Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 05:38 pm BST

PDB ID	:	8S1U
EMDB ID	:	EMD-19641
Title	:	YlmH bound to stalled 50S subunits with RqcH and PtRNA
Authors	:	Paternoga, H.; Wilson, D.N.
Deposited on	:	2024-02-16
Resolution	:	3.40 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:

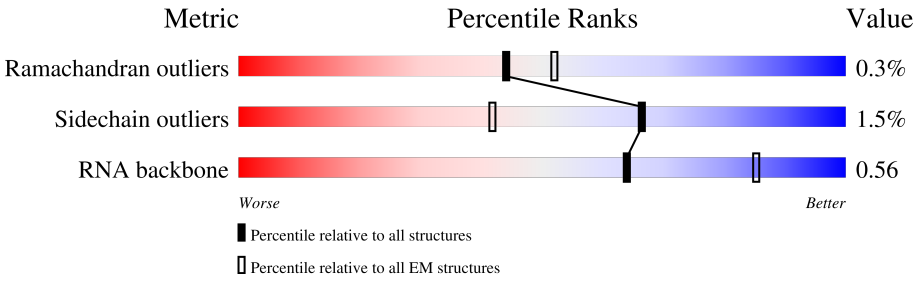
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	76	74% 50% 39% · 9%
1	c	76	87% 54% 33% 13%
2	0	59	27% 88% · 10%
3	1	49	27% 96% ·
4	2	44	· 100%
5	3	66	26% 95% · ·
6	4	37	38% 100%
7	6	66	70% 68% · 30%

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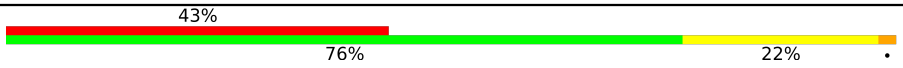
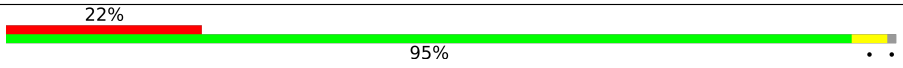
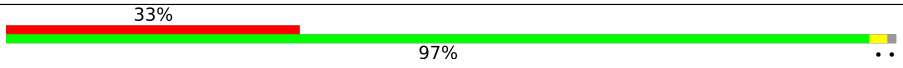
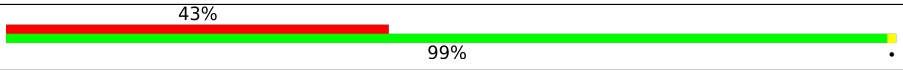
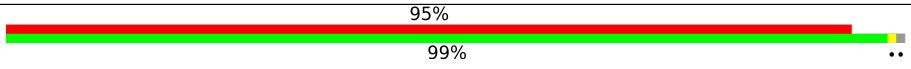
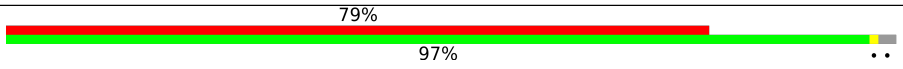
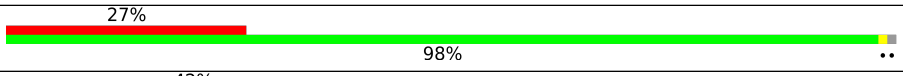
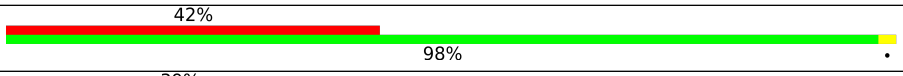
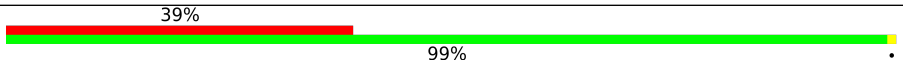
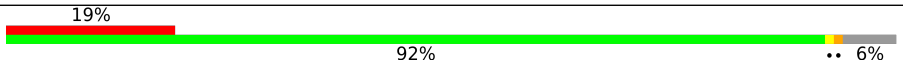
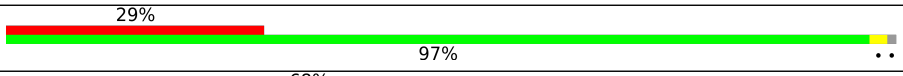
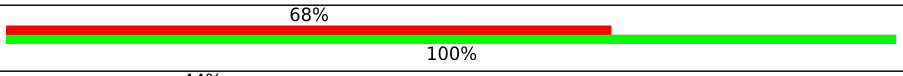
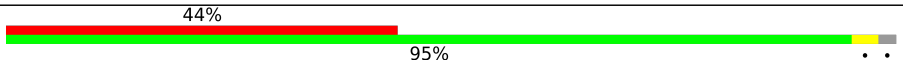
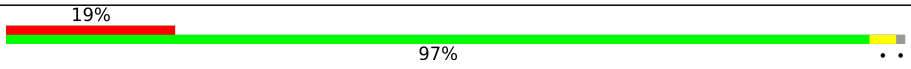
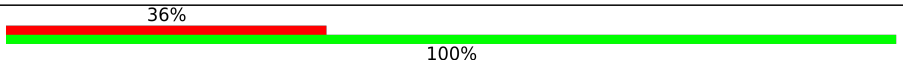
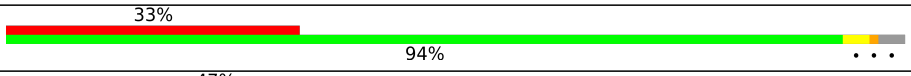
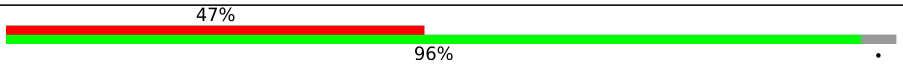
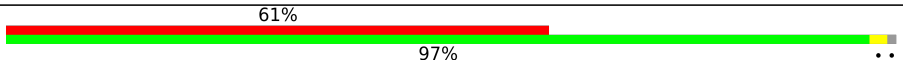
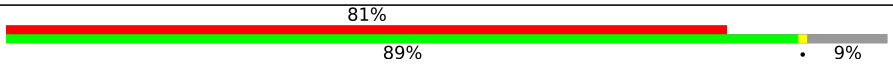
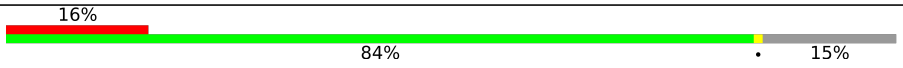
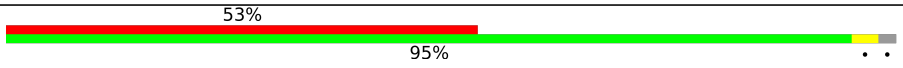
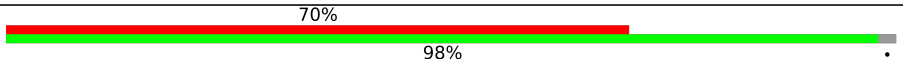
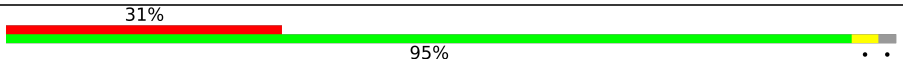
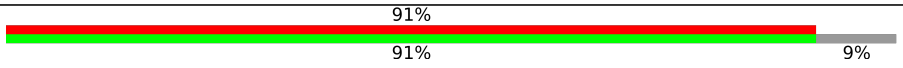
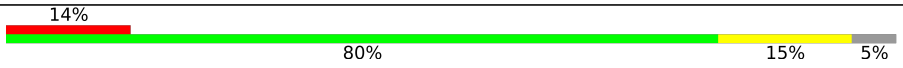
Mol	Chain	Length	Quality of chain
8	B	112	
9	C	277	
10	D	209	
11	E	207	
12	F	179	
13	G	179	
14	J	145	
15	K	122	
16	L	146	
17	M	144	
18	N	120	
19	O	120	
20	P	115	
21	Q	119	
22	R	102	
23	S	113	
24	T	95	
25	U	103	
26	V	275	
27	W	94	
28	X	62	
29	Y	66	
30	Z	59	
31	H	570	
32	A	2928	

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 93269 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 P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	66	Total	C	N	O	P	0	0
			1413	628	254	465	66		
1	a	69	Total	C	N	O	P	0	0
			1477	657	268	483	69		

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 3 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	49	Total	C	N	O	S	0	0
			411	250	82	75	4		

- Molecule 4 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 5 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 6 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	46	Total	C	N	O	S	0	0
			356	222	63	66	5		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	273	Total	C	N	O	S	0	0
			2094	1302	412	374	6		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	178	Total	C	N	O	S	0	0
			1405	893	245	260	7		

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	143	Total	C	N	O	S	0	0
			1131	714	207	205	5		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	113	Total	C	N	O	S	0	0
			922	588	177	156	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	118	Total	C	N	O	S	0	0
			950	597	191	158	4		

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	102	Total	C	N	O	S	0	0
			795	506	140	148	1		

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	110	Total	C	N	O	S	0	0
			850	530	165	151	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	91	Total	C	N	O	S	0	0
			733	458	135	137	3		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	102	Total	C	N	O	S	0	0
			770	482	143	141	4		

- Molecule 26 is a protein called Putative RNA-binding protein YlmH.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	249	Total	C	N	O	S	0	0
			1988	1256	350	376	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	258	GLY	-	expression tag	UNP P71020
V	259	SER	-	expression tag	UNP P71020
V	260	GLY	-	expression tag	UNP P71020
V	261	SER	-	expression tag	UNP P71020
V	262	GLY	-	expression tag	UNP P71020
V	263	SER	-	expression tag	UNP P71020
V	264	GLY	-	expression tag	UNP P71020
V	265	SER	-	expression tag	UNP P71020
V	266	GLY	-	expression tag	UNP P71020
V	267	SER	-	expression tag	UNP P71020
V	268	ASP	-	expression tag	UNP P71020
V	269	TYR	-	expression tag	UNP P71020
V	270	LYS	-	expression tag	UNP P71020
V	271	ASP	-	expression tag	UNP P71020
V	272	ASP	-	expression tag	UNP P71020
V	273	ASP	-	expression tag	UNP P71020
V	274	ASP	-	expression tag	UNP P71020
V	275	LYS	-	expression tag	UNP P71020

- Molecule 27 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	W	80	Total	C	N	O	0	0
			611	378	119	114		

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	61	Total	C	N	O	S	0	0
			468	289	98	79	2		

- Molecule 29 is a protein called 50S ribosomal protein L29.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 31 is a protein called Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	H	518	Total	C	N	O	0	0
			2567	1530	518	519		

- Molecule 32 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A	2789	Total	C	N	O	P	0	0
			59910	26733	11076	19313	2788		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

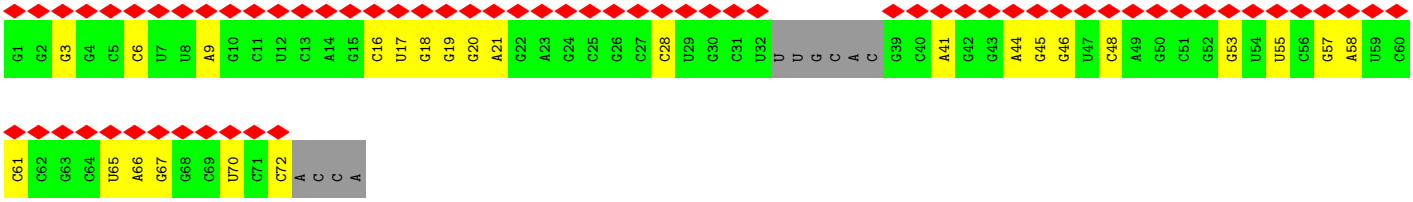
Mol	Chain	Residues	Atoms		AltConf
33	A	15	Total	K	0
			15	15	

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.

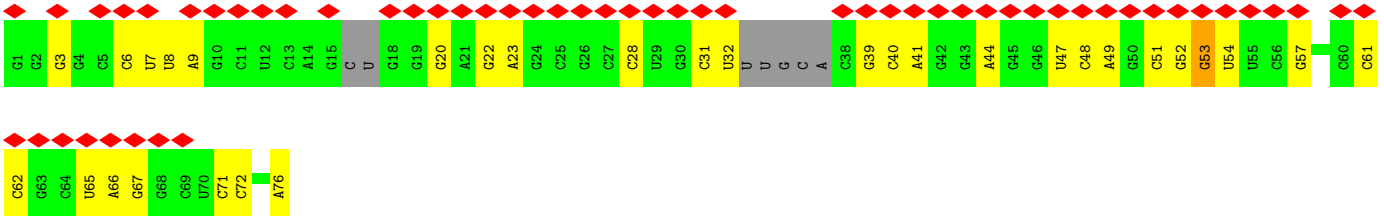
• Molecule 1: P-tRNA

Chain c:



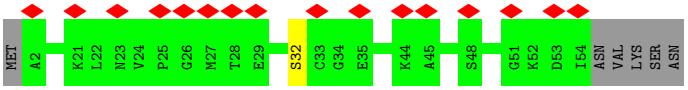
• Molecule 1: P-tRNA

Chain a:



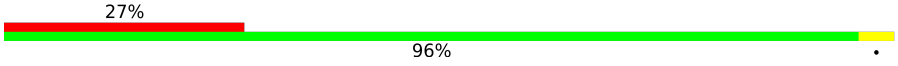
• Molecule 2: 50S ribosomal protein L32

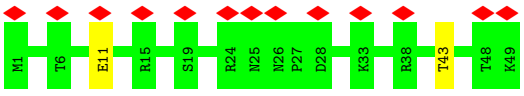
Chain 0:



• Molecule 3: 50S ribosomal protein L33 1

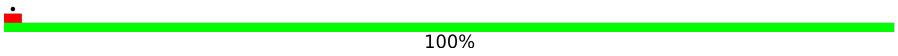
Chain 1:





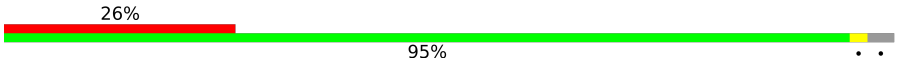
• Molecule 4: 50S ribosomal protein L34

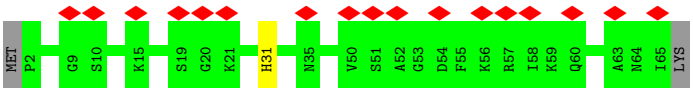
Chain 2:



• Molecule 5: 50S ribosomal protein L35

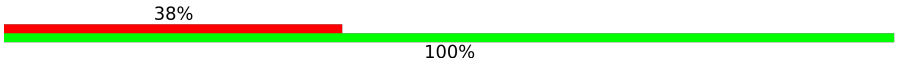
Chain 3:

