Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 07:05 am BST

PDB ID	:	8QPP
EMDB ID	:	EMD-18558
Title	:	Bacillus subtilis MutS2-collided disome complex (stalled 70S)
Authors	:	Park, E.; Mackens-Kiani, T.; Berhane, R.; Esser, H.; Erdenebat, C.; Burroughs, A.M.; Berninghausen, O.; Aravind, L.; Beckmann, R.; Green, R.; Buskirk, A.R.
Deposited on	:	2023-10-02
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:

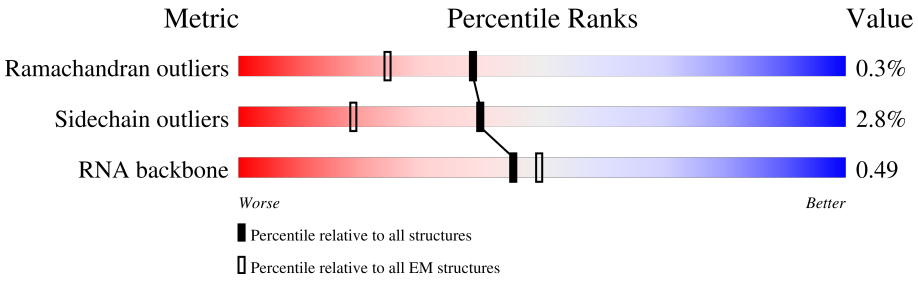
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	59	88% · 8%
2	1	48	8% 98% ·
3	2	44	· 100%
4	3	66	94% · ·
5	4	37	· 100%
6	6	64	9% 97% · ·
7	B	246	10% 85% · 11%
8	C	218	· 92% · 6%

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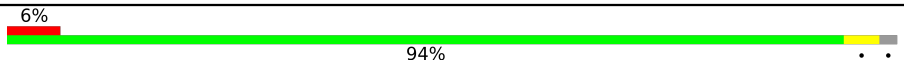
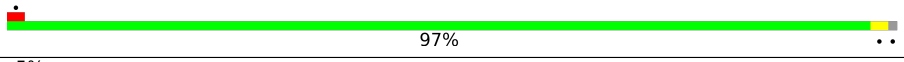
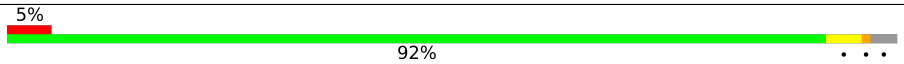
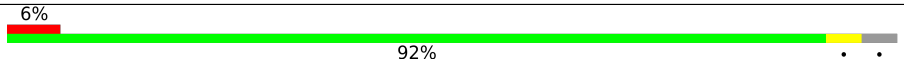
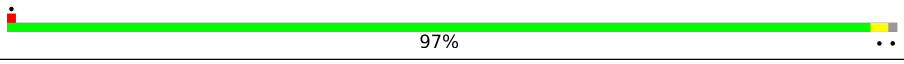
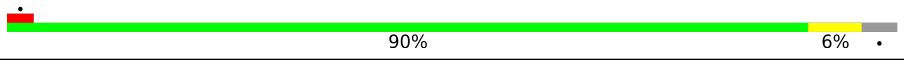
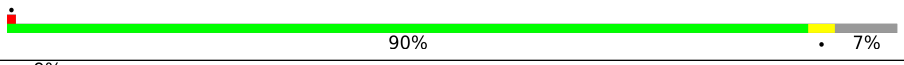
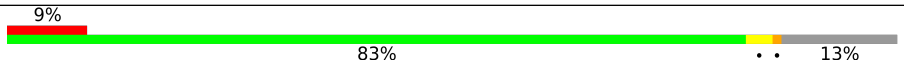
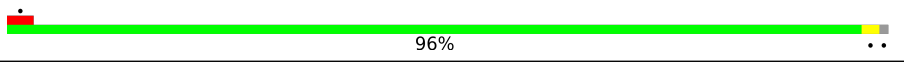
Mol	Chain	Length	Quality of chain
9	D	200	
10	E	166	
11	F	95	
12	G	156	
13	H	132	
14	I	130	
15	J	102	
16	K	131	
17	L	138	
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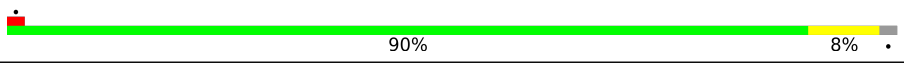
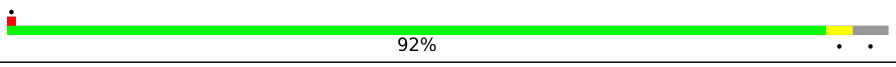
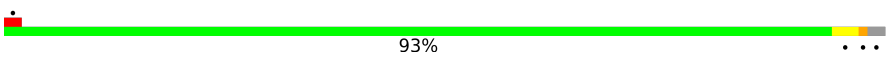
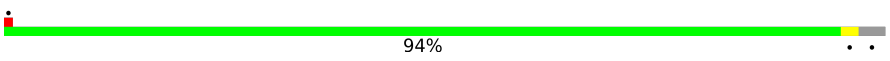
19	N	61	
20	O	89	
21	P	90	
22	Q	87	
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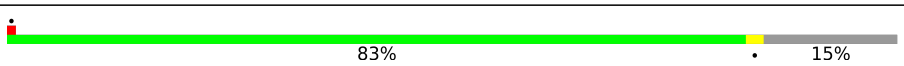
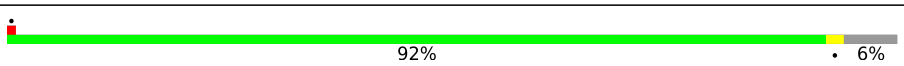
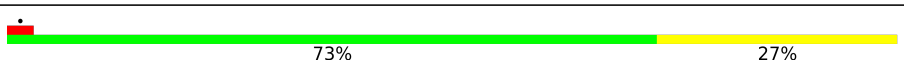
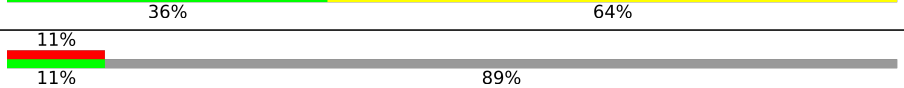
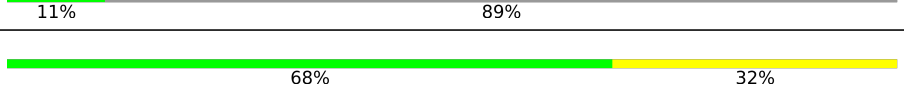
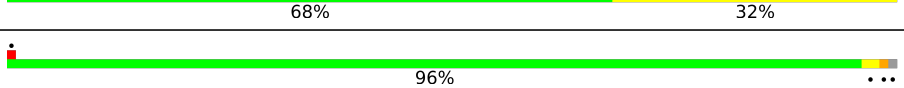
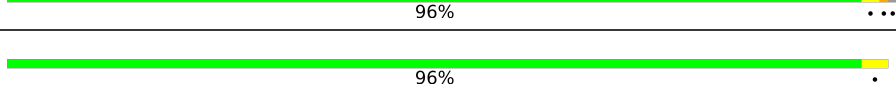
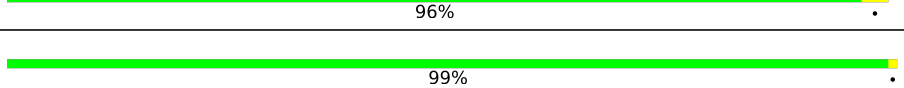
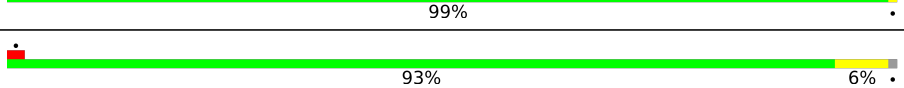
24	S	92	
25	T	88	
26	U	77	
27	V	33	
28	W	785	
29	Y	112	
30	Z	275	
31	a	207	
32	b	205	
33	c	178	

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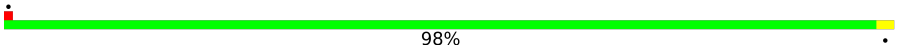
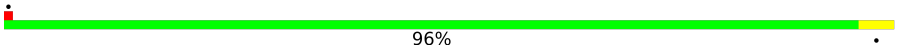
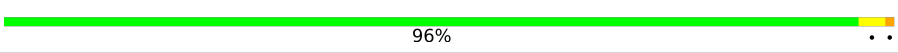
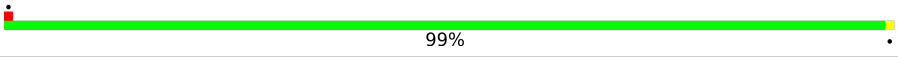
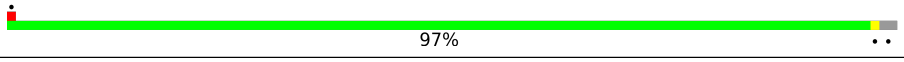
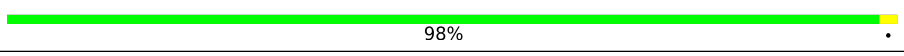
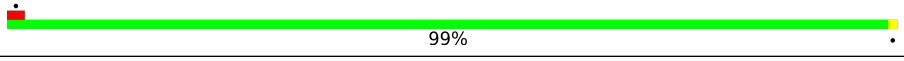
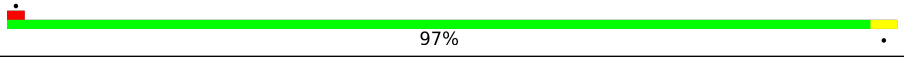
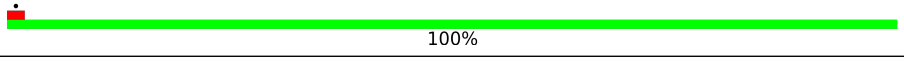
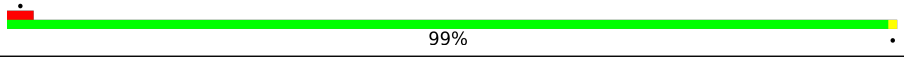
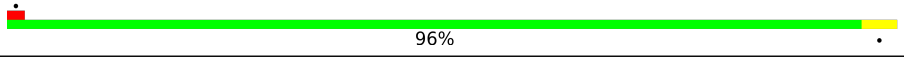
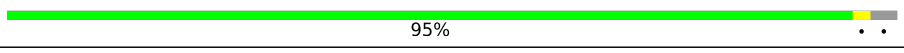
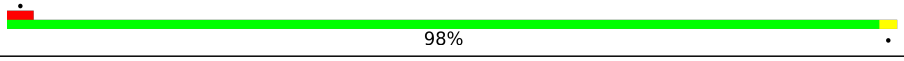
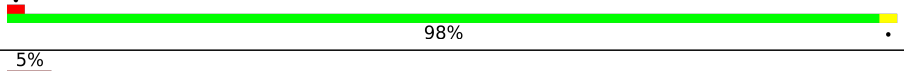
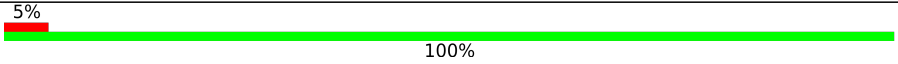
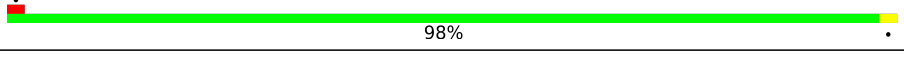
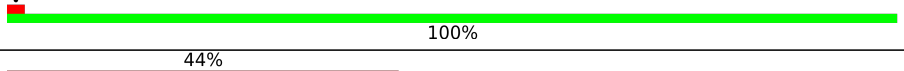
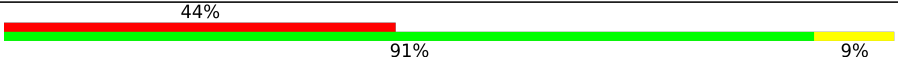
Mol	Chain	Length	Quality of chain
34	d	175	
35	e	142	
36	f	122	
37	i	146	
38	j	138	
39	k	119	
40	l	120	
41	m	115	
42	n	117	
43	o	101	
44	r	109	
45	s	93	
46	t	101	
47	u	82	
48	v	58	
49	w	65	
50	x	58	
51	9	149	
52	X	2928	
53	A	1533	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 237112 atoms, of which 94493 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	0	54	872	262	446	86	71	7	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	1	48	815	244	413	80	74	4	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2	44	778	222	410	89	55	2	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	3	64	1075	321	563	107	82	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	48	SER	ALA	conflict	UNP A0A063XFQ7

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	4	37	639	186	342	60	46	5	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	6	63	Total	C	H	N	O	S	0	0
			990	312	491	91	91	5		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	B	218	Total	C	H	N	O	S	0	0
			3588	1119	1831	309	323	6		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	C	206	Total	C	H	N	O	S	0	0
			3278	1011	1659	304	301	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	D	195	Total	C	H	N	O	S	0	0
			3174	991	1605	291	285	2		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	E	164	Total	C	H	N	O	S	0	0
			2520	767	1301	225	225	2		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	F	92	Total	C	H	N	O	S	0	0
			1502	476	747	132	146	1		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	G	149	Total	C	H	N	O	S	0	0
			2417	740	1236	220	215	6		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	H	131	Total	C	H	N	O	S	0	0
			2133	655	1096	191	188	3		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	I	125	Total	C	H	N	O	S	0	0
			1972	599	1006	191	175	1		

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	J	95	Total	C	H	N	O	S	0	0
			1557	479	796	139	141	2		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	K	114	Total	C	H	N	O	S	0	0
			1694	516	855	164	157	2		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	L	136	Total	C	H	N	O	S	0	0
			2164	653	1112	211	186	2		

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	108	Total	C	H	N	O	0	0
			1794	534	926	176	158		

- Molecule 19 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	N	60	Total	C	H	N	O	S	0	0
			1030	317	532	98	78	5		

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	O	85	Total	C	H	N	O	S	0	0
			1446	436	736	144	129	1		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	P	88	Total	C	H	N	O	S	0	0
			1417	441	722	128	124	2		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Q	84	Total	C	H	N	O	S	0	0
			1420	435	729	128	126	2		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	R	64	Total	C	H	N	O	S	0	0
			1074	332	556	96	88	2		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	S	78	Total	C	H	N	O	S	0	0
			1283	409	650	112	110	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	T	83	Total	C	H	N	O	S	0	0
			1334	390	697	130	116	1		

- Molecule 26 is a RNA chain called tRNA (77-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
26	U	77	Total	C	H	N	O	P	0	0
			2474	731	831	290	545	77		

- Molecule 27 is a RNA chain called mRNA (33-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
27	V	33	Total	C	H	N	O	P	0	0
			1063	315	359	130	226	33		

- Molecule 28 is a protein called Endonuclease MutS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	86	Total	C	H	N	O	0	0
			1335	411	673	124	127		

- Molecule 29 is a RNA chain called 5S rRNA (112-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Y	112	Total	C	H	N	O	P	0	0
			3605	1068	1213	435	778	111		

- Molecule 30 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	Z	272	Total	C	H	N	O	S	0	0
			4254	1296	2171	408	373	6		

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	a	206	Total	C	H	N	O	S	0	0
			3209	985	1640	289	290	5		

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	b	205	Total	C	H	N	O	S	0	0
			3211	980	1649	289	291	2		

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	c	176	Total	C	H	N	O	S	0	0
			2835	882	1449	241	256	7		

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	d	175	Total	C	H	N	O	S	0	0
			2734	835	1391	248	258	2		

- Molecule 35 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	e	142	Total	C	H	N	O	S	0	0
			2289	710	1165	206	203	5		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	f	122	Total	C	H	N	O	S	0	0
			1898	571	977	173	173	4		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	i	146	Total	C	H	N	O	S	0	0
			2214	671	1132	207	202	2		

- Molecule 38 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	j	135	Total	C	H	N	O	S	0	0
			2221	690	1145	205	176	5		

- Molecule 39 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	k	119	Total	C	H	N	O	S	0	0
			1940	583	986	186	181	4		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	l	120	Total	C	H	N	O	S	0	0
			1860	564	947	176	172	1		

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	m	115	Total	C	H	N	O	S	0	0
			1965	600	1020	185	159	1		

- Molecule 42 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	n	117	Total	C	H	N	O	S	0	0
			1948	591	1007	189	157	4		

- Molecule 43 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	101	Total	C	H	N	O	0	0
			1616	501	829	139	147		

- Molecule 44 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	r	109	Total	C	H	N	O	S	0	0
			1745	525	902	164	151	3		

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	s	90	Total	C	H	N	O	S	0	0
			1496	452	771	134	136	3		

- Molecule 46 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	t	101	Total	C	H	N	O	S	0	0
			1584	478	821	142	139	4		

- Molecule 47 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	82	Total	C	H	N	O	0	0
			1278	390	647	123	118		

- Molecule 48 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	v	58	Total	C	H	N	O	S	0	0
			935	275	490	92	76	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	w	65	Total	C	H	N	O	S	0	0
			1099	328	568	102	99	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	x	58	Total	C	H	N	O	S	0	0
			950	281	494	89	85	1		

- Molecule 51 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	9	149	Total	C	N	O	0	0
			733	435	149	149		

- Molecule 52 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	X	2887	Total	C	H	N	O	P	0	0
			93205	27661	31200	11460	19998	2886		

- Molecule 53 is a RNA chain called 16S rRNA (1533-MER).

