



wwPDB EM Validation Summary 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 wwPDB EM Validation Summary 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:

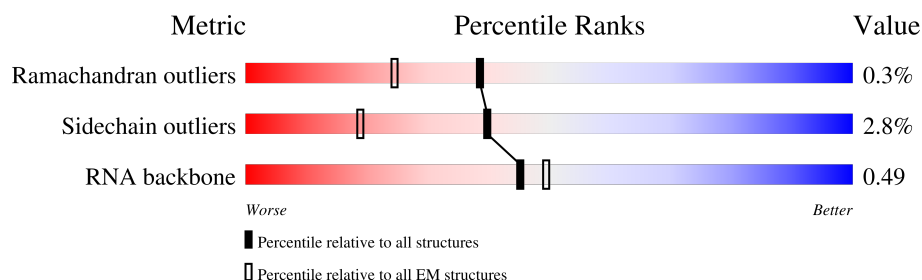
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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 $\leq 5\%$. 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	
2	1	48	
3	2	44	
4	3	66	
5	4	37	
6	6	64	
7	B	246	
8	C	218	

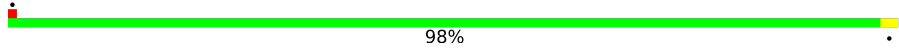
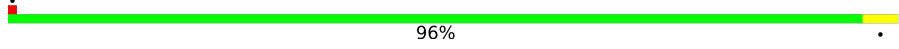
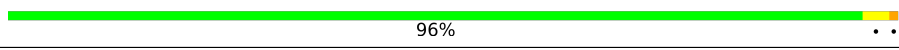
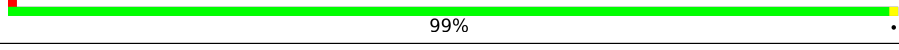
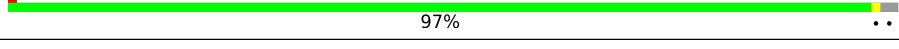
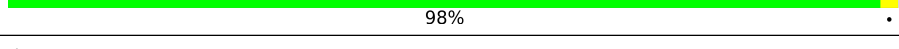
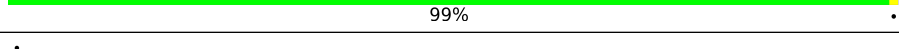
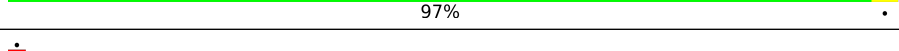
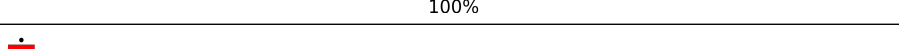
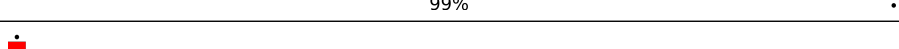
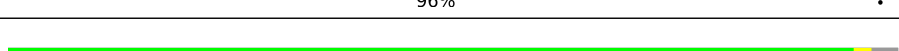
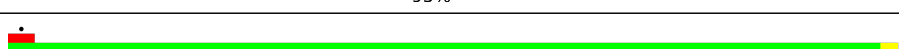

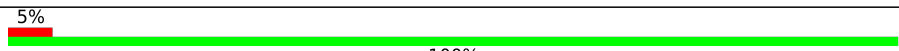
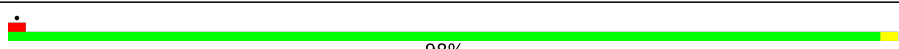
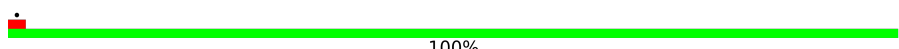
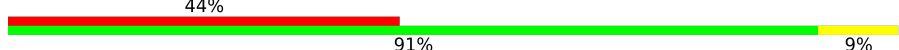



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Mol	Chain	Length	Quality of chain
9	D	200	
10	E	166	
11	F	95	
12	G	156	
13	H	132	
14	I	130	
15	J	102	
16	K	131	
17	L	138	
18	M	121	
19	N	61	
20	O	89	
21	P	90	
22	Q	87	
23	R	79	
24	S	92	
25	T	88	
26	U	77	
27	V	33	
28	W	785	
29	Y	112	
30	Z	275	
31	a	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
1	0	54	Total	C	H	N	O	S	0	0
			872	262	446	86	71	7		

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

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

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

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

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

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

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
5	4	37	Total	C	H	N	O	S	0	0
			639	186	342	60	46	5		

- 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	S	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	S	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).

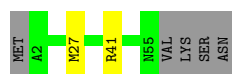
Mol	Chain	Residues	Atoms						AltConf	Trace
53	A	1533	Total	C	H	N	O	P	0	0
			49450	14667	16559	6034	10657	1533		

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.