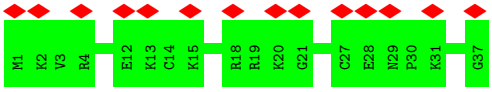




• Molecule 6: 50S ribosomal protein L36

Chain 4:



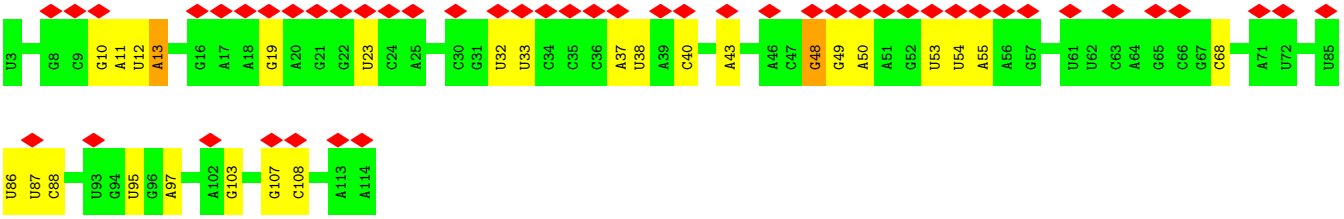


• Molecule 7: 50S ribosomal protein L31

Chain 6:

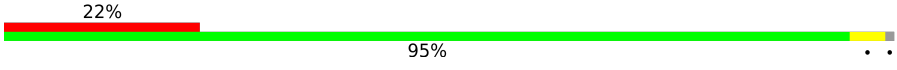
• Molecule 8: 5S rRNA

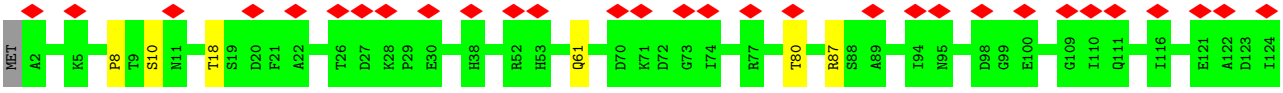
Chain B:

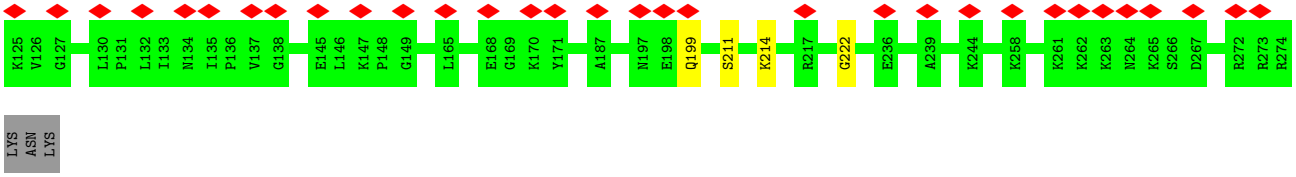


• Molecule 9: 50S ribosomal protein L2

Chain C:

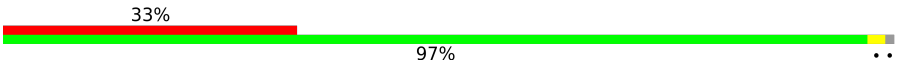


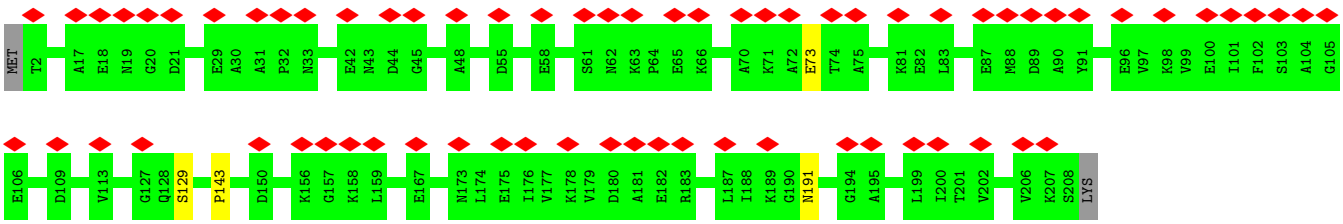




• Molecule 10: 50S ribosomal protein L3

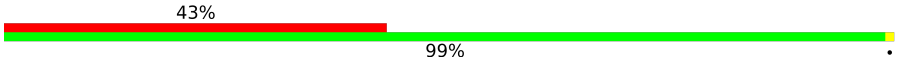
Chain D:

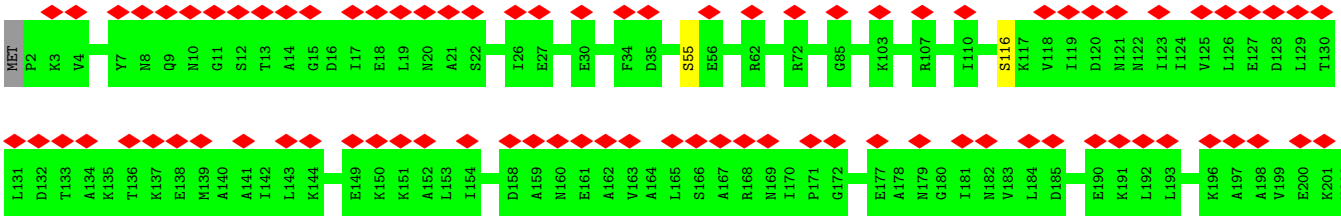




• Molecule 11: 50S ribosomal protein L4

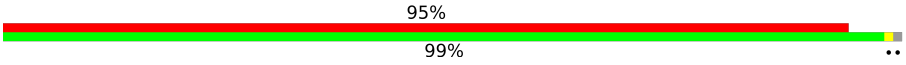
Chain E:

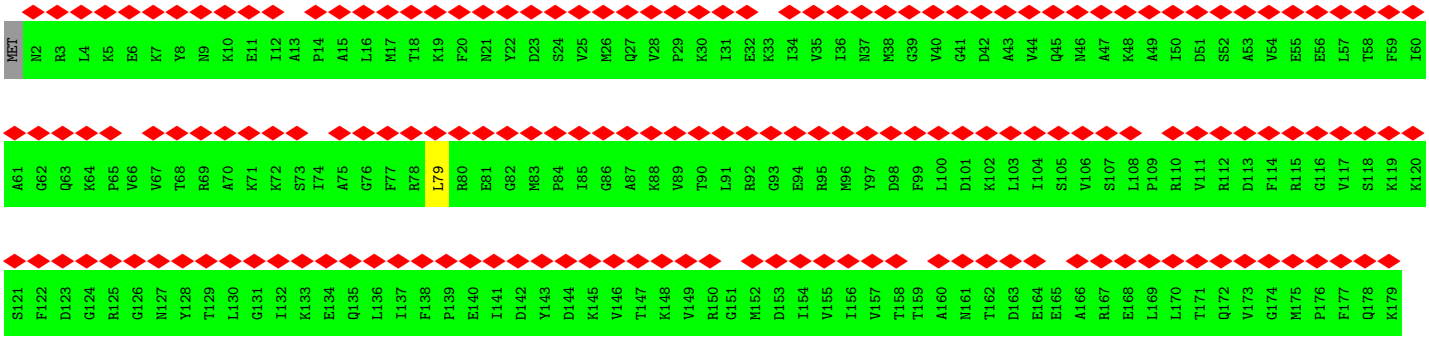




• Molecule 12: 50S ribosomal protein L5

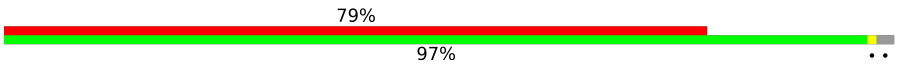
Chain F:

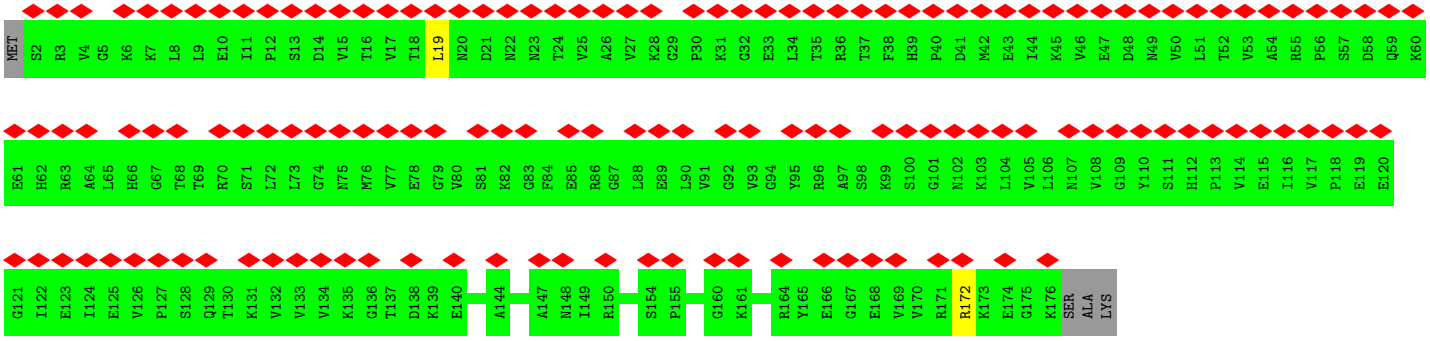




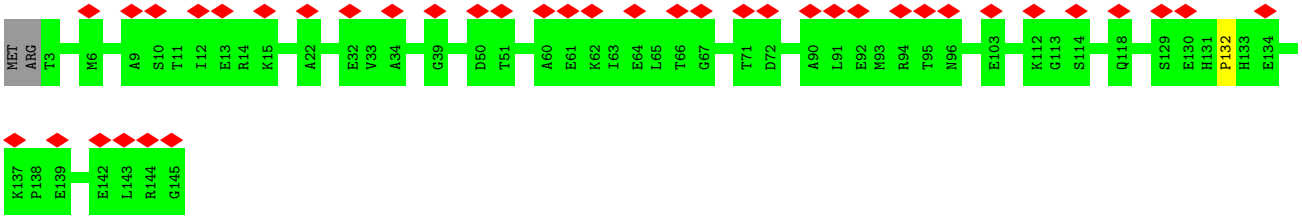
• Molecule 13: Large ribosomal subunit protein uL6

Chain G:

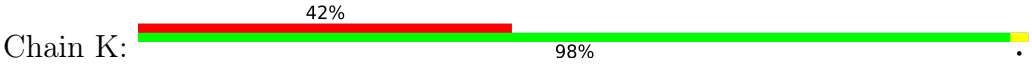


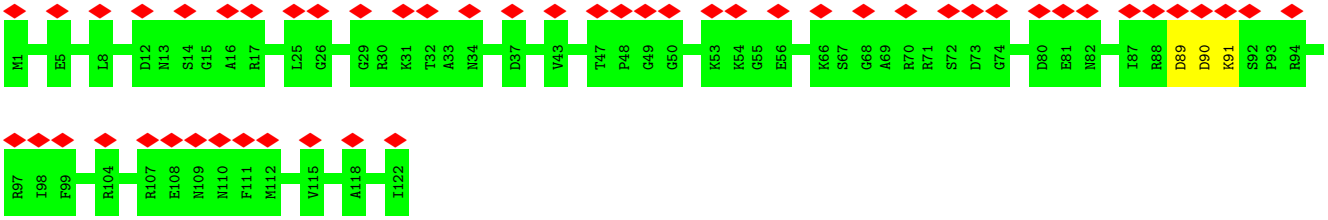


• Molecule 14: 50S ribosomal protein L13

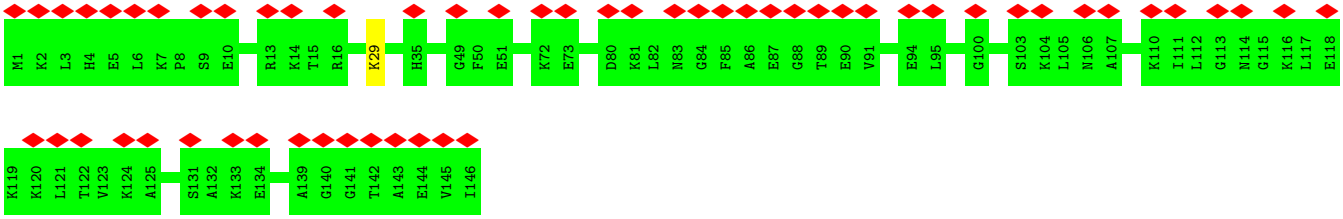


• Molecule 15: 50S ribosomal protein L14

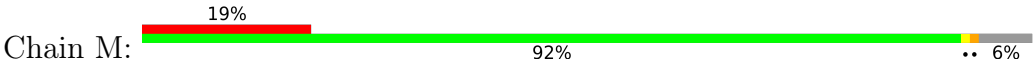


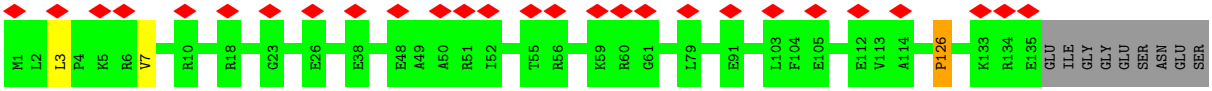


• Molecule 16: 50S ribosomal protein L15



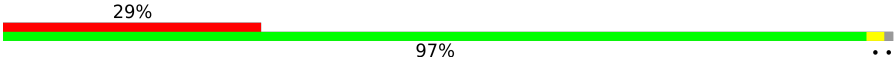
• Molecule 17: 50S ribosomal protein L16

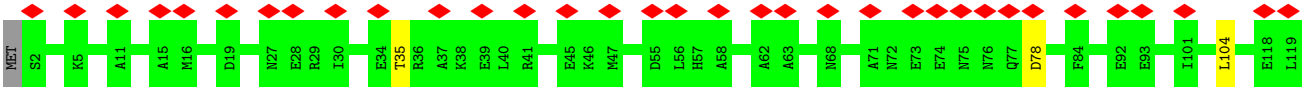




• Molecule 18: 50S ribosomal protein L17

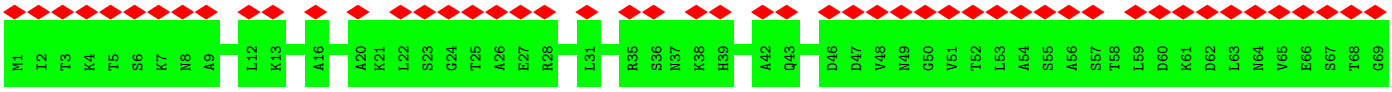
Chain N:

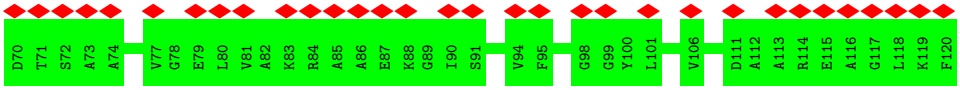




• Molecule 19: 50S ribosomal protein L18

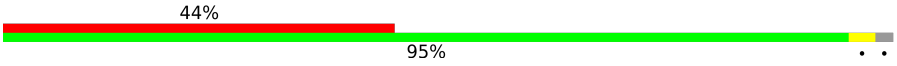
Chain O:

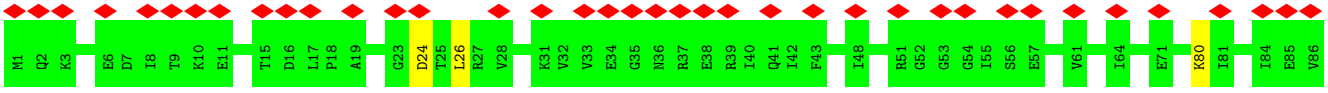


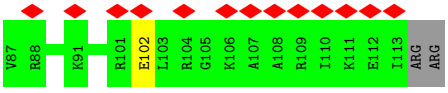


• Molecule 20: 50S ribosomal protein L19

Chain P:

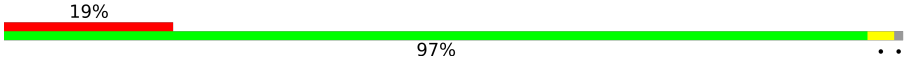


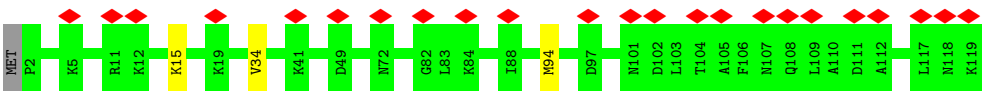




• Molecule 21: Large ribosomal subunit protein bL20

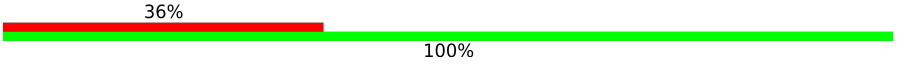
Chain Q:

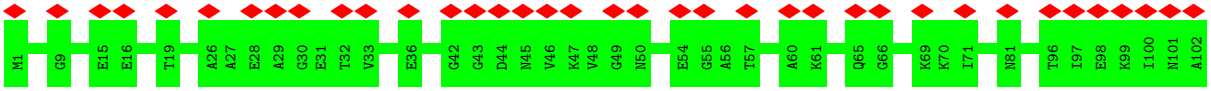




• Molecule 22: 50S ribosomal protein L21

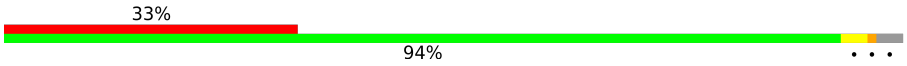
Chain R:

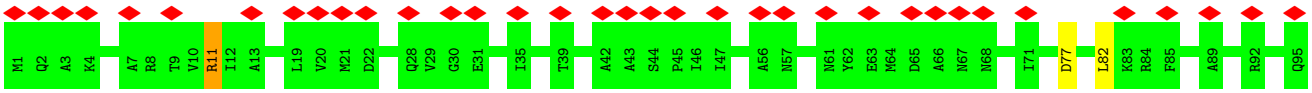


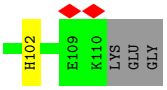


• Molecule 23: 50S ribosomal protein L22

Chain S:

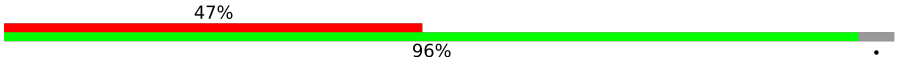


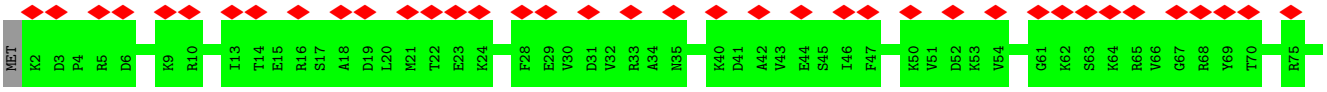


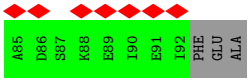


• Molecule 24: Large ribosomal subunit protein uL23

Chain T:

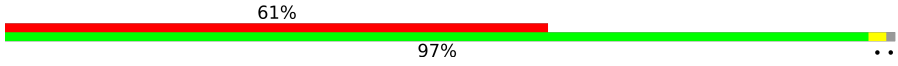


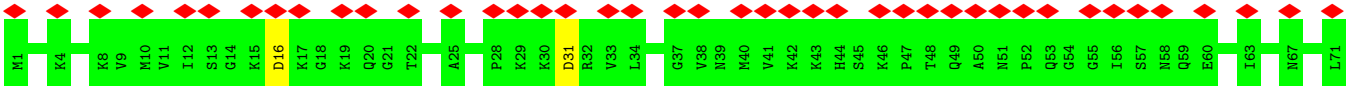


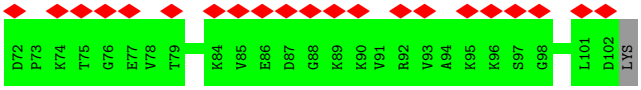


• Molecule 25: 50S ribosomal protein L24

Chain U:

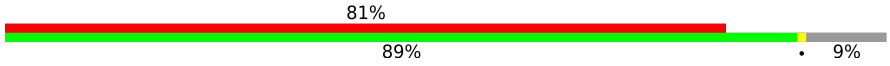


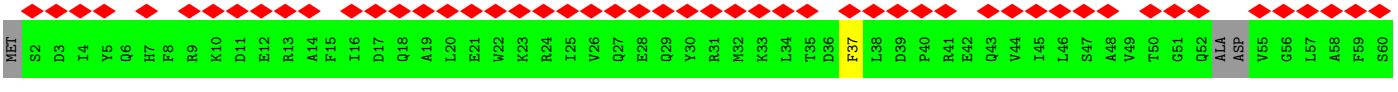


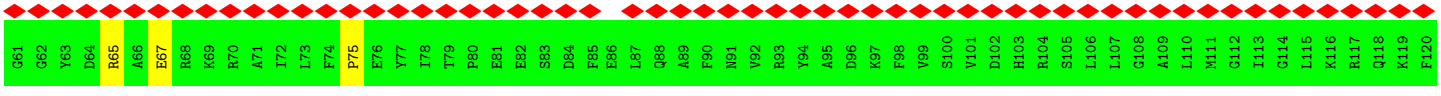


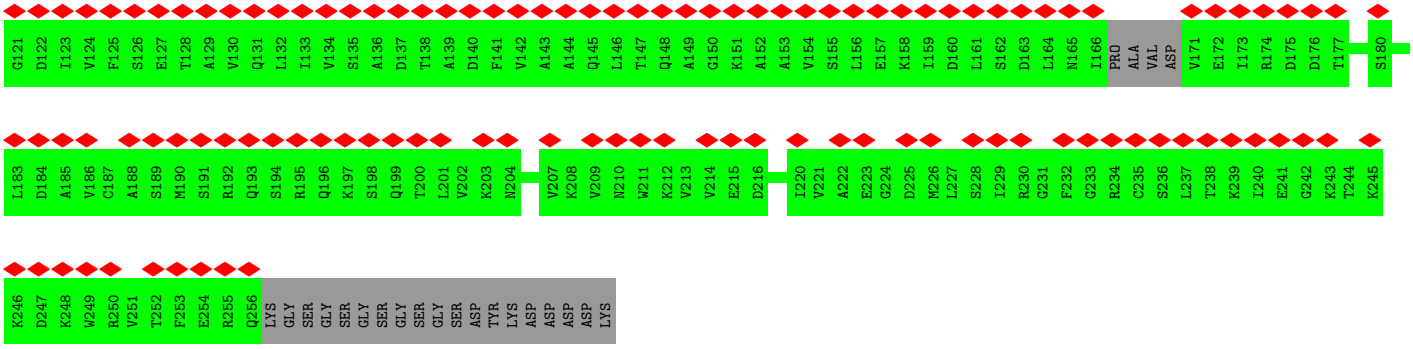
• Molecule 26: Putative RNA-binding protein YlmH

Chain V:

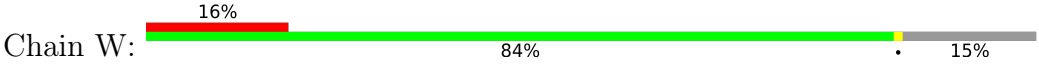


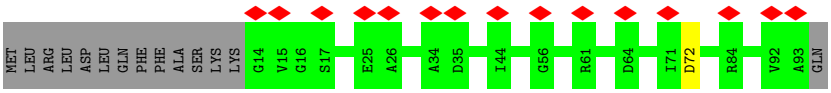




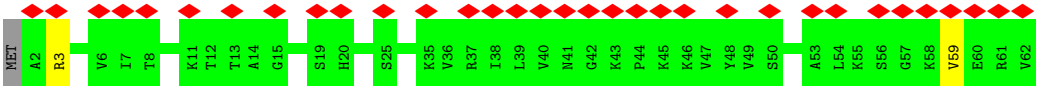


• Molecule 27: Large ribosomal subunit protein bL27

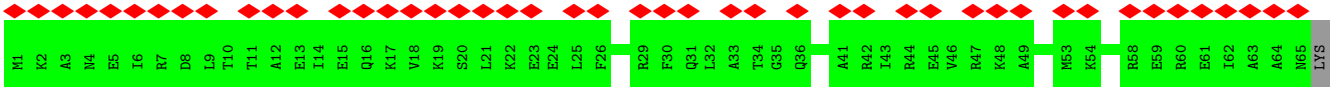




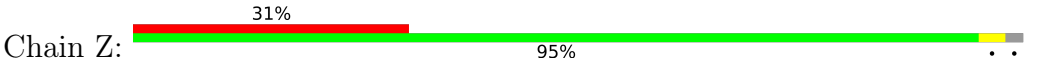
• Molecule 28: 50S ribosomal protein L28

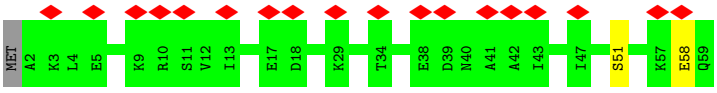


• Molecule 29: 50S ribosomal protein L29

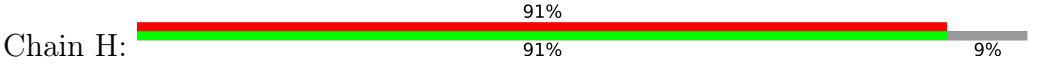


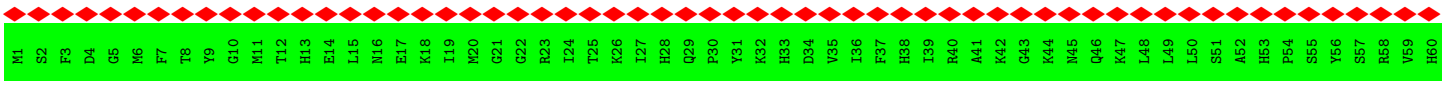
• Molecule 30: Large ribosomal subunit protein uL30