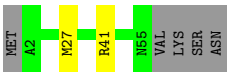
Mol	Chain	Residues	Atoms						AltConf	Trace
53	A	1533	Total	C	H	N	O	P	0	0
			49450	14667	16559	6034	10657	1533		

3 Residue-property plots (i)

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

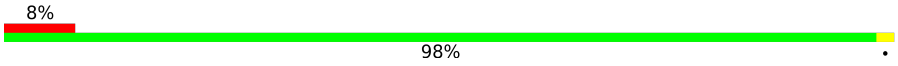
• Molecule 1: 50S ribosomal protein L32

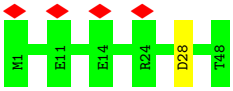
Chain 0:



• Molecule 2: Large ribosomal subunit protein bL33

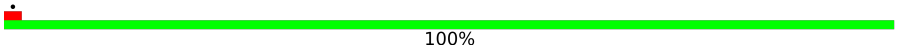
Chain 1:





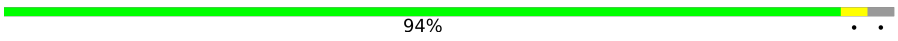
• Molecule 3: Large ribosomal subunit protein bL34

Chain 2:



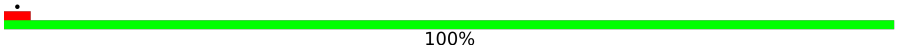
• Molecule 4: Large ribosomal subunit protein bL35

Chain 3:



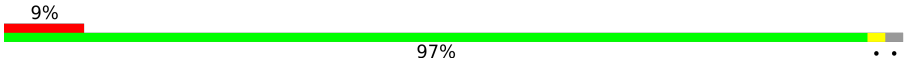
• Molecule 5: 50S ribosomal protein L36

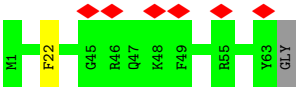
Chain 4:



• Molecule 6: Large ribosomal subunit protein bL31

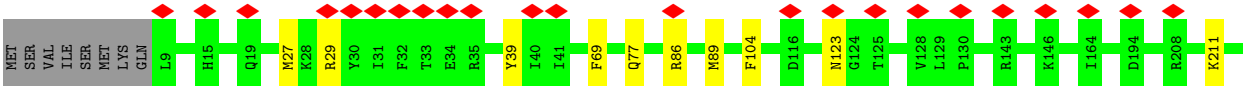
Chain 6:

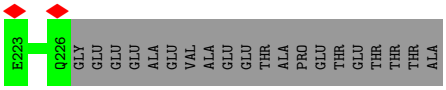




• Molecule 7: 30S ribosomal protein S2

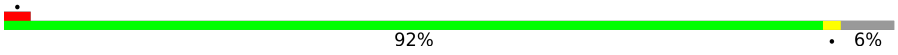
Chain B:

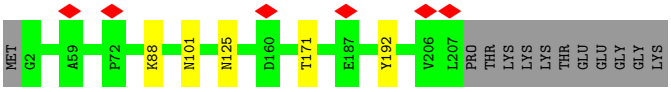




• Molecule 8: 30S ribosomal protein S3

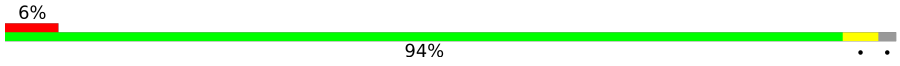
Chain C:

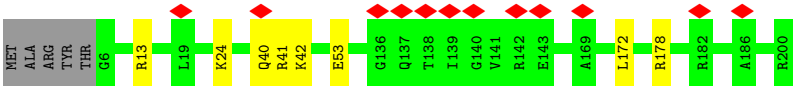




• Molecule 9: 30S ribosomal protein S4

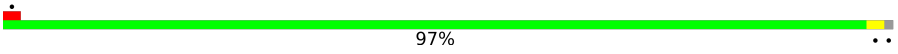
Chain D:

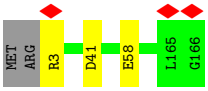




• Molecule 10: 30S ribosomal protein S5

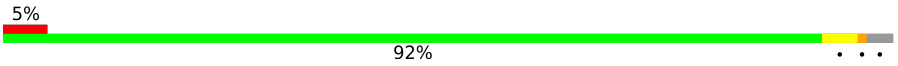
Chain E:

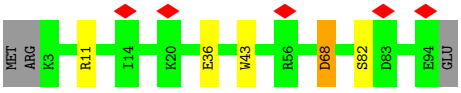




• Molecule 11: 30S ribosomal protein S6

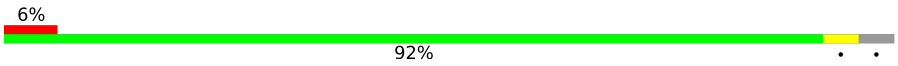
Chain F:

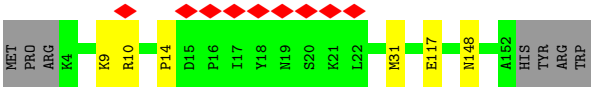




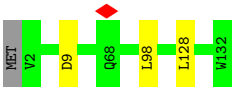
• Molecule 12: 30S ribosomal protein S7

Chain G:

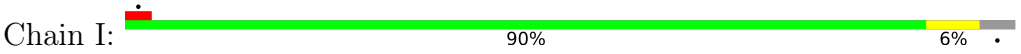


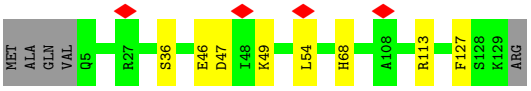


• Molecule 13: 30S ribosomal protein S8

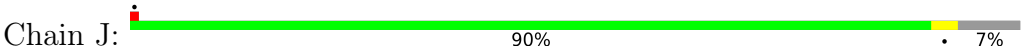


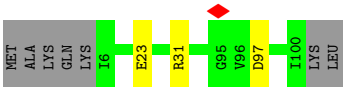
• Molecule 14: 30S ribosomal protein S9



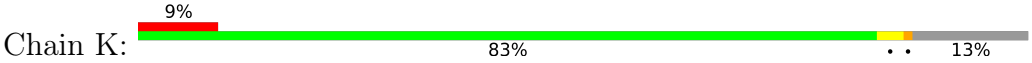


• Molecule 15: 30S ribosomal protein S10



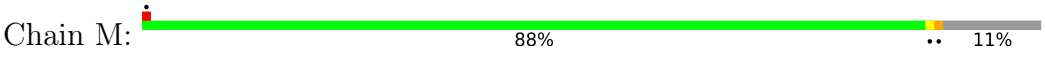


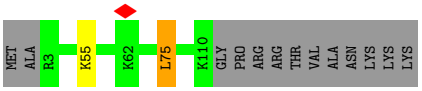
• Molecule 16: 30S ribosomal protein S11



• Molecule 17: 30S ribosomal protein S12

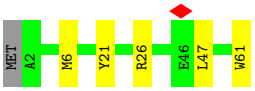
• Molecule 18: 30S ribosomal protein S13





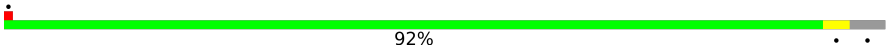
• Molecule 19: 30S ribosomal protein S14 type Z

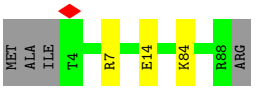
Chain N:



• Molecule 20: 30S ribosomal protein S15

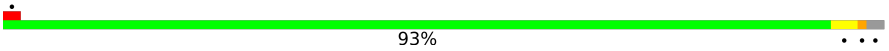
Chain O:

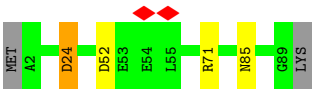




• Molecule 21: 30S ribosomal protein S16

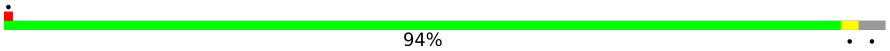
Chain P:

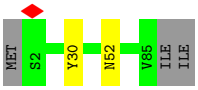




• Molecule 22: 30S ribosomal protein S17

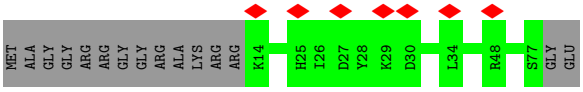
Chain Q:





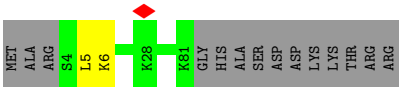
• Molecule 23: 30S ribosomal protein S18

Chain R:



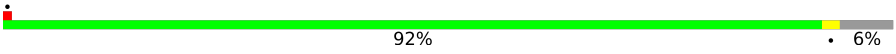
• Molecule 24: 30S ribosomal protein S19

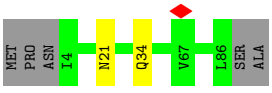
Chain S:



• Molecule 25: 30S ribosomal protein S20

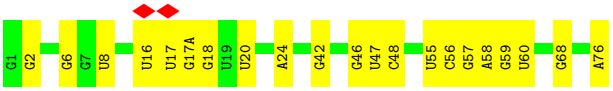
Chain T:





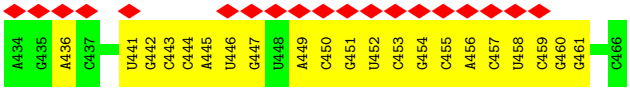
• Molecule 26: tRNA (77-MER)

Chain U:



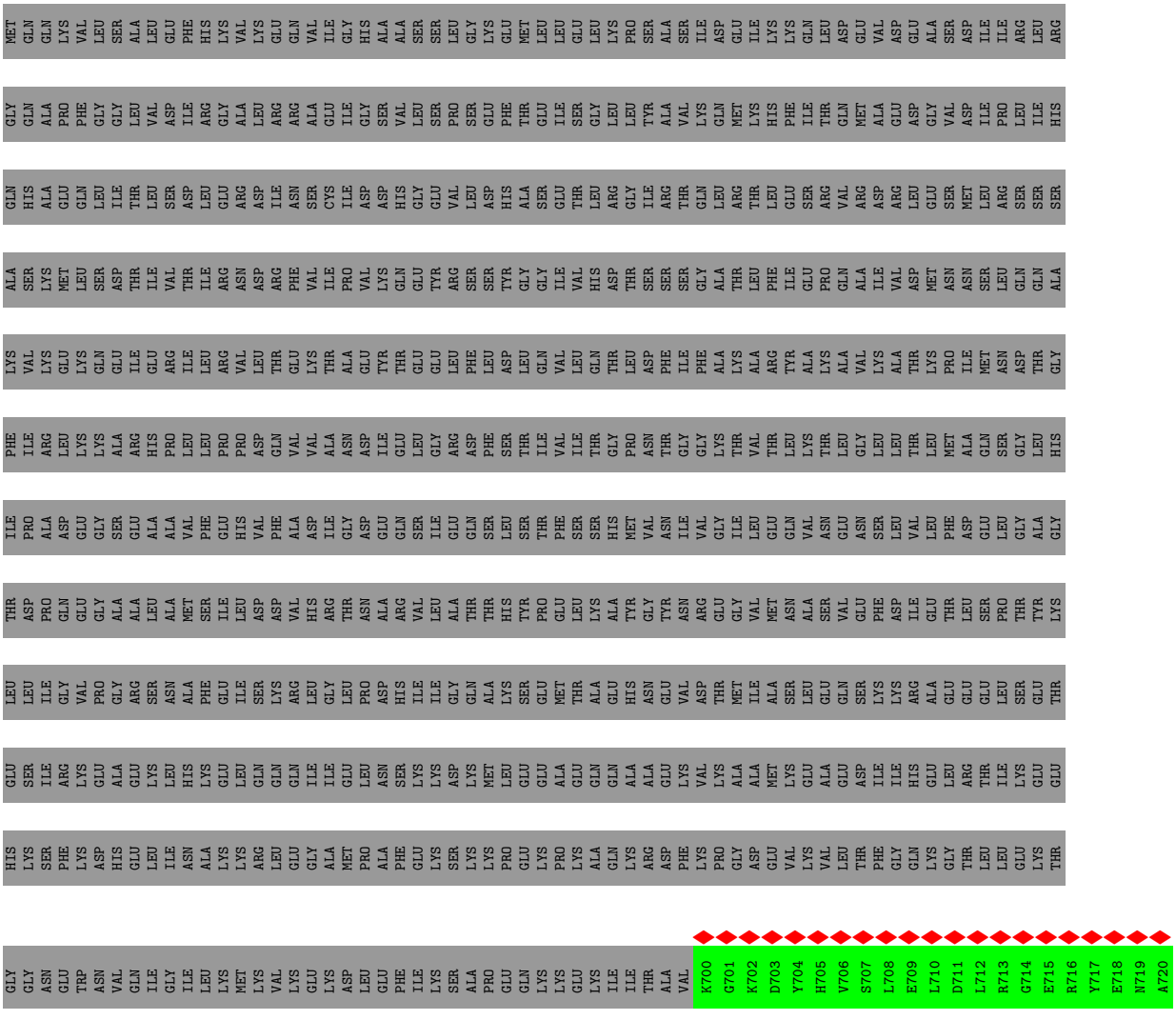
• Molecule 27: mRNA (33-MER)

Chain V:



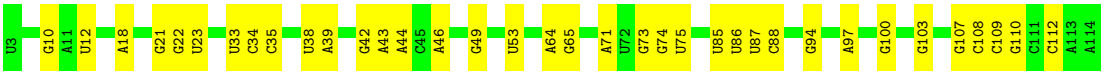
• Molecule 28: Endonuclease MutS2

Chain W:



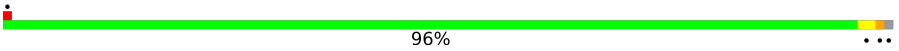
• Molecule 29: 5S rRNA (112-MER)

Chain Y:



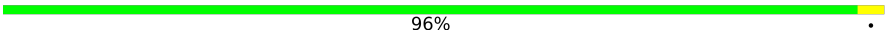
• Molecule 30: Large ribosomal subunit protein uL2

Chain Z:



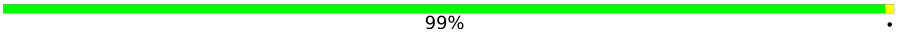
• Molecule 31: Large ribosomal subunit protein uL3

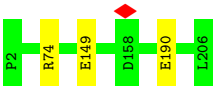
Chain a:



• Molecule 32: Large ribosomal subunit protein uL4

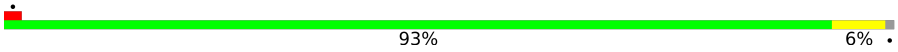
Chain b:

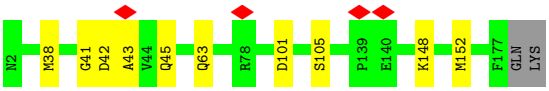




• Molecule 33: Large ribosomal subunit protein uL5

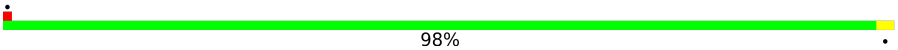
Chain c:

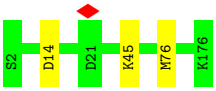




• Molecule 34: Large ribosomal subunit protein uL6

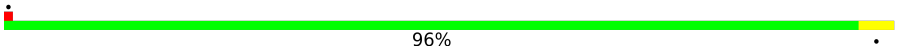
Chain d:





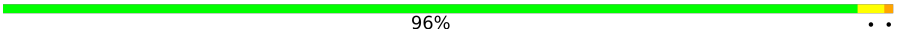
• Molecule 35: Large ribosomal subunit protein uL13

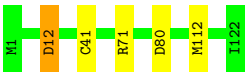
Chain e:



• Molecule 36: 50S ribosomal protein L14

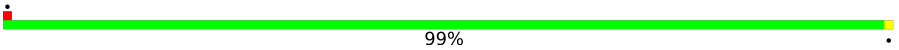
Chain f:

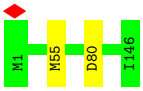




• Molecule 37: 50S ribosomal protein L15

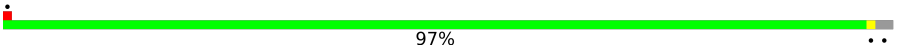
Chain i:

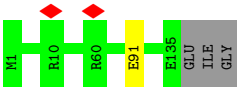




• Molecule 38: Large ribosomal subunit protein uL16

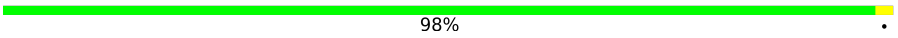
Chain j:





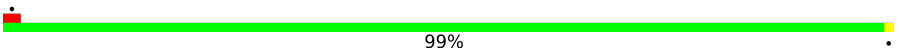
• Molecule 39: Large ribosomal subunit protein bL17

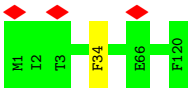
Chain k:



• Molecule 40: 50S ribosomal protein L18

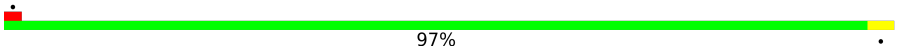
Chain l:





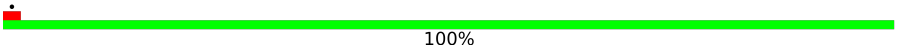
• Molecule 41: 50S ribosomal protein L19

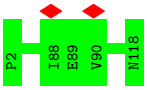
Chain m:



• Molecule 42: Large ribosomal subunit protein bL20

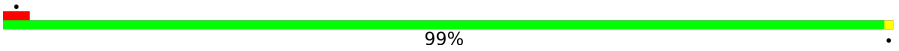
Chain n:

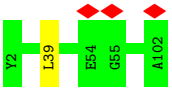




• Molecule 43: Large ribosomal subunit protein bL21

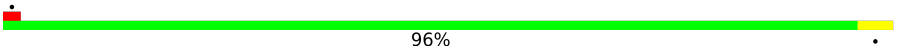
Chain o:

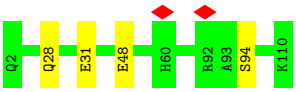




• Molecule 44: Large ribosomal subunit protein uL22

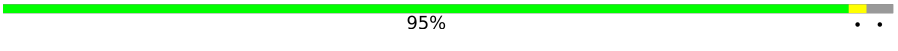
Chain r:





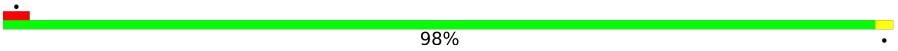
• Molecule 45: Large ribosomal subunit protein uL23

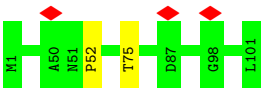
Chain s:



• Molecule 46: Large ribosomal subunit protein uL24

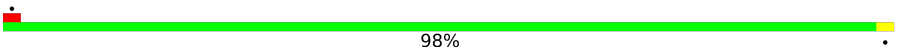
Chain t:

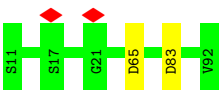




• Molecule 47: Large ribosomal subunit protein bL27

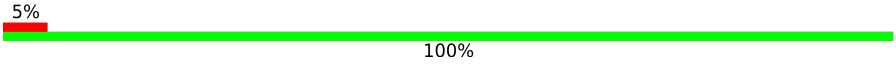
Chain u:

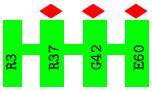




• Molecule 48: Large ribosomal subunit protein bL28

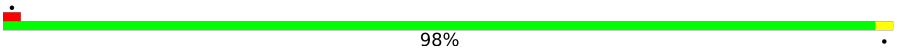
Chain v:

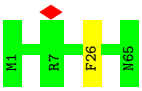




• Molecule 49: Large ribosomal subunit protein uL29

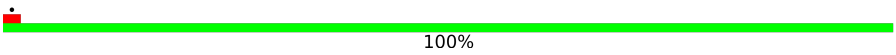
Chain w:





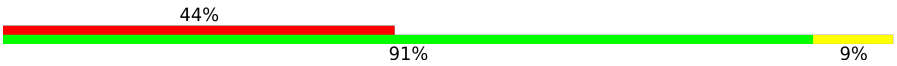
• Molecule 50: Large ribosomal subunit protein uL30

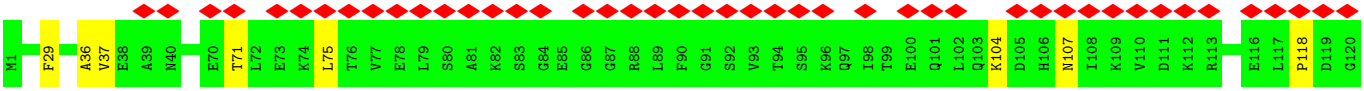
Chain x:

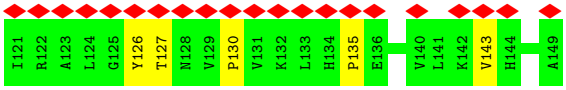


• Molecule 51: 50S ribosomal protein L9

Chain 9:

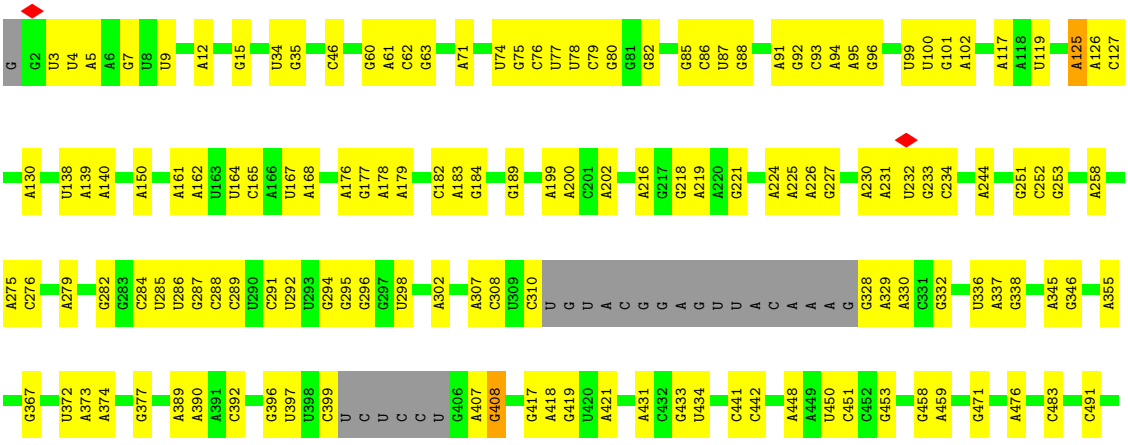


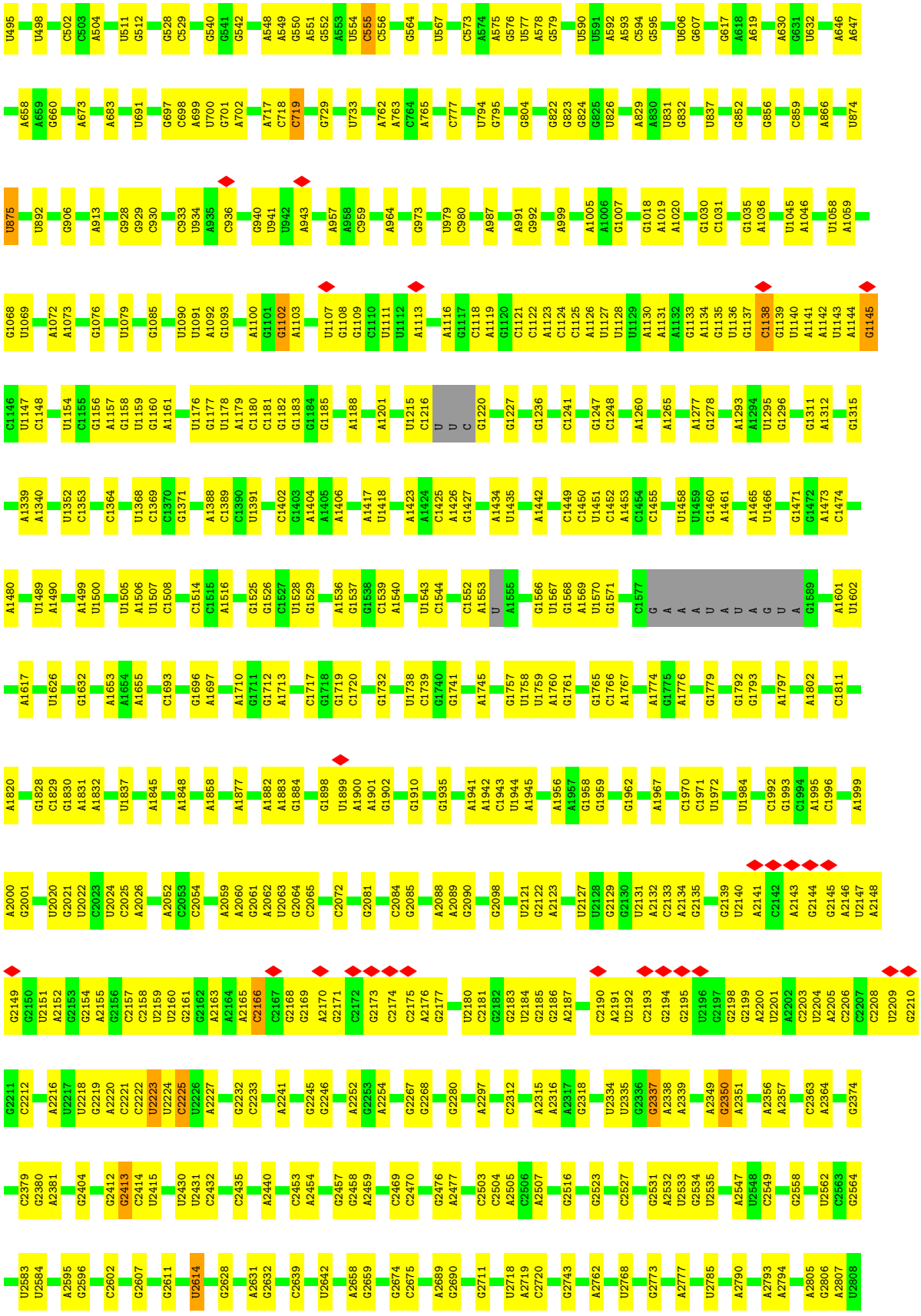


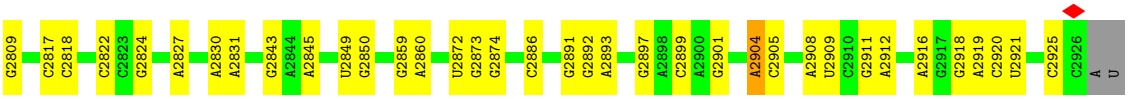


• Molecule 52: 23S ribosomal RNA

Chain X:

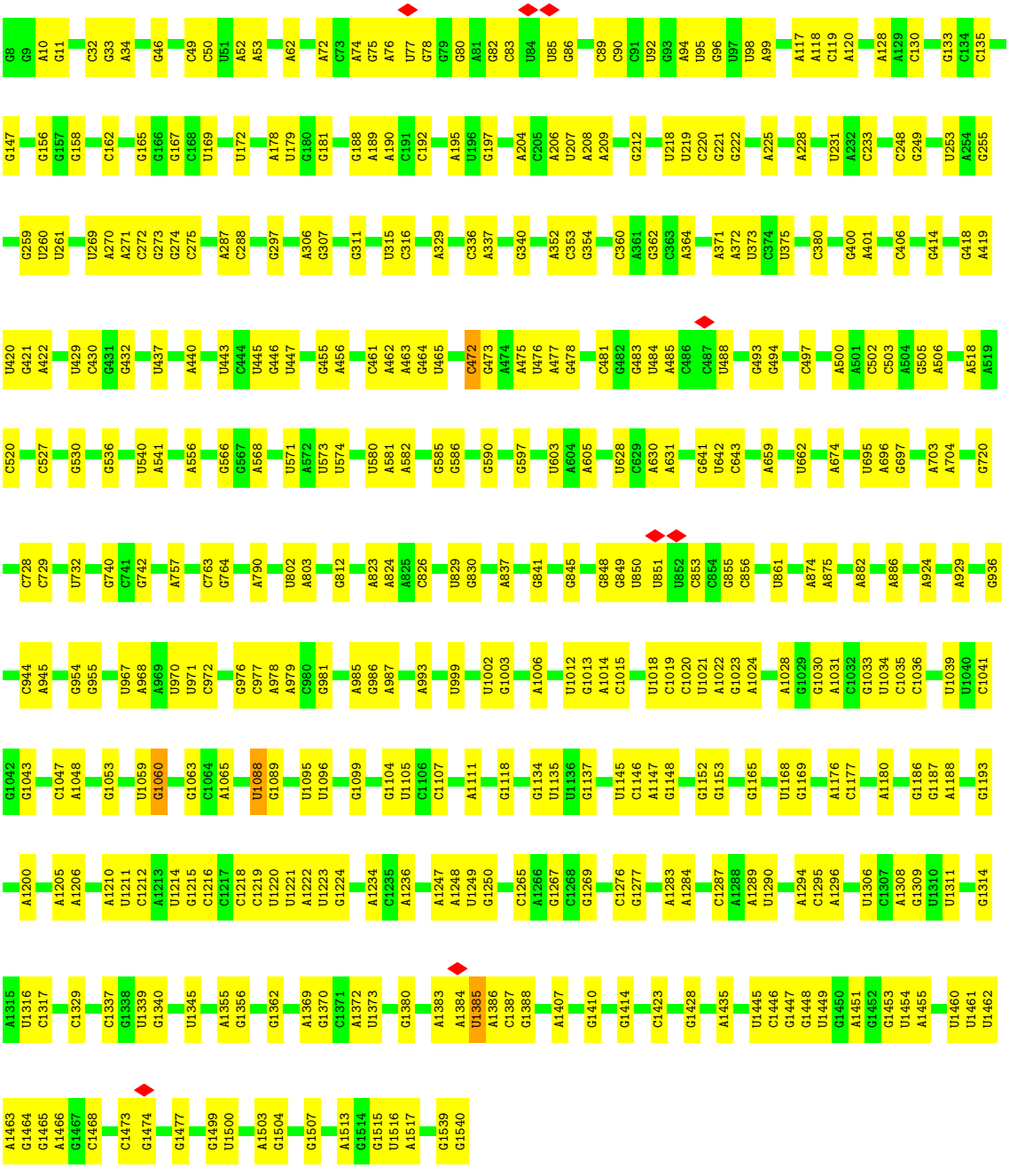






• Molecule 53: 16S rRNA (1533-MER)

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11740	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 ($e^-/Å^2$)	43.6	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.923	Depositor
Minimum map value	-0.737	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.377	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.31	0/433	0.71	0/574
2	1	0.32	0/407	0.71	0/540
3	2	0.27	0/371	0.80	0/483
4	3	0.26	0/519	0.62	0/680
5	4	0.31	0/300	0.68	0/393
6	6	0.30	0/509	0.60	0/678
7	B	0.30	0/1782	0.69	1/2392 (0.0%)
8	C	0.27	0/1641	0.65	0/2208
9	D	0.32	0/1599	0.69	0/2147
10	E	0.29	0/1231	0.65	0/1655
11	F	0.35	0/766	0.75	1/1031 (0.1%)
12	G	0.36	0/1196	0.80	1/1604 (0.1%)
13	H	0.33	0/1049	0.76	2/1407 (0.1%)
14	I	0.31	0/979	0.76	1/1315 (0.1%)
15	J	0.32	0/773	0.75	1/1044 (0.1%)
16	K	0.32	0/853	0.74	1/1153 (0.1%)
17	L	0.28	0/1069	0.67	0/1435
18	M	0.30	0/873	0.78	1/1166 (0.1%)
19	N	0.33	0/508	0.74	0/672
20	O	0.30	0/718	0.70	0/960
21	P	0.32	0/708	0.72	2/950 (0.2%)
22	Q	0.33	0/699	0.71	0/933
23	R	0.32	0/526	0.75	0/705
24	S	0.30	0/649	0.64	0/872
25	T	0.30	0/639	0.66	0/852
26	U	0.30	0/1834	0.81	0/2858
27	V	0.23	0/787	0.82	0/1224
28	W	0.25	0/670	0.58	0/894
29	Y	0.34	0/2675	0.89	2/4170 (0.0%)
30	Z	0.28	0/2120	0.67	4/2845 (0.1%)
31	a	0.28	0/1591	0.64	2/2132 (0.1%)
32	b	0.29	0/1581	0.62	0/2132
33	c	0.32	0/1405	0.64	1/1887 (0.1%)
34	d	0.30	0/1361	0.66	0/1832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	e	0.28	0/1147	0.63	0/1542
36	f	0.32	0/928	0.78	2/1245 (0.2%)
37	i	0.29	0/1094	0.61	0/1457
38	j	0.32	0/1099	0.72	0/1468
39	k	0.30	0/961	0.73	1/1284 (0.1%)
40	l	0.28	0/922	0.69	0/1236
41	m	0.30	0/958	0.74	0/1279
42	n	0.29	0/953	0.63	0/1266
43	o	0.31	0/798	0.60	0/1070
44	r	0.30	0/852	0.71	0/1146
45	s	0.34	0/731	0.74	1/974 (0.1%)
46	t	0.32	0/773	0.69	1/1032 (0.1%)
47	u	0.30	0/639	0.69	1/847 (0.1%)
48	v	0.28	0/449	0.69	0/596
49	w	0.31	0/532	0.77	0/707
50	x	0.29	0/458	0.68	0/613
51	9	0.46	0/732	0.65	0/1016
52	X	0.37	0/69451	0.86	58/108344 (0.1%)
53	A	0.35	0/36826	0.85	20/57450 (0.0%)
All	All	0.35	0/155124	0.82	104/232395 (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
33	c	0	1

There are no bond length outliers.

