Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:41 am GMT

PDB ID	:	6SJ6
EMDB ID	:	EMD-10212
Title	:	Cryo-EM structure of 50S-RsfS complex from Staphylococcus aureus
Authors	:	Khusainov, I.; Pellegrino, S.; Yusupova, G.; Yusupov, M.; Fatkhullin, B.
Deposited on	:	2019-08-12
Resolution	:	3.23 Å(reported)
Based on initial model	:	5LI0

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:

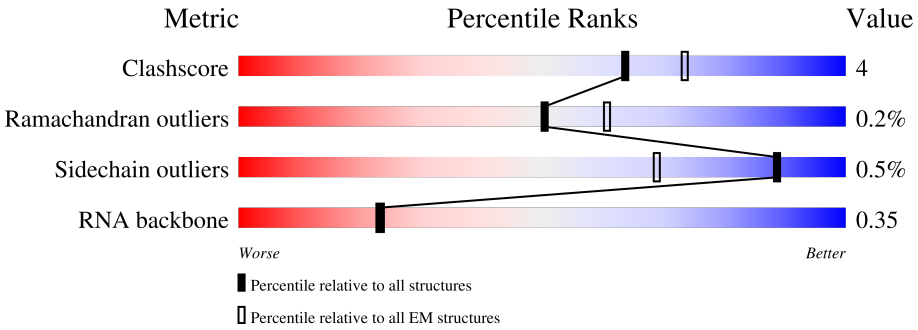
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.23 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2923	14% 50% 31% 7% 12%
2	B	115	77% 39% 43% 14% • •
3	D	277	18% 74% 12% • 13%
4	E	220	9% 87% 11% •
5	F	207	15% 86% 13% •
6	M	145	9% 94% 6%
7	N	122	17% 86% 13% •

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Mol	Chain	Length	Quality of chain
8	O	146	21% 90% 10%
9	P	144	26% 85% 10% 5%
10	Q	122	11% 80% 20%
11	R	119	93% 76% 17% 6%
12	S	116	20% 82% 7% 11%
13	T	118	8% 87% 11%
14	U	102	14% 82% 16%
15	V	117	84% 10% 6%
16	W	91	16% 87% 11%
17	X	105	30% 77% 14% 9%
18	Y	217	26% 22% 74%
19	Z	94	16% 69% 14% 17%
20	0	62	55% 58% 11% 29%
21	1	69	39% 81% 13% 6%
22	2	59	14% 85% 12%
23	4	58	19% 48% 10% 41%
24	6	45	89% 9%
25	7	66	12% 76% 18% 6%
26	9	117	84% 85% 11%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 78296 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2585	55399	24749	10151	17926	2573	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	112	2380	1066	426	778	110	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	242	1863	1161	370	329	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	216	1637	1024	301	307	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	203	1540	966	284	288	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	145	1151	717	211	220	3	0	0

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	146	Total	C	N	O	S	0	0
			1099	680	215	203	1		

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	137	Total	C	N	O	S	0	0
			1097	704	207	182	4		

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	121	Total	C	N	O	S	0	0
			956	586	183	186	1		

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	112	Total	C	N	O	0	0
			866	538	165	163		

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	103	Total	C	N	O	S	0	0
			837	528	166	142	1		

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	101	Total 791	C 501	N 141	O 149	0	0

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	110	Total 844	C 526	N 161	O 154	S 3	0	0

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	89	Total 725	C 457	N 130	O 134	S 4	0	0

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	96	Total 738	C 466	N 135	O 136	S 1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	56	Total 458	C 293	N 80	O 83	S 2	0	0

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

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

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	0	44	Total 353	C 219	N 77	O 57	0	0

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	1	65	Total	C	N	O	0	0
			536	330	101	105		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	2	57	Total	C	N	O	0	0
			441	274	83	84		

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	34	Total	C	N	O	S	0	0
			285	177	60	47	1		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	7	62	Total	C	N	O	S	0	0
			500	309	110	79	2		

- Molecule 26 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	9	112	Total	C	N	O	S	0	0
			908	568	155	181	4		

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
27	A	56	Total	Mg	0
			56	56	

- Molecule 28 is POTASSIUM ION (three-letter code: K) (formula: K).

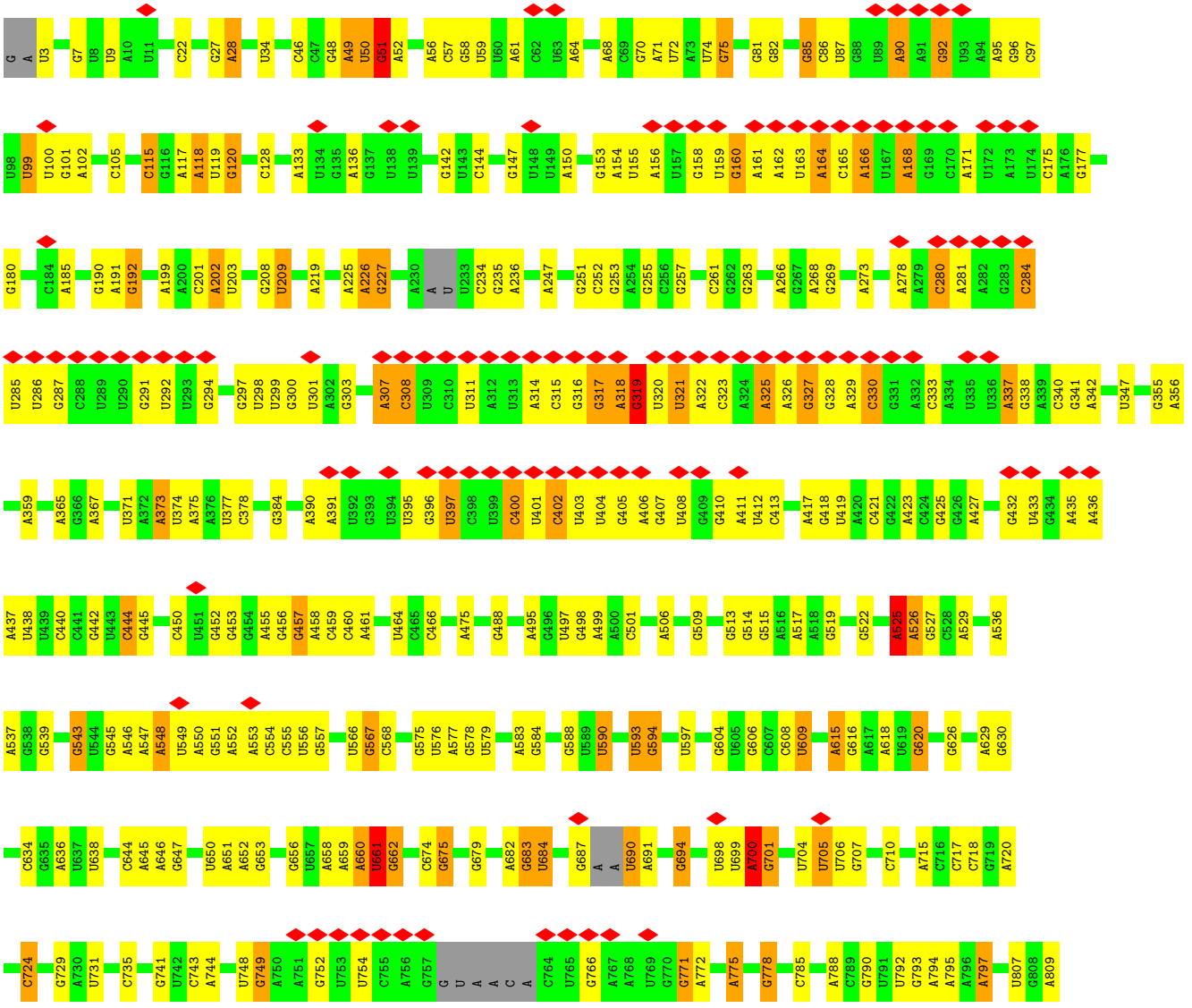
Mol	Chain	Residues	Atoms		AltConf
28	A	3	Total	K	0
			3	3	

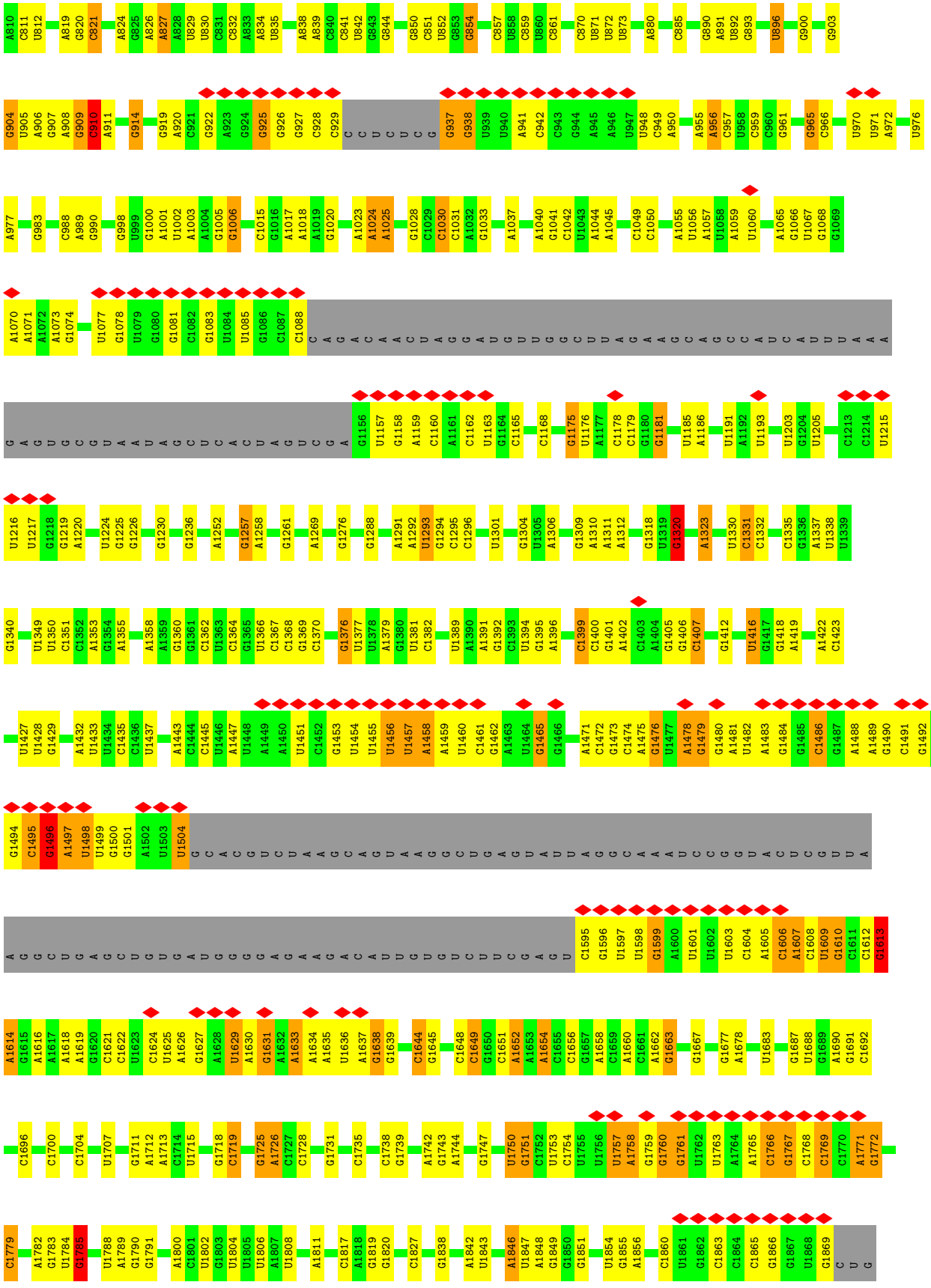
3 Residue-property plots (i)

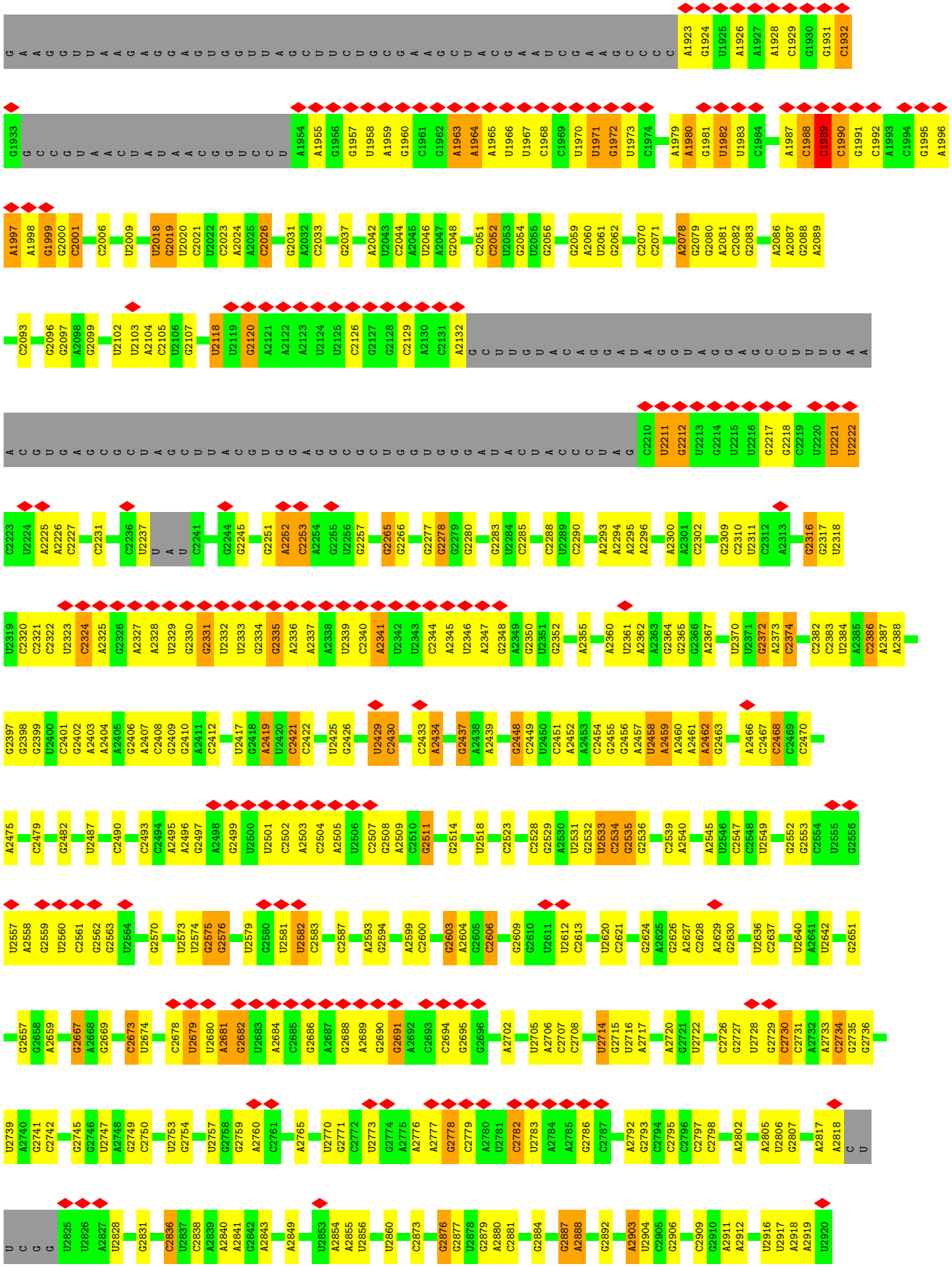
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

Chain A:

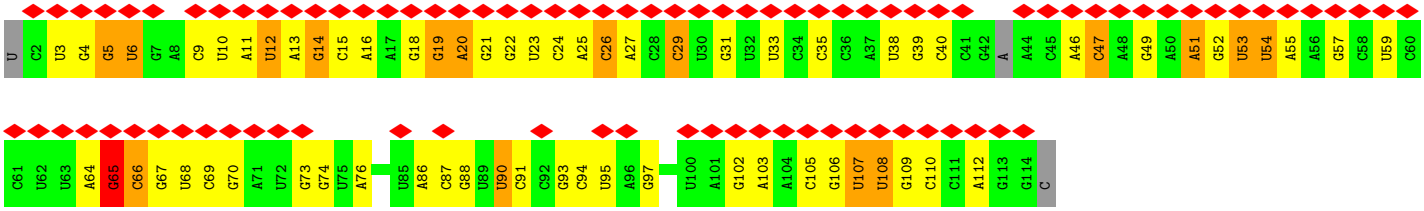






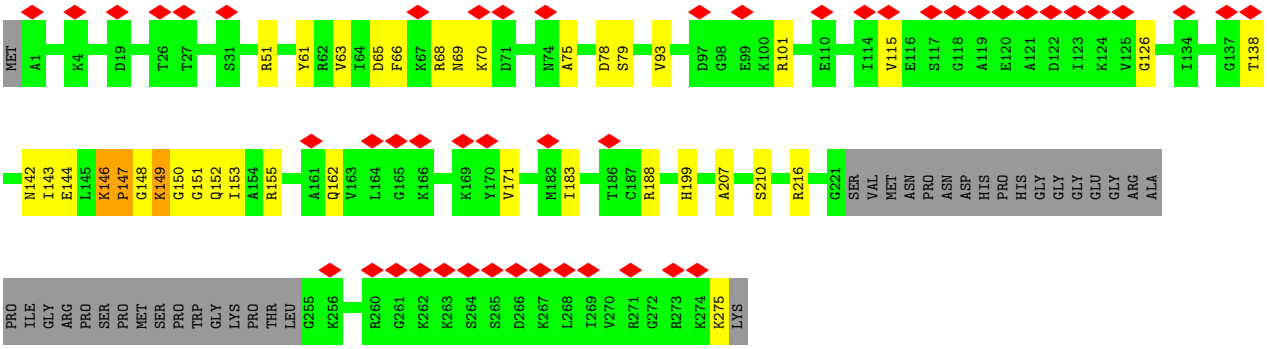
• Molecule 2: 5S ribosomal RNA

Chain B:



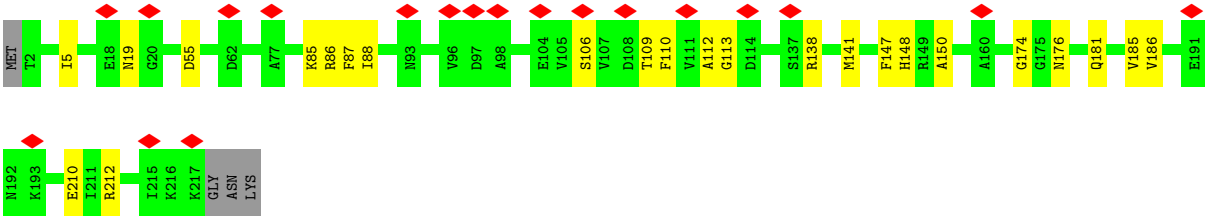
• Molecule 3: 50S ribosomal protein L2

Chain D:



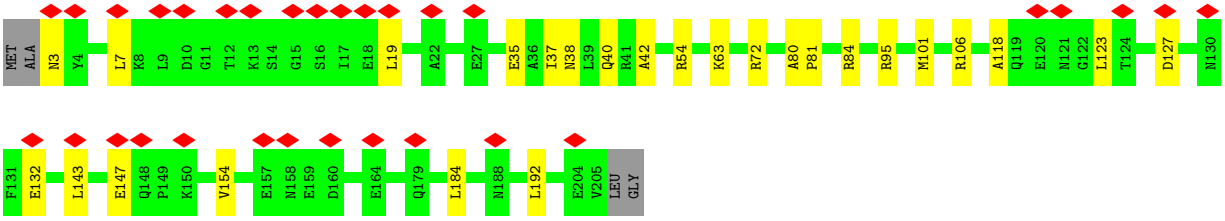
• Molecule 4: 50S ribosomal protein L3

Chain E:



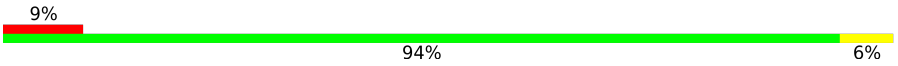
• Molecule 5: 50S ribosomal protein L4

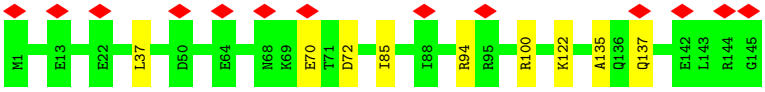
Chain F:



• Molecule 6: 50S ribosomal protein L13

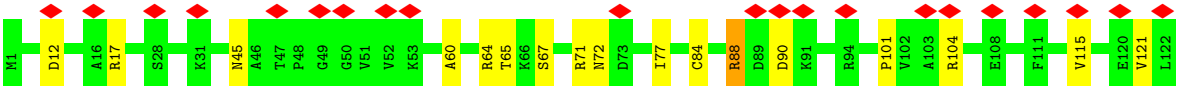
Chain M:





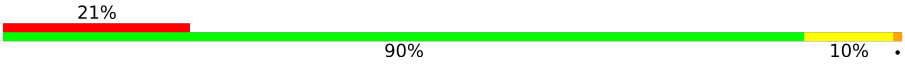
• Molecule 7: 50S ribosomal protein L14

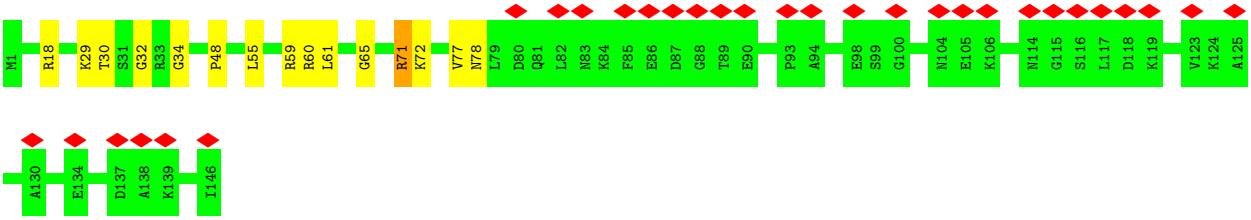
Chain N:



• Molecule 8: 50S ribosomal protein L15

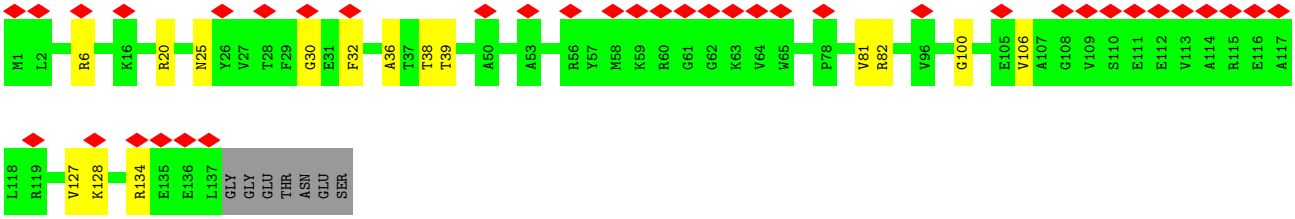
Chain O:





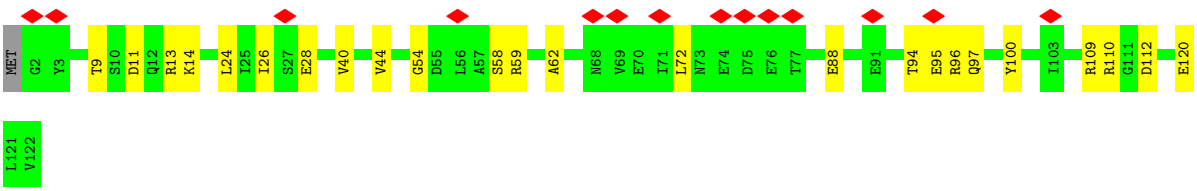
• Molecule 9: 50S ribosomal protein L16

Chain P:



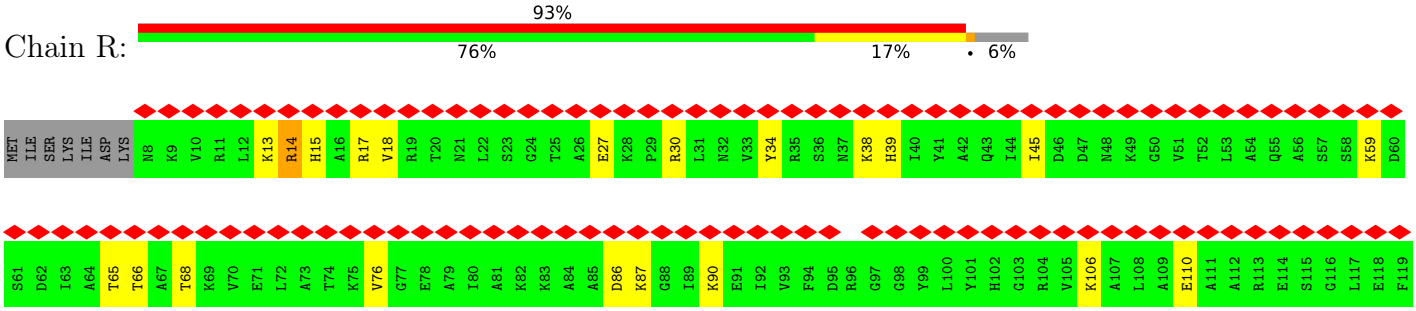
• Molecule 10: 50S ribosomal protein L17

Chain Q:



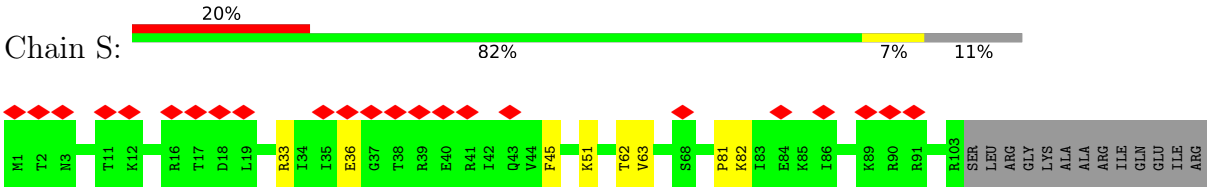
• Molecule 11: 50S ribosomal protein L18

Chain R:



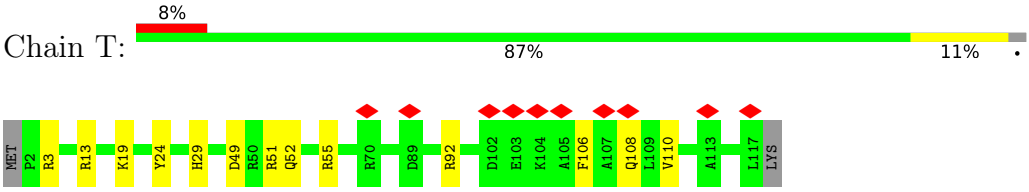
• Molecule 12: 50S ribosomal protein L19

Chain S:



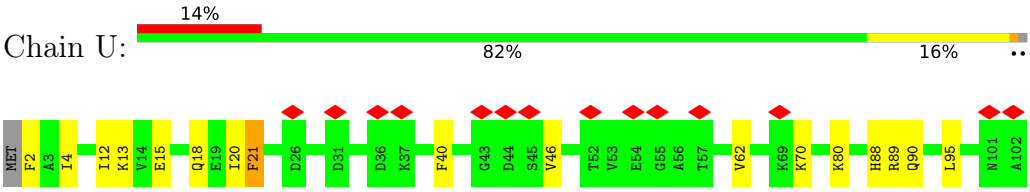
• Molecule 13: 50S ribosomal protein L20

Chain T:



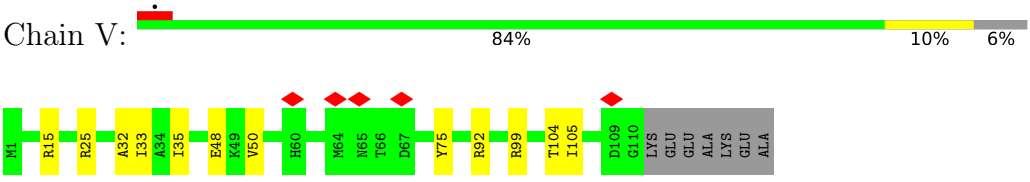
• Molecule 14: 50S ribosomal protein L21

Chain U:



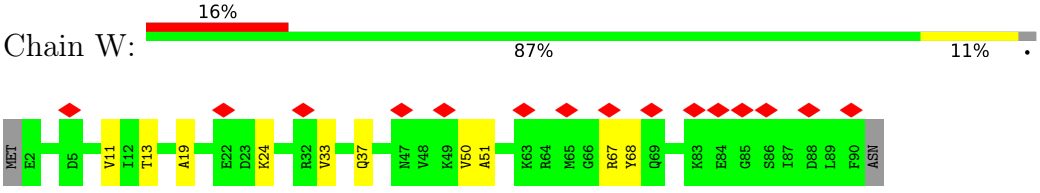
• Molecule 15: 50S ribosomal protein L22

Chain V:



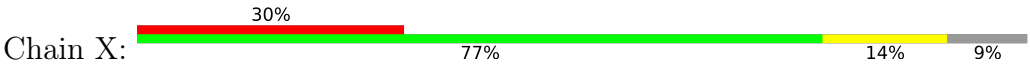
• Molecule 16: 50S ribosomal protein L23

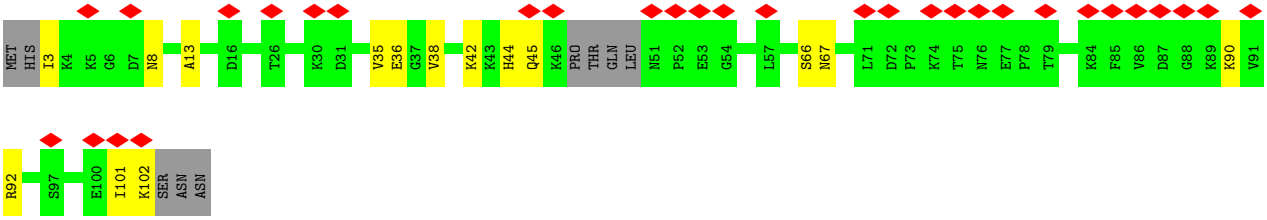
Chain W:



• Molecule 17: 50S ribosomal protein L24

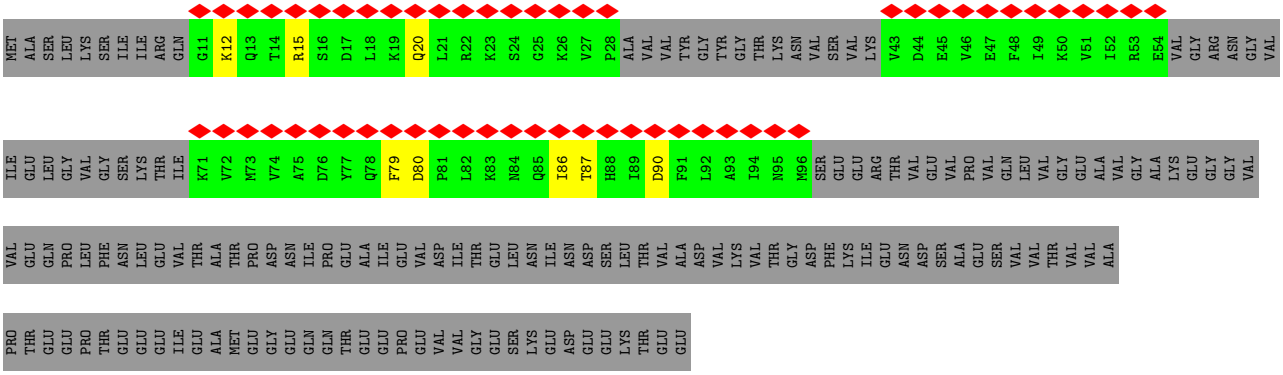
Chain X:





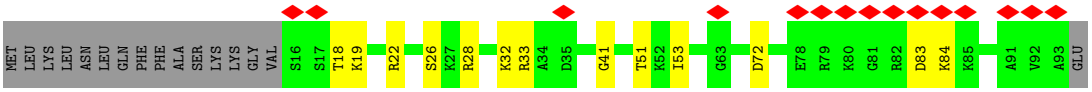
• Molecule 18: 50S ribosomal protein L25

Chain Y:



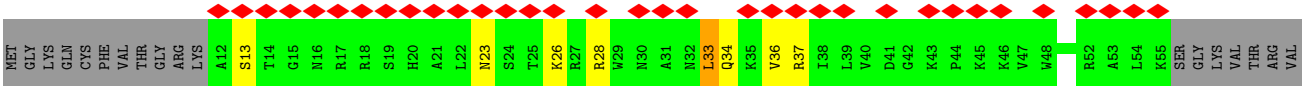
• Molecule 19: 50S ribosomal protein L27

Chain Z:



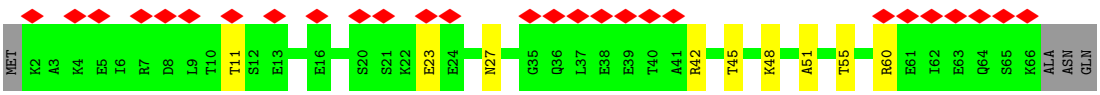
• Molecule 20: 50S ribosomal protein L28

Chain 0:



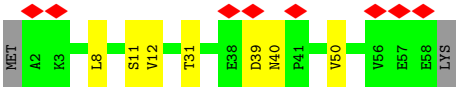
• Molecule 21: 50S ribosomal protein L29

Chain 1:



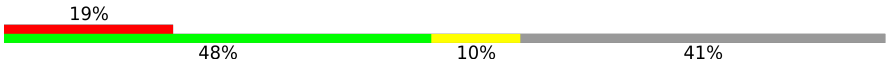
• Molecule 22: 50S ribosomal protein L30

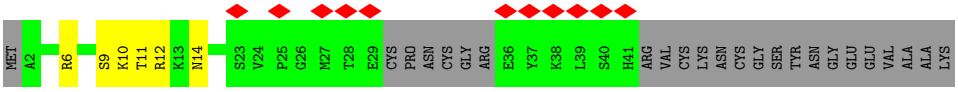
Chain 2:



• Molecule 23: 50S ribosomal protein L32

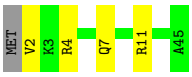
Chain 4:





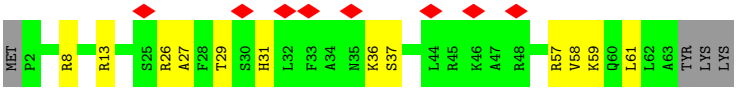
• Molecule 24: 50S ribosomal protein L34

Chain 6:



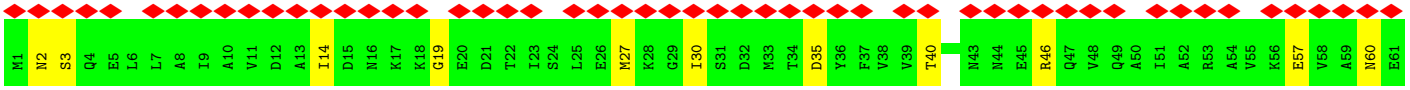
• Molecule 25: 50S ribosomal protein L35

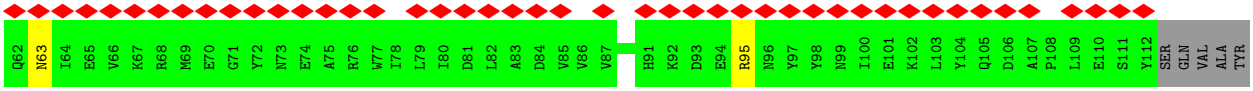
Chain 7:



• Molecule 26: Ribosomal silencing factor RsfS

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	83885	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	24.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	300.3, 300.3, 300.3	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.858, 0.858, 0.858	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.00	8/62041 (0.0%)	1.17	183/96748 (0.2%)
2	B	0.50	0/2660	1.04	3/4142 (0.1%)
3	D	0.56	0/1886	0.79	2/2522 (0.1%)
4	E	0.70	0/1661	0.70	0/2227
5	F	0.64	0/1563	0.76	0/2113
6	M	0.59	0/1173	0.73	0/1578
7	N	0.59	0/927	0.79	1/1243 (0.1%)
8	O	0.62	0/1113	0.79	1/1482 (0.1%)
9	P	0.53	0/1121	0.73	0/1504
10	Q	0.59	0/960	0.80	1/1282 (0.1%)
11	R	0.39	0/875	0.69	0/1171
12	S	0.58	0/849	0.72	0/1136
13	T	0.73	0/955	0.81	2/1265 (0.2%)
14	U	0.65	0/801	0.81	3/1070 (0.3%)
15	V	0.72	0/852	0.84	2/1148 (0.2%)
16	W	0.58	0/733	0.74	0/978
17	X	0.50	0/744	0.77	0/990
18	Y	0.36	0/462	0.66	0/615
19	Z	0.59	0/603	0.76	1/801 (0.1%)
20	0	0.43	0/358	0.82	1/479 (0.2%)
21	1	0.43	0/537	0.69	0/714
22	2	0.55	0/443	0.69	0/597
23	4	0.76	0/289	0.75	0/381
24	6	0.74	0/377	0.91	1/491 (0.2%)
25	7	0.57	0/504	0.82	0/661
26	9	0.36	0/921	0.64	0/1244
All	All	0.91	8/85408 (0.0%)	1.09	201/128582 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1296	C	N1-C6	-5.51	1.33	1.37
1	A	2037	G	N9-C8	-5.37	1.34	1.37
1	A	2470	C	N1-C6	-5.36	1.33	1.37
1	A	859	C	C4-C5	-5.33	1.38	1.43
1	A	2044	C	N1-C6	-5.27	1.33	1.37
1	A	2080	G	N9-C8	-5.23	1.34	1.37
1	A	2468	C	C4-C5	-5.22	1.38	1.43
1	A	118	A	C6-N6	-5.21	1.29	1.33

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1486	C	C2-N1-C1'	10.11	129.92	118.80
1	A	1486	C	N1-C2-O2	9.95	124.87	118.90
1	A	1486	C	N3-C2-O2	-8.82	115.72	121.90
1	A	2468	C	C5-C4-N4	-8.79	114.04	120.20
1	A	209	U	N3-C2-O2	-8.45	116.29	122.20
1	A	2468	C	N3-C4-N4	7.84	123.48	118.00
1	A	501	C	C6-N1-C2	-7.78	117.19	120.30
1	A	2348	G	C4-N9-C1'	7.49	136.23	126.50
1	A	827	A	N1-C6-N6	7.30	122.98	118.60
1	A	910	C	N1-C2-O2	7.23	123.24	118.90
1	A	1989	C	C6-N1-C2	-7.12	117.45	120.30
1	A	209	U	C6-N1-C2	-7.06	116.76	121.00
1	A	1486	C	C6-N1-C1'	-7.01	112.39	120.80
1	A	778	G	N1-C2-N2	-6.92	109.97	116.20
1	A	1331	C	C5-C4-N4	-6.85	115.41	120.20
1	A	1779	C	C5-C4-N4	-6.79	115.45	120.20
1	A	1988	C	C6-N1-C2	-6.76	117.60	120.30
1	A	859	C	C5-C4-N4	-6.75	115.47	120.20
1	A	2348	G	C8-N9-C1'	-6.75	118.22	127.00
1	A	661	U	P-O3'-C3'	6.75	127.80	119.70
1	A	832	C	C5-C4-N4	-6.75	115.48	120.20
1	A	615	A	N1-C6-N6	6.74	122.64	118.60
1	A	1648	C	C5-C4-N4	-6.66	115.54	120.20
1	A	2023	C	N3-C4-C5	6.64	124.56	121.90
1	A	1486	C	C6-N1-C2	-6.57	117.67	120.30
1	A	615	A	C5-C6-N6	-6.46	118.53	123.70
1	A	988	C	C6-N1-C2	-6.45	117.72	120.30
1	A	209	U	N1-C2-O2	6.45	127.31	122.80
1	A	2021	C	C5-C4-N4	-6.44	115.69	120.20
1	A	819	A	C5-C6-N6	-6.43	118.56	123.70
1	A	1025	A	N1-C6-N6	-6.43	114.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1376	G	C4-C5-N7	6.42	113.37	110.80
1	A	115	C	C5-C4-N4	-6.38	115.73	120.20
13	T	13	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	317	G	C4-N9-C1'	6.36	134.76	126.50
1	A	892	U	C2-N1-C1'	6.33	125.29	117.70
1	A	819	A	N1-C6-N6	6.31	122.39	118.60
1	A	557	G	O4'-C1'-N9	6.29	113.23	108.20
1	A	861	C	C5-C4-N4	-6.28	115.80	120.20
1	A	201	C	C5-C4-N4	-6.26	115.81	120.20
1	A	785	C	C5-C4-N4	-6.25	115.83	120.20
1	A	51	G	C4-N9-C1'	6.25	134.62	126.50
14	U	89	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	318	A	C5-C6-N6	-6.25	118.70	123.70
1	A	501	C	C5-C6-N1	6.24	124.12	121.00
1	A	318	A	N1-C6-N6	6.19	122.31	118.60
1	A	778	G	N3-C2-N2	6.17	124.22	119.90
10	Q	96	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	A	57	C	C5-C4-N4	-6.15	115.90	120.20
1	A	2086	A	O4'-C1'-N9	6.14	113.11	108.20
1	A	1331	C	N3-C4-N4	6.14	122.30	118.00
1	A	910	C	C2-N1-C1'	6.12	125.53	118.80
1	A	2245	G	C4-N9-C1'	6.12	134.45	126.50
1	A	1350	U	C2-N1-C1'	6.09	125.01	117.70
1	A	724	C	C5-C4-N4	-6.07	115.95	120.20
1	A	2048	G	C8-N9-C4	-6.06	103.98	106.40
1	A	1785	G	N3-C2-N2	-6.00	115.70	119.90
1	A	2604	A	C5-C6-N6	-5.99	118.91	123.70
1	A	910	C	N3-C2-O2	-5.99	117.71	121.90
15	V	99	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	2887	G	N3-C2-N2	-5.97	115.72	119.90
1	A	2294	A	N1-C6-N6	5.95	122.17	118.60
1	A	99	U	P-O3'-C3'	5.93	126.82	119.70
1	A	51	G	C8-N9-C1'	-5.93	119.30	127.00
1	A	2103	U	N3-C2-O2	-5.91	118.06	122.20
1	A	1376	G	N9-C4-C5	-5.89	103.04	105.40
1	A	2253	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1030	C	C5-C4-N4	-5.86	116.10	120.20
1	A	2348	G	N3-C4-N9	5.84	129.50	126.00
1	A	2086	A	N1-C6-N6	-5.83	115.10	118.60
1	A	1335	C	C5-C4-N4	-5.82	116.12	120.20
1	A	2103	U	N1-C2-O2	5.81	126.87	122.80
1	A	1649	C	C5-C4-N4	-5.79	116.15	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	315	C	C6-N1-C2	-5.78	117.99	120.30
13	T	13	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	1399	C	C6-N1-C2	-5.77	117.99	120.30
1	A	321	U	N3-C2-O2	-5.76	118.17	122.20
1	A	1389	U	N3-C2-O2	-5.75	118.18	122.20
1	A	998	G	N3-C2-N2	5.73	123.91	119.90
1	A	128	C	C5-C4-N4	-5.73	116.19	120.20
1	A	2730	C	N1-C2-O2	5.73	122.34	118.90
1	A	832	C	N3-C4-N4	5.71	122.00	118.00
1	A	735	C	C5-C4-N4	-5.70	116.21	120.20
1	A	2462	A	O4'-C1'-N9	5.66	112.72	108.20
1	A	421	C	C5-C4-N4	-5.64	116.25	120.20
1	A	1980	A	C8-N9-C4	-5.63	103.55	105.80
3	D	51	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	255	G	C2-N3-C4	-5.62	109.09	111.90
1	A	2387	A	C5-C6-N6	-5.61	119.21	123.70
1	A	373	A	N1-C6-N6	5.61	121.96	118.60
7	N	88	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	118	A	C5-C6-N1	5.59	120.50	117.70
1	A	827	A	C5-C6-N6	-5.59	119.23	123.70
1	A	227	G	C4-N9-C1'	5.57	133.74	126.50
1	A	1651	C	C6-N1-C2	-5.57	118.07	120.30
1	A	690	U	N3-C2-O2	-5.57	118.30	122.20
1	A	2245	G	C8-N9-C1'	-5.57	119.77	127.00
1	A	2604	A	N1-C6-N6	5.55	121.93	118.60
1	A	1644	C	C6-N1-C2	-5.54	118.08	120.30
1	A	2387	A	N1-C6-N6	5.54	121.92	118.60
1	A	2093	C	C5-C4-N4	-5.52	116.33	120.20
1	A	841	C	C5-C4-N4	-5.52	116.34	120.20
1	A	2056	G	C2-N3-C4	-5.52	109.14	111.90
1	A	1033	G	C8-N9-C4	-5.50	104.20	106.40
1	A	1351	C	C6-N1-C2	-5.50	118.10	120.30
1	A	1989	C	C5-C6-N1	5.50	123.75	121.00
1	A	2302	C	C6-N1-C2	-5.49	118.10	120.30
1	A	321	U	N1-C2-O2	5.49	126.64	122.80
1	A	501	C	N3-C4-C5	-5.48	119.71	121.90
1	A	1997	A	P-O3'-C3'	5.48	126.27	119.70
1	A	2290	C	N3-C4-N4	5.46	121.82	118.00
1	A	2511	G	N3-C4-C5	5.45	131.32	128.60
1	A	319	G	C4-N9-C1'	5.44	133.58	126.50
1	A	2750	C	C6-N1-C2	-5.44	118.12	120.30
1	A	615	A	C4-C5-N7	5.43	113.42	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2419	A	O4'-C1'-N9	5.43	112.55	108.20
1	A	2730	C	P-O3'-C3'	5.42	126.21	119.70
1	A	2335	G	N3-C2-N2	-5.40	116.12	119.90
1	A	317	G	C8-N9-C1'	-5.39	119.99	127.00
1	A	1648	C	N3-C4-C5	5.39	124.06	121.90
1	A	1779	C	N3-C4-N4	5.39	121.78	118.00
1	A	700	A	P-O3'-C3'	5.37	126.15	119.70
1	A	1750	U	P-O3'-C3'	5.37	126.15	119.70
1	A	1382	C	C5-C4-N4	-5.37	116.44	120.20
1	A	1498	U	C6-N1-C1'	5.36	128.71	121.20
1	A	2606	C	N3-C4-C5	5.36	124.04	121.90
1	A	457	G	P-O3'-C3'	5.36	126.13	119.70
1	A	1382	C	N3-C4-N4	5.35	121.75	118.00
15	V	25	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	1416	U	C6-N1-C2	-5.33	117.80	121.00
1	A	2019	G	C8-N9-C4	-5.33	104.27	106.40
1	A	1175	G	N3-C2-N2	-5.32	116.17	119.90
1	A	1751	G	C4-N9-C1'	5.32	133.41	126.50
1	A	1719	C	C5-C4-N4	-5.31	116.48	120.20
1	A	615	A	C5-N7-C8	-5.30	101.25	103.90
1	A	497	U	O4'-C1'-N1	5.30	112.44	108.20
1	A	1382	C	C6-N1-C2	-5.29	118.18	120.30
1	A	1980	A	N7-C8-N9	5.29	116.44	113.80
1	A	1713	A	C8-N9-C4	-5.28	103.69	105.80
1	A	497	U	C6-N1-C2	-5.28	117.83	121.00
1	A	1932	C	C2-N1-C1'	5.27	124.60	118.80
1	A	257	G	C2-N3-C4	-5.26	109.27	111.90
1	A	1654	A	C5-N7-C8	-5.26	101.27	103.90
19	Z	22	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	498	G	N1-C2-N2	-5.24	111.49	116.20
1	A	457	G	OP2-P-O3'	5.23	116.71	105.20
1	A	2876	G	N3-C4-N9	-5.23	122.86	126.00
1	A	2288	C	C5-C4-N4	-5.23	116.54	120.20
1	A	1704	C	C5-C4-N4	-5.22	116.55	120.20
2	B	76	A	N7-C8-N9	5.21	116.41	113.80
1	A	1785	G	N3-C4-N9	-5.21	122.87	126.00
1	A	1376	G	C5-C6-O6	-5.21	125.47	128.60
1	A	2245	G	N3-C4-N9	5.21	129.12	126.00
1	A	555	C	C5-C4-N4	-5.19	116.56	120.20
8	O	18	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	525	A	N1-C6-N6	-5.18	115.49	118.60
1	A	1817	C	N3-C4-N4	5.18	121.63	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1719	C	N3-C4-N4	5.18	121.63	118.00
1	A	2290	C	C5-C4-N4	-5.17	116.58	120.20
1	A	2528	C	N1-C2-O2	5.16	121.99	118.90
1	A	998	G	N1-C2-N2	-5.15	111.56	116.20
14	U	21	PHE	CB-CG-CD1	5.15	124.41	120.80
2	B	65	G	C4-N9-C1'	5.15	133.19	126.50
1	A	2708	C	C5-C4-N4	-5.14	116.60	120.20
1	A	2433	C	C6-N1-C1'	5.14	126.97	120.80
1	A	192	G	C4-C5-N7	5.13	112.85	110.80
1	A	788	A	C5-C6-N6	-5.13	119.60	123.70
1	A	2419	A	C6-C5-N7	-5.13	128.71	132.30
1	A	2750	C	C5-C4-N4	-5.11	116.62	120.20
1	A	1496	G	C2-N3-C4	5.11	114.46	111.90
20	0	28	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	202	A	C4-C5-C6	-5.10	114.45	117.00
1	A	2052	C	C5-C4-N4	-5.10	116.63	120.20
1	A	2888	A	N7-C8-N9	5.10	116.35	113.80
1	A	1320	G	N1-C2-N2	-5.09	111.62	116.20
1	A	690	U	C6-N1-C2	-5.08	117.95	121.00
1	A	501	C	N3-C4-N4	5.08	121.56	118.00
1	A	700	A	C4-C5-N7	5.08	113.24	110.70
14	U	89	ARG	NE-CZ-NH2	-5.08	117.76	120.30
3	D	146	LYS	C-N-CD	5.07	139.05	128.40
1	A	2078	A	C5-C6-N6	-5.06	119.65	123.70
1	A	717	C	C5-C4-N4	-5.06	116.66	120.20
1	A	998	G	C4-C5-N7	5.05	112.82	110.80
1	A	2316	G	C4-N9-C1'	5.05	133.07	126.50
1	A	57	C	N3-C4-C5	5.05	123.92	121.90
1	A	2606	C	C5-C4-N4	-5.05	116.67	120.20
2	B	76	A	C8-N9-C4	-5.05	103.78	105.80
1	A	2750	C	N3-C4-N4	5.04	121.53	118.00
1	A	319	G	N3-C4-C5	-5.04	126.08	128.60
1	A	1613	G	C6-C5-N7	-5.03	127.38	130.40
1	A	497	U	C5-C6-N1	5.03	125.22	122.70
1	A	626	G	N7-C8-N9	5.03	115.61	113.10
1	A	821	C	C5-C4-N4	5.02	123.71	120.20
1	A	965	G	N3-C4-N9	-5.02	122.99	126.00
1	A	1025	A	C8-N9-C4	-5.01	103.80	105.80
1	A	1989	C	P-O3'-C3'	5.01	125.71	119.70
1	A	1613	G	C4-N9-C1'	5.00	133.01	126.50
24	6	11	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	A	937	G	C4-N9-C1'	5.00	133.00	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1332	C	C5-C4-N4	-5.00	116.70	120.20
1	A	2078	A	C5-N7-C8	-5.00	101.40	103.90