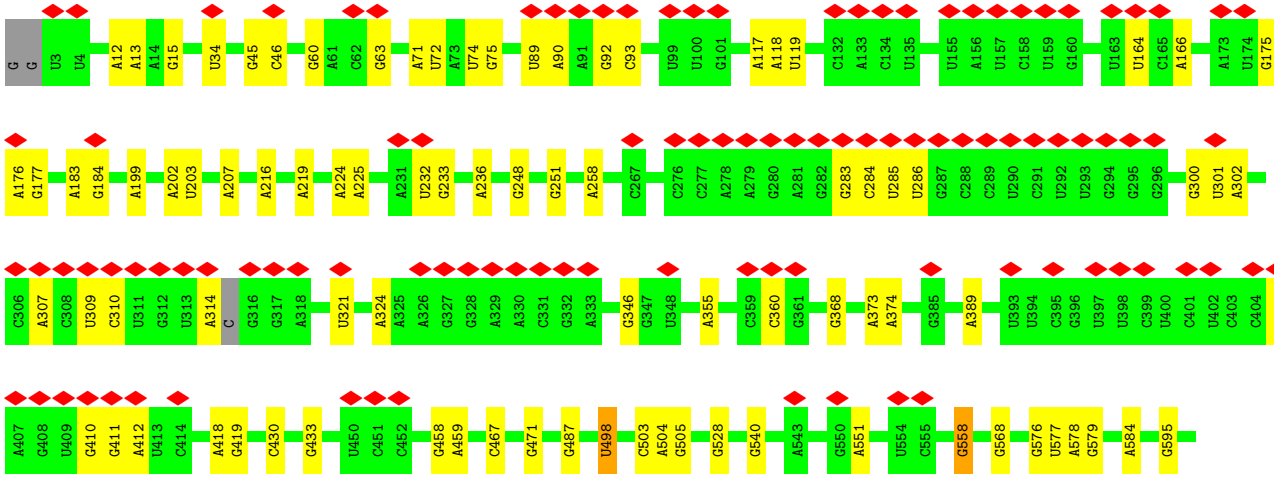
• Molecule 31: Rqc2 homolog RqcH

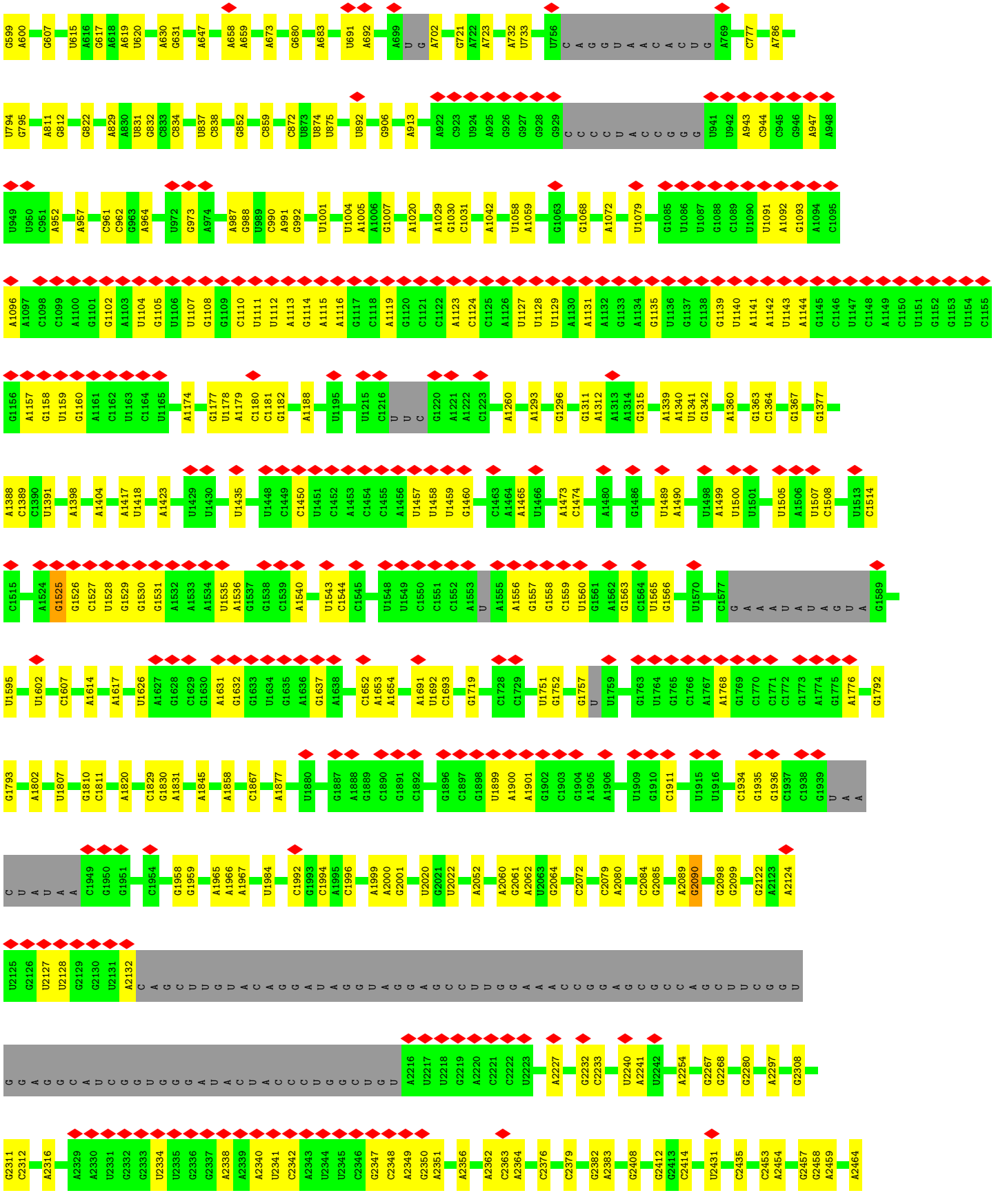


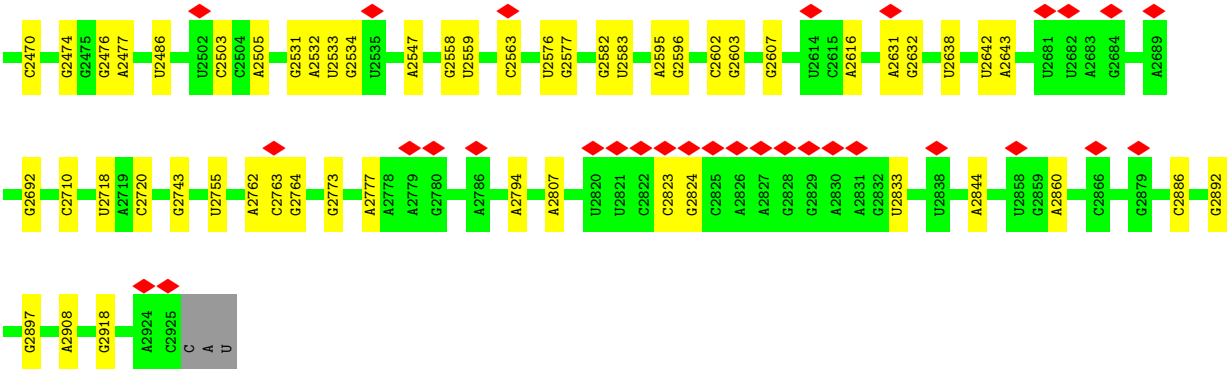


- Molecule 32: 23S rRNA

Chain A:



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G2534
U2535
A2547
G2558
U2559
C2563
U2576
G2577
G2582
U2583
A2595
G2596
C2602
G2603
G2607
U2614
C2615
A2616
A2631
G2632
U2638
U2642
A2643
U2681
U2682
A2683
G2684
A2689
G2692
C2710
U2718
A2719
C2720
G2743
U2755
A2762
C2763
G2764
G2773
A2777
A2778
A2779
G2780
A2786
A2794
A2807
U2820
U2821
C2822
C2823
G2824
C2825
A2826
A2827
G2828
G2829
A2830
A2831
G2832
U2833
U2838
A2844
U2858
G2859
A2860
C2866
G2879
C2886
G2892
G2897
A2908
G2918
A2924
C2925
C
A
U

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3770	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0235	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 2MG, OMG, PSU, 5MU, H2U, K, 2MA

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	0.62	0/1648	1.10	3/2564 (0.1%)
1	c	0.62	0/1577	1.03	1/2456 (0.0%)
2	0	0.43	0/425	0.75	0/563
3	1	0.42	0/416	0.83	0/551
4	2	0.51	0/371	0.84	0/483
5	3	0.44	0/519	0.76	0/680
6	4	0.42	0/300	0.77	0/393
7	6	0.40	0/363	0.56	0/485
8	B	0.57	0/2675	1.04	4/4170 (0.1%)
9	C	0.42	0/2131	0.77	0/2859
10	D	0.42	0/1597	0.76	0/2140
11	E	0.36	0/1586	0.70	0/2139
12	F	0.38	0/1424	0.64	0/1910
13	G	0.39	0/1360	0.66	0/1832
14	J	0.45	0/1154	0.72	0/1552
15	K	0.41	0/928	0.76	0/1245
16	L	0.41	0/1094	0.70	0/1457
17	M	0.41	0/1099	0.78	1/1468 (0.1%)
18	N	0.38	0/961	0.73	0/1284
19	O	0.38	0/922	0.71	0/1236
20	P	0.38	0/935	0.73	0/1251
21	Q	0.41	0/962	0.77	1/1277 (0.1%)
22	R	0.39	0/806	0.71	0/1080
23	S	0.39	0/859	0.75	1/1156 (0.1%)
24	T	0.42	0/739	0.78	0/985
25	U	0.38	0/780	0.68	0/1043
26	V	0.39	0/2016	0.67	0/2709
27	W	0.45	0/619	0.77	0/824
28	X	0.39	0/472	0.71	0/627
29	Y	0.35	0/531	0.71	0/707
30	Z	0.38	0/458	0.77	0/613
31	H	0.34	0/2564	0.50	0/3569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
32	A	0.61	0/66810	1.00	34/104210 (0.0%)
All	All	0.56	0/101101	0.94	45/151518 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	C	0	1
20	P	0	1
23	S	0	1
All	All	0	3

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	1177	G	O3'-P-O5'	-6.51	91.62	104.00
32	A	207	A	O3'-P-O5'	-6.28	92.08	104.00
1	a	51	C	C2'-C3'-O3'	6.24	123.69	113.70
32	A	795	G	C1'-O4'-C4'	-6.07	105.04	109.90
32	A	2080	A	O3'-P-O5'	-6.01	92.58	104.00
32	A	1398	A	O3'-P-O5'	-5.91	92.77	104.00
32	A	2347	G	O3'-P-O5'	-5.91	92.78	104.00
8	B	86	U	O3'-P-O5'	-5.89	92.81	104.00
32	A	721	G	O3'-P-O5'	-5.83	92.92	104.00
32	A	1417	A	O3'-P-O5'	-5.81	92.95	104.00
1	a	71	C	O3'-P-O5'	-5.71	93.16	104.00
23	S	11	ARG	CG-CD-NE	-5.69	99.85	111.80
32	A	2476	G	OP1-P-O3'	5.68	117.69	105.20
32	A	1810	G	O3'-P-O5'	-5.66	93.25	104.00
32	A	786	A	O3'-P-O5'	-5.65	93.27	104.00
32	A	2090	G	O3'-P-O5'	-5.57	93.41	104.00
32	A	988	G	OP2-P-O3'	5.55	117.42	105.20
32	A	1363	G	O3'-P-O5'	-5.55	93.46	104.00
32	A	2643	A	O3'-P-O5'	-5.52	93.51	104.00
32	A	2710	C	O3'-P-O5'	-5.48	93.58	104.00
32	A	2382	G	O3'-P-O5'	-5.45	93.64	104.00
32	A	1965	A	C1'-O4'-C4'	-5.43	105.56	109.90
8	B	48	G	C2'-C3'-O3'	5.43	122.38	113.70
32	A	2079	C	O3'-P-O5'	-5.42	93.70	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	2616	A	OP2-P-O3'	5.41	117.11	105.20
32	A	872	C	OP1-P-O3'	5.34	116.96	105.20
32	A	2340	A	O3'-P-O5'	-5.33	93.87	104.00
32	A	834	C	O5'-P-OP1	5.32	117.08	110.70
17	M	126	PRO	N-CA-CB	-5.29	96.78	102.60
1	a	53	G	O3'-P-O5'	-5.28	93.98	104.00
1	c	58	A	O3'-P-O5'	-5.21	94.10	104.00
32	A	2844	A	O3'-P-O5'	-5.21	94.10	104.00
8	B	68	C	O3'-P-O5'	-5.18	94.15	104.00
32	A	72	U	C3'-C2'-C1'	-5.18	97.36	101.50
32	A	1807	U	O3'-P-O5'	-5.16	94.20	104.00
32	A	2383	A	O3'-P-O5'	-5.15	94.21	104.00
32	A	498	U	C1'-O4'-C4'	-5.11	105.81	109.90
32	A	723	A	O3'-P-O5'	-5.11	94.30	104.00
21	Q	94	MET	CG-SD-CE	5.10	108.36	100.20
32	A	558	G	O4'-C1'-N9	5.10	112.28	108.20
32	A	1367	G	O3'-P-O5'	-5.09	94.33	104.00
8	B	13	A	C3'-C2'-C1'	-5.05	97.46	101.50
32	A	1934	C	O3'-P-O5'	-5.05	94.41	104.00
32	A	1525	G	C2'-C3'-O3'	5.03	121.74	113.70
32	A	505	G	C3'-C2'-C1'	-5.00	97.50	101.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	C	80	THR	Peptide
20	P	26	LEU	Peptide
23	S	11	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	0	51/59 (86%)	44 (86%)	6 (12%)	1 (2%)	7 30
3	1	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	7 30
4	2	42/44 (96%)	40 (95%)	2 (5%)	0	100 100
5	3	62/66 (94%)	56 (90%)	6 (10%)	0	100 100
6	4	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
7	6	44/66 (67%)	44 (100%)	0	0	100 100
9	C	271/277 (98%)	254 (94%)	16 (6%)	1 (0%)	34 67
10	D	205/209 (98%)	187 (91%)	17 (8%)	1 (0%)	29 61
11	E	204/207 (99%)	193 (95%)	11 (5%)	0	100 100
12	F	176/179 (98%)	172 (98%)	4 (2%)	0	100 100
13	G	173/179 (97%)	168 (97%)	5 (3%)	0	100 100
14	J	141/145 (97%)	139 (99%)	2 (1%)	0	100 100
15	K	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19 51
16	L	144/146 (99%)	133 (92%)	10 (7%)	1 (1%)	22 55
17	M	133/144 (92%)	120 (90%)	13 (10%)	0	100 100
18	N	117/120 (98%)	108 (92%)	9 (8%)	0	100 100
19	O	118/120 (98%)	113 (96%)	5 (4%)	0	100 100
20	P	111/115 (96%)	104 (94%)	7 (6%)	0	100 100
21	Q	116/119 (98%)	108 (93%)	8 (7%)	0	100 100
22	R	100/102 (98%)	99 (99%)	1 (1%)	0	100 100
23	S	108/113 (96%)	105 (97%)	3 (3%)	0	100 100
24	T	89/95 (94%)	85 (96%)	4 (4%)	0	100 100
25	U	100/103 (97%)	91 (91%)	9 (9%)	0	100 100
26	V	243/275 (88%)	225 (93%)	14 (6%)	4 (2%)	9 34
27	W	78/94 (83%)	73 (94%)	5 (6%)	0	100 100
28	X	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3 21
29	Y	63/66 (96%)	62 (98%)	1 (2%)	0	100 100
30	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100 100
31	H	512/570 (90%)	502 (98%)	10 (2%)	0	100 100
All	All	3718/3942 (94%)	3513 (94%)	193 (5%)	12 (0%)	44 72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	222	GLY
10	D	73	GLU
26	V	37	PHE
26	V	65	ARG
2	0	32	SER
26	V	67	GLU
3	1	11	GLU
16	L	29	LYS
28	X	3	ARG
15	K	91	LYS
26	V	75	PRO
28	X	59	VAL

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	
2	0	47/53 (89%)	47 (100%)	0	100	100
3	1	47/47 (100%)	46 (98%)	1 (2%)	53	76
4	2	39/39 (100%)	39 (100%)	0	100	100
5	3	54/56 (96%)	53 (98%)	1 (2%)	57	78
6	4	35/35 (100%)	35 (100%)	0	100	100
7	6	39/55 (71%)	38 (97%)	1 (3%)	46	72
9	C	221/225 (98%)	213 (96%)	8 (4%)	35	63
10	D	168/170 (99%)	165 (98%)	3 (2%)	59	79
11	E	169/170 (99%)	167 (99%)	2 (1%)	71	85
12	F	153/154 (99%)	152 (99%)	1 (1%)	84	92
13	G	148/151 (98%)	146 (99%)	2 (1%)	67	83
14	J	121/123 (98%)	120 (99%)	1 (1%)	81	91
15	K	101/101 (100%)	99 (98%)	2 (2%)	55	77
16	L	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	M	109/116 (94%)	106 (97%)	3 (3%)	43 70
18	N	99/100 (99%)	96 (97%)	3 (3%)	41 68
19	O	93/93 (100%)	93 (100%)	0	100 100
20	P	98/100 (98%)	95 (97%)	3 (3%)	40 68
21	Q	97/98 (99%)	95 (98%)	2 (2%)	53 76
22	R	84/84 (100%)	84 (100%)	0	100 100
23	S	91/93 (98%)	88 (97%)	3 (3%)	38 66
24	T	82/85 (96%)	82 (100%)	0	100 100
25	U	86/87 (99%)	84 (98%)	2 (2%)	50 74
26	V	215/234 (92%)	215 (100%)	0	100 100
27	W	61/74 (82%)	60 (98%)	1 (2%)	62 81
28	X	49/50 (98%)	49 (100%)	0	100 100
29	Y	56/57 (98%)	56 (100%)	0	100 100
30	Z	52/53 (98%)	50 (96%)	2 (4%)	33 61
All	All	2724/2813 (97%)	2683 (98%)	41 (2%)	66 82

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1	43	THR
5	3	31	HIS
7	6	26	SER
9	C	8	PRO
9	C	10	SER
9	C	18	THR
9	C	61	GLN
9	C	87	ARG
9	C	199	GLN
9	C	211	SER
9	C	214	LYS
10	D	129	SER
10	D	143	PRO
10	D	191	ASN
11	E	55	SER
11	E	116	SER
12	F	79	LEU
13	G	19	LEU