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	X	138	U	OP1-P-O3'	-35.75	26.55	105.20
52	X	139	A	OP1-P-OP2	-13.65	99.13	119.60
46	t	52	PRO	CA-N-CD	-9.60	98.06	111.50
52	X	1970	C	C2-N1-C1'	8.98	128.68	118.80
53	A	1107	C	N3-C2-O2	-8.78	115.75	121.90
52	X	2166	C	C6-N1-C2	-8.72	116.81	120.30
29	Y	35	C	C6-N1-C2	-8.20	117.02	120.30
52	X	718	C	N1-C2-O2	8.07	123.74	118.90
52	X	1970	C	N1-C2-O2	7.79	123.57	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	472	C	N3-C2-O2	-7.71	116.50	121.90
52	X	167	U	C2-N1-C1'	7.46	126.65	117.70
52	X	1970	C	N3-C2-O2	-7.36	116.75	121.90
52	X	2614	U	C2-N1-C1'	7.31	126.47	117.70
53	A	1219	C	N3-C2-O2	-7.22	116.84	121.90
53	A	1060	G	N1-C6-O6	-7.11	115.63	119.90
52	X	328	G	OP1-P-OP2	-7.04	109.04	119.60
21	P	24	ASP	CB-CG-OD1	6.90	124.51	118.30
7	B	27	MET	CA-CB-CG	6.82	124.90	113.30
52	X	1220	G	OP1-P-OP2	-6.82	109.37	119.60
52	X	138	U	OP2-P-O3'	6.81	120.18	105.20
53	A	1385	U	N3-C2-O2	-6.77	117.46	122.20
52	X	2225	C	N3-C2-O2	-6.75	117.18	121.90
52	X	2503	C	C6-N1-C2	-6.73	117.61	120.30
52	X	1970	C	C6-N1-C2	-6.67	117.63	120.30
52	X	1352	U	C2-N1-C1'	6.57	125.59	117.70
53	A	1060	G	C5-C6-O6	6.54	132.52	128.60
52	X	1138	C	C6-N1-C2	-6.51	117.69	120.30
36	f	12	ASP	CB-CG-OD1	6.51	124.16	118.30
52	X	875	U	C2-N1-C1'	6.45	125.44	117.70
53	A	1047	C	C6-N1-C2	-6.36	117.76	120.30
11	F	68	ASP	CB-CG-OD1	6.34	124.00	118.30
52	X	2817	C	N3-C2-O2	-6.31	117.48	121.90
16	K	114	ASP	CB-CG-OD1	6.28	123.95	118.30
18	M	75	LEU	CA-CB-CG	6.20	129.56	115.30
14	I	47	ASP	CB-CG-OD1	6.19	123.88	118.30
52	X	1145	G	C4-N9-C1'	6.08	134.41	126.50
52	X	718	C	N3-C2-O2	-6.08	117.64	121.90
52	X	1970	C	C6-N1-C1'	-6.03	113.56	120.80
52	X	2212	C	N3-C2-O2	-5.98	117.71	121.90
52	X	1145	G	C8-N9-C1'	-5.96	119.26	127.00
52	X	1138	C	C5-C6-N1	5.94	123.97	121.00
52	X	719	C	C6-N1-C2	-5.93	117.93	120.30
52	X	1720	C	N1-C2-O2	5.82	122.39	118.90
53	A	1099	G	C5-C6-O6	5.82	132.09	128.60
53	A	1423	C	N3-C2-O2	-5.80	117.84	121.90
13	H	98	LEU	CA-CB-CG	5.79	128.63	115.30
52	X	719	C	N3-C2-O2	-5.79	117.85	121.90
53	A	1099	G	N1-C6-O6	-5.79	116.42	119.90
52	X	2357	A	N7-C8-N9	5.77	116.68	113.80
52	X	2614	U	N1-C2-O2	5.76	126.83	122.80
31	a	150	ASP	CB-CG-OD1	5.71	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	X	3	U	C2-N1-C1'	5.69	124.53	117.70
52	X	856	G	N1-C6-O6	-5.66	116.50	119.90
30	Z	66	ASP	CB-CG-OD1	5.63	123.36	118.30
52	X	2225	C	N1-C2-O2	5.63	122.28	118.90
52	X	856	G	C5-C6-O6	5.61	131.97	128.60
53	A	1219	C	C6-N1-C2	-5.61	118.06	120.30
36	f	71	ARG	NE-CZ-NH1	5.58	123.09	120.30
52	X	167	U	N3-C2-O2	-5.55	118.32	122.20
12	G	31	MET	CA-CB-CG	5.51	122.67	113.30
52	X	555	C	C6-N1-C2	-5.50	118.10	120.30
53	A	1385	U	C2-N1-C1'	5.49	124.29	117.70
53	A	1219	C	N1-C2-N3	5.49	123.04	119.20
52	X	167	U	N1-C2-O2	5.46	126.63	122.80
52	X	1720	C	N3-C2-O2	-5.46	118.08	121.90
30	Z	267	ASP	CB-CG-OD1	5.44	123.20	118.30
21	P	52	ASP	CB-CG-OD1	5.42	123.18	118.30
52	X	2337	G	P-O3'-C3'	5.42	126.21	119.70
30	Z	98	ASP	CB-CG-OD1	5.42	123.17	118.30
47	u	83	ASP	CB-CG-OD1	5.41	123.17	118.30
52	X	2413	G	P-O3'-C3'	5.39	126.17	119.70
52	X	2223	U	C2-N1-C1'	5.38	124.15	117.70
52	X	2614	U	N3-C2-O2	-5.36	118.44	122.20
52	X	2166	C	N3-C2-O2	-5.36	118.15	121.90
52	X	1102	G	O4'-C1'-N9	5.36	112.49	108.20
53	A	763	C	C2-N1-C1'	5.34	124.67	118.80
52	X	408	G	C8-N9-C1'	5.34	133.94	127.00
52	X	1145	G	N3-C4-N9	5.33	129.20	126.00
52	X	2357	A	C8-N9-C4	-5.32	103.67	105.80
53	A	472	C	C6-N1-C2	-5.32	118.17	120.30
53	A	1107	C	N1-C2-O2	5.30	122.08	118.90
52	X	1138	C	N1-C2-O2	5.29	122.07	118.90
39	k	78	ASP	CB-CG-OD1	5.28	123.06	118.30
29	Y	35	C	N3-C2-O2	-5.27	118.21	121.90
33	c	152	MET	CA-CB-CG	5.26	122.25	113.30
53	A	1088	U	C5-C6-N1	5.22	125.31	122.70
52	X	125	A	O4'-C1'-N9	-5.21	104.03	108.20
52	X	2221	C	O4'-C1'-N1	-5.21	104.03	108.20
52	X	167	U	C6-N1-C1'	-5.20	113.93	121.20
52	X	719	C	N1-C2-N3	5.19	122.83	119.20
13	H	9	ASP	CB-CG-OD1	5.18	122.96	118.30
45	s	19	ASP	CB-CG-OD1	5.17	122.96	118.30
53	A	1385	U	N1-C2-O2	5.13	126.39	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	X	979	U	O4'-C1'-N1	5.12	112.29	108.20
52	X	856	G	N3-C4-N9	-5.11	122.93	126.00
52	X	1247	G	O4'-C1'-N9	5.10	112.28	108.20
15	J	97	ASP	CB-CG-OD1	5.09	122.88	118.30
52	X	2904	A	P-O3'-C3'	5.07	125.78	119.70
53	A	472	C	N1-C2-O2	5.06	121.94	118.90
31	a	54	ASP	CB-CG-OD1	5.04	122.84	118.30
30	Z	20	ASP	CB-CG-OD1	5.04	122.83	118.30
52	X	2350	G	N3-C4-C5	-5.03	126.08	128.60
53	A	1385	U	C6-N1-C2	-5.02	117.99	121.00
52	X	2614	U	C6-N1-C1'	-5.02	114.17	121.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	c	43	ALA	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	52/59 (88%)	50 (96%)	2 (4%)	0	100	100
2	1	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
3	2	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
4	3	62/66 (94%)	58 (94%)	4 (6%)	0	100	100
5	4	35/37 (95%)	33 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	61/64 (95%)	52 (85%)	9 (15%)	0	100	100
7	B	216/246 (88%)	199 (92%)	17 (8%)	0	100	100
8	C	204/218 (94%)	189 (93%)	15 (7%)	0	100	100
9	D	193/200 (96%)	171 (89%)	22 (11%)	0	100	100
10	E	162/166 (98%)	148 (91%)	14 (9%)	0	100	100
11	F	90/95 (95%)	84 (93%)	6 (7%)	0	100	100
12	G	147/156 (94%)	126 (86%)	21 (14%)	0	100	100
13	H	129/132 (98%)	119 (92%)	10 (8%)	0	100	100
14	I	123/130 (95%)	113 (92%)	10 (8%)	0	100	100
15	J	93/102 (91%)	87 (94%)	6 (6%)	0	100	100
16	K	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
17	L	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
18	M	106/121 (88%)	95 (90%)	11 (10%)	0	100	100
19	N	58/61 (95%)	48 (83%)	10 (17%)	0	100	100
20	O	83/89 (93%)	75 (90%)	8 (10%)	0	100	100
21	P	86/90 (96%)	80 (93%)	6 (7%)	0	100	100
22	Q	82/87 (94%)	79 (96%)	3 (4%)	0	100	100
23	R	62/79 (78%)	57 (92%)	5 (8%)	0	100	100
24	S	76/92 (83%)	67 (88%)	9 (12%)	0	100	100
25	T	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
28	W	84/785 (11%)	78 (93%)	6 (7%)	0	100	100
30	Z	270/275 (98%)	253 (94%)	17 (6%)	0	100	100
31	a	204/207 (99%)	190 (93%)	14 (7%)	0	100	100
32	b	203/205 (99%)	186 (92%)	17 (8%)	0	100	100
33	c	174/178 (98%)	160 (92%)	13 (8%)	1 (1%)	22	50
34	d	173/175 (99%)	154 (89%)	19 (11%)	0	100	100
35	e	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
36	f	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
37	i	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
38	j	133/138 (96%)	123 (92%)	10 (8%)	0	100	100
39	k	117/119 (98%)	113 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	l	118/120 (98%)	104 (88%)	14 (12%)	0	100	100
41	m	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
42	n	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
43	o	99/101 (98%)	87 (88%)	12 (12%)	0	100	100
44	r	107/109 (98%)	99 (92%)	8 (8%)	0	100	100
45	s	88/93 (95%)	81 (92%)	7 (8%)	0	100	100
46	t	99/101 (98%)	88 (89%)	11 (11%)	0	100	100
47	u	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
48	v	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
49	w	63/65 (97%)	57 (90%)	6 (10%)	0	100	100
50	x	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
51	9	147/149 (99%)	107 (73%)	27 (18%)	13 (9%)	0	4
All	All	5438/6399 (85%)	4977 (92%)	447 (8%)	14 (0%)	38	66

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	9	37	VAL
51	9	107	ASN
51	9	130	PRO
51	9	135	PRO
51	9	104	LYS
51	9	126	TYR
51	9	127	THR
51	9	29	PHE
51	9	71	THR
51	9	118	PRO
51	9	143	VAL
51	9	36	ALA
51	9	75	LEU
33	c	41	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	48/53 (91%)	46 (96%)	2 (4%)	25	51
2	1	46/46 (100%)	45 (98%)	1 (2%)	47	68
3	2	39/39 (100%)	39 (100%)	0	100	100
4	3	54/57 (95%)	52 (96%)	2 (4%)	29	54
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	53/53 (100%)	52 (98%)	1 (2%)	52	71
7	B	189/212 (89%)	180 (95%)	9 (5%)	21	48
8	C	168/178 (94%)	163 (97%)	5 (3%)	36	61
9	D	169/173 (98%)	161 (95%)	8 (5%)	22	49
10	E	128/130 (98%)	125 (98%)	3 (2%)	45	67
11	F	81/84 (96%)	76 (94%)	5 (6%)	15	40
12	G	125/132 (95%)	120 (96%)	5 (4%)	27	52
13	H	111/112 (99%)	110 (99%)	1 (1%)	75	86
14	I	98/102 (96%)	91 (93%)	7 (7%)	12	37
15	J	86/92 (94%)	84 (98%)	2 (2%)	45	67
16	K	86/100 (86%)	81 (94%)	5 (6%)	17	42
17	L	114/116 (98%)	111 (97%)	3 (3%)	41	64
18	M	94/104 (90%)	92 (98%)	2 (2%)	48	69
19	N	53/54 (98%)	48 (91%)	5 (9%)	7	25
20	O	80/83 (96%)	77 (96%)	3 (4%)	28	54
21	P	74/76 (97%)	71 (96%)	3 (4%)	26	51
22	Q	77/80 (96%)	75 (97%)	2 (3%)	41	64
23	R	56/64 (88%)	56 (100%)	0	100	100
24	S	70/81 (86%)	68 (97%)	2 (3%)	37	61
25	T	66/70 (94%)	64 (97%)	2 (3%)	36	61
28	W	69/673 (10%)	69 (100%)	0	100	100
30	Z	220/223 (99%)	214 (97%)	6 (3%)	40	63
31	a	167/168 (99%)	162 (97%)	5 (3%)	36	61
32	b	169/169 (100%)	166 (98%)	3 (2%)	54	73
33	c	151/153 (99%)	144 (95%)	7 (5%)	23	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	d	148/148 (100%)	145 (98%)	3 (2%)	50 70
35	e	120/120 (100%)	115 (96%)	5 (4%)	25 51
36	f	101/101 (100%)	97 (96%)	4 (4%)	27 52
37	i	110/110 (100%)	108 (98%)	2 (2%)	54 73
38	j	109/111 (98%)	108 (99%)	1 (1%)	75 86
39	k	99/99 (100%)	98 (99%)	1 (1%)	73 83
40	l	93/93 (100%)	92 (99%)	1 (1%)	70 81
41	m	100/100 (100%)	97 (97%)	3 (3%)	36 61
42	n	96/96 (100%)	96 (100%)	0	100 100
43	o	83/83 (100%)	82 (99%)	1 (1%)	67 80
44	r	90/90 (100%)	86 (96%)	4 (4%)	24 50
45	s	81/84 (96%)	80 (99%)	1 (1%)	67 80
46	t	85/85 (100%)	84 (99%)	1 (1%)	67 80
47	u	64/64 (100%)	63 (98%)	1 (2%)	58 75
48	v	47/47 (100%)	47 (100%)	0	100 100
49	w	56/56 (100%)	55 (98%)	1 (2%)	54 73
50	x	52/52 (100%)	52 (100%)	0	100 100
All	All	4510/5251 (86%)	4382 (97%)	128 (3%)	40 62

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	27	MET
1	0	41	ARG
2	1	28	ASP
4	3	61	MET
4	3	64	ASN
6	6	22	PHE
7	B	29	ARG
7	B	39	TYR
7	B	69	PHE
7	B	77	GLN
7	B	86	ARG
7	B	89	MET
7	B	104	PHE
7	B	123	ASN

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Mol	Chain	Res	Type
7	B	211	LYS
8	C	88	LYS
8	C	101	ASN
8	C	125	ASN
8	C	171	THR
8	C	192	TYR
9	D	13	ARG
9	D	24	LYS
9	D	40	GLN
9	D	41	ARG
9	D	42	LYS
9	D	53	GLU
9	D	172	LEU
9	D	178	ARG
10	E	3	ARG
10	E	41	ASP
10	E	58	GLU
11	F	11	ARG
11	F	36	GLU
11	F	43	TRP
11	F	68	ASP
11	F	82	SER
12	G	9	LYS
12	G	10	ARG
12	G	14	PRO
12	G	117	GLU
12	G	148	ASN
13	H	128	LEU
14	I	36	SER
14	I	46	GLU
14	I	49	LYS
14	I	54	LEU
14	I	68	HIS
14	I	113	ARG
14	I	127	PHE
15	J	23	GLU
15	J	31	ARG
16	K	66	GLN
16	K	82	LYS
16	K	114	ASP
16	K	121	ASN
16	K	128	ARG

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Mol	Chain	Res	Type
17	L	30	SER
17	L	31	PHE
17	L	63	ARG
18	M	55	LYS
18	M	75	LEU
19	N	6	MET
19	N	21	TYR
19	N	26	ARG
19	N	47	LEU
19	N	61	TRP
20	O	7	ARG
20	O	14	GLU
20	O	84	LYS
21	P	24	ASP
21	P	71	ARG
21	P	85	ASN
22	Q	30	TYR
22	Q	52	ASN
24	S	5	LEU
24	S	6	LYS
25	T	21	ASN
25	T	34	GLN
30	Z	20	ASP
30	Z	98	ASP
30	Z	194	GLN
30	Z	221	ARG
30	Z	257	PHE
30	Z	272	ARG
31	a	51	LEU
31	a	61	SER
31	a	130	ARG
31	a	137	SER
31	a	152	ASN
32	b	74	ARG
32	b	149	GLU
32	b	190	GLU
33	c	38	MET
33	c	42	ASP
33	c	45	GLN
33	c	63	GLN
33	c	101	ASP
33	c	105	SER