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	55399	0	27886	252	0
2	B	2380	0	1210	22	0
3	D	1863	0	1992	26	0
4	E	1637	0	1680	13	0
5	F	1540	0	1577	18	0
6	M	1151	0	1145	7	0
7	N	920	0	981	8	0
8	O	1099	0	1142	13	0
9	P	1097	0	1166	10	0
10	Q	956	0	1002	15	0
11	R	866	0	899	15	0
12	S	837	0	902	6	0
13	T	943	0	1014	8	0
14	U	791	0	824	11	0
15	V	844	0	901	6	0
16	W	725	0	761	5	0
17	X	738	0	800	10	0
18	Y	458	0	477	7	0
19	Z	597	0	607	7	0
20	0	353	0	381	8	0
21	1	536	0	567	6	0
22	2	441	0	478	4	0
23	4	285	0	305	4	0
24	6	373	0	420	3	0
25	7	500	0	564	15	0
26	9	908	0	884	7	0
27	A	56	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	3	0	0	0	0
All	All	78296	0	50565	437	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 (437) 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)
8:O:48:PRO:O	25:7:59:LYS:NZ	1.89	1.04
3:D:142:ASN:OD1	3:D:151:GLY:HA3	1.62	0.98
1:A:1865:C:HO2'	1:A:1923:A:HO5'	0.95	0.92
3:D:142:ASN:OD1	3:D:151:GLY:CA	2.24	0.85
1:A:674:C:O2	1:A:684:U:O2'	1.94	0.84
1:A:705:U:O4	5:F:95:ARG:NH1	2.12	0.81
1:A:1400:C:OP1	20:0:37:ARG:NH1	2.13	0.81
1:A:1609:U:O2'	1:A:1610:G:O5'	1.99	0.81
1:A:1445:C:N4	1:A:1638:G:O6	2.14	0.80
1:A:1753:U:O2	1:A:2879:G:N2	2.15	0.80
1:A:1017:A:OP2	14:U:80:LYS:NZ	2.11	0.80
1:A:983:G:OP1	25:7:57:ARG:NH1	2.15	0.79
7:N:104:ARG:NH2	12:S:36:GLU:OE2	2.15	0.79
1:A:2828:U:O2	1:A:2911:A:N6	2.17	0.78
1:A:161:A:OP1	1:A:163:U:O2'	2.02	0.78
1:A:700:A:O2'	1:A:701:G:O5'	2.01	0.77
3:D:66:PHE:HB3	3:D:151:GLY:H	1.49	0.77
1:A:1964:A:O2'	1:A:1966:U:OP1	2.02	0.77
3:D:65:ASP:OD2	3:D:101:ARG:NH2	2.18	0.77
1:A:2680:U:O2	1:A:2695:G:N2	2.18	0.76
1:A:2778:G:O2'	1:A:2779:C:O4'	2.03	0.76
1:A:896:U:O4	1:A:972:A:N6	2.17	0.76
1:A:1006:G:O2'	1:A:2523:C:O2'	2.04	0.76
1:A:2849:A:OP1	4:E:86:ARG:NH2	2.18	0.76
2:B:107:U:O2'	2:B:108:U:O4'	2.03	0.76
1:A:2479:C:N4	1:A:2531:U:O4	2.18	0.75
10:Q:26:ILE:HD12	10:Q:72:LEU:HD11	1.68	0.75
2:B:12:U:OP2	2:B:68:U:O2'	2.05	0.75
5:F:101:MET:O	5:F:106:ARG:NH2	2.20	0.74
19:Z:51:THR:OG1	19:Z:53:ILE:O	2.04	0.74
1:A:1658:A:N6	15:V:92:ARG:O	2.20	0.74
1:A:937:G:O2'	1:A:938:G:O4'	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:C:N4	1:A:1181:G:O6	2.20	0.73
1:A:2107:G:O2'	20:0:23:ASN:ND2	2.22	0.73
1:A:3:U:O4	1:A:2919:A:N6	2.20	0.73
1:A:568:C:O2	1:A:597:U:O2'	2.07	0.72
1:A:661:U:O2'	1:A:662:G:OP2	2.05	0.72
1:A:526:A:O2'	17:X:42:LYS:O	2.07	0.72
1:A:1606:C:O2'	1:A:1607:A:O4'	2.06	0.71
2:B:93:G:N7	18:Y:15:ARG:NH2	2.38	0.71
5:F:3:ASN:N	5:F:19:LEU:O	2.22	0.71
21:1:23:GLU:O	21:1:27:ASN:ND2	2.23	0.71
2:B:27:A:N6	2:B:53:U:O4	2.20	0.71
3:D:68:ARG:O	3:D:188:ARG:NH1	2.23	0.71
1:A:105:C:HO2'	1:A:337:A:HO2'	1.39	0.71
1:A:1960:G:O2'	1:A:2000:G:O2'	2.04	0.71
1:A:1612:C:O2'	1:A:1613:G:O5'	2.07	0.70
1:A:347:U:O4	1:A:356:A:N6	2.17	0.70
1:A:1459:A:N6	1:A:1631:G:OP1	2.25	0.70
1:A:705:U:O2'	1:A:707:G:OP2	2.08	0.70
2:B:22:G:N2	2:B:26:C:O2	2.25	0.70
2:B:20:A:O2'	2:B:21:G:O4'	2.08	0.70
1:A:253:G:OP1	8:O:59:ARG:NH1	2.26	0.69
1:A:2458:U:O2'	1:A:2459:A:OP1	2.10	0.69
1:A:1595:C:O5'	1:A:1598:U:O4	2.10	0.69
1:A:593:U:O2'	1:A:594:G:OP1	2.10	0.69
1:A:2448:G:N7	25:7:31:HIS:NE2	2.31	0.69
1:A:2836:C:O2	1:A:2903:A:O2'	2.11	0.69
1:A:2659:A:O2'	1:A:2831:G:O2'	2.08	0.68
1:A:319:G:N2	1:A:321:U:OP1	2.26	0.68
7:N:64:ARG:NH1	7:N:101:PRO:O	2.26	0.68
1:A:160:G:O2'	1:A:166:A:N7	2.26	0.68
1:A:1073:A:OP1	9:P:128:LYS:NZ	2.26	0.67
4:E:141:MET:SD	4:E:148:HIS:ND1	2.68	0.67
10:Q:54:GLY:O	10:Q:59:ARG:NH1	2.27	0.67
8:O:61:LEU:O	25:7:13:ARG:NH1	2.27	0.67
10:Q:94:THR:OG1	10:Q:95:GLU:OE1	2.08	0.66
10:Q:109:ARG:NH2	10:Q:112:ASP:OD2	2.28	0.66
1:A:297:G:N2	1:A:298:U:O4	2.29	0.66
14:U:62:VAL:HG12	14:U:95:LEU:HD23	1.77	0.66
1:A:495:A:O2'	13:T:3:ARG:NH1	2.29	0.65
2:B:90:U:OP1	18:Y:20:GLN:NE2	2.29	0.65
14:U:2:PHE:N	14:U:15:GLU:OE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1972:G:N2	1:A:1989:C:O2'	2.29	0.65
1:A:2285:C:O2'	1:A:2454:C:OP2	2.15	0.65
1:A:75:G:O2'	21:1:48:LYS:NZ	2.30	0.65
1:A:2257:G:H1'	20:0:33:LEU:HD23	1.77	0.65
4:E:19:ASN:O	12:S:82:LYS:NZ	2.29	0.65
5:F:143:LEU:O	5:F:147:GLU:N	2.30	0.65
1:A:340:C:OP1	17:X:90:LYS:NZ	2.29	0.65
1:A:1757:U:O2'	1:A:1758:A:O4'	2.15	0.64
1:A:2917:U:O2'	6:M:135:ALA:O	2.15	0.64
1:A:2682:G:O2'	1:A:2691:G:O6	2.10	0.64
1:A:1451:U:N3	1:A:1633:A:N7	2.46	0.64
1:A:1353:A:O4'	1:A:1429:G:N2	2.31	0.63
1:A:914:G:O3'	9:P:6:ARG:NH1	2.31	0.63
2:B:94:C:OP2	18:Y:12:LYS:NZ	2.24	0.63
3:D:151:GLY:O	3:D:152:GLN:HG2	1.98	0.63
1:A:1379:A:O2'	1:A:1381:U:OP2	2.15	0.63
1:A:660:A:N7	5:F:40:GLN:NE2	2.46	0.63
1:A:1501:G:N2	1:A:1504:U:O4'	2.31	0.63
3:D:152:GLN:O	3:D:153:ILE:HD13	1.97	0.63
4:E:210:GLU:OE2	4:E:212:ARG:NH2	2.32	0.63
1:A:529:A:OP1	17:X:45:GLN:NE2	2.31	0.63
1:A:2132:A:O4'	1:A:2212:G:N2	2.32	0.63
17:X:35:VAL:HG13	17:X:38:VAL:HG21	1.81	0.63
1:A:826:A:OP1	3:D:216:ARG:NH2	2.31	0.62
3:D:199:HIS:ND1	3:D:199:HIS:O	2.33	0.62
1:A:903:G:N2	1:A:2296:A:OP2	2.31	0.62
11:R:30:ARG:N	11:R:45:ILE:O	2.31	0.62
12:S:33:ARG:NH2	12:S:81:PRO:O	2.33	0.62
1:A:325:A:H61	1:A:402:C:HO2'	1.48	0.62
1:A:2681:A:H62	1:A:2694:C:H41	1.46	0.62
9:P:32:PHE:O	9:P:106:VAL:N	2.32	0.61
1:A:2226:A:N1	1:A:2252:A:N6	2.48	0.61
1:A:2388:A:OP2	25:7:26:ARG:NH1	2.32	0.61
7:N:12:ASP:O	7:N:17:ARG:NH2	2.32	0.61
2:B:26:C:O2'	2:B:57:G:N2	2.33	0.61
1:A:2382:C:OP1	19:Z:33:ARG:NH2	2.34	0.61
1:A:1843:U:HO2'	3:D:61:TYR:HH	1.49	0.61
1:A:609:U:O2'	1:A:854:G:OP2	2.17	0.61
1:A:579:U:O2'	13:T:49:ASP:OD2	2.11	0.61
1:A:2603:G:O2'	1:A:2606:C:OP2	2.18	0.61
8:O:71:ARG:NH1	8:O:72:LYS:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:G:O2'	1:A:102:A:N1	2.26	0.60
1:A:2132:A:O2'	1:A:2211:U:O2	2.07	0.60
1:A:1637:A:O2'	1:A:1638:G:O5'	2.15	0.60
8:O:48:PRO:C	25:7:59:LYS:HZ2	2.05	0.60
19:Z:41:GLY:N	19:Z:72:ASP:OD1	2.34	0.60
3:D:144:GLU:HG2	3:D:150:GLY:O	2.01	0.60
14:U:88:HIS:NE2	14:U:90:GLN:OE1	2.32	0.60
21:1:51:ALA:O	21:1:55:THR:OG1	2.18	0.60
1:A:1175:G:N2	1:A:1176:U:O4	2.35	0.59
2:B:6:U:OP1	11:R:34:TYR:OH	2.14	0.59
25:7:36:LYS:O	25:7:37:SER:OG	2.20	0.59
1:A:1758:A:H62	1:A:1769:C:H42	1.51	0.59
1:A:2060:A:O2'	1:A:2062:G:OP2	2.20	0.59
10:Q:44:VAL:O	10:Q:100:TYR:OH	2.19	0.59
1:A:1597:U:OP1	1:A:1599:G:N2	2.35	0.59
8:O:48:PRO:C	25:7:59:LYS:NZ	2.54	0.59
1:A:2382:C:O2'	19:Z:32:LYS:NZ	2.36	0.59
1:A:191:A:OP1	20:0:13:SER:OG	2.20	0.59
14:U:62:VAL:HG12	14:U:95:LEU:CD2	2.33	0.58
1:A:1497:A:N6	1:A:1501:G:O6	2.36	0.58
1:A:1609:U:HO2'	1:A:1610:G:P	2.26	0.58
1:A:284:C:O2'	1:A:287:G:N2	2.26	0.58
1:A:909:G:O2'	1:A:910:C:OP1	2.22	0.58
14:U:15:GLU:N	14:U:18:GLN:OE1	2.35	0.57
1:A:273:A:OP2	1:A:297:G:N2	2.27	0.57
1:A:2046:U:OP2	23:4:6:ARG:NH2	2.38	0.57
3:D:138:THR:N	3:D:162:GLN:OE1	2.38	0.57
5:F:118:ALA:HA	5:F:123:LEU:HD12	1.85	0.57
6:M:72:ASP:OD1	6:M:72:ASP:N	2.36	0.57
16:W:19:ALA:HB1	16:W:24:LYS:HB2	1.86	0.57
1:A:1175:G:HO2'	1:A:2052:C:HO2'	1.49	0.56
7:N:88:ARG:NH1	7:N:90:ASP:OD2	2.38	0.56
1:A:741:G:H1	1:A:811:C:H42	1.54	0.56
1:A:2499:G:N2	1:A:2504:C:OP1	2.39	0.56
7:N:60:ALA:HB1	7:N:84:CYS:SG	2.46	0.56
10:Q:58:SER:O	10:Q:62:ALA:N	2.38	0.56
8:O:55:LEU:O	8:O:60:ARG:NH2	2.38	0.56
1:A:192:G:OP2	20:0:26:LYS:NZ	2.21	0.56
9:P:38:THR:HG22	9:P:39:THR:H	1.70	0.56
1:A:1031:C:O2'	1:A:1044:A:N3	2.39	0.56
1:A:2372:G:HO2'	1:A:2408:C:HO2'	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:G:N1	1:A:548:A:OP2	2.38	0.56
1:A:1711:G:O2'	1:A:2018:U:O4	2.24	0.56
1:A:2026:C:O2	1:A:2714:U:O2'	2.23	0.56
19:Z:83:ASP:OD1	19:Z:84:LYS:N	2.39	0.56
1:A:2120:G:N3	1:A:2252:A:N6	2.54	0.55
5:F:132:GLU:N	5:F:132:GLU:OE1	2.40	0.55
1:A:1475:A:O2'	1:A:1476:G:O5'	2.18	0.55
5:F:37:ILE:HG23	5:F:184:LEU:HD13	1.87	0.55
1:A:1766:C:OP1	1:A:1767:G:N2	2.40	0.55
10:Q:40:VAL:O	10:Q:44:VAL:HG12	2.07	0.55
3:D:149:LYS:HE3	3:D:152:GLN:HE22	1.72	0.55
1:A:1459:A:N6	1:A:1631:G:O4'	2.41	0.54
11:R:65:THR:HG22	11:R:66:THR:H	1.73	0.54
26:9:14:ILE:O	26:9:19:GLY:N	2.39	0.54
1:A:1649:C:O2	1:A:1654:A:O2'	2.15	0.54
3:D:69:ASN:OD1	3:D:70:LYS:N	2.40	0.54
1:A:674:C:O2'	1:A:684:U:O2	2.26	0.54
1:A:1037:A:OP2	13:T:51:ARG:NH2	2.40	0.54
1:A:1458:A:N6	1:A:1631:G:OP2	2.41	0.54
1:A:1475:A:HO2'	1:A:1476:G:P	2.31	0.54
1:A:2318:U:O2'	1:A:2401:C:O2	2.25	0.54
1:A:158:G:N7	1:A:160:G:N1	2.56	0.54
1:A:904:G:O2'	1:A:961:G:O6	2.24	0.54
1:A:1663:G:HO2'	24:6:2:VAL:N	2.06	0.54
1:A:1979:A:O2'	1:A:2587:C:O2'	2.26	0.54
1:A:2493:C:H42	1:A:2511:G:H1	1.56	0.54
1:A:955:A:O2'	1:A:956:A:O5'	2.24	0.54
1:A:1652:A:O2'	1:A:1654:A:OP2	2.25	0.54
1:A:456:G:O2'	1:A:2434:A:OP1	2.25	0.54
12:S:51:LYS:HB3	12:S:62:THR:HG22	1.90	0.54
3:D:115:VAL:HG13	3:D:126:GLY:O	2.08	0.53
1:A:247:A:OP2	25:7:8:ARG:NH2	2.41	0.53
14:U:12:ILE:HG21	14:U:20:ILE:HD11	1.89	0.53
1:A:49:A:OP1	1:A:51:G:N2	2.41	0.53
1:A:517:A:OP1	5:F:84:ARG:NH1	2.41	0.53
26:9:40:THR:O	26:9:95:ARG:NH1	2.42	0.53
1:A:278:A:H61	1:A:294:G:H1	1.56	0.53
1:A:1726:A:OP1	1:A:1743:G:N2	2.41	0.53
3:D:142:ASN:OD1	3:D:151:GLY:HA2	2.07	0.53
4:E:112:ALA:HB1	4:E:186:VAL:O	2.09	0.53
7:N:115:VAL:HG13	7:N:121:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:G:N2	1:A:976:U:O2	2.39	0.53
1:A:1963:A:N6	1:A:1990:C:H41	2.06	0.53
2:B:6:U:O2'	11:R:30:ARG:NH2	2.40	0.53
1:A:1394:U:O2	1:A:1412:G:N2	2.41	0.53
1:A:2684:A:H62	1:A:2691:G:H21	1.56	0.53
1:A:1980:A:H2	1:A:2576:G:H21	1.57	0.52
1:A:159:U:O4	1:A:168:A:N6	2.42	0.52
16:W:67:ARG:NH2	16:W:68:TYR:OH	2.42	0.52
1:A:300:G:O6	1:A:450:C:N4	2.43	0.52
1:A:2324:C:N3	1:A:2360:A:N6	2.52	0.52
3:D:148:GLY:O	3:D:149:LYS:HG3	2.09	0.52
1:A:1806:U:OP2	1:A:1811:A:N6	2.43	0.52
1:A:1478:A:O2'	1:A:1479:G:O5'	2.20	0.52
5:F:80:ALA:HB1	5:F:81:PRO:HD2	1.90	0.52
1:A:329:A:O2'	1:A:330:C:OP2	2.22	0.52
1:A:1612:C:HO2'	1:A:1613:G:P	2.32	0.52
1:A:2736:G:OP1	10:Q:14:LYS:NZ	2.31	0.52
1:A:327:G:O2'	1:A:328:G:O4'	2.24	0.52
1:A:2717:A:OP2	10:Q:13:ARG:NH2	2.43	0.52
1:A:644:C:N3	1:A:701:G:N2	2.53	0.52
17:X:3:ILE:O	17:X:92:ARG:NH2	2.43	0.52
4:E:55:ASP:OD1	4:E:85:LYS:NZ	2.36	0.51
1:A:797:A:OP1	24:6:4:ARG:NH2	2.42	0.51
1:A:1496:G:N2	1:A:1500:G:O6	2.44	0.51
8:O:48:PRO:HB2	25:7:59:LYS:HE3	1.92	0.51
1:A:2535:G:O2'	1:A:2582:U:OP1	2.14	0.51
1:A:2667:G:OP1	6:M:100:ARG:NH1	2.44	0.51
13:T:24:TYR:O	13:T:29:HIS:ND1	2.38	0.51
1:A:590:U:OP1	1:A:1257:G:O2'	2.26	0.51
1:A:2702:A:H61	1:A:2759:G:H1	1.57	0.51
26:9:27:MET:HA	26:9:30:ILE:HD13	1.92	0.51
4:E:174:GLY:O	4:E:176:ASN:N	2.42	0.51
19:Z:26:SER:O	19:Z:28:ARG:NH1	2.43	0.51
1:A:319:G:O2'	1:A:325:A:N6	2.44	0.50
1:A:2421:C:N4	1:A:2459:A:N1	2.58	0.50
2:B:31:G:H1	2:B:47:C:H42	1.59	0.50
2:B:66:C:H41	2:B:67:G:H21	1.57	0.50
1:A:1495:C:O2	1:A:1501:G:N1	2.40	0.50
10:Q:9:THR:HG23	10:Q:11:ASP:OD1	2.12	0.50
9:P:36:ALA:HB1	9:P:127:VAL:HG22	1.93	0.50
5:F:154:VAL:HG12	5:F:192:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:U:N3	1:A:327:G:OP2	2.43	0.50
18:Y:86:ILE:HG23	18:Y:86:ILE:O	2.11	0.50
1:A:1304:G:O5'	15:V:15:ARG:NH2	2.45	0.50
1:A:1725:G:O2'	1:A:1789:A:O2'	2.27	0.50
10:Q:120:GLU:N	10:Q:120:GLU:OE1	2.45	0.50
11:R:27:GLU:O	11:R:90:LYS:NZ	2.27	0.50
1:A:2321:C:OP1	11:R:14:ARG:NE	2.45	0.49
1:A:1078:G:H1	1:A:1165:C:H42	1.60	0.49
21:1:11:THR:OG1	21:1:60:ARG:NH1	2.46	0.49
1:A:2681:A:H62	1:A:2694:C:N4	2.10	0.49
1:A:522:G:N1	1:A:525:A:OP2	2.45	0.49
9:P:36:ALA:HB1	9:P:127:VAL:CG2	2.42	0.49
1:A:307:A:N7	1:A:308:C:N4	2.60	0.49
1:A:1963:A:H61	1:A:1990:C:H41	1.60	0.49
1:A:2330:G:N2	1:A:2341:A:O5'	2.45	0.49
1:A:48:G:N2	1:A:49:A:N1	2.61	0.49
1:A:280:C:N4	1:A:291:G:O6	2.47	0.48
1:A:325:A:N6	1:A:402:C:HO2'	2.10	0.48
11:R:13:LYS:O	11:R:17:ARG:NE	2.41	0.48
1:A:1637:A:HO2'	1:A:1638:G:P	2.35	0.48
1:A:1758:A:N6	1:A:1767:G:OP2	2.45	0.48
2:B:19:G:O2'	2:B:20:A:OP1	2.28	0.48
9:P:30:GLY:O	9:P:134:ARG:NH1	2.46	0.48
1:A:252:C:OP2	1:A:2421:C:O2'	2.26	0.48
1:A:1757:U:O2'	1:A:1758:A:O5'	2.23	0.48
1:A:2877:G:N2	1:A:2880:A:OP2	2.47	0.48
1:A:327:G:O2'	1:A:400:C:O2	2.32	0.48
1:A:608:C:O2	1:A:620:G:N2	2.46	0.48
2:B:66:C:N4	2:B:67:G:H21	2.11	0.48
1:A:2678:C:N3	1:A:2679:U:N3	2.62	0.48
7:N:65:THR:OG1	7:N:67:SER:O	2.19	0.48
9:P:25:ASN:ND2	9:P:100:GLY:O	2.45	0.48
1:A:2118:U:O2'	20:0:34:GLN:NE2	2.47	0.48
1:A:2325:A:P	1:A:2341:A:H61	2.37	0.48
24:6:4:ARG:O	24:6:7:GLN:NE2	2.42	0.47
1:A:2322:C:O2	1:A:2365:G:N2	2.47	0.47
1:A:133:A:N3	1:A:147:G:N2	2.62	0.47
25:7:58:VAL:O	25:7:59:LYS:HB2	2.14	0.47
1:A:50:U:N3	1:A:120:G:OP2	2.47	0.47
1:A:1613:G:O2'	1:A:1614:A:O5'	2.24	0.47
8:O:77:VAL:HG12	8:O:78:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:42:ARG:O	21:1:45:THR:OG1	2.29	0.47
1:A:2533:U:O2'	1:A:2534:C:OP2	2.33	0.47
11:R:39:HIS:HD1	11:R:59:LYS:HE2	1.80	0.47
1:A:82:G:N1	1:A:102:A:OP2	2.42	0.47
1:A:325:A:N6	1:A:402:C:O2'	2.35	0.47
1:A:1996:A:H2'	1:A:1999:G:H21	1.80	0.47
1:A:2293:A:N6	1:A:2300:A:OP2	2.44	0.47
2:B:5:G:N2	2:B:110:C:O2	2.48	0.47
4:E:106:SER:O	4:E:109:THR:HG22	2.14	0.47
1:A:2860:U:O2'	10:Q:97:GLN:NE2	2.48	0.47
3:D:63:VAL:O	3:D:63:VAL:HG13	2.15	0.47
1:A:2680:U:H5	1:A:2681:A:HO2'	1.62	0.47
9:P:20:ARG:NH2	18:Y:79:PHE:O	2.48	0.47
12:S:45:PHE:HE2	12:S:63:VAL:HG23	1.80	0.47
23:4:11:THR:OG1	23:4:12:ARG:N	2.48	0.47
25:7:27:ALA:O	25:7:29:THR:N	2.48	0.47
1:A:2673:C:OP2	1:A:2759:G:O2'	2.32	0.46
17:X:66:SER:OG	17:X:66:SER:O	2.33	0.46
1:A:2873:C:H42	1:A:2884:G:H1	1.63	0.46
10:Q:24:LEU:O	10:Q:28:GLU:N	2.40	0.46
11:R:76:VAL:HG12	11:R:76:VAL:O	2.15	0.46
1:A:86:C:H42	1:A:96:G:H1	1.64	0.46
22:2:50:VAL:HG23	22:2:50:VAL:O	2.14	0.46
1:A:2495:A:O2'	1:A:2496:A:O4'	2.33	0.46
3:D:75:ALA:HB1	3:D:93:VAL:HG23	1.96	0.46
19:Z:18:THR:HG22	19:Z:19:LYS:H	1.80	0.46
1:A:2429:U:HO2'	1:A:2430:C:P	2.38	0.46
1:A:2104:A:OP1	1:A:2265:G:N2	2.26	0.46
9:P:81:VAL:HG22	9:P:82:ARG:H	1.81	0.46
1:A:1456:U:OP1	1:A:1629:U:N3	2.49	0.46
4:E:87:PHE:O	4:E:88:ILE:HD13	2.17	0.45
11:R:30:ARG:O	11:R:45:ILE:N	2.49	0.45
1:A:1293:U:N3	5:F:72:ARG:O	2.49	0.45
26:9:60:ASN:O	26:9:63:ASN:ND2	2.49	0.45
1:A:566:U:O2'	1:A:567:G:N7	2.42	0.45
1:A:909:G:HO2'	1:A:910:C:P	2.36	0.45
1:A:2429:U:O2'	1:A:2430:C:O5'	2.33	0.45
1:A:2702:A:H61	1:A:2759:G:H22	1.64	0.45
23:4:11:THR:O	23:4:14:ASN:N	2.45	0.45
1:A:444:C:P	20:0:33:LEU:HD11	2.56	0.45
1:A:1501:G:H21	1:A:1504:U:C4'	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:VAL:N	3:D:183:ILE:O	2.47	0.45
15:V:75:TYR:OH	15:V:104:THR:HG21	2.16	0.45
15:V:50:VAL:HG12	15:V:105:ILE:HD12	1.99	0.45
1:A:1257:G:OP2	13:T:19:LYS:NZ	2.40	0.45
11:R:106:LYS:O	11:R:110:GLU:N	2.50	0.45
1:A:645:A:HO2'	1:A:647:G:HO2'	1.61	0.45
14:U:12:ILE:HG22	14:U:13:LYS:N	2.32	0.45
20:0:36:VAL:HG22	20:0:37:ARG:H	1.82	0.45
1:A:636:A:O2'	25:7:61:LEU:HD13	2.17	0.44
1:A:2331:G:N2	1:A:2340:C:O2'	2.50	0.44
3:D:146:LYS:HB3	3:D:147:PRO:CD	2.47	0.44
4:E:147:PHE:CE1	4:E:150:ALA:HB3	2.52	0.44
5:F:7:LEU:HD21	5:F:127:ASP:OD1	2.18	0.44
8:O:29:LYS:HG3	8:O:30:THR:HG23	2.00	0.44
1:A:460:C:O2	1:A:2437:G:N2	2.51	0.44
1:A:1784:U:H3'	1:A:1785:G:C5'	2.48	0.44
1:A:2384:U:O2'	1:A:2386:C:OP2	2.19	0.44
2:B:14:G:O6	2:B:66:C:N4	2.50	0.44
8:O:48:PRO:HB2	25:7:59:LYS:CE	2.46	0.44
2:B:73:G:N2	18:Y:90:ASP:OD1	2.49	0.44
22:2:8:LEU:HD23	22:2:31:THR:HA	2.00	0.44
1:A:1457:U:HO2'	1:A:1458:A:H8	1.64	0.44
1:A:1605:A:O2'	1:A:1606:C:O4'	2.29	0.44
12:S:45:PHE:CE2	12:S:63:VAL:HG23	2.52	0.44
13:T:106:PHE:O	13:T:110:VAL:HG22	2.18	0.44
16:W:50:VAL:HG22	16:W:51:ALA:O	2.18	0.44
5:F:35:GLU:OE1	5:F:35:GLU:N	2.47	0.44
1:A:27:G:O2'	1:A:28:A:OP2	2.29	0.43
1:A:396:G:O2'	1:A:397:U:O5'	2.34	0.43
1:A:1865:C:O2'	1:A:1923:A:O5'	2.01	0.43
26:9:57:GLU:O	26:9:60:ASN:N	2.51	0.43
1:A:908:A:H2'	1:A:909:G:H5'	2.00	0.43
1:A:1320:G:N2	1:A:1323:A:OP2	2.45	0.43
1:A:2373:A:O2'	1:A:2374:C:OP1	2.35	0.43
1:A:1364:C:O2'	10:Q:110:ARG:NH2	2.44	0.43
1:A:2918:A:OP1	6:M:137:GLN:NE2	2.51	0.43
11:R:15:HIS:O	11:R:18:VAL:HG22	2.19	0.43
1:A:1996:A:O2'	1:A:1999:G:N3	2.40	0.43
1:A:2702:A:N6	1:A:2759:G:H22	2.17	0.43
8:O:48:PRO:HB2	25:7:59:LYS:NZ	2.33	0.43
1:A:226:A:O2'	1:A:466:C:O2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:C:N4	1:A:397:U:O4	2.52	0.43
1:A:1760:G:O2'	1:A:1761:G:OP1	2.34	0.43
5:F:38:ASN:O	5:F:42:ALA:N	2.50	0.43
16:W:11:VAL:HG12	16:W:13:THR:HG23	1.99	0.43
17:X:36:GLU:OE1	17:X:36:GLU:N	2.52	0.43
1:A:2277:G:O2'	1:A:2278:G:OP2	2.35	0.43
21:1:55:THR:O	21:1:55:THR:HG22	2.18	0.43
1:A:2372:G:O2'	1:A:2408:C:O2'	2.25	0.43
10:Q:88:GLU:N	10:Q:88:GLU:OE1	2.52	0.43
1:A:161:A:OP2	1:A:166:A:N6	2.52	0.43
1:A:2727:G:H1	1:A:2734:C:H42	1.67	0.43
3:D:143:ILE:HG22	3:D:144:GLU:N	2.34	0.43
15:V:32:ALA:HA	15:V:35:ILE:HG22	2.01	0.43
1:A:1023:A:H3'	1:A:1024:A:C5'	2.49	0.43
1:A:2221:U:O2'	1:A:2222:U:OP1	2.34	0.43
2:B:21:G:O6	2:B:54:U:O2'	2.28	0.43
1:A:675:G:OP1	1:A:694:G:N2	2.46	0.42
1:A:683:G:O2'	1:A:684:U:O5'	2.32	0.42
1:A:2575:G:H1	1:A:2587:C:H42	1.65	0.42
4:E:5:ILE:HD12	4:E:110:PHE:CE2	2.53	0.42
6:M:70:GLU:OE1	6:M:94:ARG:NH2	2.53	0.42
26:9:27:MET:N	26:9:35:ASP:O	2.49	0.42
4:E:113:GLY:N	4:E:185:VAL:O	2.50	0.42
16:W:33:VAL:HG13	16:W:37:GLN:OE1	2.19	0.42
1:A:720:A:OP1	5:F:63:LYS:NZ	2.41	0.42
1:A:775:A:OP1	1:A:1802:U:O2'	2.38	0.42
3:D:78:ASP:OD1	3:D:79:SER:N	2.53	0.42
11:R:86:ASP:OD1	11:R:87:LYS:N	2.52	0.42
17:X:13:ALA:HB3	17:X:67:ASN:HB2	2.01	0.42
2:B:15:C:H42	2:B:65:G:H22	1.67	0.42
1:A:90:A:O2'	1:A:92:G:O6	2.35	0.42
1:A:1465:G:H1	1:A:1624:C:H42	1.67	0.42
11:R:68:THR:O	11:R:68:THR:HG23	2.19	0.42
1:A:163:U:O2'	1:A:164:A:OP2	2.38	0.42
6:M:85:ILE:O	6:M:85:ILE:HG23	2.20	0.42
1:A:2684:A:H62	1:A:2691:G:N2	2.18	0.42
1:A:718:C:OP1	5:F:54:ARG:NH1	2.53	0.42
1:A:749:G:O2'	1:A:771:G:N2	2.43	0.42
1:A:2000:G:H3'	1:A:2001:C:H5"	2.02	0.42
3:D:207:ALA:O	3:D:210:SER:OG	2.13	0.42
1:A:543:G:O2'	17:X:44:HIS:NE2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:80:ASP:OD2	18:Y:87:THR:HG21	2.20	0.41
1:A:375:A:O2'	1:A:377:U:OP2	2.31	0.41
1:A:1083:G:H22	1:A:1160:C:H2'	1.85	0.41
1:A:2757:U:O2'	4:E:181:GLN:O	2.38	0.41
13:T:52:GLN:HA	13:T:55:ARG:HE	1.84	0.41
15:V:33:ILE:HG23	15:V:48:GLU:OE2	2.20	0.41
1:A:1219:G:O2'	1:A:1220:A:N7	2.31	0.41
1:A:1261:G:N7	14:U:70:LYS:NZ	2.68	0.41
1:A:2782:C:HO2'	1:A:2783:U:H6	1.68	0.41
22:2:39:ASP:OD1	22:2:40:ASN:N	2.54	0.41
17:X:101:ILE:HG22	17:X:102:LYS:N	2.36	0.41
22:2:11:SER:OG	22:2:12:VAL:N	2.53	0.41
1:A:925:G:O6	1:A:941:A:N6	2.53	0.41
1:A:1771:A:O2'	1:A:1772:G:O5'	2.36	0.41
1:A:2324:C:H5'	1:A:2341:A:H62	1.86	0.41
1:A:2419:A:H2	1:A:2451:C:H42	1.69	0.41
2:B:29:C:H1'	2:B:51:A:H61	1.86	0.41
3:D:75:ALA:HB1	3:D:93:VAL:CG2	2.51	0.41
7:N:77:ILE:HG23	7:N:77:ILE:O	2.20	0.41
14:U:4:ILE:HD12	14:U:40:PHE:CD2	2.56	0.41
5:F:7:LEU:HD21	5:F:127:ASP:CG	2.41	0.41
26:9:2:ASN:OD1	26:9:3:SER:N	2.54	0.41
13:T:108:GLN:OE1	14:U:46:VAL:HG11	2.21	0.40
1:A:1846:A:OP1	3:D:155:ARG:N	2.54	0.40
1:A:1971:U:N3	1:A:1982:U:OP2	2.47	0.40
23:4:9:SER:OG	23:4:10:LYS:N	2.55	0.40
1:A:687:G:N2	1:A:690:U:O5'	2.55	0.40
1:A:904:G:O2'	1:A:905:U:OP2	2.40	0.40
1:A:2715:G:N1	1:A:2747:U:OP2	2.45	0.40
2:B:14:G:N2	2:B:67:G:O2'	2.55	0.40
8:O:32:GLY:O	8:O:34:GLY:N	2.54	0.40
11:R:38:LYS:HZ1	11:R:65:THR:H	1.68	0.40
1:A:1360:G:H1	1:A:1368:C:H42	1.69	0.40
1:A:1407:C:O2'	1:A:1838:G:O2'	2.38	0.40
1:A:1484:G:N1	1:A:1599:G:O2'	2.48	0.40
6:M:37:LEU:HD22	6:M:122:LYS:HG3	2.02	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
3	D	238/277 (86%)	193 (81%)	43 (18%)	2 (1%)	19 55
4	E	214/220 (97%)	174 (81%)	40 (19%)	0	100 100
5	F	201/207 (97%)	158 (79%)	43 (21%)	0	100 100
6	M	143/145 (99%)	119 (83%)	24 (17%)	0	100 100
7	N	120/122 (98%)	94 (78%)	26 (22%)	0	100 100
8	O	144/146 (99%)	121 (84%)	22 (15%)	1 (1%)	22 58
9	P	135/144 (94%)	118 (87%)	17 (13%)	0	100 100
10	Q	119/122 (98%)	97 (82%)	22 (18%)	0	100 100
11	R	110/119 (92%)	89 (81%)	21 (19%)	0	100 100
12	S	101/116 (87%)	89 (88%)	12 (12%)	0	100 100
13	T	114/118 (97%)	100 (88%)	14 (12%)	0	100 100
14	U	99/102 (97%)	86 (87%)	13 (13%)	0	100 100
15	V	108/117 (92%)	95 (88%)	13 (12%)	0	100 100
16	W	87/91 (96%)	70 (80%)	17 (20%)	0	100 100
17	X	92/105 (88%)	67 (73%)	25 (27%)	0	100 100
18	Y	50/217 (23%)	38 (76%)	12 (24%)	0	100 100
19	Z	76/94 (81%)	61 (80%)	15 (20%)	0	100 100
20	0	42/62 (68%)	27 (64%)	14 (33%)	1 (2%)	6 30
21	1	63/69 (91%)	57 (90%)	6 (10%)	0	100 100
22	2	55/59 (93%)	44 (80%)	11 (20%)	0	100 100
23	4	30/58 (52%)	26 (87%)	4 (13%)	0	100 100
24	6	42/45 (93%)	36 (86%)	6 (14%)	0	100 100
25	7	60/66 (91%)	46 (77%)	14 (23%)	0	100 100
26	9	110/117 (94%)	93 (84%)	17 (16%)	0	100 100
All	All	2553/2938 (87%)	2098 (82%)	451 (18%)	4 (0%)	50 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	149	LYS
20	0	33	LEU
8	O	65	GLY
3	D	147	PRO