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Mol	Chain	Res	Type
13	G	172	ARG
14	J	132	PRO
15	K	89	ASP
15	K	90	ASP
17	M	3	LEU
17	M	7	VAL
17	M	126	PRO
18	N	35	THR
18	N	78	ASP
18	N	104	LEU
20	P	24	ASP
20	P	80	LYS
20	P	102	GLU
21	Q	15	LYS
21	Q	34	VAL
23	S	77	ASP
23	S	82	LEU
23	S	102	HIS
25	U	16	ASP
25	U	31	ASP
27	W	72	ASP
30	Z	51	SER
30	Z	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	0	40	HIS
5	3	31	HIS
5	3	35	ASN
5	3	60	GLN
9	C	194	GLN
10	D	126	HIS
11	E	49	HIS
14	J	136	GLN
15	K	3	GLN
15	K	4	GLN
15	K	110	ASN
23	S	73	GLN
24	T	58	ASN
25	U	99	GLN
26	V	7	HIS

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Mol	Chain	Res	Type
26	V	52	GLN
26	V	204	ASN
28	X	17	ASN
28	X	23	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	66/76 (86%)	29 (43%)	0
1	c	64/76 (84%)	24 (37%)	0
32	A	2778/2928 (94%)	372 (13%)	53 (1%)
8	B	111/112 (99%)	24 (21%)	5 (4%)
All	All	3019/3192 (94%)	449 (14%)	58 (1%)

All (449) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	c	3	G
1	c	6	C
1	c	9	A
1	c	16	C
1	c	17	U
1	c	18	G
1	c	19	G
1	c	20	G
1	c	21	A
1	c	28	C
1	c	41	A
1	c	44	A
1	c	45	G
1	c	46	G
1	c	48	C
1	c	53	G
1	c	55	U
1	c	57	G
1	c	61	C
1	c	65	U
1	c	66	A
1	c	67	G
1	c	70	U
1	c	72	C

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Mol	Chain	Res	Type
8	B	10	G
8	B	11	A
8	B	12	U
8	B	13	A
8	B	19	G
8	B	23	U
8	B	32	U
8	B	33	U
8	B	38	U
8	B	40	C
8	B	43	A
8	B	48	G
8	B	49	G
8	B	50	A
8	B	53	U
8	B	54	U
8	B	55	A
8	B	87	U
8	B	88	C
8	B	95	U
8	B	97	A
8	B	103	G
8	B	107	G
8	B	108	C
1	a	3	G
1	a	6	C
1	a	7	U
1	a	8	U
1	a	9	A
1	a	20	G
1	a	22	G
1	a	23	A
1	a	28	C
1	a	31	C
1	a	32	U
1	a	39	G
1	a	40	C
1	a	41	A
1	a	44	A
1	a	47	U
1	a	48	C
1	a	49	A

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Mol	Chain	Res	Type
1	a	52	G
1	a	53	G
1	a	54	U
1	a	57	G
1	a	61	C
1	a	62	C
1	a	65	U
1	a	66	A
1	a	67	G
1	a	72	C
1	a	76	A
32	A	12	A
32	A	13	A
32	A	15	G
32	A	34	U
32	A	45	G
32	A	46	C
32	A	60	G
32	A	63	G
32	A	71	A
32	A	74	U
32	A	75	G
32	A	89	U
32	A	90	A
32	A	93	C
32	A	117	A
32	A	118	A
32	A	119	U
32	A	164	U
32	A	166	A
32	A	175	G
32	A	176	A
32	A	177	G
32	A	183	A
32	A	184	G
32	A	199	A
32	A	202	A
32	A	203	U
32	A	216	A
32	A	219	A
32	A	224	A
32	A	225	A

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Mol	Chain	Res	Type
32	A	232	U
32	A	233	G
32	A	236	A
32	A	248	G
32	A	251	G
32	A	258	A
32	A	283	G
32	A	284	C
32	A	285	U
32	A	286	U
32	A	300	G
32	A	301	U
32	A	302	A
32	A	307	A
32	A	309	U
32	A	310	C
32	A	314	A
32	A	321	U
32	A	324	A
32	A	346	G
32	A	355	A
32	A	360	C
32	A	368	G
32	A	373	A
32	A	374	A
32	A	405	U
32	A	410	G
32	A	411	G
32	A	412	A
32	A	418	A
32	A	419	G
32	A	430	C
32	A	433	G
32	A	458	G
32	A	459	A
32	A	467	C
32	A	471	G
32	A	487	G
32	A	498	U
32	A	503	C
32	A	504	A
32	A	528	G

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Mol	Chain	Res	Type
32	A	540	G
32	A	551	A
32	A	568	G
32	A	576	G
32	A	577	U
32	A	578	A
32	A	579	G
32	A	584	A
32	A	595	G
32	A	600	A
32	A	607	G
32	A	617	G
32	A	619	A
32	A	630	A
32	A	631	G
32	A	647	A
32	A	658	A
32	A	659	A
32	A	673	A
32	A	680	G
32	A	683	A
32	A	691	U
32	A	692	A
32	A	733	U
32	A	777	C
32	A	794	5MU
32	A	811	A
32	A	812	G
32	A	822	G
32	A	829	A
32	A	831	U
32	A	832	G
32	A	837	U
32	A	838	C
32	A	852	G
32	A	859	C
32	A	874	U
32	A	875	U
32	A	892	U
32	A	906	G
32	A	913	A
32	A	943	A

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Mol	Chain	Res	Type
32	A	944	C
32	A	947	A
32	A	952	A
32	A	957	A
32	A	961	C
32	A	962	C
32	A	964	A
32	A	973	G
32	A	987	A
32	A	991	A
32	A	992	G
32	A	1004	U
32	A	1005	A
32	A	1007	G
32	A	1020	A
32	A	1029	A
32	A	1030	G
32	A	1031	C
32	A	1042	A
32	A	1058	U
32	A	1059	A
32	A	1068	G
32	A	1072	A
32	A	1079	U
32	A	1091	U
32	A	1092	A
32	A	1093	G
32	A	1096	A
32	A	1102	G
32	A	1104	U
32	A	1105	G
32	A	1107	U
32	A	1108	G
32	A	1110	C
32	A	1112	U
32	A	1113	A
32	A	1114	G
32	A	1115	A
32	A	1116	A
32	A	1119	A
32	A	1123	A
32	A	1124	C

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Mol	Chain	Res	Type
32	A	1127	U
32	A	1128	U
32	A	1129	U
32	A	1131	A
32	A	1135	G
32	A	1139	G
32	A	1140	U
32	A	1141	A
32	A	1142	A
32	A	1143	U
32	A	1144	A
32	A	1157	A
32	A	1158	G
32	A	1159	U
32	A	1160	G
32	A	1174	A
32	A	1178	U
32	A	1179	A
32	A	1180	C
32	A	1181	C
32	A	1182	G
32	A	1188	A
32	A	1260	A
32	A	1293	A
32	A	1296	G
32	A	1311	G
32	A	1312	A
32	A	1315	G
32	A	1339	A
32	A	1340	A
32	A	1341	U
32	A	1342	G
32	A	1360	A
32	A	1364	C
32	A	1377	G
32	A	1388	A
32	A	1389	C
32	A	1391	U
32	A	1404	A
32	A	1418	U
32	A	1423	A
32	A	1435	U

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Mol	Chain	Res	Type
32	A	1450	C
32	A	1457	U
32	A	1458	U
32	A	1459	U
32	A	1460	G
32	A	1465	A
32	A	1473	A
32	A	1474	C
32	A	1489	U
32	A	1490	A
32	A	1499	A
32	A	1500	U
32	A	1505	U
32	A	1507	U
32	A	1508	C
32	A	1514	C
32	A	1525	G
32	A	1526	G
32	A	1527	C
32	A	1528	U
32	A	1529	G
32	A	1531	G
32	A	1536	A
32	A	1540	A
32	A	1544	C
32	A	1556	A
32	A	1557	G
32	A	1558	G
32	A	1559	C
32	A	1560	U
32	A	1563	G
32	A	1566	G
32	A	1595	U
32	A	1607	C
32	A	1614	A
32	A	1617	A
32	A	1626	U
32	A	1631	A
32	A	1632	G
32	A	1637	G
32	A	1653	A
32	A	1654	A

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Mol	Chain	Res	Type
32	A	1691	A
32	A	1693	C
32	A	1719	G
32	A	1752	G
32	A	1757	G
32	A	1768	A
32	A	1776	A
32	A	1792	G
32	A	1793	G
32	A	1802	A
32	A	1811	C
32	A	1820	A
32	A	1829	C
32	A	1830	G
32	A	1831	A
32	A	1845	A
32	A	1858	A
32	A	1867	C
32	A	1877	A
32	A	1899	U
32	A	1900	A
32	A	1901	A
32	A	1911	C
32	A	1935	G
32	A	1936	G
32	A	1958	G
32	A	1959	G
32	A	1966	A
32	A	1967	A
32	A	1984	U
32	A	1992	C
32	A	1994	C
32	A	1996	C
32	A	1999	A
32	A	2000	A
32	A	2001	G
32	A	2020	U
32	A	2022	U
32	A	2052	A
32	A	2060	A
32	A	2061	G
32	A	2062	A

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Mol	Chain	Res	Type
32	A	2072	C
32	A	2084	C
32	A	2085	G
32	A	2089	A
32	A	2090	G
32	A	2098	G
32	A	2099	G
32	A	2122	G
32	A	2124	A
32	A	2128	U
32	A	2132	A
32	A	2227	A
32	A	2232	G
32	A	2233	C
32	A	2240	U
32	A	2241	A
32	A	2254	A
32	A	2267	G
32	A	2268	G
32	A	2297	A
32	A	2308	G
32	A	2312	C
32	A	2316	A
32	A	2334	U
32	A	2338	A
32	A	2341	U
32	A	2342	C
32	A	2348	C
32	A	2349	A
32	A	2350	G
32	A	2351	A
32	A	2356	A
32	A	2362	A
32	A	2363	C
32	A	2364	A
32	A	2376	C
32	A	2379	C
32	A	2408	G
32	A	2412	G
32	A	2414	C
32	A	2431	U
32	A	2435	C

Continued on next page...

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Mol	Chain	Res	Type
32	A	2453	C
32	A	2454	A
32	A	2457	G
32	A	2458	G
32	A	2459	A
32	A	2464	A
32	A	2470	C
32	A	2477	A
32	A	2503	C
32	A	2505	A
32	A	2531	G
32	A	2534	G
32	A	2547	A
32	A	2558	G
32	A	2559	U
32	A	2563	C
32	A	2577	G
32	A	2583	U
32	A	2595	A
32	A	2596	G
32	A	2602	C
32	A	2607	G
32	A	2631	A
32	A	2632	G
32	A	2638	U
32	A	2642	U
32	A	2692	G
32	A	2718	U
32	A	2720	C
32	A	2743	G
32	A	2755	U
32	A	2762	A
32	A	2763	C
32	A	2764	G
32	A	2773	G
32	A	2777	A
32	A	2794	A
32	A	2807	A
32	A	2823	C
32	A	2824	G
32	A	2833	U
32	A	2860	A

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Mol	Chain	Res	Type
32	A	2886	C
32	A	2892	G
32	A	2897	G
32	A	2908	A
32	A	2918	G

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	B	32	U
8	B	37	A
8	B	48	G
8	B	49	G
8	B	107	G
32	A	12	A
32	A	92	G
32	A	118	A
32	A	175	G
32	A	183	A
32	A	202	A
32	A	224	A
32	A	389	A
32	A	558	G
32	A	599	G
32	A	615	U
32	A	691	U
32	A	702	A
32	A	732	A
32	A	811	A
32	A	831	U
32	A	837	U
32	A	913	A
32	A	990	C
32	A	1004	U
32	A	1030	G
32	A	1111	U
32	A	1179	A
32	A	1339	A
32	A	1364	C
32	A	1507	U
32	A	1525	G
32	A	1527	C

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Mol	Chain	Res	Type
32	A	1530	G
32	A	1535	U
32	A	1536	A
32	A	1543	U
32	A	1558	G
32	A	1565	U
32	A	1602	U
32	A	1631	A
32	A	1652	C
32	A	1653	A
32	A	1692	U
32	A	1751	U
32	A	2064	G
32	A	2127	U
32	A	2311	G
32	A	2316	A
32	A	2348	C
32	A	2349	A
32	A	2362	A
32	A	2459	A
32	A	2558	G
32	A	2576	U
32	A	2631	A
32	A	2823	C
32	A	2892	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	PSU	A	2533	33,32	18,21,22	1.00	1 (5%)	22,30,33	0.75	0
32	2MA	A	2532	33,32	17,25,26	1.06	2 (11%)	17,37,40	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	G7M	A	2603	32	20,26,27	0.99	1 (5%)	17,39,42	0.44	0
32	OMG	A	2280	33,32,1	18,26,27	1.14	3 (16%)	19,38,41	0.80	0
32	PSU	A	2486	32	18,21,22	0.97	1 (5%)	22,30,33	0.67	0
32	5MU	A	620	33,32	19,22,23	0.36	0	28,32,35	0.66	2 (7%)
32	2MG	A	2474	32	18,26,27	1.17	3 (16%)	16,38,41	0.77	0
32	H2U	A	2478	32	18,21,22	0.66	0	21,30,33	0.74	0
32	5MU	A	794	32	19,22,23	0.28	0	28,32,35	0.33	0
32	5MU	A	1968	32	19,22,23	0.49	0	28,32,35	0.47	0
32	PSU	A	1001	32	18,21,22	0.83	1 (5%)	22,30,33	0.72	0
32	OMG	A	2582	32	18,26,27	1.04	3 (16%)	19,38,41	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	A	2533	33,32	-	0/7/25/26	0/2/2/2
32	2MA	A	2532	33,32	-	2/3/25/26	0/3/3/3
32	G7M	A	2603	32	-	0/3/25/26	0/3/3/3
32	OMG	A	2280	33,32,1	-	0/5/27/28	0/3/3/3
32	PSU	A	2486	32	-	0/7/25/26	0/2/2/2
32	5MU	A	620	33,32	-	0/7/25/26	0/2/2/2
32	2MG	A	2474	32	-	0/5/27/28	0/3/3/3
32	H2U	A	2478	32	-	0/7/38/39	0/2/2/2
32	5MU	A	794	32	-	0/7/25/26	0/2/2/2
32	5MU	A	1968	32	-	0/7/25/26	0/2/2/2
32	PSU	A	1001	32	-	0/7/25/26	0/2/2/2
32	OMG	A	2582	32	-	0/5/27/28	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	2533	PSU	C6-C5	3.82	1.39	1.35
32	A	2486	PSU	C6-C5	3.74	1.39	1.35
32	A	2603	G7M	C8-N9	3.13	1.38	1.33
32	A	1001	PSU	C6-C5	3.11	1.38	1.35
32	A	2280	OMG	C5-C6	-3.04	1.41	1.47
32	A	2474	2MG	C5-C6	-2.77	1.41	1.47
32	A	2532	2MA	C2-N3	2.72	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	2582	OMG	C5-C6	-2.72	1.41	1.47
32	A	2280	OMG	C8-N7	-2.42	1.30	1.35
32	A	2474	2MG	C5-C4	-2.40	1.37	1.43
32	A	2532	2MA	C5-C4	-2.30	1.37	1.43
32	A	2474	2MG	C8-N7	-2.17	1.31	1.35
32	A	2582	OMG	C8-N7	-2.13	1.31	1.35
32	A	2280	OMG	C5-C4	-2.09	1.37	1.43
32	A	2582	OMG	C5-C4	-2.01	1.38	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	2532	2MA	CM2-C2-N1	2.84	122.54	116.23
32	A	620	5MU	O3'-C3'-C4'	-2.33	104.30	111.05
32	A	620	5MU	O3'-C3'-C2'	2.05	118.44	111.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	2532	2MA	C4'-C5'-O5'-P
32	A	2532	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

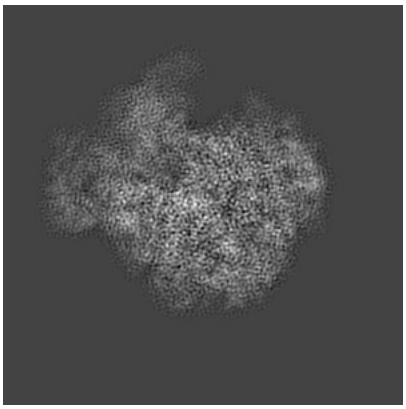
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19641. These allow visual inspection of the internal detail of the map and identification of artifacts.