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Mol	Chain	Res	Type
33	c	148	LYS
34	d	14	ASP
34	d	45	LYS
34	d	76	MET
35	e	53	ASP
35	e	93	MET
35	e	114	SER
35	e	117	ARG
35	e	119	MET
36	f	12	ASP
36	f	41	CYS
36	f	80	ASP
36	f	112	MET
37	i	55	MET
37	i	80	ASP
38	j	91	GLU
39	k	98	TYR
40	l	34	PHE
41	m	56	SER
41	m	99	TYR
41	m	106	LYS
43	o	39	LEU
44	r	28	GLN
44	r	31	GLU
44	r	48	GLU
44	r	94	SER
45	s	38	GLU
46	t	75	THR
47	u	65	ASP
49	w	26	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	40	GLN
5	4	34	GLN
8	C	136	GLN
9	D	82	HIS
9	D	96	ASN
11	F	13	ASN
11	F	33	ASN
14	I	32	ASN

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Mol	Chain	Res	Type
14	I	50	GLN
17	L	35	HIS
17	L	122	ASN
18	M	101	ASN
20	O	5	GLN
34	d	22	ASN
35	e	8	ASN
36	f	3	GLN
39	k	72	ASN
40	l	43	GLN
43	o	50	ASN
43	o	81	ASN
45	s	55	ASN
48	v	23	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	U	76/77 (98%)	21 (27%)	0
27	V	32/33 (96%)	21 (65%)	0
29	Y	111/112 (99%)	35 (31%)	3 (2%)
52	X	2881/2928 (98%)	684 (23%)	36 (1%)
53	A	1532/1533 (99%)	384 (25%)	20 (1%)
All	All	4632/4683 (98%)	1145 (24%)	59 (1%)

All (1145) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	U	2	G
26	U	6	G
26	U	8	U
26	U	16	U
26	U	17	U
26	U	17(A)	G
26	U	18	G
26	U	20	U
26	U	24	A
26	U	42	G
26	U	46	G
26	U	47	U
26	U	48	C

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Mol	Chain	Res	Type
26	U	55	U
26	U	56	C
26	U	57	G
26	U	58	A
26	U	59	G
26	U	60	U
26	U	68	G
26	U	76	A
27	V	436	A
27	V	441	U
27	V	442	G
27	V	443	C
27	V	444	C
27	V	445	A
27	V	446	U
27	V	447	G
27	V	449	A
27	V	450	C
27	V	451	G
27	V	452	U
27	V	453	C
27	V	454	G
27	V	455	C
27	V	456	A
27	V	457	C
27	V	458	U
27	V	459	C
27	V	460	G
27	V	461	G
29	Y	10	G
29	Y	12	U
29	Y	18	A
29	Y	21	G
29	Y	22	G
29	Y	23	U
29	Y	33	U
29	Y	34	C
29	Y	38	U
29	Y	39	A
29	Y	42	G
29	Y	43	A
29	Y	44	A

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Mol	Chain	Res	Type
29	Y	46	A
29	Y	49	G
29	Y	53	U
29	Y	64	A
29	Y	65	G
29	Y	71	A
29	Y	73	G
29	Y	74	G
29	Y	75	U
29	Y	85	U
29	Y	86	U
29	Y	87	U
29	Y	88	C
29	Y	94	G
29	Y	97	A
29	Y	100	G
29	Y	103	G
29	Y	107	G
29	Y	108	C
29	Y	109	C
29	Y	110	G
29	Y	112	C
52	X	4	U
52	X	5	A
52	X	7	G
52	X	9	U
52	X	12	A
52	X	15	G
52	X	34	U
52	X	35	G
52	X	46	C
52	X	60	G
52	X	61	A
52	X	62	C
52	X	63	G
52	X	71	A
52	X	74	U
52	X	75	G
52	X	76	C
52	X	77	U
52	X	78	U
52	X	79	C

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Mol	Chain	Res	Type
52	X	80	G
52	X	82	G
52	X	85	G
52	X	86	C
52	X	87	U
52	X	88	G
52	X	91	A
52	X	92	G
52	X	93	C
52	X	94	A
52	X	95	A
52	X	96	G
52	X	99	U
52	X	100	U
52	X	101	G
52	X	102	A
52	X	117	A
52	X	119	U
52	X	125	A
52	X	126	A
52	X	127	C
52	X	130	A
52	X	140	A
52	X	150	A
52	X	161	A
52	X	162	A
52	X	164	U
52	X	165	C
52	X	168	A
52	X	176	A
52	X	177	G
52	X	178	A
52	X	179	A
52	X	182	C
52	X	183	A
52	X	184	G
52	X	189	G
52	X	199	A
52	X	200	A
52	X	202	A
52	X	216	A
52	X	218	G

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Mol	Chain	Res	Type
52	X	219	A
52	X	221	G
52	X	224	A
52	X	225	A
52	X	226	A
52	X	227	G
52	X	230	A
52	X	231	A
52	X	232	U
52	X	233	G
52	X	234	C
52	X	244	A
52	X	251	G
52	X	252	C
52	X	253	G
52	X	258	A
52	X	275	A
52	X	276	C
52	X	279	A
52	X	282	G
52	X	284	C
52	X	285	U
52	X	286	U
52	X	287	G
52	X	288	C
52	X	289	C
52	X	291	C
52	X	292	U
52	X	294	G
52	X	295	G
52	X	296	G
52	X	298	U
52	X	302	A
52	X	307	A
52	X	308	C
52	X	310	C
52	X	329	A
52	X	330	A
52	X	332	G
52	X	336	U
52	X	337	A
52	X	338	G

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Mol	Chain	Res	Type
52	X	345	A
52	X	346	G
52	X	355	A
52	X	367	G
52	X	372	U
52	X	373	A
52	X	374	A
52	X	377	G
52	X	389	A
52	X	390	A
52	X	392	C
52	X	396	G
52	X	397	U
52	X	399	C
52	X	407	A
52	X	408	G
52	X	417	G
52	X	418	A
52	X	419	G
52	X	421	A
52	X	431	A
52	X	433	G
52	X	434	U
52	X	442	C
52	X	448	A
52	X	450	U
52	X	451	C
52	X	453	G
52	X	458	G
52	X	459	A
52	X	471	G
52	X	476	A
52	X	483	C
52	X	491	C
52	X	495	U
52	X	498	U
52	X	502	C
52	X	504	A
52	X	512	G
52	X	528	G
52	X	529	C
52	X	540	G

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Mol	Chain	Res	Type
52	X	542	G
52	X	548	A
52	X	550	G
52	X	551	A
52	X	552	G
52	X	554	U
52	X	555	C
52	X	556	C
52	X	564	G
52	X	567	U
52	X	573	C
52	X	575	A
52	X	576	G
52	X	577	U
52	X	578	A
52	X	579	G
52	X	590	U
52	X	592	A
52	X	593	A
52	X	594	C
52	X	595	G
52	X	606	U
52	X	607	G
52	X	617	G
52	X	619	A
52	X	630	A
52	X	632	U
52	X	646	A
52	X	647	A
52	X	658	A
52	X	660	G
52	X	673	A
52	X	683	A
52	X	691	U
52	X	697	G
52	X	698	C
52	X	699	A
52	X	700	U
52	X	701	G
52	X	702	A
52	X	717	A
52	X	719	C

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Mol	Chain	Res	Type
52	X	729	G
52	X	733	U
52	X	762	A
52	X	763	A
52	X	765	A
52	X	777	C
52	X	794	U
52	X	795	G
52	X	804	G
52	X	822	G
52	X	823	G
52	X	824	G
52	X	826	U
52	X	829	A
52	X	831	U
52	X	832	G
52	X	837	U
52	X	852	G
52	X	859	C
52	X	866	A
52	X	874	U
52	X	875	U
52	X	892	U
52	X	906	G
52	X	913	A
52	X	928	G
52	X	929	G
52	X	930	C
52	X	933	C
52	X	934	U
52	X	936	C
52	X	940	G
52	X	941	U
52	X	943	A
52	X	957	A
52	X	959	C
52	X	964	A
52	X	973	G
52	X	980	C
52	X	987	A
52	X	991	A
52	X	992	G

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Mol	Chain	Res	Type
52	X	999	A
52	X	1005	A
52	X	1007	G
52	X	1018	G
52	X	1019	A
52	X	1020	A
52	X	1030	G
52	X	1031	C
52	X	1036	A
52	X	1046	A
52	X	1058	U
52	X	1059	A
52	X	1068	G
52	X	1069	U
52	X	1072	A
52	X	1073	A
52	X	1076	G
52	X	1079	U
52	X	1085	G
52	X	1090	U
52	X	1091	U
52	X	1092	A
52	X	1093	G
52	X	1100	A
52	X	1102	G
52	X	1103	A
52	X	1107	U
52	X	1108	G
52	X	1109	G
52	X	1111	U
52	X	1113	A
52	X	1116	A
52	X	1118	C
52	X	1119	A
52	X	1121	C
52	X	1122	C
52	X	1123	A
52	X	1124	C
52	X	1125	C
52	X	1126	A
52	X	1127	U
52	X	1128	U

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Mol	Chain	Res	Type
52	X	1130	A
52	X	1131	A
52	X	1133	G
52	X	1134	A
52	X	1135	G
52	X	1136	U
52	X	1137	G
52	X	1138	C
52	X	1139	G
52	X	1140	U
52	X	1141	A
52	X	1142	A
52	X	1143	U
52	X	1144	A
52	X	1145	G
52	X	1147	U
52	X	1148	C
52	X	1154	U
52	X	1157	A
52	X	1158	G
52	X	1159	U
52	X	1160	G
52	X	1161	A
52	X	1177	G
52	X	1178	U
52	X	1179	A
52	X	1180	C
52	X	1181	C
52	X	1182	G
52	X	1183	G
52	X	1185	G
52	X	1188	A
52	X	1201	A
52	X	1215	U
52	X	1216	C
52	X	1227	G
52	X	1236	G
52	X	1241	C
52	X	1248	C
52	X	1260	A
52	X	1265	A
52	X	1277	A

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Mol	Chain	Res	Type
52	X	1278	G
52	X	1293	A
52	X	1295	U
52	X	1296	G
52	X	1311	G
52	X	1312	A
52	X	1315	G
52	X	1339	A
52	X	1340	A
52	X	1353	C
52	X	1364	C
52	X	1368	U
52	X	1369	C
52	X	1371	G
52	X	1388	A
52	X	1389	C
52	X	1391	U
52	X	1402	C
52	X	1404	A
52	X	1406	A
52	X	1417	A
52	X	1418	U
52	X	1423	A
52	X	1425	C
52	X	1426	A
52	X	1427	G
52	X	1434	A
52	X	1435	U
52	X	1442	A
52	X	1449	C
52	X	1450	C
52	X	1452	C
52	X	1453	A
52	X	1455	C
52	X	1458	U
52	X	1460	G
52	X	1461	A
52	X	1465	A
52	X	1466	U
52	X	1471	G
52	X	1473	A
52	X	1474	C

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Mol	Chain	Res	Type
52	X	1480	A
52	X	1489	U
52	X	1490	A
52	X	1499	A
52	X	1500	U
52	X	1505	U
52	X	1506	A
52	X	1507	U
52	X	1508	C
52	X	1514	C
52	X	1516	A
52	X	1525	G
52	X	1526	G
52	X	1528	U
52	X	1529	G
52	X	1536	A
52	X	1537	G
52	X	1539	C
52	X	1540	A
52	X	1543	U
52	X	1544	C
52	X	1552	C
52	X	1553	A
52	X	1566	G
52	X	1568	G
52	X	1569	A
52	X	1570	U
52	X	1571	G
52	X	1601	A
52	X	1602	U
52	X	1617	A
52	X	1626	U
52	X	1632	G
52	X	1653	A
52	X	1655	A
52	X	1693	C
52	X	1696	G
52	X	1697	A
52	X	1710	A
52	X	1713	A
52	X	1717	C
52	X	1719	G

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Mol	Chain	Res	Type
52	X	1732	G
52	X	1738	U
52	X	1739	C
52	X	1741	G
52	X	1745	A
52	X	1757	G
52	X	1758	U
52	X	1759	U
52	X	1760	A
52	X	1761	G
52	X	1765	G
52	X	1767	A
52	X	1774	A
52	X	1776	A
52	X	1779	G
52	X	1792	G
52	X	1793	G
52	X	1797	A
52	X	1802	A
52	X	1811	C
52	X	1820	A
52	X	1828	G
52	X	1829	C
52	X	1830	G
52	X	1831	A
52	X	1832	A
52	X	1837	U
52	X	1845	A
52	X	1848	A
52	X	1858	A
52	X	1877	A
52	X	1882	A
52	X	1883	A
52	X	1884	G
52	X	1898	G
52	X	1899	U
52	X	1900	A
52	X	1901	A
52	X	1902	G
52	X	1910	G
52	X	1935	G
52	X	1941	A

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Mol	Chain	Res	Type
52	X	1942	A
52	X	1943	C
52	X	1944	U
52	X	1945	A
52	X	1956	A
52	X	1958	G
52	X	1959	G
52	X	1962	G
52	X	1967	A
52	X	1971	C
52	X	1972	U
52	X	1984	U
52	X	1992	C
52	X	1993	G
52	X	1995	A
52	X	1996	C
52	X	1999	A
52	X	2000	A
52	X	2001	G
52	X	2020	U
52	X	2021	G
52	X	2022	U
52	X	2024	U
52	X	2025	C
52	X	2026	A
52	X	2052	A
52	X	2054	C
52	X	2059	A
52	X	2060	A
52	X	2061	G
52	X	2062	A
52	X	2063	U
52	X	2064	G
52	X	2065	C
52	X	2072	C
52	X	2081	G
52	X	2084	C
52	X	2085	G
52	X	2088	A
52	X	2089	A
52	X	2090	G
52	X	2098	G

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Mol	Chain	Res	Type
52	X	2121	U
52	X	2122	G
52	X	2123	A
52	X	2127	U
52	X	2129	G
52	X	2131	U
52	X	2132	A
52	X	2133	C
52	X	2134	A
52	X	2135	G
52	X	2139	G
52	X	2140	U
52	X	2141	A
52	X	2143	A
52	X	2144	G
52	X	2145	G
52	X	2146	A
52	X	2147	U
52	X	2148	A
52	X	2149	G
52	X	2151	U
52	X	2152	A
52	X	2154	G
52	X	2155	A
52	X	2157	C
52	X	2158	C
52	X	2159	U
52	X	2160	U
52	X	2161	G
52	X	2163	A
52	X	2165	A
52	X	2166	C
52	X	2168	G
52	X	2169	G
52	X	2170	A
52	X	2171	G
52	X	2173	G
52	X	2174	C
52	X	2175	C
52	X	2176	A
52	X	2177	G
52	X	2181	C

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Mol	Chain	Res	Type
52	X	2183	G
52	X	2184	U
52	X	2185	G
52	X	2186	G
52	X	2187	A
52	X	2190	C
52	X	2191	A
52	X	2193	C
52	X	2194	G
52	X	2195	G
52	X	2198	G
52	X	2199	G
52	X	2200	A
52	X	2201	U
52	X	2203	C
52	X	2204	U
52	X	2205	A
52	X	2206	C
52	X	2208	C
52	X	2209	U
52	X	2210	G
52	X	2216	A
52	X	2218	U
52	X	2219	G
52	X	2220	A
52	X	2222	C
52	X	2223	U
52	X	2224	U
52	X	2225	C
52	X	2227	A
52	X	2232	G
52	X	2233	C
52	X	2241	A
52	X	2245	G
52	X	2246	G
52	X	2252	A
52	X	2254	A
52	X	2267	G
52	X	2268	G
52	X	2280	G
52	X	2297	A
52	X	2312	C

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Mol	Chain	Res	Type
52	X	2315	A
52	X	2316	A
52	X	2318	G
52	X	2334	U
52	X	2335	U
52	X	2338	A
52	X	2339	A
52	X	2349	A
52	X	2350	G
52	X	2351	A
52	X	2356	A
52	X	2363	C
52	X	2364	A
52	X	2374	G
52	X	2379	C
52	X	2381	A
52	X	2404	G
52	X	2412	G
52	X	2414	C
52	X	2415	U
52	X	2430	U
52	X	2431	U
52	X	2432	C
52	X	2435	C
52	X	2440	A
52	X	2453	C
52	X	2454	A
52	X	2457	G
52	X	2458	G
52	X	2459	A
52	X	2469	C
52	X	2470	C
52	X	2476	G
52	X	2477	A
52	X	2504	C
52	X	2505	A
52	X	2507	A
52	X	2516	G
52	X	2523	G
52	X	2527	C
52	X	2531	G
52	X	2532	A

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Mol	Chain	Res	Type
52	X	2533	U
52	X	2534	G
52	X	2535	U
52	X	2547	A
52	X	2549	C
52	X	2558	G
52	X	2562	U
52	X	2564	G
52	X	2583	U
52	X	2584	U
52	X	2595	A
52	X	2596	G
52	X	2602	C
52	X	2607	G
52	X	2611	G
52	X	2614	U
52	X	2628	G
52	X	2631	A
52	X	2632	G
52	X	2639	C
52	X	2642	U
52	X	2658	A
52	X	2659	G
52	X	2674	G
52	X	2675	C
52	X	2689	A
52	X	2690	G
52	X	2711	G
52	X	2718	U
52	X	2719	A
52	X	2720	C
52	X	2743	G
52	X	2762	A
52	X	2768	U
52	X	2773	G
52	X	2777	A
52	X	2785	U
52	X	2790	A
52	X	2793	A
52	X	2794	A
52	X	2806	G
52	X	2807	A