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
3	D	196/224 (88%)	195 (100%)	1 (0%)	88 94
4	E	174/177 (98%)	173 (99%)	1 (1%)	86 93
5	F	163/169 (96%)	163 (100%)	0	100 100
6	M	123/123 (100%)	123 (100%)	0	100 100
7	N	100/100 (100%)	97 (97%)	3 (3%)	41 70
8	O	112/112 (100%)	111 (99%)	1 (1%)	78 89
9	P	114/119 (96%)	114 (100%)	0	100 100
10	Q	101/102 (99%)	101 (100%)	0	100 100
11	R	88/95 (93%)	87 (99%)	1 (1%)	73 87
12	S	92/102 (90%)	92 (100%)	0	100 100
13	T	96/98 (98%)	95 (99%)	1 (1%)	76 88
14	U	85/86 (99%)	84 (99%)	1 (1%)	71 86
15	V	89/94 (95%)	89 (100%)	0	100 100
16	W	80/82 (98%)	80 (100%)	0	100 100
17	X	81/90 (90%)	80 (99%)	1 (1%)	71 86
18	Y	52/190 (27%)	52 (100%)	0	100 100
19	Z	61/75 (81%)	61 (100%)	0	100 100
20	0	37/52 (71%)	37 (100%)	0	100 100
21	1	59/62 (95%)	59 (100%)	0	100 100
22	2	51/53 (96%)	51 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	4	32/51 (63%)	32 (100%)	0	100 100
24	6	39/40 (98%)	39 (100%)	0	100 100
25	7	53/57 (93%)	53 (100%)	0	100 100
26	9	98/102 (96%)	97 (99%)	1 (1%)	76 88
All	All	2176/2455 (89%)	2165 (100%)	11 (0%)	89 94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	275	LYS
4	E	138	ARG
7	N	45	ASN
7	N	71	ARG
7	N	72	ASN
8	O	71	ARG
11	R	14	ARG
13	T	92	ARG
14	U	21	PHE
17	X	8	ASN
26	9	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	85	ASN
3	D	152	GLN
4	E	76	HIS
5	F	188	ASN
7	N	4	GLN
7	N	45	ASN
10	Q	97	GLN
12	S	31	HIS
17	X	8	ASN
17	X	45	GLN
17	X	51	ASN
18	Y	88	HIS
20	0	23	ASN
20	0	34	GLN
21	1	27	ASN
26	9	63	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2573/2923 (88%)	849 (32%)	22 (0%)
2	B	110/115 (95%)	52 (47%)	2 (1%)
All	All	2683/3038 (88%)	901 (33%)	24 (0%)