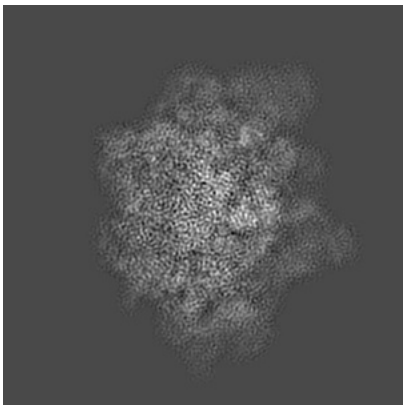
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

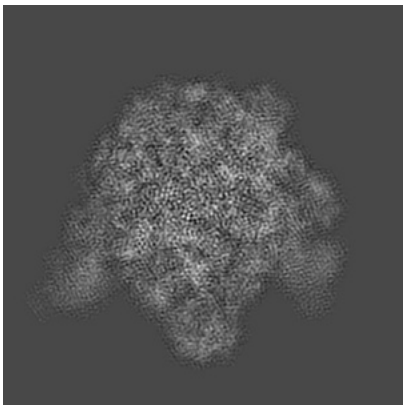
6.1.1 Primary map



X

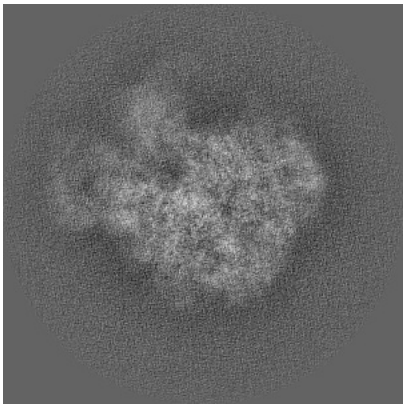


Y

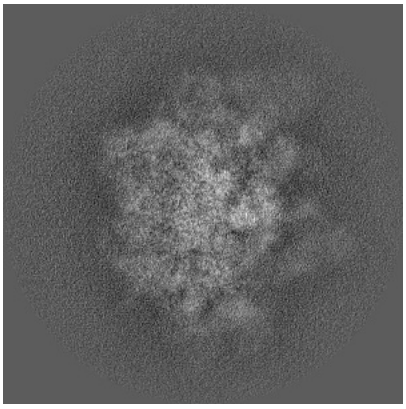


Z

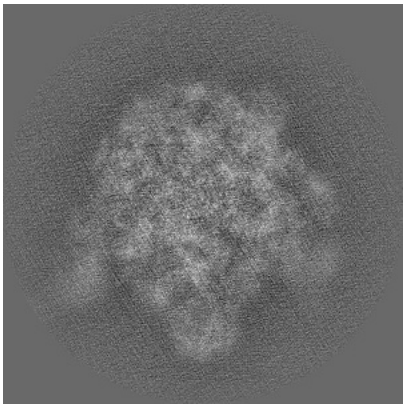
6.1.2 Raw map



X



Y

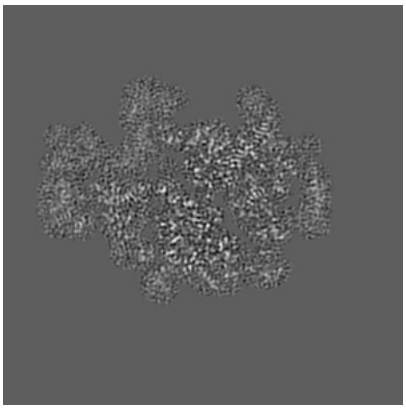


Z

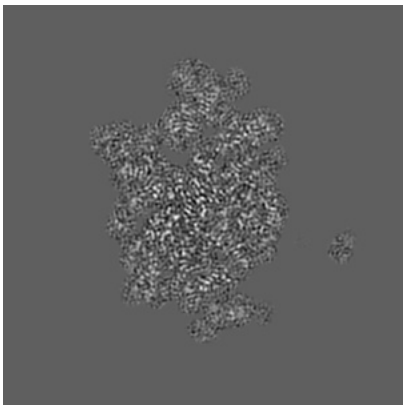
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

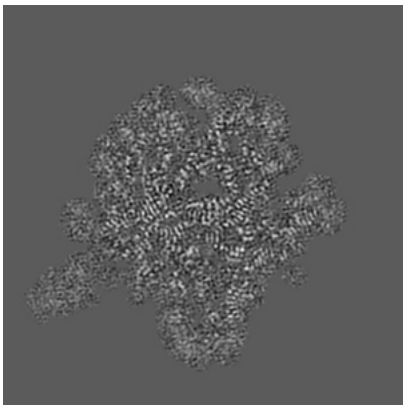
6.2.1 Primary map



X Index: 192

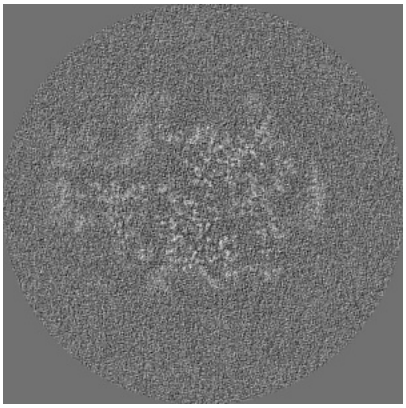


Y Index: 192

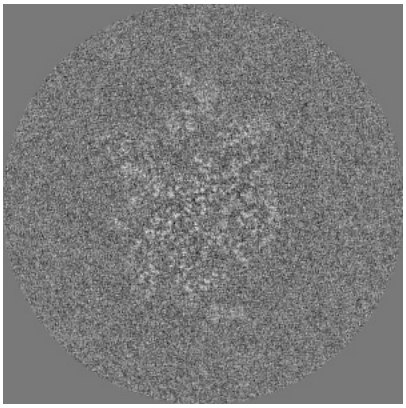


Z Index: 192

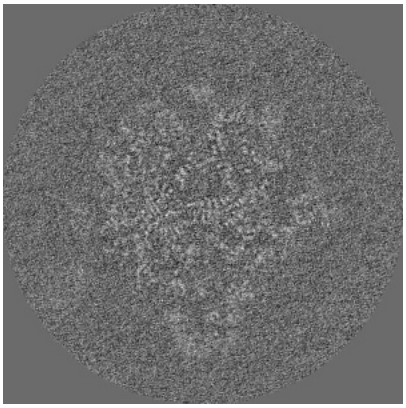
6.2.2 Raw map



X Index: 192



Y Index: 192

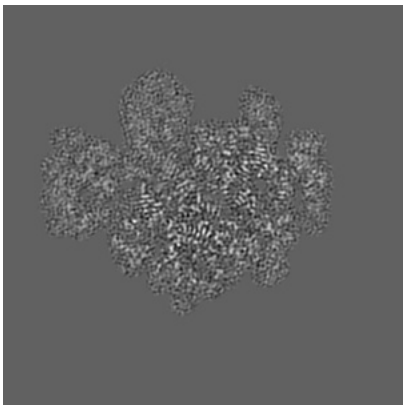


Z Index: 192

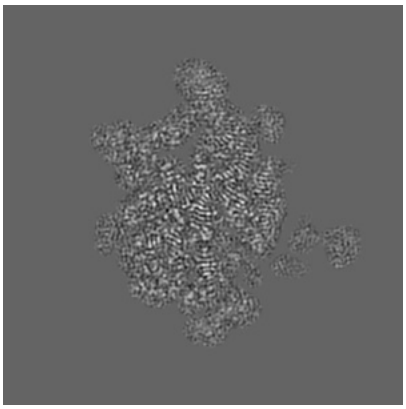
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

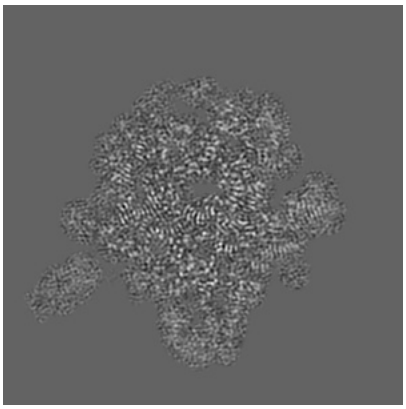
6.3.1 Primary map



X Index: 180

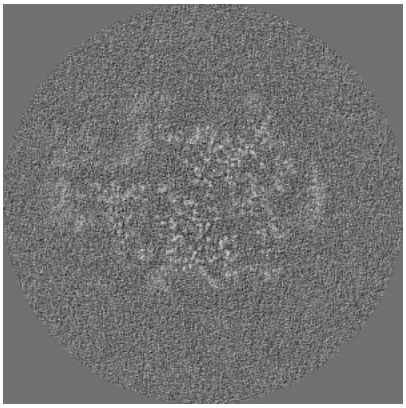


Y Index: 184

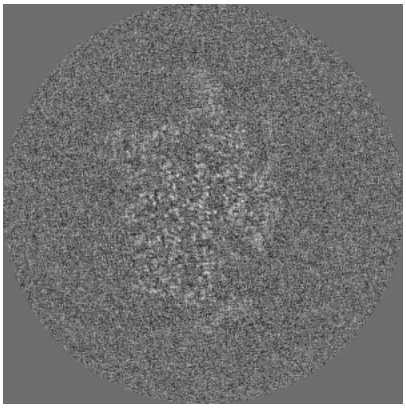


Z Index: 195

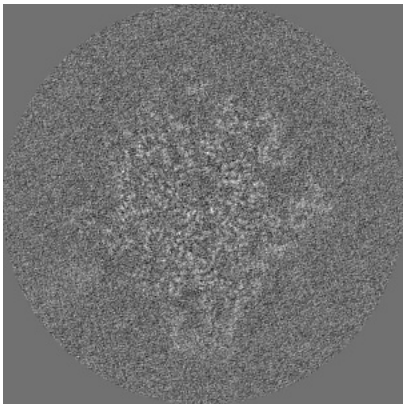
6.3.2 Raw map



X Index: 192



Y Index: 184

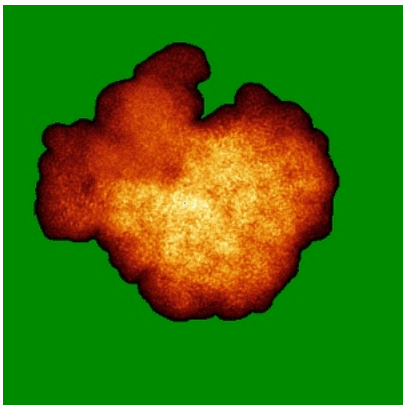


Z Index: 196

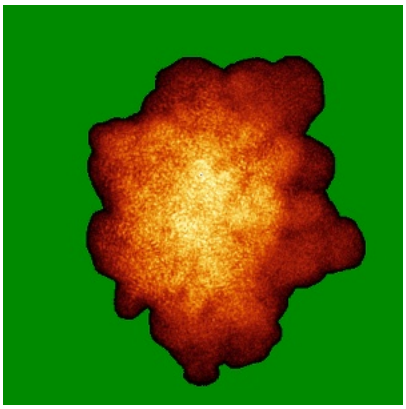
The images above show the largest variance slices of the map in three orthogonal directions.