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Mol	Chain	Res	Type
52	X	2809	G
52	X	2818	C
52	X	2822	C
52	X	2824	G
52	X	2827	A
52	X	2830	A
52	X	2831	A
52	X	2843	G
52	X	2845	A
52	X	2849	U
52	X	2850	G
52	X	2859	G
52	X	2860	A
52	X	2872	U
52	X	2873	G
52	X	2874	G
52	X	2886	C
52	X	2891	G
52	X	2892	G
52	X	2893	A
52	X	2897	G
52	X	2899	C
52	X	2901	G
52	X	2905	C
52	X	2908	A
52	X	2909	U
52	X	2911	G
52	X	2912	A
52	X	2916	A
52	X	2918	G
52	X	2919	A
52	X	2920	C
52	X	2921	U
52	X	2925	C
53	A	10	A
53	A	11	G
53	A	32	C
53	A	33	G
53	A	34	A
53	A	46	G
53	A	49	C
53	A	50	C

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Mol	Chain	Res	Type
53	A	52	A
53	A	53	A
53	A	62	A
53	A	72	A
53	A	74	A
53	A	75	G
53	A	76	A
53	A	77	U
53	A	78	G
53	A	80	G
53	A	82	G
53	A	83	C
53	A	85	U
53	A	86	G
53	A	89	C
53	A	90	C
53	A	92	U
53	A	94	A
53	A	95	U
53	A	96	G
53	A	98	U
53	A	99	A
53	A	117	A
53	A	118	A
53	A	119	C
53	A	120	A
53	A	128	A
53	A	130	C
53	A	133	G
53	A	135	C
53	A	147	G
53	A	156	G
53	A	158	G
53	A	162	C
53	A	165	G
53	A	167	G
53	A	169	U
53	A	172	U
53	A	178	A
53	A	179	U
53	A	181	G
53	A	188	G

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Mol	Chain	Res	Type
53	A	189	A
53	A	190	A
53	A	192	C
53	A	195	A
53	A	197	G
53	A	204	A
53	A	206	A
53	A	207	U
53	A	208	A
53	A	209	A
53	A	212	G
53	A	218	U
53	A	219	U
53	A	220	C
53	A	221	G
53	A	222	G
53	A	225	A
53	A	228	A
53	A	231	U
53	A	233	C
53	A	248	C
53	A	249	G
53	A	253	U
53	A	255	G
53	A	259	G
53	A	260	U
53	A	261	U
53	A	269	U
53	A	270	A
53	A	271	A
53	A	272	C
53	A	273	G
53	A	274	G
53	A	275	C
53	A	287	A
53	A	288	C
53	A	297	G
53	A	307	G
53	A	311	G
53	A	316	C
53	A	329	A
53	A	336	C

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Mol	Chain	Res	Type
53	A	337	A
53	A	340	G
53	A	352	A
53	A	353	C
53	A	354	G
53	A	360	C
53	A	362	G
53	A	364	A
53	A	371	A
53	A	373	U
53	A	375	U
53	A	380	C
53	A	400	G
53	A	401	A
53	A	406	C
53	A	414	G
53	A	418	G
53	A	419	A
53	A	420	U
53	A	421	G
53	A	422	A
53	A	429	U
53	A	430	C
53	A	432	G
53	A	437	U
53	A	440	A
53	A	443	U
53	A	445	U
53	A	446	G
53	A	447	U
53	A	456	A
53	A	461	C
53	A	462	A
53	A	463	A
53	A	464	G
53	A	465	U
53	A	472	C
53	A	473	G
53	A	475	A
53	A	476	U
53	A	477	A
53	A	478	G

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Mol	Chain	Res	Type
53	A	481	C
53	A	483	G
53	A	484	U
53	A	485	A
53	A	488	U
53	A	493	G
53	A	494	G
53	A	497	C
53	A	500	A
53	A	502	C
53	A	503	C
53	A	505	G
53	A	506	A
53	A	518	A
53	A	520	C
53	A	527	C
53	A	530	G
53	A	536	G
53	A	540	U
53	A	541	A
53	A	556	A
53	A	566	G
53	A	568	A
53	A	571	U
53	A	573	U
53	A	574	U
53	A	580	U
53	A	581	A
53	A	582	A
53	A	585	G
53	A	586	G
53	A	590	G
53	A	597	G
53	A	603	U
53	A	605	A
53	A	628	U
53	A	630	A
53	A	631	A
53	A	641	G
53	A	642	U
53	A	643	C
53	A	659	A

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Mol	Chain	Res	Type
53	A	662	U
53	A	674	A
53	A	695	U
53	A	696	A
53	A	697	G
53	A	703	A
53	A	704	A
53	A	720	G
53	A	728	C
53	A	729	C
53	A	732	U
53	A	740	G
53	A	742	G
53	A	757	A
53	A	764	G
53	A	790	A
53	A	802	U
53	A	803	A
53	A	812	G
53	A	823	A
53	A	824	A
53	A	826	C
53	A	829	U
53	A	830	G
53	A	837	A
53	A	841	G
53	A	845	G
53	A	849	G
53	A	850	U
53	A	851	U
53	A	853	C
53	A	856	C
53	A	861	U
53	A	874	A
53	A	875	A
53	A	882	A
53	A	886	A
53	A	924	A
53	A	929	A
53	A	936	G
53	A	944	C
53	A	945	A

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Mol	Chain	Res	Type
53	A	954	G
53	A	955	G
53	A	967	U
53	A	968	A
53	A	970	U
53	A	971	U
53	A	972	C
53	A	976	G
53	A	977	C
53	A	978	A
53	A	979	A
53	A	981	G
53	A	985	A
53	A	986	G
53	A	987	A
53	A	993	A
53	A	999	U
53	A	1002	U
53	A	1003	G
53	A	1006	A
53	A	1012	U
53	A	1013	G
53	A	1014	A
53	A	1015	C
53	A	1018	U
53	A	1019	C
53	A	1020	C
53	A	1021	U
53	A	1022	A
53	A	1023	G
53	A	1024	A
53	A	1028	A
53	A	1030	G
53	A	1031	A
53	A	1033	G
53	A	1034	U
53	A	1035	C
53	A	1036	C
53	A	1039	U
53	A	1041	C
53	A	1043	G
53	A	1048	A

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Mol	Chain	Res	Type
53	A	1053	G
53	A	1059	U
53	A	1060	G
53	A	1063	G
53	A	1065	A
53	A	1088	U
53	A	1089	G
53	A	1095	U
53	A	1096	U
53	A	1104	G
53	A	1105	U
53	A	1111	A
53	A	1118	G
53	A	1134	G
53	A	1135	U
53	A	1137	G
53	A	1145	U
53	A	1146	C
53	A	1148	G
53	A	1152	G
53	A	1153	G
53	A	1165	G
53	A	1168	U
53	A	1169	G
53	A	1176	A
53	A	1177	C
53	A	1180	A
53	A	1186	G
53	A	1187	G
53	A	1188	A
53	A	1193	G
53	A	1200	A
53	A	1205	A
53	A	1206	A
53	A	1210	A
53	A	1211	U
53	A	1212	C
53	A	1214	U
53	A	1215	G
53	A	1216	C
53	A	1218	C
53	A	1220	U

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Mol	Chain	Res	Type
53	A	1221	U
53	A	1222	A
53	A	1223	U
53	A	1224	G
53	A	1234	A
53	A	1236	A
53	A	1247	A
53	A	1248	A
53	A	1249	U
53	A	1250	G
53	A	1265	C
53	A	1267	G
53	A	1269	G
53	A	1277	G
53	A	1283	A
53	A	1284	A
53	A	1287	C
53	A	1289	A
53	A	1290	U
53	A	1294	A
53	A	1295	C
53	A	1296	A
53	A	1306	U
53	A	1308	A
53	A	1309	G
53	A	1311	U
53	A	1314	G
53	A	1317	C
53	A	1329	C
53	A	1337	C
53	A	1339	U
53	A	1340	G
53	A	1345	U
53	A	1355	A
53	A	1356	G
53	A	1362	G
53	A	1369	A
53	A	1370	G
53	A	1372	A
53	A	1373	U
53	A	1380	G
53	A	1383	A

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Mol	Chain	Res	Type
53	A	1384	A
53	A	1385	U
53	A	1386	A
53	A	1387	C
53	A	1388	G
53	A	1407	A
53	A	1410	G
53	A	1414	G
53	A	1428	G
53	A	1435	A
53	A	1445	U
53	A	1446	C
53	A	1447	G
53	A	1448	G
53	A	1449	U
53	A	1451	A
53	A	1453	G
53	A	1454	U
53	A	1455	A
53	A	1460	U
53	A	1461	U
53	A	1462	U
53	A	1463	A
53	A	1464	G
53	A	1465	G
53	A	1466	A
53	A	1468	C
53	A	1473	C
53	A	1474	G
53	A	1477	G
53	A	1500	U
53	A	1503	A
53	A	1504	G
53	A	1507	G
53	A	1513	A
53	A	1515	G
53	A	1516	U
53	A	1517	A
53	A	1539	G
53	A	1540	G

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	Y	21	G
29	Y	33	U
29	Y	38	U
52	X	101	G
52	X	164	U
52	X	252	C
52	X	407	A
52	X	441	C
52	X	450	U
52	X	511	U
52	X	528	G
52	X	549	A
52	X	762	A
52	X	1035	G
52	X	1045	U
52	X	1156	G
52	X	1176	U
52	X	1451	U
52	X	1507	U
52	X	1525	G
52	X	1567	U
52	X	1712	G
52	X	1766	C
52	X	1882	A
52	X	1900	A
52	X	2131	U
52	X	2133	C
52	X	2180	U
52	X	2192	U
52	X	2219	G
52	X	2223	U
52	X	2334	U
52	X	2337	G
52	X	2380	G
52	X	2413	G
52	X	2469	C
52	X	2534	G
52	X	2805	A
52	X	2904	A
53	A	206	A
53	A	306	A
53	A	315	U
53	A	372	A

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Mol	Chain	Res	Type
53	A	455	G
53	A	483	G
53	A	642	U
53	A	728	C
53	A	848	G
53	A	855	G
53	A	1022	A
53	A	1088	U
53	A	1147	A
53	A	1211	U
53	A	1276	C
53	A	1316	U
53	A	1369	A
53	A	1460	U
53	A	1463	A
53	A	1499	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

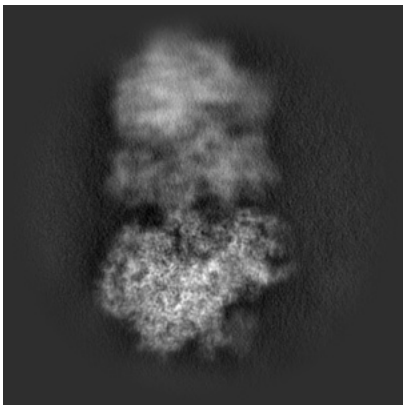
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18558. These allow visual inspection of the internal detail of the map and identification of artifacts.

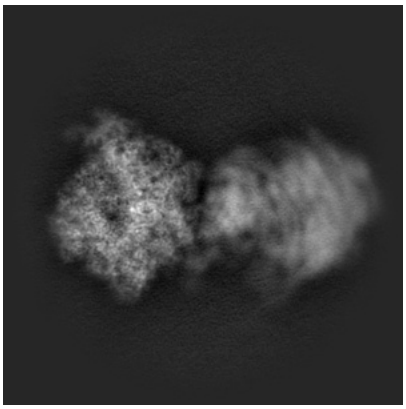
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

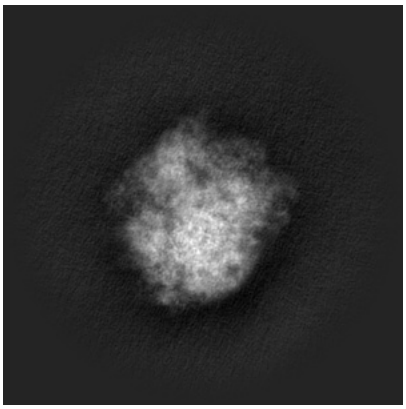
6.1.1 Primary map



X

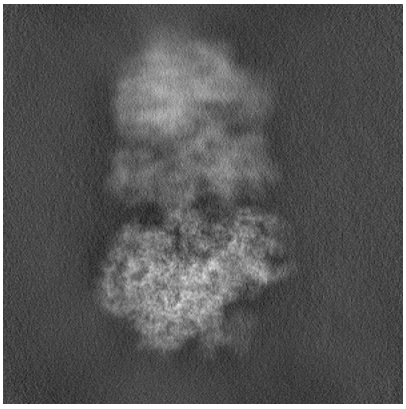


Y

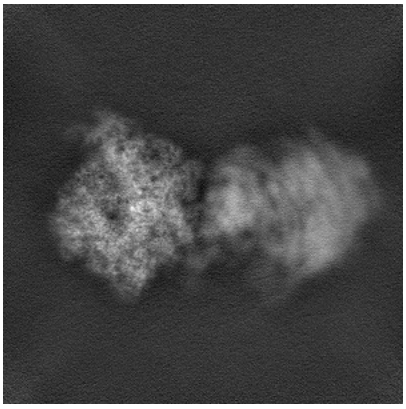


Z

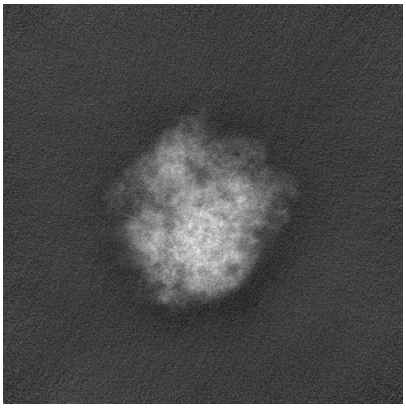
6.1.2 Raw map



X



Y

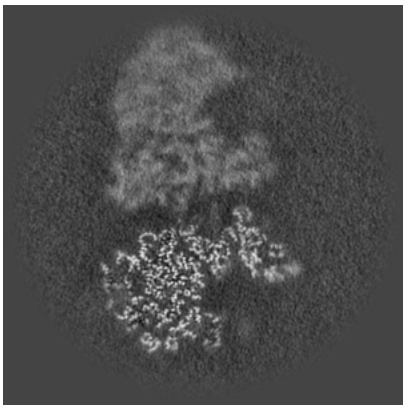


Z

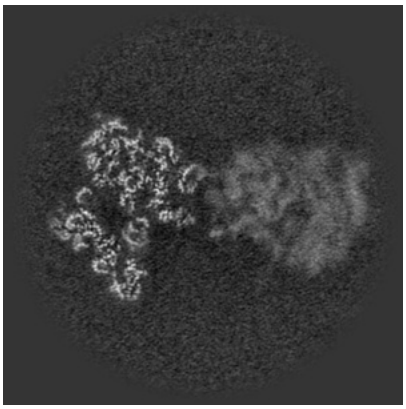
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

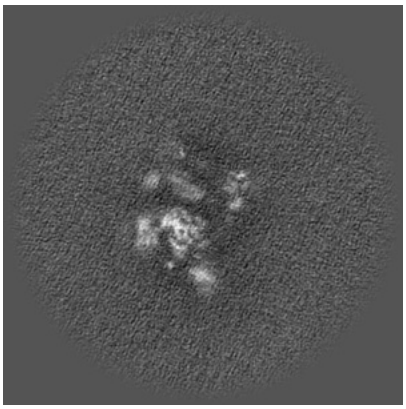
6.2.1 Primary map



X Index: 250

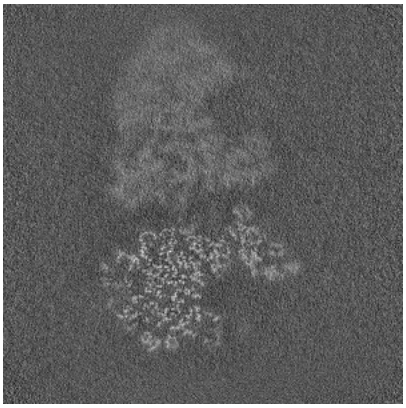


Y Index: 250

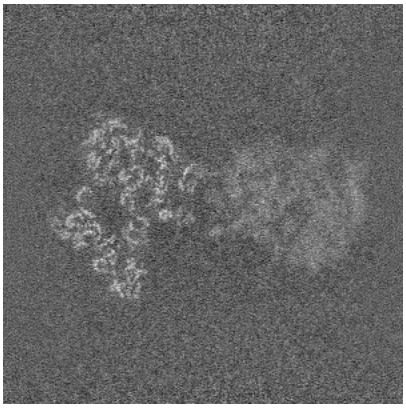


Z Index: 250

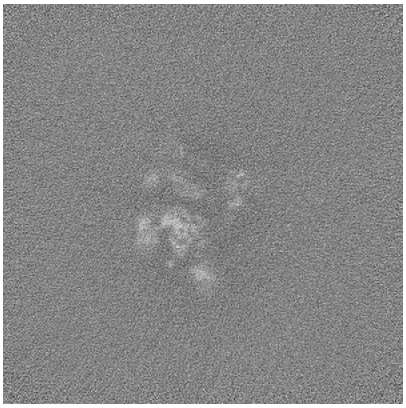
6.2.2 Raw map



X Index: 250



Y Index: 250

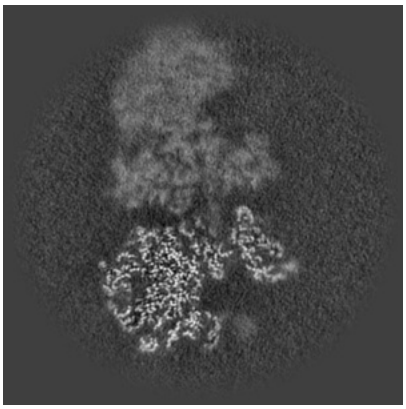


Z Index: 250

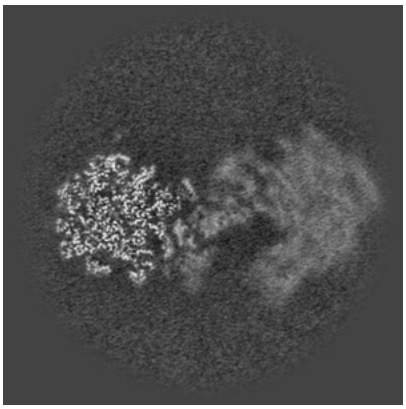
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