All (901) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	U
1	A	22	C
1	A	28	A
1	A	34	U
1	A	46	C
1	A	49	A
1	A	50	U
1	A	51	G
1	A	52	A
1	A	56	A
1	A	58	G
1	A	59	U
1	A	61	A
1	A	64	A
1	A	68	A
1	A	70	G
1	A	71	A
1	A	72	U
1	A	74	U
1	A	75	G
1	A	81	G
1	A	85	G
1	A	87	U
1	A	90	A
1	A	92	G
1	A	95	A
1	A	97	C
1	A	99	U
1	A	100	U
1	A	101	G
1	A	115	C
1	A	117	A
1	A	118	A

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Mol	Chain	Res	Type
1	A	119	U
1	A	120	G
1	A	136	A
1	A	142	G
1	A	144	C
1	A	150	A
1	A	153	G
1	A	154	A
1	A	155	U
1	A	156	A
1	A	160	G
1	A	162	A
1	A	164	A
1	A	165	C
1	A	166	A
1	A	168	A
1	A	171	A
1	A	175	C
1	A	177	G
1	A	180	G
1	A	185	A
1	A	190	G
1	A	199	A
1	A	202	A
1	A	203	U
1	A	208	G
1	A	209	U
1	A	219	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	234	C
1	A	235	G
1	A	236	A
1	A	251	G
1	A	261	C
1	A	263	G
1	A	266	A
1	A	268	A
1	A	269	G
1	A	280	C
1	A	281	A

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Mol	Chain	Res	Type
1	A	284	C
1	A	285	U
1	A	286	U
1	A	292	U
1	A	299	U
1	A	301	U
1	A	303	G
1	A	307	A
1	A	308	C
1	A	311	U
1	A	314	A
1	A	316	G
1	A	317	G
1	A	318	A
1	A	319	G
1	A	320	U
1	A	322	A
1	A	323	C
1	A	325	A
1	A	326	A
1	A	327	G
1	A	330	C
1	A	333	C
1	A	337	A
1	A	338	G
1	A	341	G
1	A	342	A
1	A	355	G
1	A	359	A
1	A	365	A
1	A	367	A
1	A	371	U
1	A	373	A
1	A	374	U
1	A	378	C
1	A	384	G
1	A	390	A
1	A	391	A
1	A	395	U
1	A	397	U
1	A	400	C
1	A	401	U

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Mol	Chain	Res	Type
1	A	402	C
1	A	403	U
1	A	404	U
1	A	405	G
1	A	406	A
1	A	407	G
1	A	408	U
1	A	410	G
1	A	411	A
1	A	412	U
1	A	413	C
1	A	417	A
1	A	418	G
1	A	419	U
1	A	423	A
1	A	425	G
1	A	427	A
1	A	432	G
1	A	433	U
1	A	435	A
1	A	436	A
1	A	437	A
1	A	438	U
1	A	440	C
1	A	442	G
1	A	444	C
1	A	445	G
1	A	452	G
1	A	453	G
1	A	455	A
1	A	457	G
1	A	458	A
1	A	459	C
1	A	461	A
1	A	464	U
1	A	475	A
1	A	488	G
1	A	499	A
1	A	506	A
1	A	509	G
1	A	513	G
1	A	514	G

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Mol	Chain	Res	Type
1	A	515	G
1	A	519	G
1	A	525	A
1	A	526	A
1	A	527	G
1	A	536	A
1	A	537	A
1	A	539	G
1	A	543	G
1	A	546	A
1	A	547	A
1	A	549	U
1	A	550	A
1	A	551	G
1	A	552	A
1	A	553	A
1	A	554	C
1	A	556	U
1	A	567	G
1	A	575	G
1	A	576	U
1	A	577	A
1	A	578	G
1	A	583	A
1	A	584	G
1	A	588	G
1	A	590	U
1	A	593	U
1	A	594	G
1	A	604	G
1	A	606	G
1	A	609	U
1	A	615	A
1	A	616	G
1	A	618	A
1	A	620	G
1	A	629	A
1	A	630	G
1	A	634	C
1	A	638	U
1	A	646	A
1	A	650	U

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Mol	Chain	Res	Type
1	A	651	A
1	A	652	A
1	A	653	G
1	A	656	G
1	A	658	A
1	A	659	A
1	A	660	A
1	A	661	U
1	A	662	G
1	A	675	G
1	A	679	G
1	A	682	A
1	A	683	G
1	A	684	U
1	A	691	A
1	A	694	G
1	A	698	U
1	A	699	U
1	A	700	A
1	A	701	G
1	A	704	U
1	A	705	U
1	A	706	U
1	A	710	C
1	A	715	A
1	A	724	C
1	A	729	G
1	A	731	U
1	A	743	C
1	A	744	A
1	A	748	U
1	A	749	G
1	A	752	G
1	A	754	U
1	A	766	G
1	A	771	G
1	A	772	A
1	A	775	A
1	A	778	G
1	A	790	G
1	A	792	U
1	A	793	G

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Mol	Chain	Res	Type
1	A	794	A
1	A	795	A
1	A	797	A
1	A	807	U
1	A	809	A
1	A	812	U
1	A	820	G
1	A	821	C
1	A	824	A
1	A	827	A
1	A	829	U
1	A	830	U
1	A	834	A
1	A	835	U
1	A	838	A
1	A	839	A
1	A	842	U
1	A	844	G
1	A	850	G
1	A	851	C
1	A	852	U
1	A	854	G
1	A	857	C
1	A	870	C
1	A	871	U
1	A	872	U
1	A	873	U
1	A	880	A
1	A	885	C
1	A	890	G
1	A	891	A
1	A	896	U
1	A	900	G
1	A	904	G
1	A	906	A
1	A	907	G
1	A	909	G
1	A	910	C
1	A	911	A
1	A	914	G
1	A	919	G
1	A	920	A

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Mol	Chain	Res	Type
1	A	922	G
1	A	925	G
1	A	926	G
1	A	927	G
1	A	928	C
1	A	929	C
1	A	938	G
1	A	942	C
1	A	948	U
1	A	949	C
1	A	950	A
1	A	956	A
1	A	957	C
1	A	959	C
1	A	965	G
1	A	966	C
1	A	970	U
1	A	971	U
1	A	977	A
1	A	989	A
1	A	990	G
1	A	1000	G
1	A	1001	A
1	A	1002	U
1	A	1003	A
1	A	1005	G
1	A	1006	G
1	A	1015	C
1	A	1018	A
1	A	1020	G
1	A	1024	A
1	A	1025	A
1	A	1028	G
1	A	1030	C
1	A	1040	A
1	A	1041	G
1	A	1042	C
1	A	1045	A
1	A	1049	C
1	A	1055	A
1	A	1056	U
1	A	1057	A

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Mol	Chain	Res	Type
1	A	1059	A
1	A	1060	U
1	A	1065	A
1	A	1066	G
1	A	1067	U
1	A	1068	G
1	A	1070	A
1	A	1071	A
1	A	1074	G
1	A	1077	U
1	A	1081	G
1	A	1085	U
1	A	1088	C
1	A	1157	U
1	A	1158	G
1	A	1159	A
1	A	1162	C
1	A	1163	U
1	A	1168	C
1	A	1178	C
1	A	1179	C
1	A	1181	G
1	A	1185	U
1	A	1186	A
1	A	1191	U
1	A	1193	U
1	A	1203	U
1	A	1205	U
1	A	1215	U
1	A	1216	U
1	A	1217	U
1	A	1225	G
1	A	1226	G
1	A	1230	G
1	A	1236	G
1	A	1252	A
1	A	1257	G
1	A	1258	A
1	A	1269	A
1	A	1276	G
1	A	1288	G
1	A	1291	A

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Mol	Chain	Res	Type
1	A	1292	A
1	A	1293	U
1	A	1294	G
1	A	1295	C
1	A	1301	U
1	A	1306	A
1	A	1309	G
1	A	1310	A
1	A	1311	A
1	A	1312	A
1	A	1318	G
1	A	1320	G
1	A	1323	A
1	A	1330	U
1	A	1331	C
1	A	1337	A
1	A	1338	U
1	A	1340	G
1	A	1349	U
1	A	1355	A
1	A	1358	A
1	A	1362	C
1	A	1366	U
1	A	1367	C
1	A	1369	G
1	A	1370	C
1	A	1376	G
1	A	1377	U
1	A	1391	A
1	A	1392	G
1	A	1395	G
1	A	1396	A
1	A	1399	C
1	A	1401	G
1	A	1402	A
1	A	1405	G
1	A	1406	G
1	A	1407	C
1	A	1416	U
1	A	1418	G
1	A	1419	A
1	A	1422	A

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Mol	Chain	Res	Type
1	A	1423	C
1	A	1427	U
1	A	1428	U
1	A	1432	A
1	A	1433	U
1	A	1435	C
1	A	1437	U
1	A	1443	A
1	A	1447	A
1	A	1453	G
1	A	1454	U
1	A	1455	U
1	A	1456	U
1	A	1457	U
1	A	1458	A
1	A	1460	U
1	A	1461	C
1	A	1462	G
1	A	1465	G
1	A	1471	A
1	A	1472	C
1	A	1473	G
1	A	1474	C
1	A	1476	G
1	A	1478	A
1	A	1479	G
1	A	1480	G
1	A	1481	A
1	A	1482	U
1	A	1483	A
1	A	1486	C
1	A	1488	A
1	A	1489	A
1	A	1490	G
1	A	1491	C
1	A	1492	G
1	A	1494	G
1	A	1495	C
1	A	1496	G
1	A	1497	A
1	A	1498	U
1	A	1499	U

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Mol	Chain	Res	Type
1	A	1504	U
1	A	1596	G
1	A	1599	G
1	A	1601	U
1	A	1603	U
1	A	1604	C
1	A	1606	C
1	A	1607	A
1	A	1609	U
1	A	1610	G
1	A	1613	G
1	A	1614	A
1	A	1616	A
1	A	1618	A
1	A	1619	A
1	A	1621	C
1	A	1622	C
1	A	1625	U
1	A	1626	A
1	A	1627	G
1	A	1629	U
1	A	1630	A
1	A	1631	G
1	A	1633	A
1	A	1634	A
1	A	1635	A
1	A	1636	U
1	A	1638	G
1	A	1639	G
1	A	1644	C
1	A	1645	G
1	A	1652	A
1	A	1656	C
1	A	1660	A
1	A	1662	A
1	A	1663	G
1	A	1667	G
1	A	1677	G
1	A	1678	A
1	A	1683	U
1	A	1687	G
1	A	1688	U

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Mol	Chain	Res	Type
1	A	1690	A
1	A	1691	G
1	A	1692	C
1	A	1696	C
1	A	1700	C
1	A	1707	U
1	A	1712	A
1	A	1715	U
1	A	1718	G
1	A	1719	C
1	A	1725	G
1	A	1726	A
1	A	1728	C
1	A	1731	G
1	A	1735	C
1	A	1738	C
1	A	1739	G
1	A	1742	A
1	A	1744	A
1	A	1747	G
1	A	1751	G
1	A	1754	C
1	A	1757	U
1	A	1758	A
1	A	1759	G
1	A	1761	G
1	A	1763	U
1	A	1765	A
1	A	1766	C
1	A	1767	G
1	A	1768	C
1	A	1769	C
1	A	1771	A
1	A	1772	G
1	A	1779	C
1	A	1782	A
1	A	1783	G
1	A	1785	G
1	A	1788	U
1	A	1790	G
1	A	1791	G
1	A	1800	A

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Mol	Chain	Res	Type
1	A	1804	U
1	A	1808	U
1	A	1819	G
1	A	1820	G
1	A	1827	C
1	A	1842	A
1	A	1846	A
1	A	1847	U
1	A	1848	A
1	A	1849	G
1	A	1851	G
1	A	1854	U
1	A	1855	G
1	A	1856	A
1	A	1860	C
1	A	1863	C
1	A	1866	G
1	A	1869	G
1	A	1924	G
1	A	1926	A
1	A	1928	A
1	A	1929	C
1	A	1931	G
1	A	1932	C
1	A	1955	A
1	A	1957	G
1	A	1958	U
1	A	1959	A
1	A	1963	A
1	A	1964	A
1	A	1965	A
1	A	1967	U
1	A	1968	C
1	A	1970	U
1	A	1971	U
1	A	1972	G
1	A	1973	U
1	A	1981	G
1	A	1982	U
1	A	1983	U
1	A	1987	A
1	A	1989	C

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Mol	Chain	Res	Type
1	A	1990	C
1	A	1991	G
1	A	1992	C
1	A	1995	G
1	A	1997	A
1	A	1998	A
1	A	1999	G
1	A	2001	C
1	A	2006	C
1	A	2009	U
1	A	2018	U
1	A	2019	G
1	A	2020	U
1	A	2024	A
1	A	2026	C
1	A	2031	G
1	A	2033	C
1	A	2042	A
1	A	2051	C
1	A	2054	G
1	A	2059	G
1	A	2061	U
1	A	2070	C
1	A	2071	C
1	A	2078	A
1	A	2079	G
1	A	2081	A
1	A	2082	C
1	A	2083	G
1	A	2087	A
1	A	2088	G
1	A	2089	A
1	A	2096	G
1	A	2097	G
1	A	2099	G
1	A	2102	U
1	A	2105	C
1	A	2118	U
1	A	2120	G
1	A	2126	C
1	A	2129	C
1	A	2211	U

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Mol	Chain	Res	Type
1	A	2212	G
1	A	2217	G
1	A	2218	G
1	A	2222	U
1	A	2225	A
1	A	2227	C
1	A	2231	C
1	A	2237	U
1	A	2251	G
1	A	2252	A
1	A	2253	C
1	A	2265	G
1	A	2266	G
1	A	2278	G
1	A	2280	G
1	A	2283	G
1	A	2295	A
1	A	2309	G
1	A	2310	C
1	A	2311	U
1	A	2316	G
1	A	2317	G
1	A	2320	C
1	A	2323	U
1	A	2324	C
1	A	2327	A
1	A	2328	A
1	A	2329	U
1	A	2331	G
1	A	2332	U
1	A	2333	U
1	A	2334	G
1	A	2335	G
1	A	2336	A
1	A	2337	A
1	A	2339	U
1	A	2341	A
1	A	2344	C
1	A	2345	A
1	A	2346	U
1	A	2347	A
1	A	2350	G

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Mol	Chain	Res	Type
1	A	2352	G
1	A	2355	A
1	A	2361	U
1	A	2362	A
1	A	2364	G
1	A	2367	A
1	A	2370	U
1	A	2372	G
1	A	2374	C
1	A	2383	C
1	A	2386	C
1	A	2397	G
1	A	2398	G
1	A	2399	G
1	A	2402	G
1	A	2403	A
1	A	2404	A
1	A	2406	G
1	A	2407	A
1	A	2409	G
1	A	2410	G
1	A	2412	C
1	A	2417	U
1	A	2421	C
1	A	2422	C
1	A	2425	U
1	A	2426	G
1	A	2429	U
1	A	2430	C
1	A	2434	A
1	A	2437	G
1	A	2439	A
1	A	2448	G
1	A	2449	C
1	A	2452	A
1	A	2455	G
1	A	2456	G
1	A	2457	A
1	A	2459	A
1	A	2460	A
1	A	2461	A
1	A	2462	A

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Mol	Chain	Res	Type
1	A	2463	G
1	A	2466	A
1	A	2467	C
1	A	2468	C
1	A	2475	A
1	A	2482	G
1	A	2487	U
1	A	2490	C
1	A	2497	G
1	A	2501	U
1	A	2502	C
1	A	2503	A
1	A	2505	A
1	A	2507	C
1	A	2508	G
1	A	2509	A
1	A	2514	G
1	A	2518	U
1	A	2529	G
1	A	2532	G
1	A	2533	U
1	A	2534	C
1	A	2535	G
1	A	2536	G
1	A	2539	C
1	A	2540	A
1	A	2545	A
1	A	2547	C
1	A	2549	U
1	A	2552	G
1	A	2553	G
1	A	2557	U
1	A	2558	A
1	A	2559	G
1	A	2560	U
1	A	2561	C
1	A	2562	G
1	A	2563	G
1	A	2570	G
1	A	2573	U
1	A	2574	U
1	A	2575	G

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Mol	Chain	Res	Type
1	A	2576	G
1	A	2579	U
1	A	2581	U
1	A	2582	U
1	A	2583	C
1	A	2593	A
1	A	2594	G
1	A	2599	A
1	A	2600	C
1	A	2603	G
1	A	2609	G
1	A	2612	U
1	A	2613	C
1	A	2620	U
1	A	2621	C
1	A	2624	G
1	A	2626	G
1	A	2627	A
1	A	2628	C
1	A	2629	A
1	A	2630	G
1	A	2636	U
1	A	2637	C
1	A	2640	U
1	A	2642	U
1	A	2651	G
1	A	2657	G
1	A	2667	G
1	A	2669	G
1	A	2673	C
1	A	2674	U
1	A	2679	U
1	A	2681	A
1	A	2682	G
1	A	2686	G
1	A	2688	G
1	A	2689	A
1	A	2690	G
1	A	2691	G
1	A	2705	U
1	A	2706	A
1	A	2707	C

Continued on next page...