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

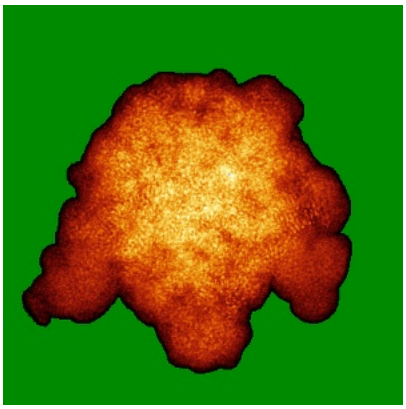
6.4.1 Primary map



X

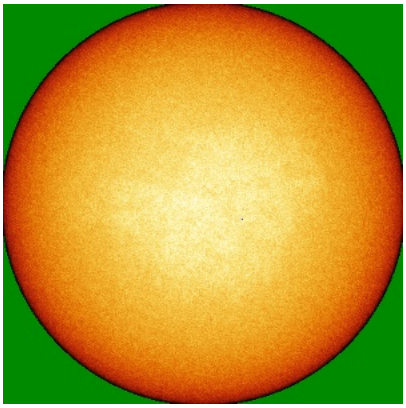


Y

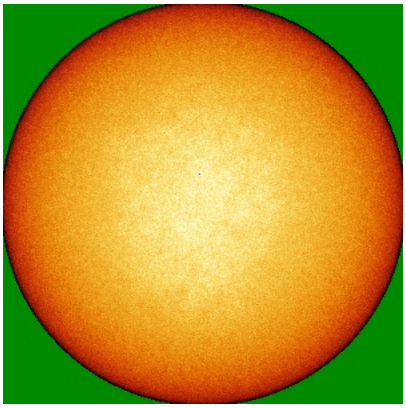


Z

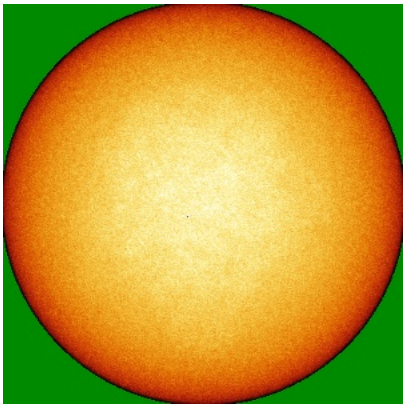
6.4.2 Raw map



X



Y

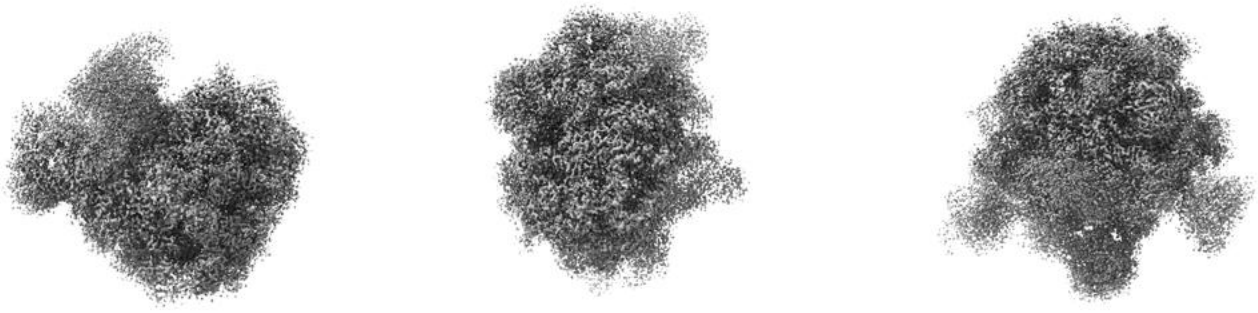


Z

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)

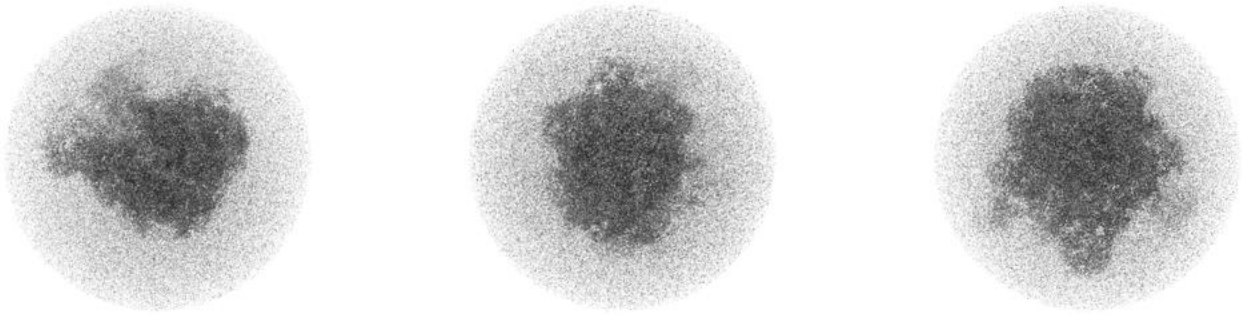
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0235. 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.

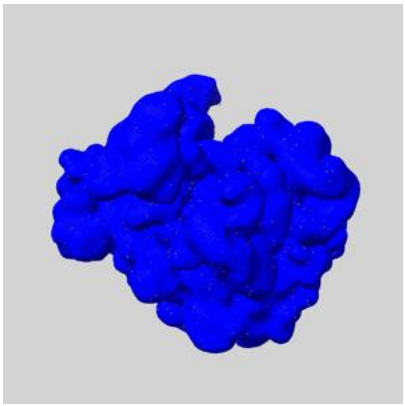
6.6 Mask visualisation (i)

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

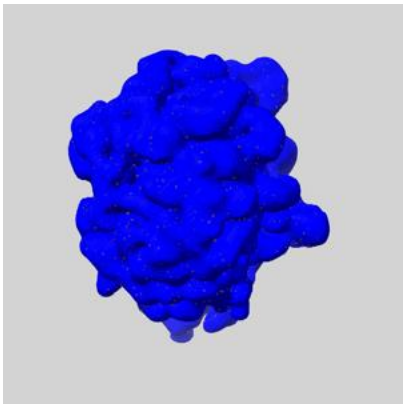
A mask typically either:

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

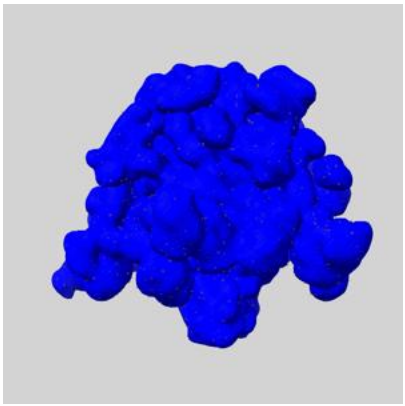
6.6.1 emd_19641_msk_1.map (i)



X



Y

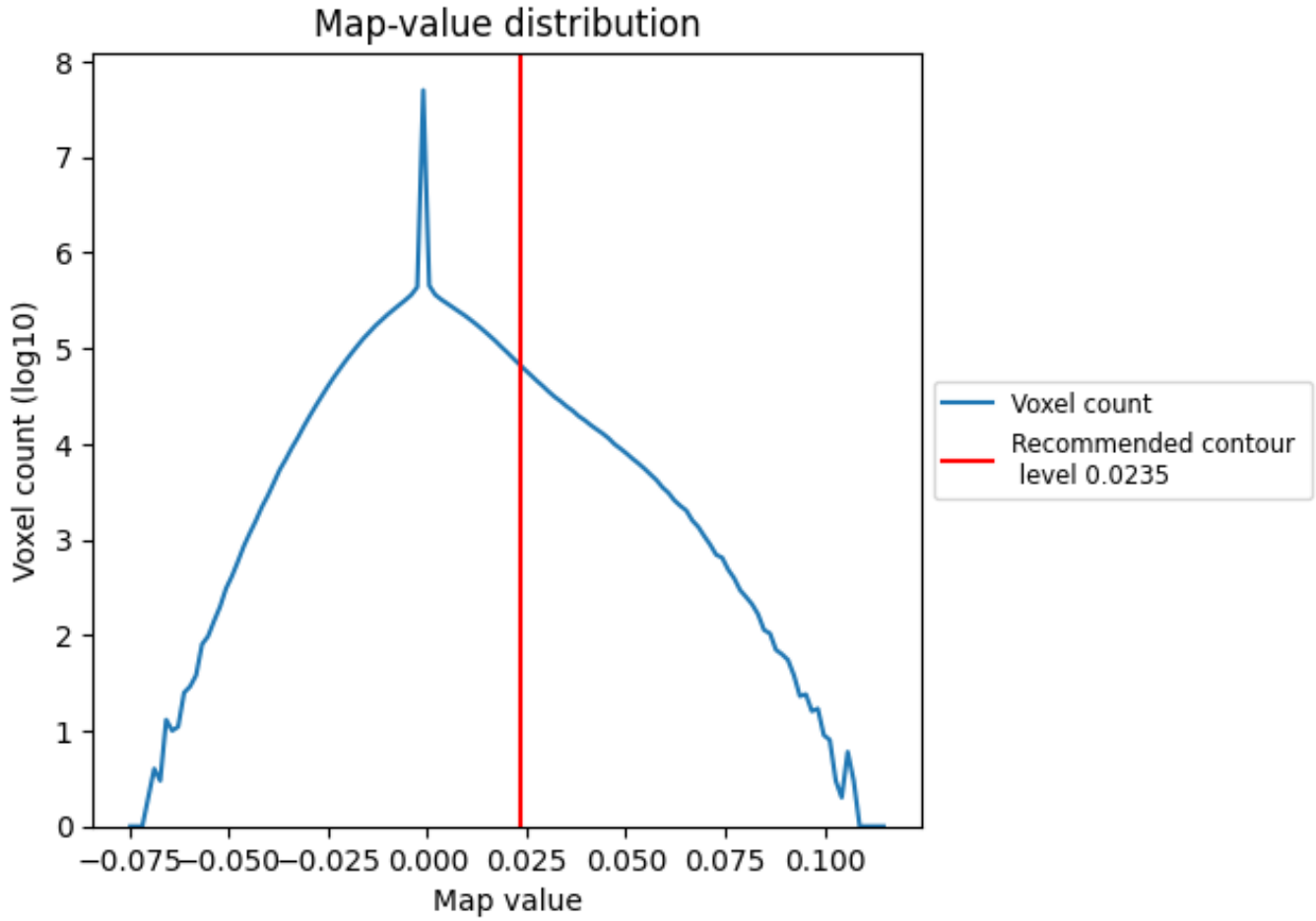


Z

7 Map analysis

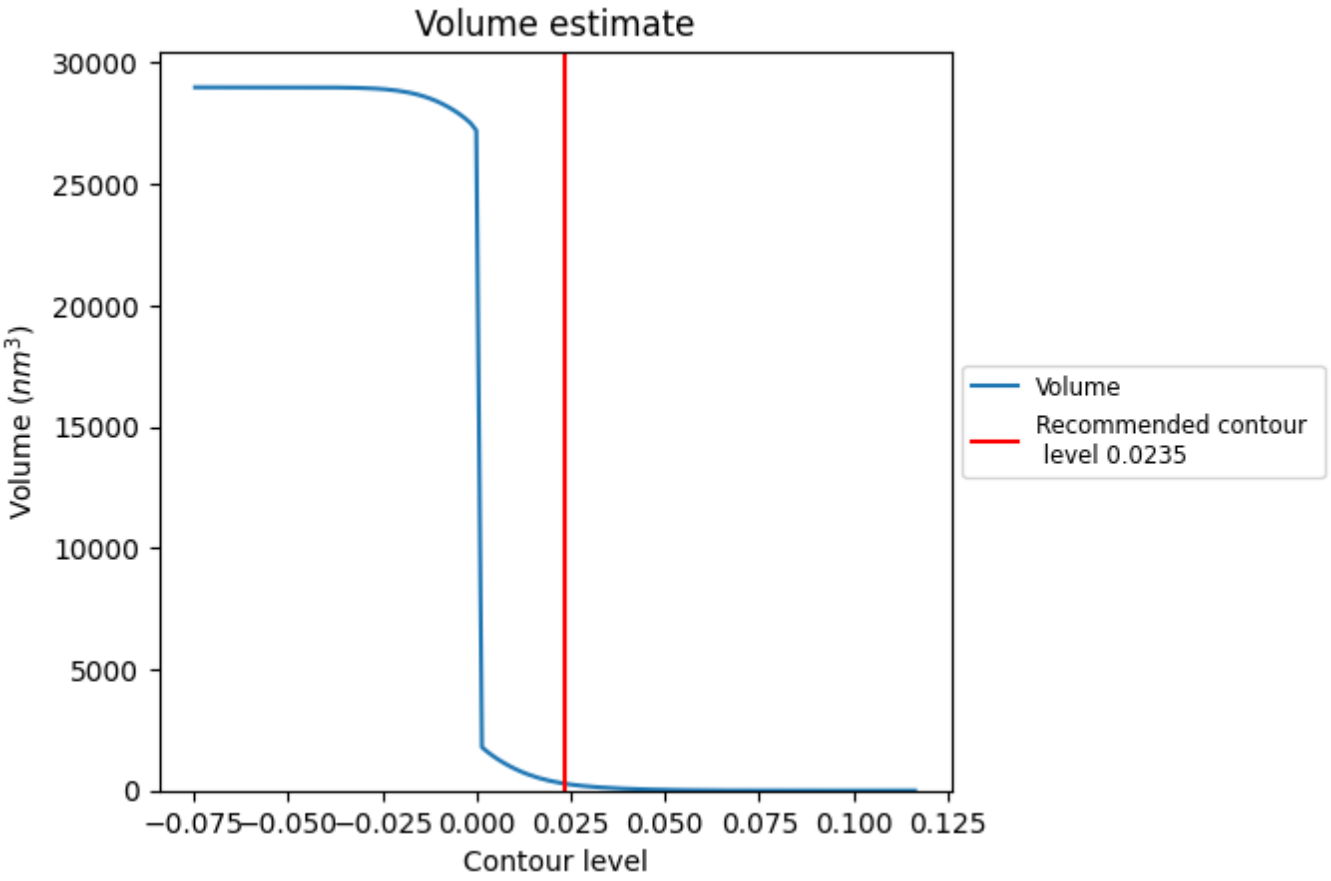
This section contains the results of statistical analysis of the map.

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.

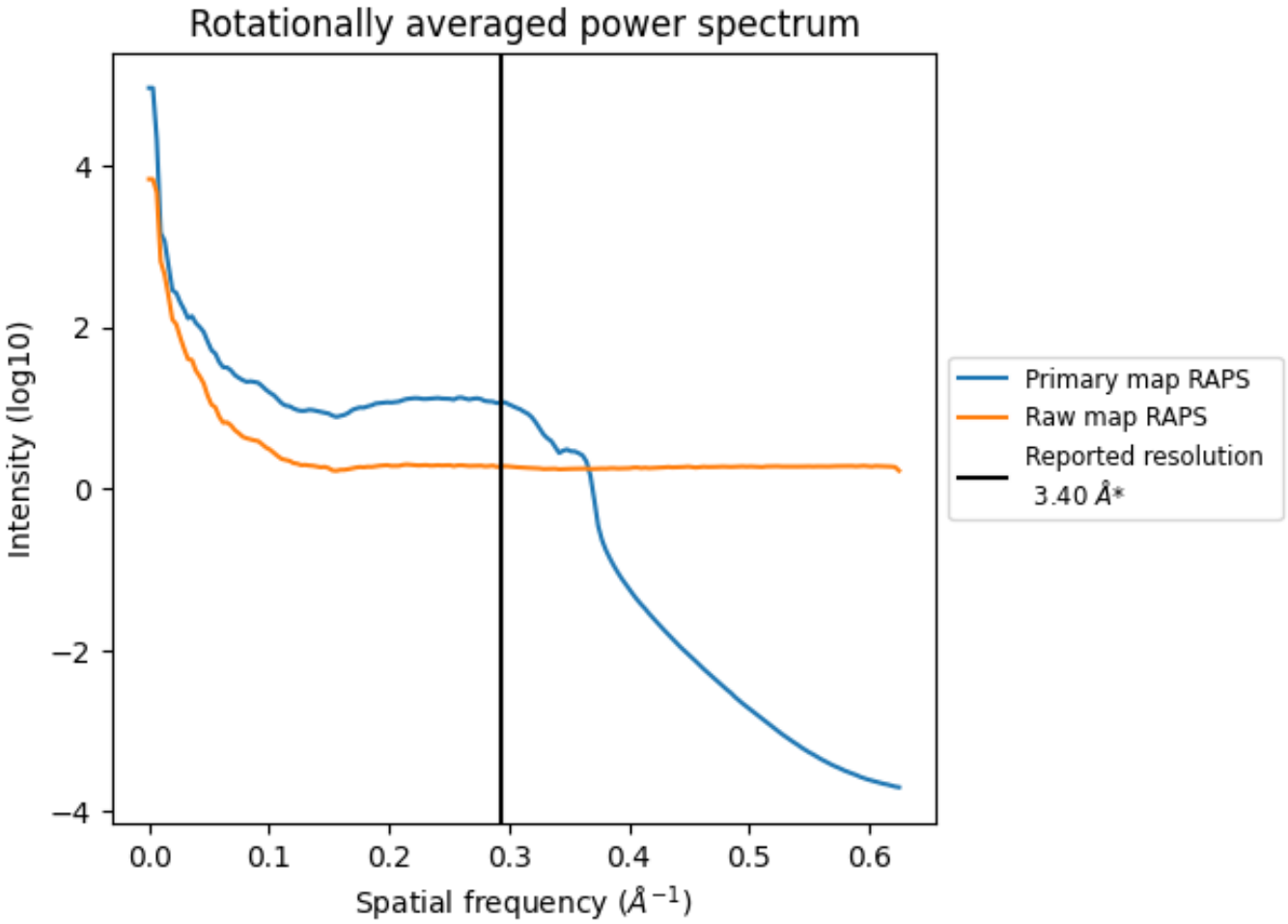
7.2 Volume estimate



The volume at the recommended contour level is 284 nm^3; this corresponds to an approximate mass of 257 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)