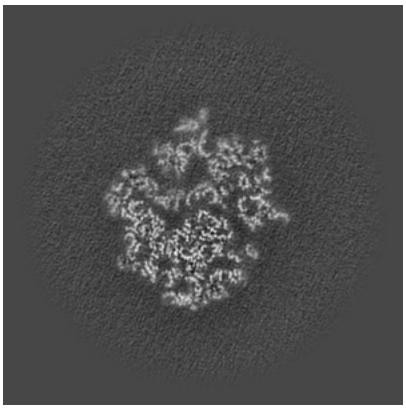
6.3.1 Primary map



X Index: 246

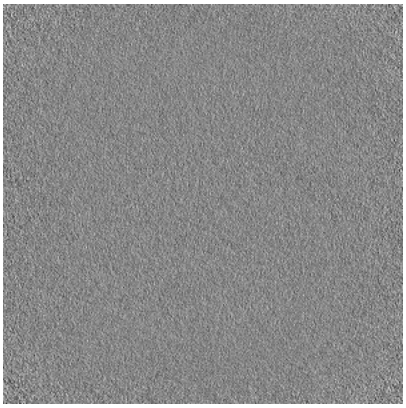


Y Index: 210

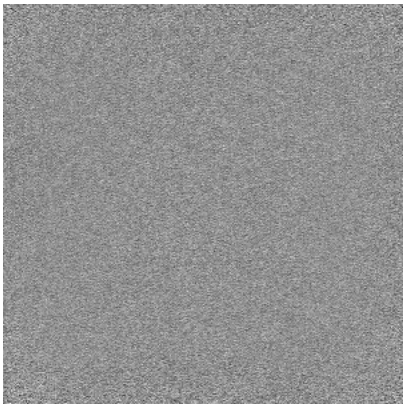


Z Index: 167

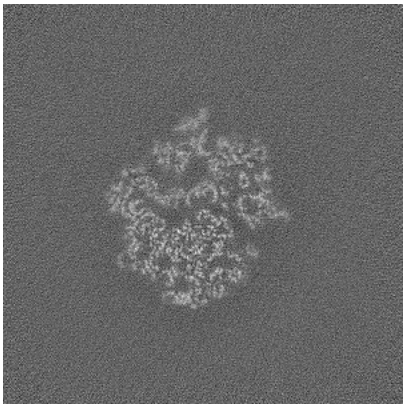
6.3.2 Raw map



X Index: 0



Y Index: 0

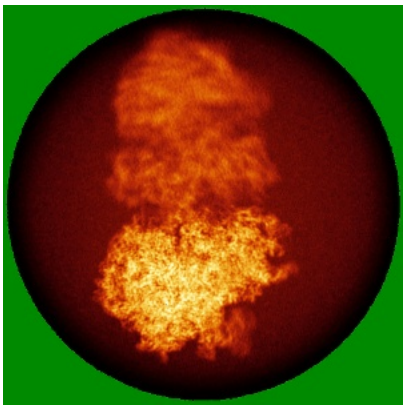


Z Index: 168

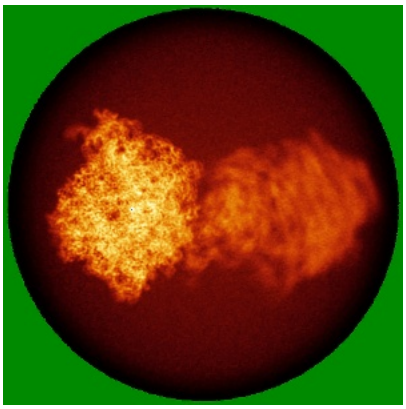
The images above show the largest variance slices of the map in three orthogonal directions.

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

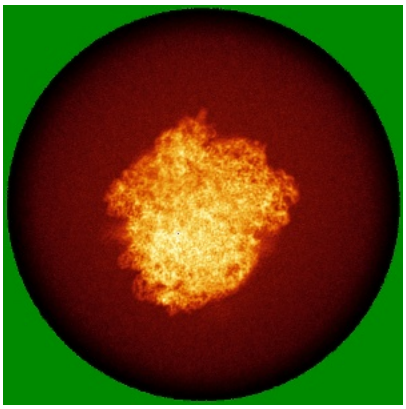
6.4.1 Primary map



X

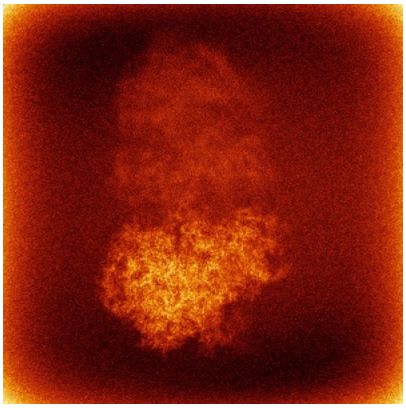


Y

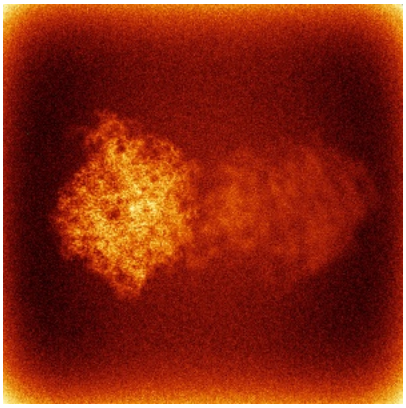


Z

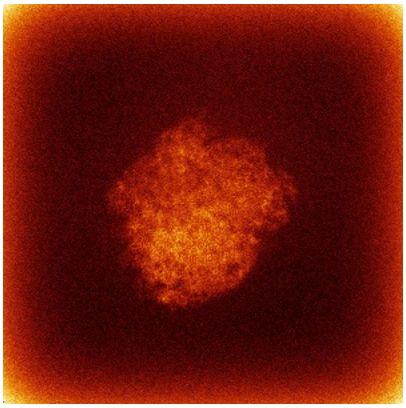
6.4.2 Raw map



X



Y

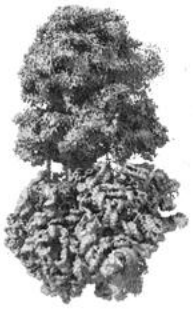


Z

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



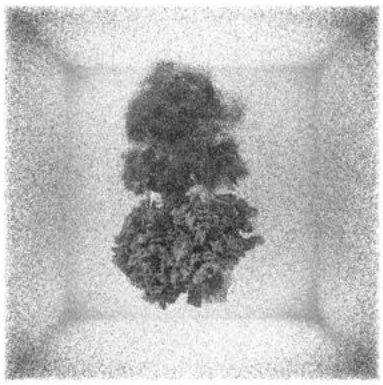
X

Y

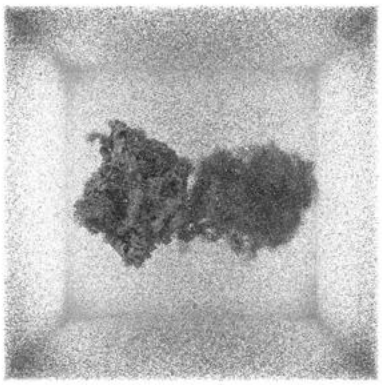
Z

The images above show the 3D surface view of the map at the recommended contour level 0.377. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

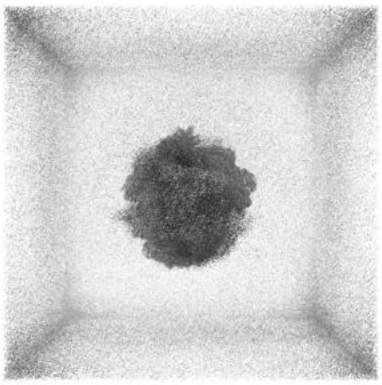
6.5.2 Raw map



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.

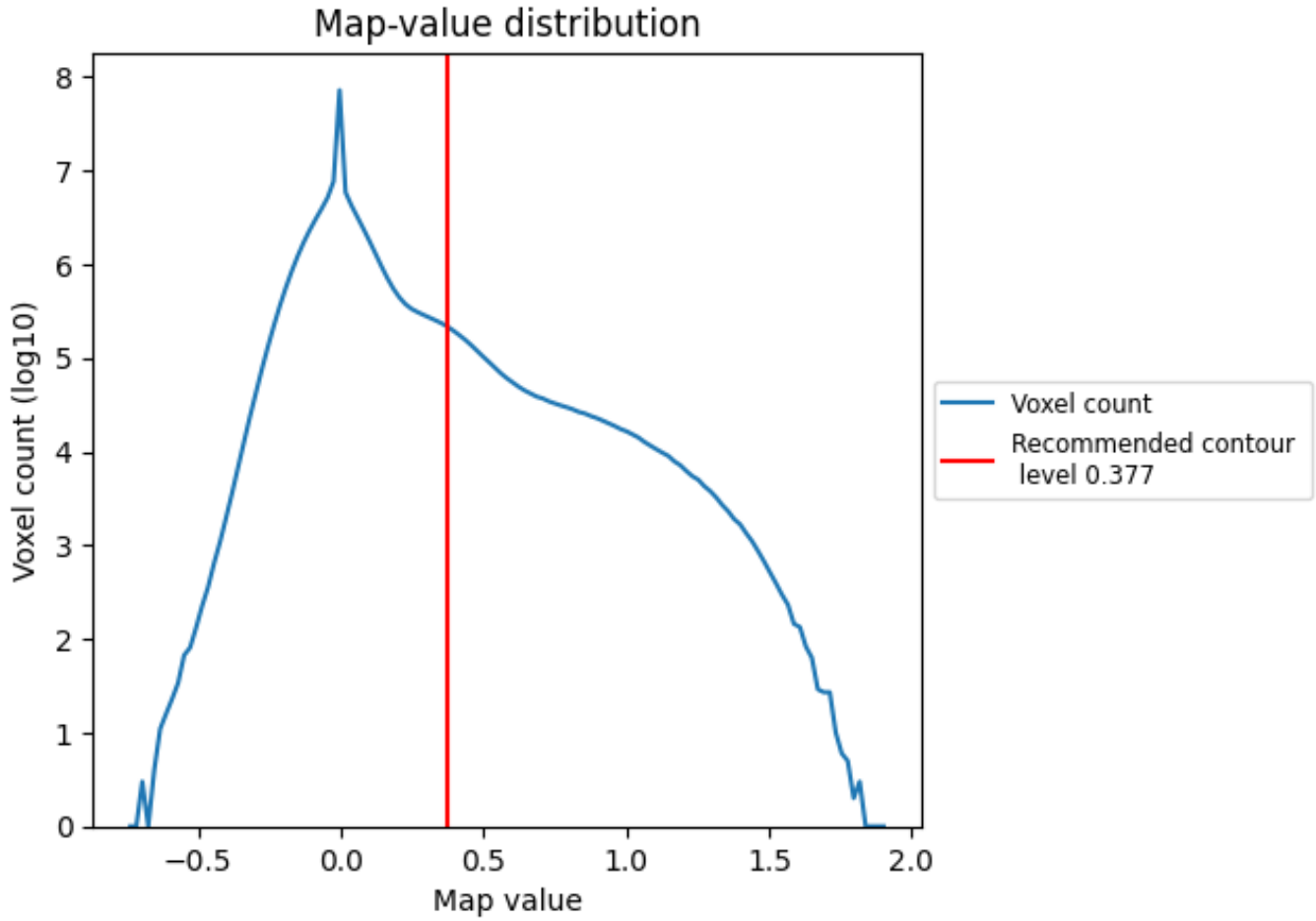
6.6 Mask visualisation (i)

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

7 Map analysis

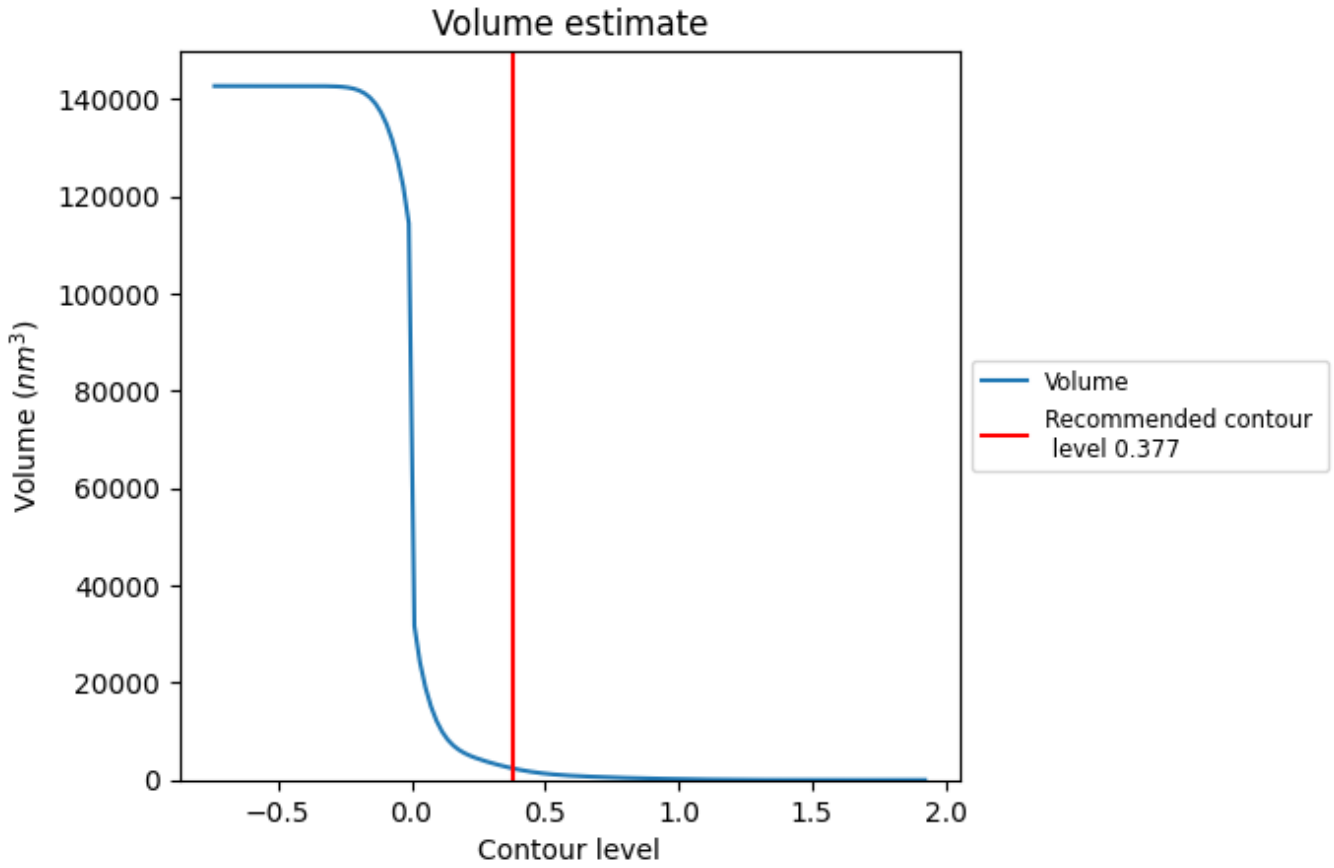
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

