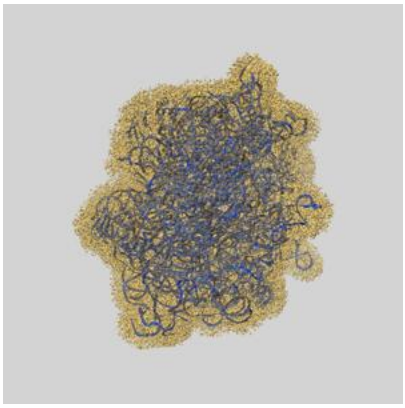
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26125 and PDB model 7TTW. Per-residue inclusion information can be found in section 3 on page 9.

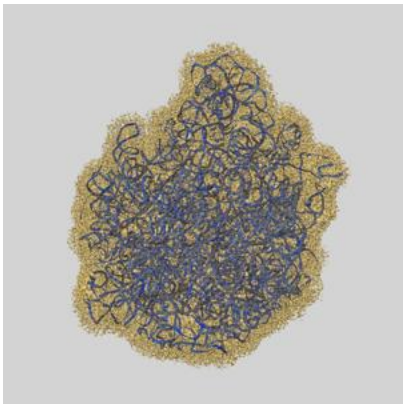
9.1 Map-model overlay



X



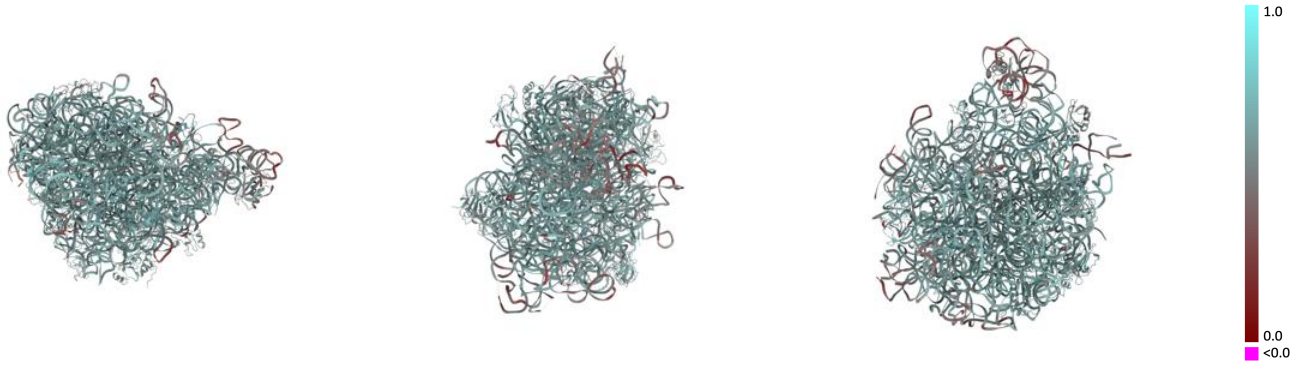
Y



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.

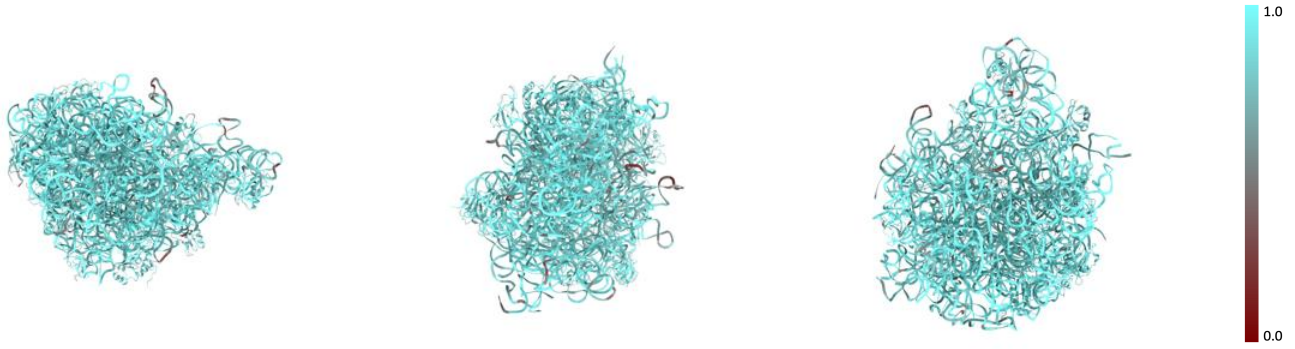
9.2 Q-score mapped to coordinate model



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.