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Mol	Chain	Res	Type
1	A	2714	U
1	A	2716	U
1	A	2720	A
1	A	2722	U
1	A	2726	C
1	A	2728	U
1	A	2729	G
1	A	2730	C
1	A	2731	C
1	A	2733	A
1	A	2734	C
1	A	2735	G
1	A	2739	U
1	A	2741	G
1	A	2742	C
1	A	2745	G
1	A	2749	G
1	A	2753	U
1	A	2754	G
1	A	2760	A
1	A	2765	A
1	A	2770	U
1	A	2771	G
1	A	2773	U
1	A	2776	A
1	A	2777	A
1	A	2778	G
1	A	2782	C
1	A	2786	G
1	A	2792	A
1	A	2793	G
1	A	2795	C
1	A	2797	C
1	A	2798	C
1	A	2802	A
1	A	2805	A
1	A	2806	U
1	A	2807	G
1	A	2817	A
1	A	2818	A
1	A	2836	C
1	A	2838	C

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Mol	Chain	Res	Type
1	A	2840	A
1	A	2841	A
1	A	2843	A
1	A	2854	A
1	A	2855	A
1	A	2856	U
1	A	2876	G
1	A	2881	C
1	A	2887	G
1	A	2888	A
1	A	2892	G
1	A	2903	A
1	A	2904	U
1	A	2906	G
1	A	2909	C
1	A	2912	A
1	A	2916	U
2	B	3	U
2	B	5	G
2	B	6	U
2	B	9	C
2	B	10	U
2	B	11	A
2	B	12	U
2	B	13	A
2	B	14	G
2	B	16	A
2	B	18	G
2	B	20	A
2	B	23	U
2	B	24	C
2	B	25	A
2	B	26	C
2	B	29	C
2	B	33	U
2	B	35	C
2	B	38	U
2	B	39	G
2	B	40	C
2	B	46	A
2	B	47	C
2	B	49	G

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Mol	Chain	Res	Type
2	B	51	A
2	B	52	G
2	B	53	U
2	B	54	U
2	B	55	A
2	B	59	U
2	B	64	A
2	B	65	G
2	B	66	C
2	B	69	C
2	B	70	G
2	B	74	G
2	B	86	A
2	B	87	C
2	B	88	G
2	B	90	U
2	B	91	C
2	B	95	U
2	B	97	G
2	B	102	G
2	B	103	A
2	B	105	C
2	B	106	G
2	B	107	U
2	B	108	U
2	B	109	G
2	B	112	A

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	99	U
1	A	411	A
1	A	457	G
1	A	548	A
1	A	661	U
1	A	700	A
1	A	909	G
1	A	1224	U
1	A	1491	C
1	A	1608	C
1	A	1750	U

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Mol	Chain	Res	Type
1	A	1760	G
1	A	1988	C
1	A	1989	C
1	A	1997	A
1	A	2221	U
1	A	2458	U
1	A	2459	A
1	A	2507	C
1	A	2560	U
1	A	2730	C
1	A	2887	G
2	B	4	G
2	B	19	G

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 59 ligands modelled in this entry, 59 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

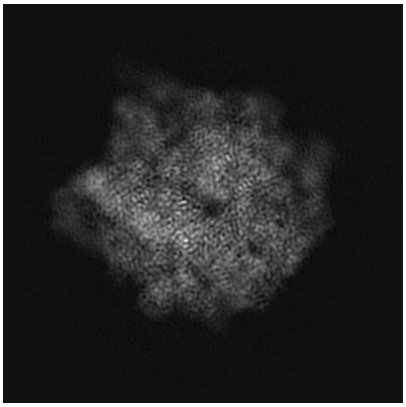
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10212. These allow visual inspection of the internal detail of the map and identification of artifacts.

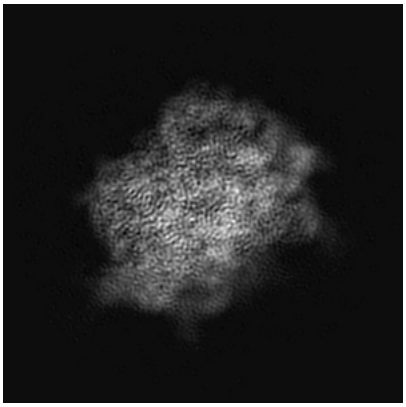
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

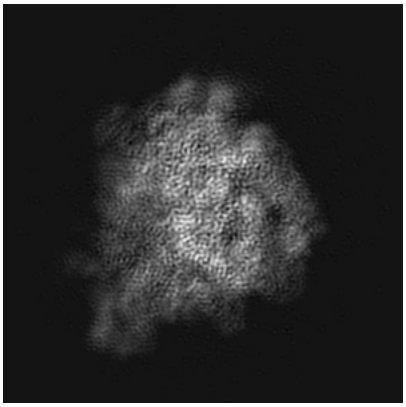
6.1.1 Primary map



X



Y

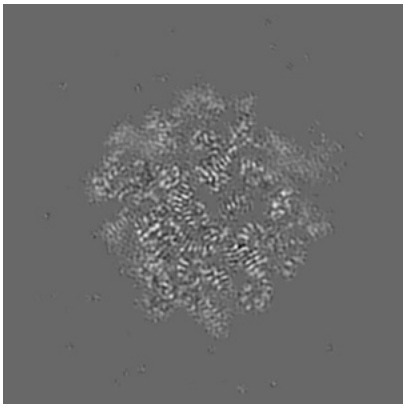


Z

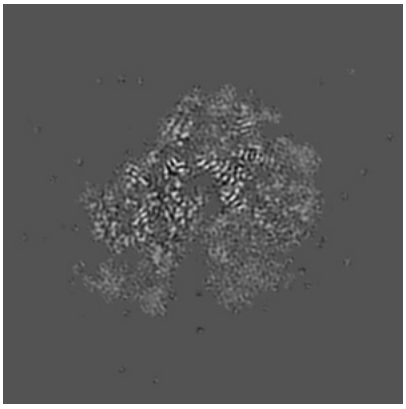
The images above show the map projected in three orthogonal directions.

6.2 Central slices

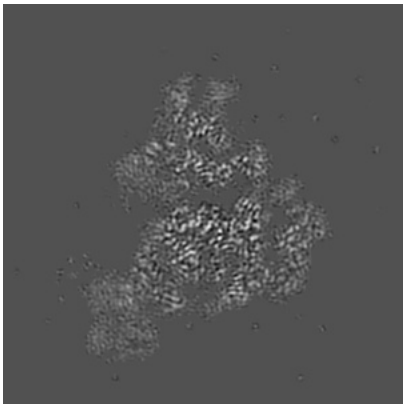
6.2.1 Primary map



X Index: 175



Y Index: 175

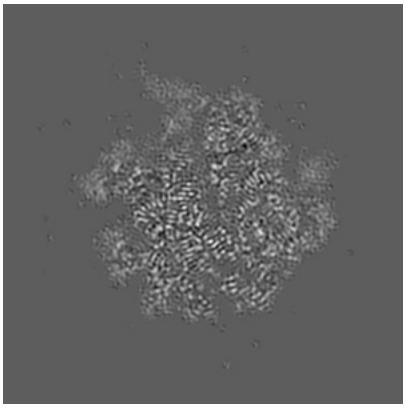


Z Index: 175

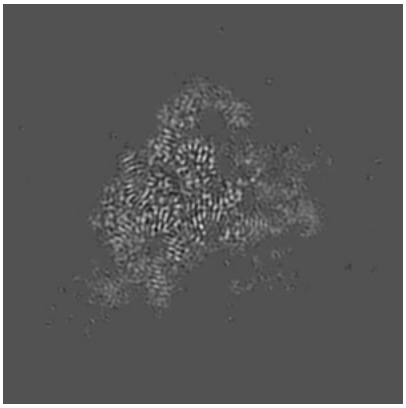
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

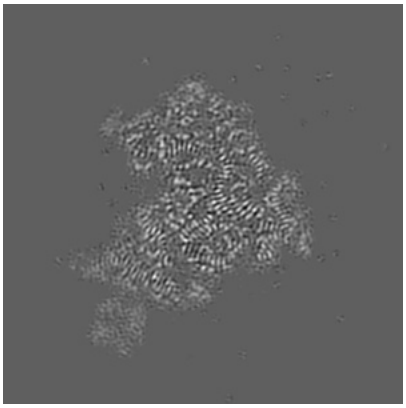
6.3.1 Primary map



X Index: 162



Y Index: 159

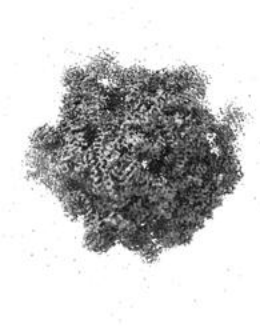


Z Index: 150

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 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

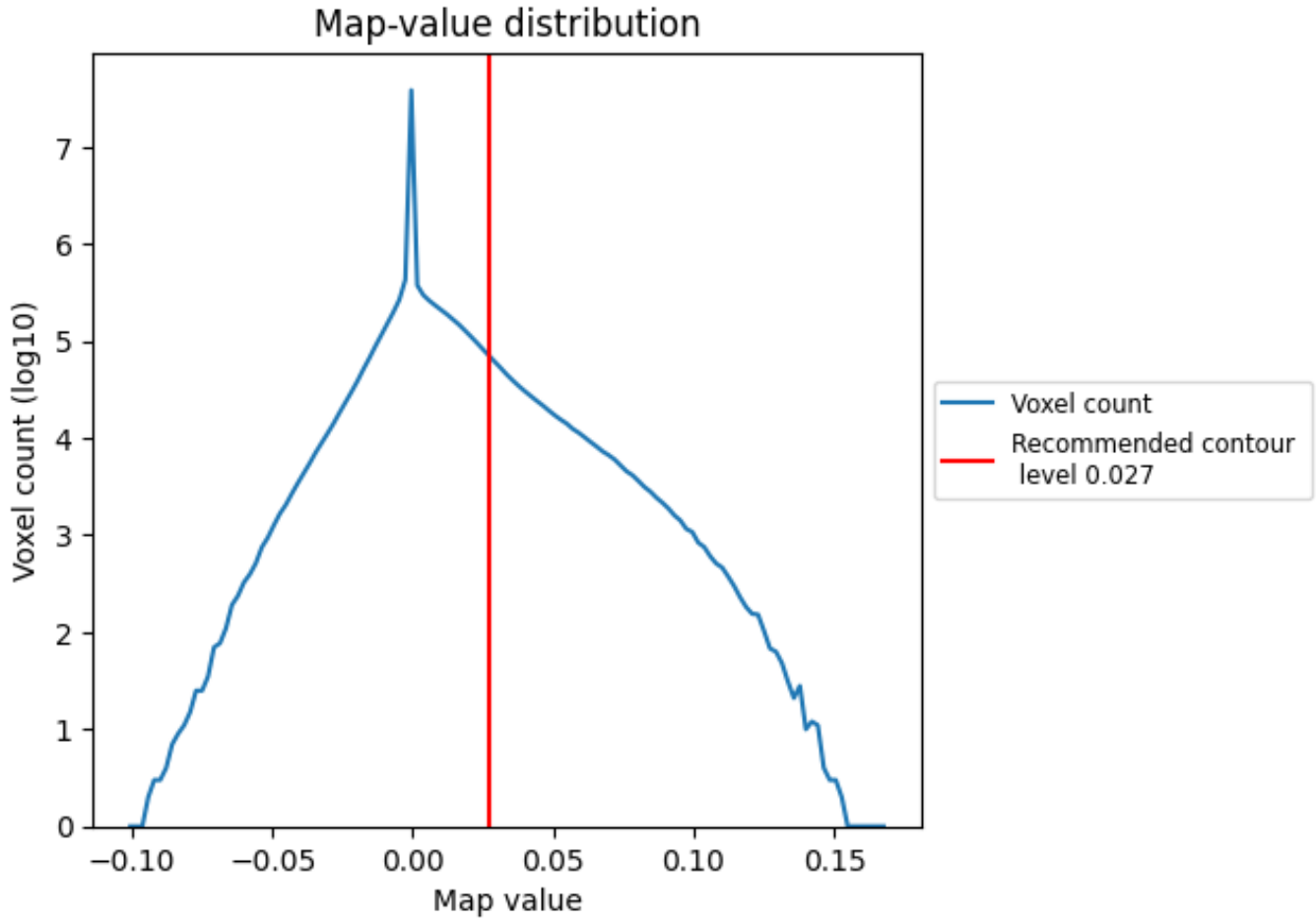
6.5 Mask visualisation (i)

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

7 Map analysis

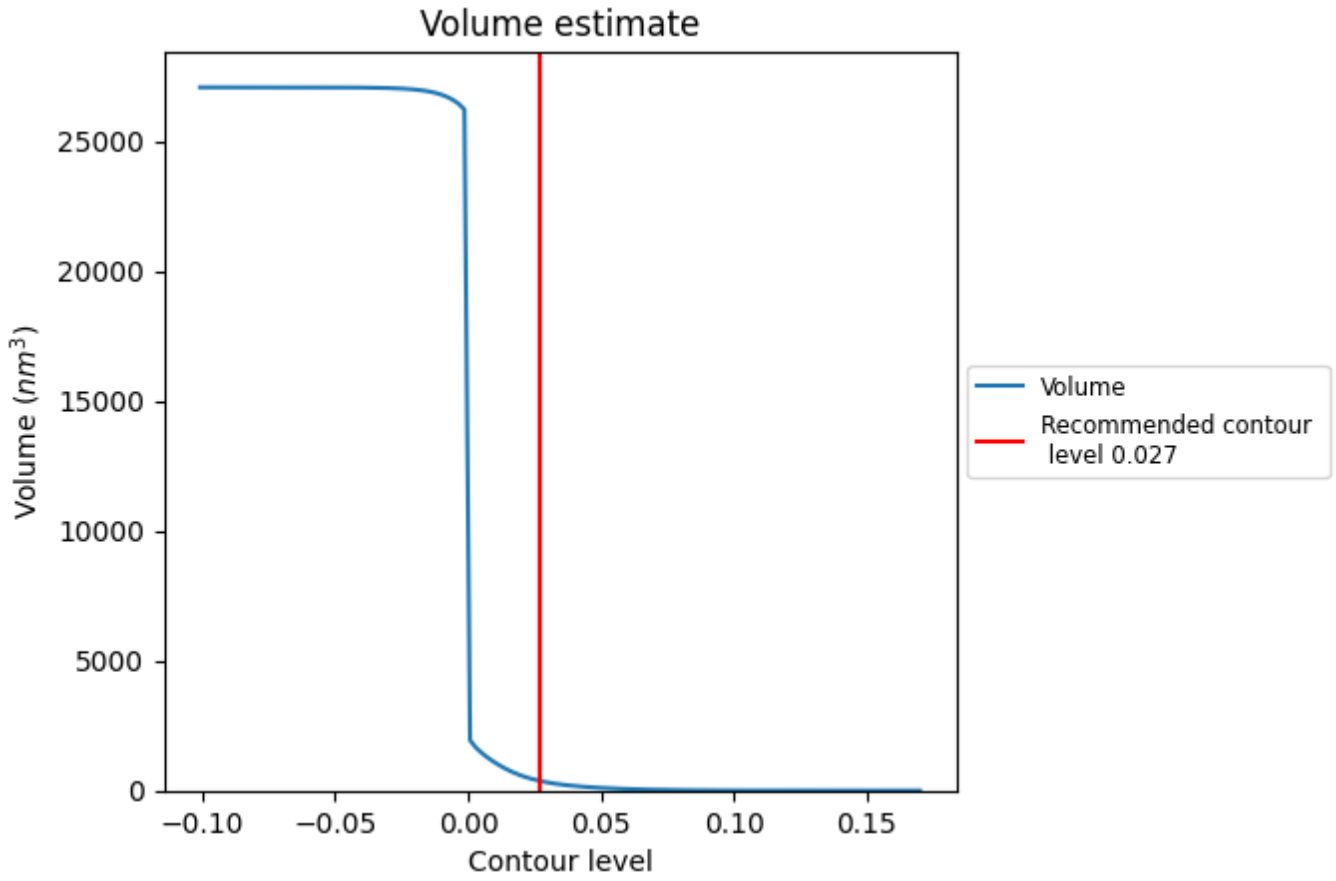
This section contains the results of statistical analysis of the map.