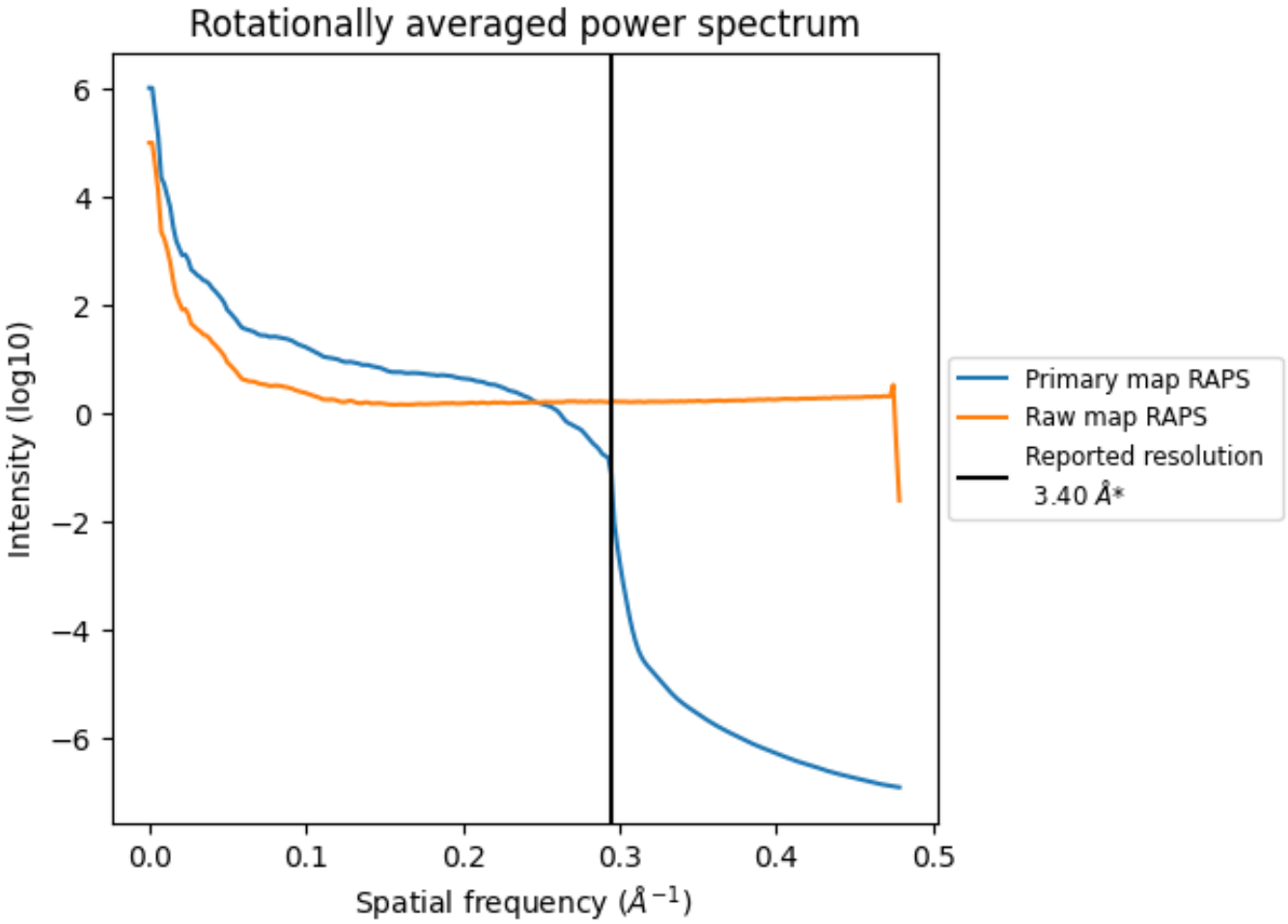
7.2 Volume estimate



The volume at the recommended contour level is 2415 nm^3; this corresponds to an approximate mass of 2182 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)

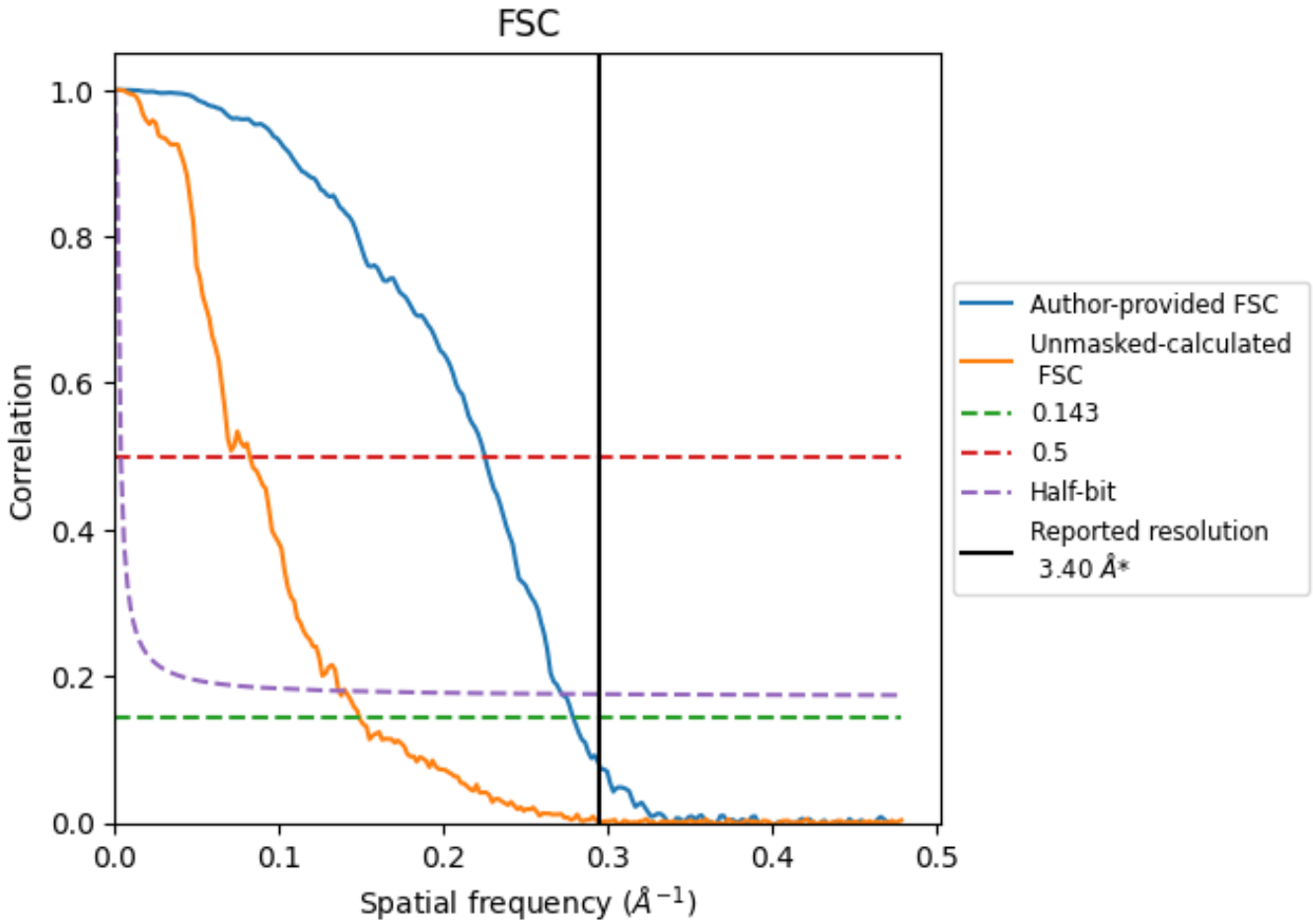


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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)

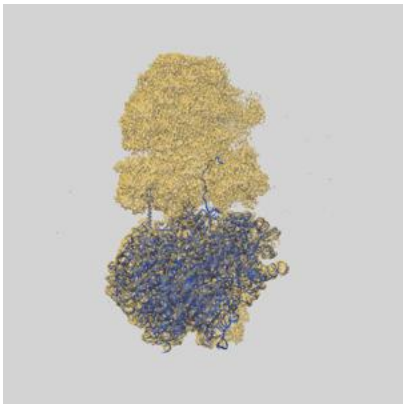
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.59	4.44	3.68
Unmasked-calculated*	6.72	12.17	7.33

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

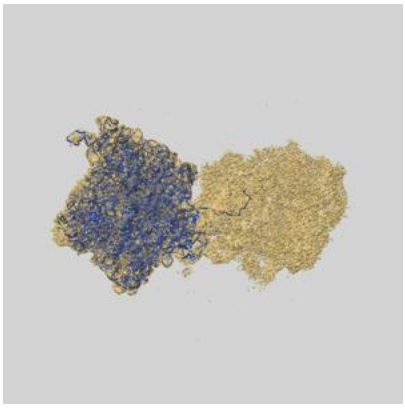
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18558 and PDB model 8QPP. Per-residue inclusion information can be found in section 3 on page 13.

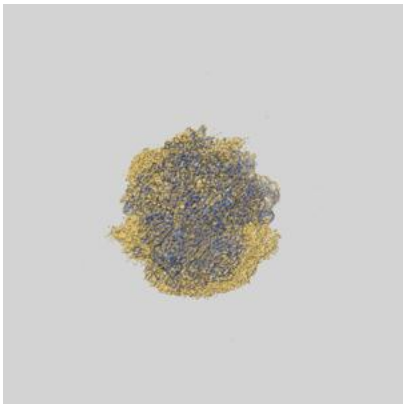
9.1 Map-model overlay



X



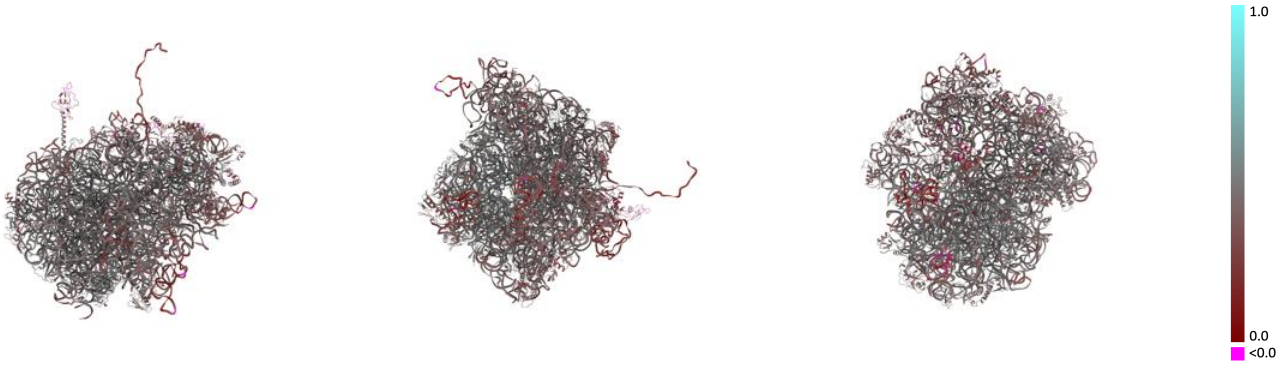
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.377 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.

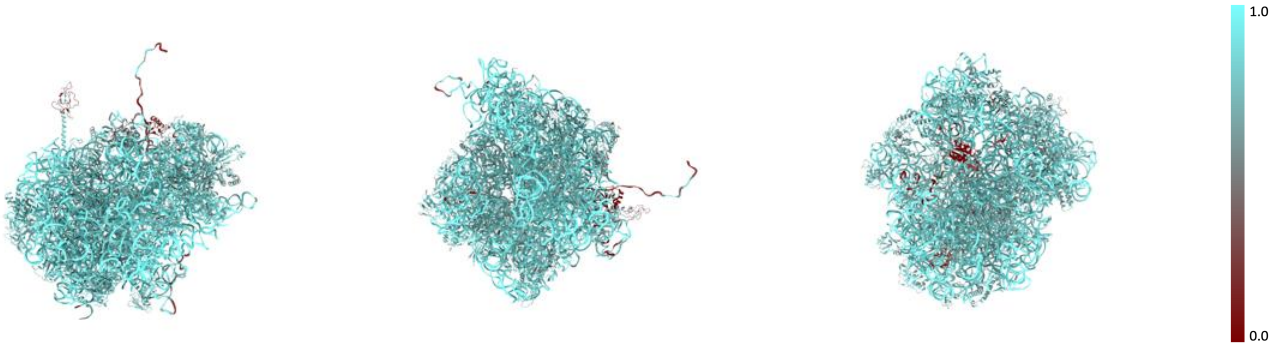
9.2 Q-score mapped to coordinate model (i)



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.

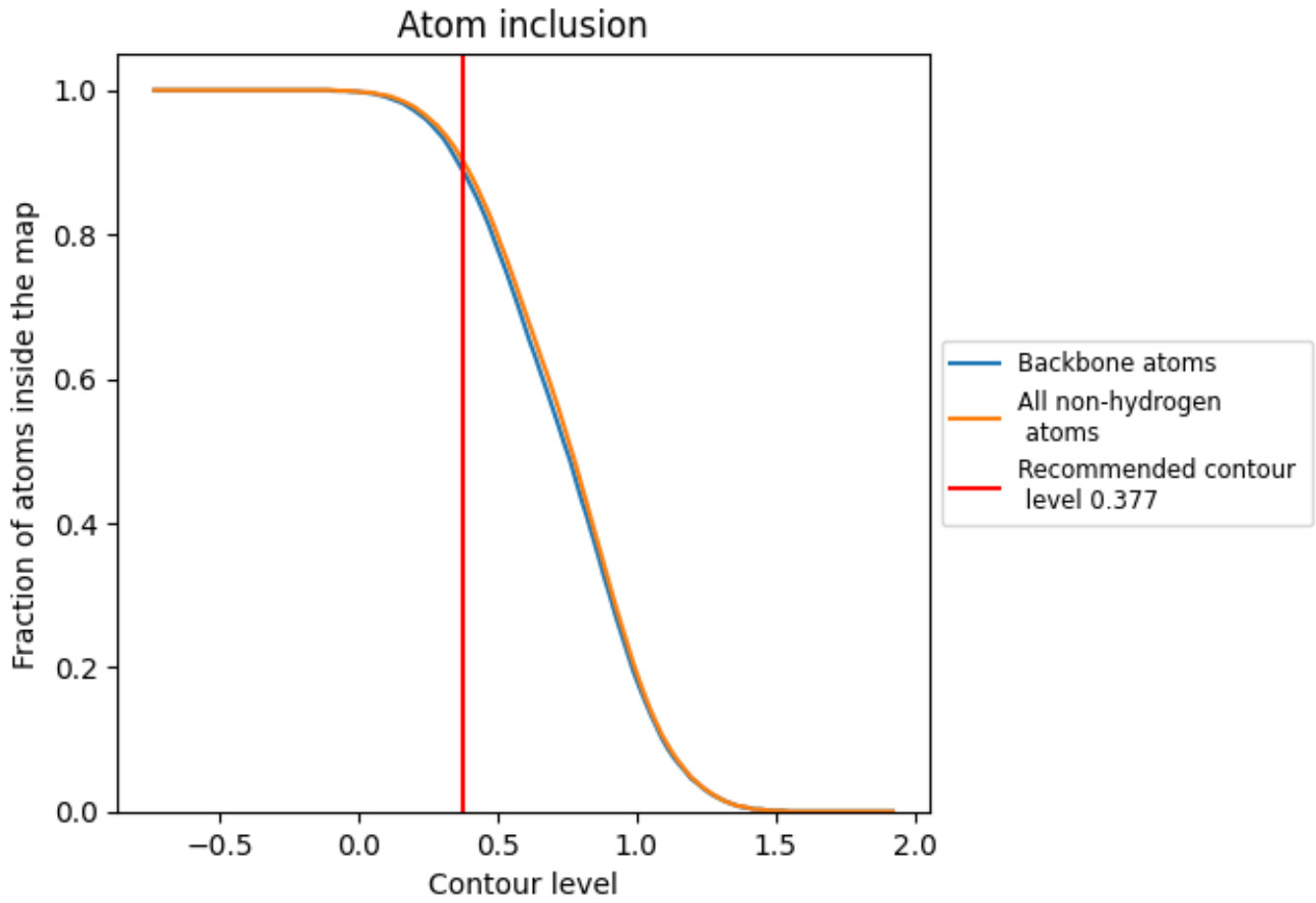
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.377).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.377) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.4150
0	0.8620	0.4680
1	0.7450	0.4240
2	0.8320	0.4800
3	0.8140	0.4790
4	0.8140	0.4590
6	0.7400	0.3390
9	0.5360	0.2560
A	0.9600	0.4070
B	0.6580	0.3500
C	0.7330	0.3860
D	0.7510	0.3620
E	0.7770	0.4390
F	0.7150	0.4120
G	0.6980	0.3620
H	0.7770	0.4350
I	0.7700	0.3840
J	0.7740	0.3920
K	0.6850	0.4160
L	0.7930	0.4390
M	0.8270	0.3850
N	0.8360	0.4190
O	0.7820	0.4000
P	0.8080	0.4190
Q	0.7520	0.4330
R	0.6690	0.4040
S	0.8650	0.3990
T	0.7800	0.3800
U	0.9190	0.3930
V	0.4590	0.2680
W	0.0260	0.2270
X	0.9550	0.4240
Y	0.9720	0.3960
Z	0.8020	0.4740
a	0.8480	0.4720

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Chain	Atom inclusion	Q-score
b	0.8030	0.4310
c	0.7640	0.3650
d	0.7960	0.3910
e	0.8560	0.4410
f	0.7740	0.4660
i	0.8040	0.4450
j	0.8200	0.4580
k	0.8310	0.4530
l	0.7970	0.3890
m	0.8150	0.4560
n	0.8500	0.4220
o	0.8250	0.4430
r	0.8130	0.4490
s	0.7850	0.4590
t	0.7920	0.4180
u	0.8300	0.4560
v	0.7110	0.4600
w	0.7920	0.3810
x	0.8270	0.4360