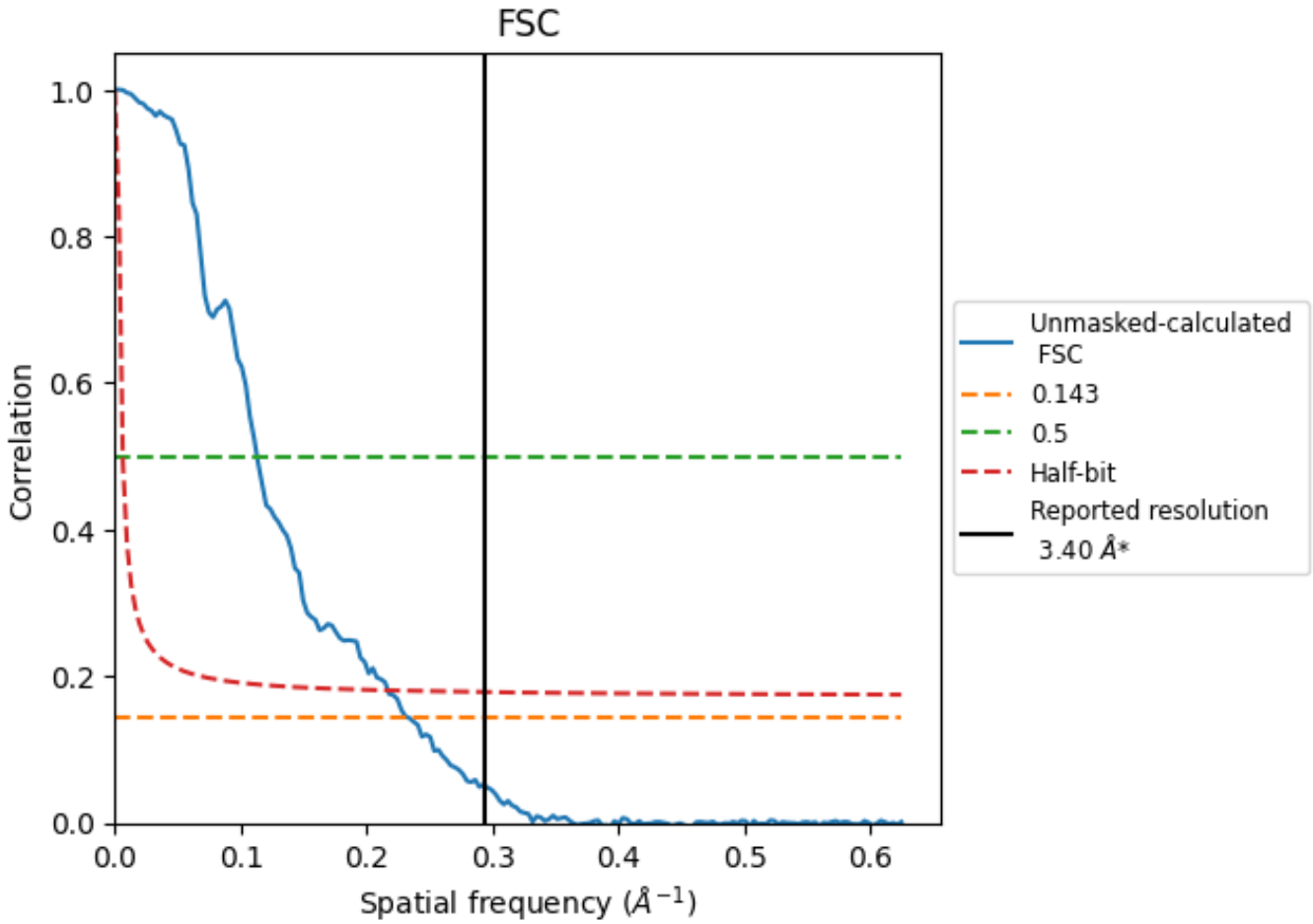


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

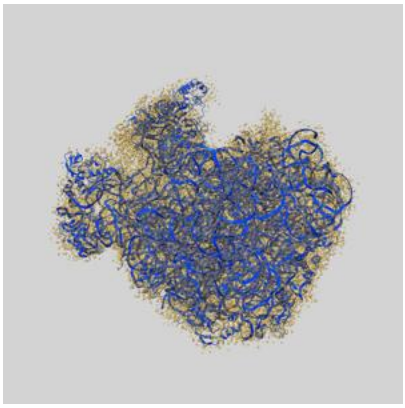
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	8.85	4.61

*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 4.28 differs from the reported value 3.4 by more than 10 %

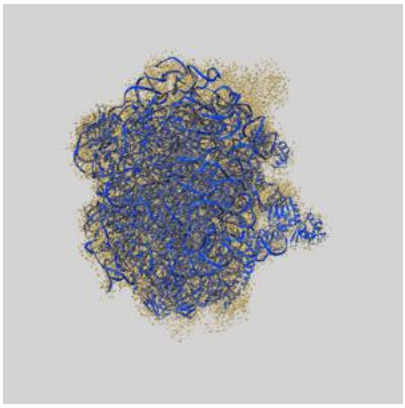
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19641 and PDB model 8S1U. Per-residue inclusion information can be found in section 3 on page 10.

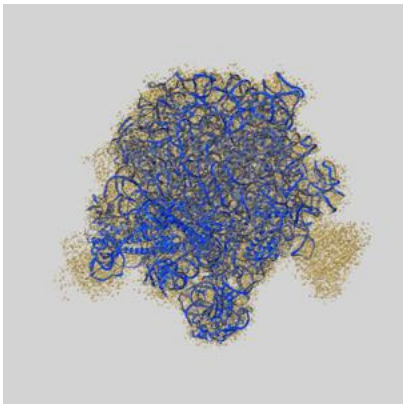
9.1 Map-model overlay



X



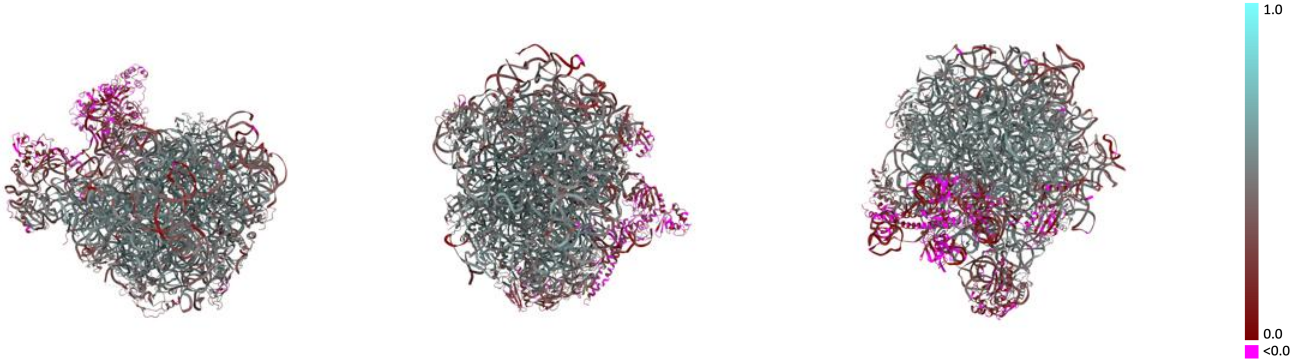
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0235 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.

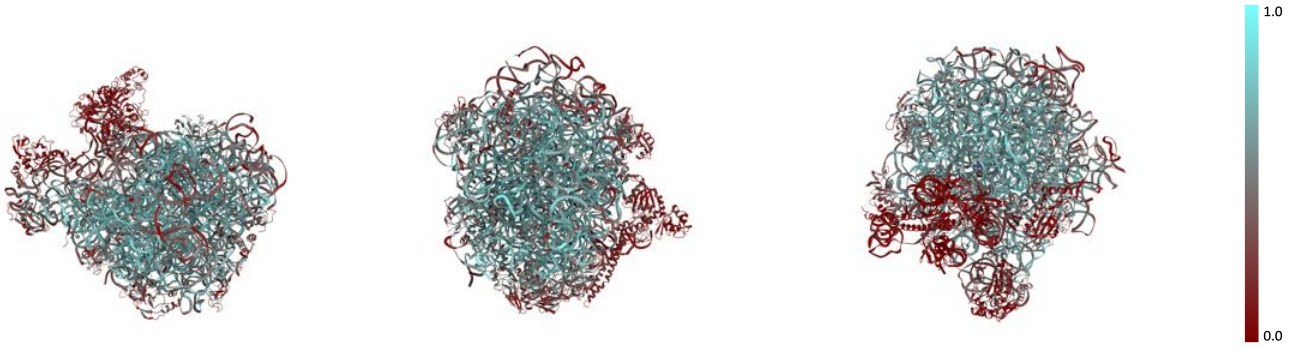
9.2 Q-score mapped to coordinate model (i)



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.

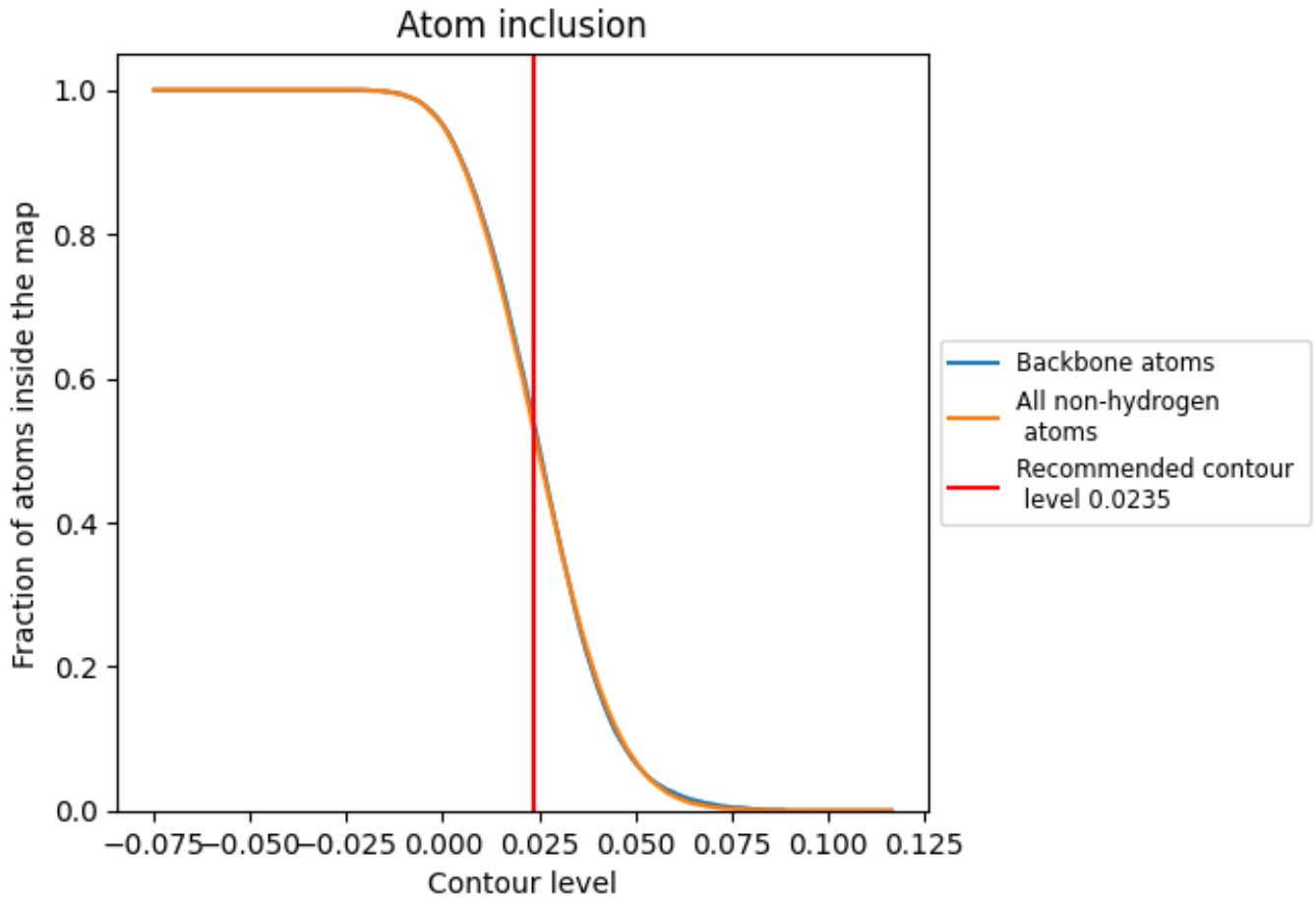
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0235).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 53% 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 (0.0235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5340	0.4480
0	0.5360	0.4960
1	0.5090	0.4580
2	0.6530	0.5460
3	0.5610	0.5390
4	0.4910	0.5090
6	0.0170	0.0400
A	0.6240	0.4940
B	0.4530	0.4040
C	0.5440	0.5060
D	0.5200	0.4970
E	0.4690	0.4550
F	0.1080	0.1600
G	0.2240	0.2630
H	0.0370	0.0380
J	0.5510	0.4940
K	0.4540	0.4820
L	0.4790	0.4650
M	0.5360	0.4880
N	0.5230	0.4850
O	0.3280	0.3710
P	0.4280	0.4350
Q	0.5880	0.5220
R	0.4650	0.4590
S	0.5010	0.5090
T	0.4130	0.4250
U	0.3360	0.3740
V	0.1560	0.1900
W	0.5640	0.4970
X	0.3920	0.4570
Y	0.3190	0.3850
Z	0.5090	0.4560
a	0.2490	0.2530
c	0.0570	0.1180