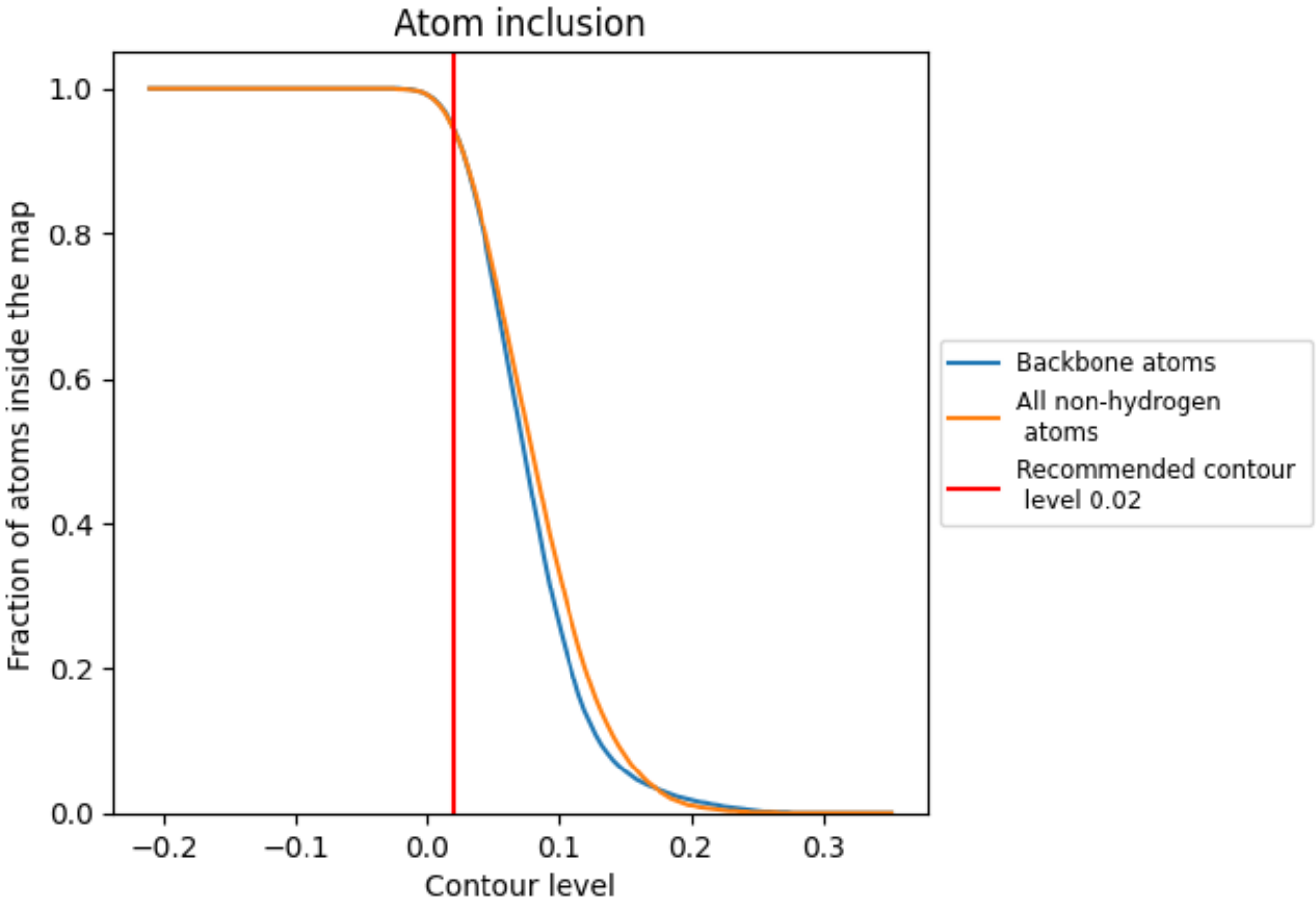
9.3 Atom inclusion mapped to coordinate model



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, 94% of all backbone atoms, 94% 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	0.9430	0.5980
1	0.9500	0.6020
2	0.8650	0.4830
A	0.9110	0.5880
B	0.9680	0.6240
C	0.9650	0.6380
D	0.9260	0.5990
E	0.9540	0.6290
F	0.9220	0.5850
G	0.8840	0.5430
H	0.8470	0.5360
I	0.9430	0.6180
J	0.9240	0.5720
K	0.8440	0.5290
L	0.9520	0.6220
M	0.9530	0.6190
N	0.9530	0.6100
O	0.8750	0.5630
P	0.9890	0.6630
Q	0.9820	0.6550
R	0.9340	0.5850
S	0.9310	0.5990
V	0.9600	0.6270
W	0.9130	0.5790
X	0.9270	0.6020
Y	0.9290	0.6030
Z	0.9360	0.6050
a	0.8660	0.5170