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.

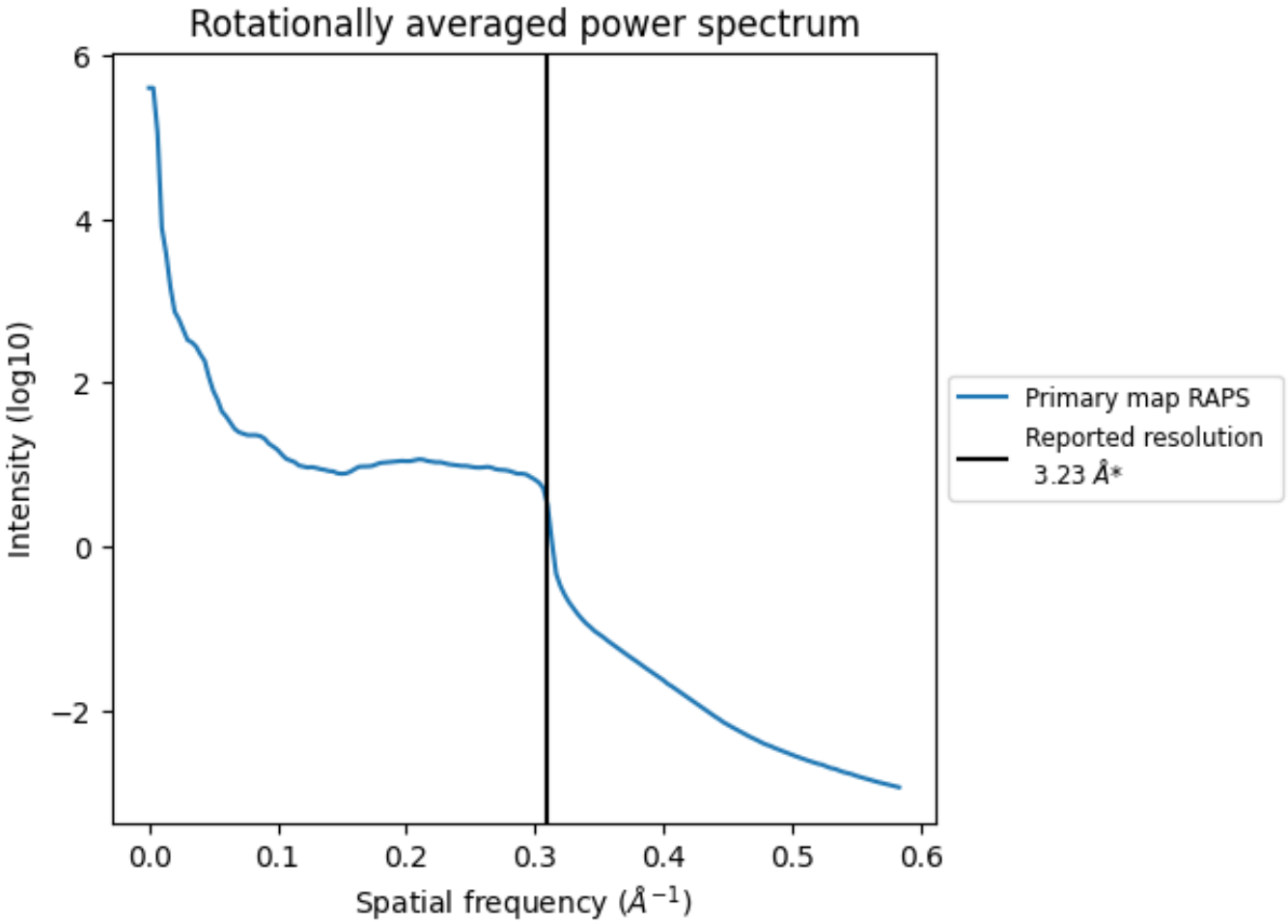
7.2 Volume estimate (i)



The volume at the recommended contour level is 372 nm^3; this corresponds to an approximate mass of 336 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)

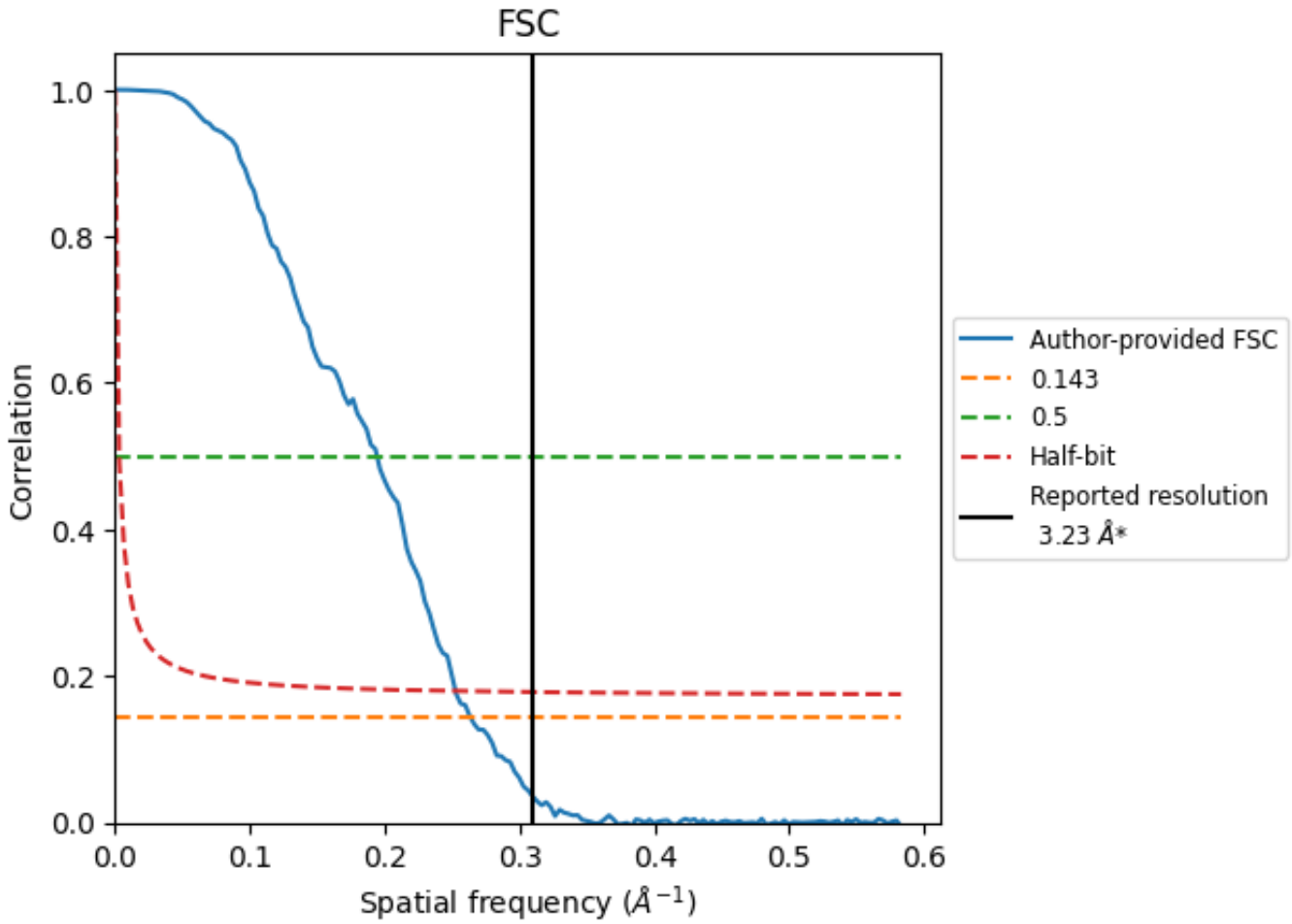


*Reported resolution corresponds to spatial frequency of 0.310 Å^{-1}

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 0.310 Å^{-1}

8.2 Resolution estimates (i)

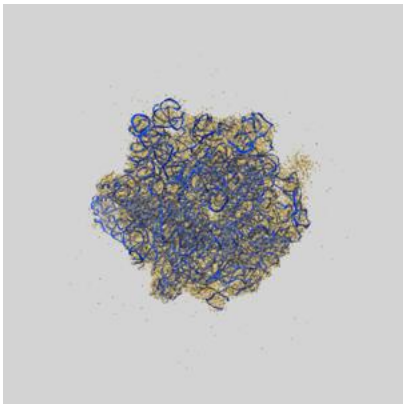
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.79	5.15	3.96
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 3.23 by more than 10 %

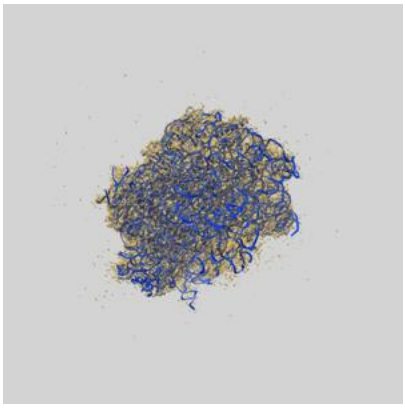
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10212 and PDB model 6SJ6. Per-residue inclusion information can be found in section 3 on page 9.

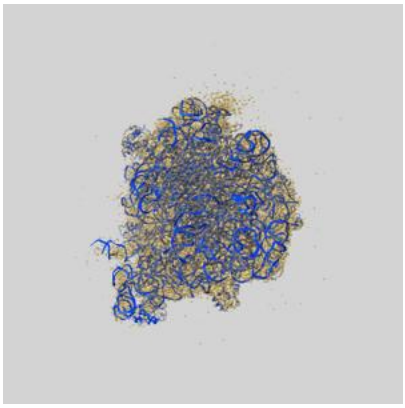
9.1 Map-model overlay



X



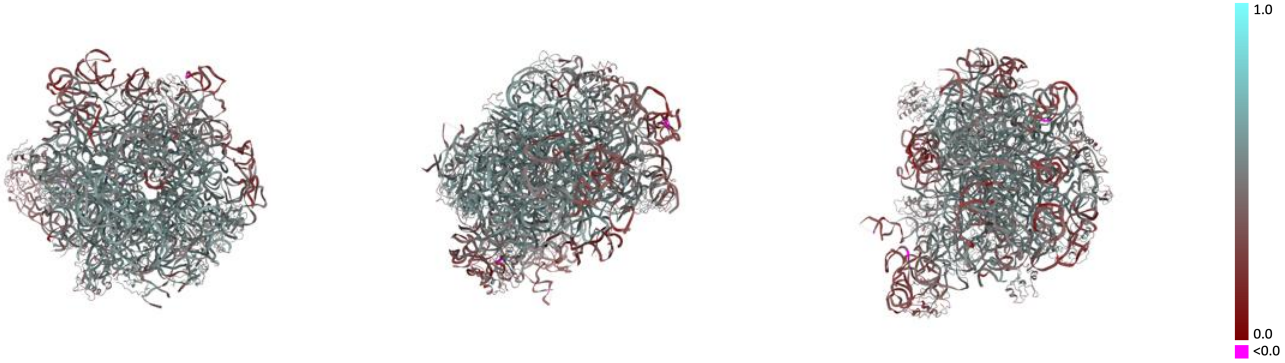
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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.

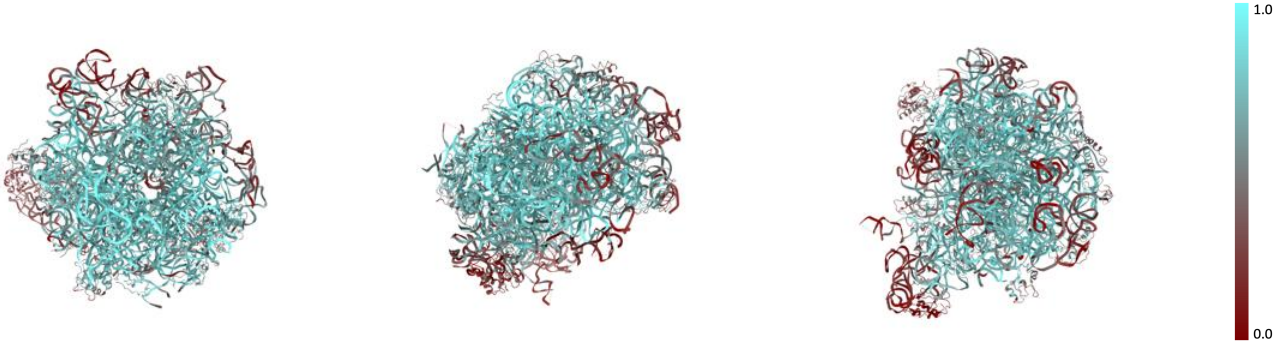
9.2 Q-score mapped to coordinate model (i)



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.

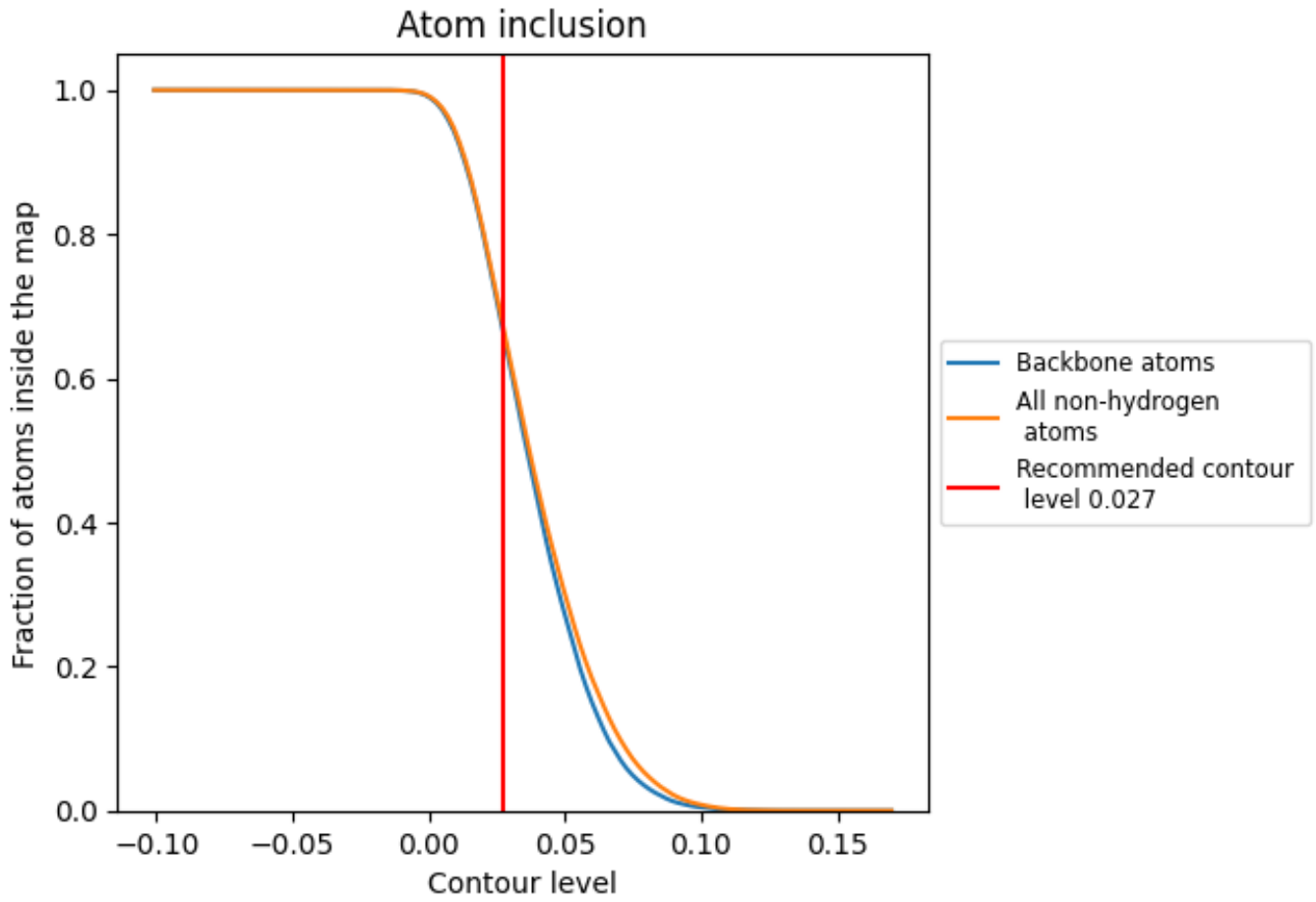
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 68% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6782	0.4800
0	0.2419	0.3870
1	0.4712	0.4250
2	0.6651	0.4880
4	0.5803	0.4890
6	0.8068	0.5580
7	0.6639	0.4940
9	0.2177	0.3740
A	0.7309	0.4890
B	0.2563	0.3010
D	0.6236	0.4790
E	0.7024	0.5320
F	0.6720	0.5150
M	0.6741	0.5140
N	0.6276	0.4980
O	0.6255	0.4950
P	0.5433	0.4570
Q	0.6804	0.5080
R	0.0723	0.2740
S	0.6000	0.4910
T	0.7429	0.5270
U	0.6688	0.5030
V	0.7445	0.5370
W	0.6040	0.4740
X	0.4966	0.4400
Y	0.0887	0.2920
Z	0.6505	0.4930