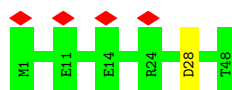
- Molecule 1: 50S ribosomal protein L32

Chain 0:  88% 8%



- Molecule 2: Large ribosomal subunit protein bL33

Chain 1:  8% 98%



- Molecule 3: Large ribosomal subunit protein bL34

Chain 2:  100%



- Molecule 4: Large ribosomal subunit protein bL35

Chain 3:  94%



- Molecule 5: 50S ribosomal protein L36

Chain 4:  100%



- Molecule 6: Large ribosomal subunit protein bL31

Chain 6:

Chain B:

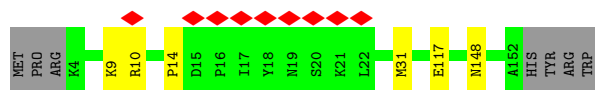
Chain C:

Chain D:

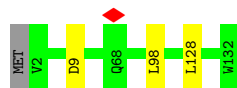
Chain E:

Chain F:

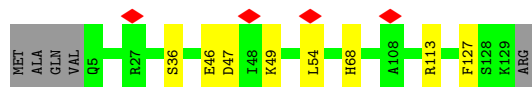
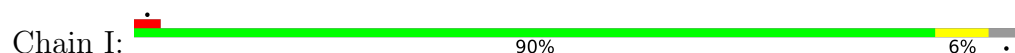
Chain G:



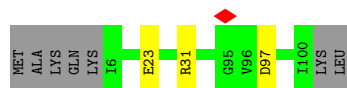
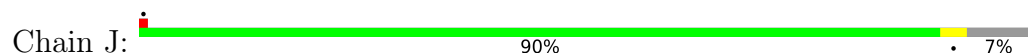
- Molecule 13: 30S ribosomal protein S8



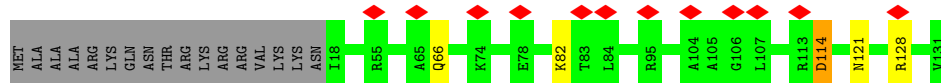
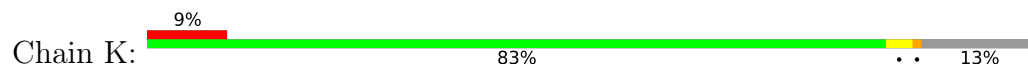
- Molecule 14: 30S ribosomal protein S9



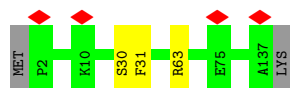
- Molecule 15: 30S ribosomal protein S10



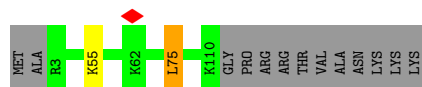
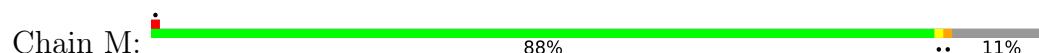
- Molecule 16: 30S ribosomal protein S11



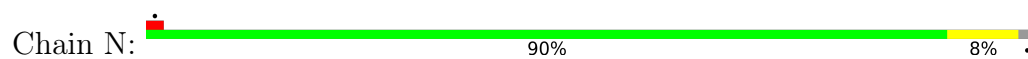
- Molecule 17: 30S ribosomal protein S12



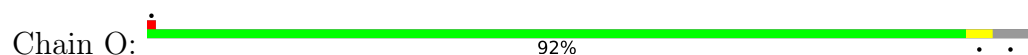
- Molecule 18: 30S ribosomal protein S13



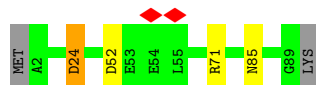
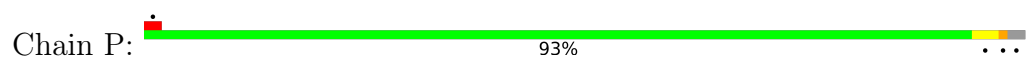
- Molecule 19: 30S ribosomal protein S14 type Z



- Molecule 20: 30S ribosomal protein S15



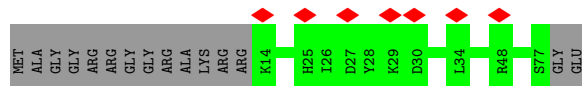
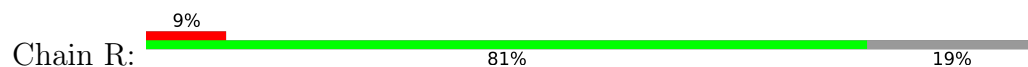
- Molecule 21: 30S ribosomal protein S16



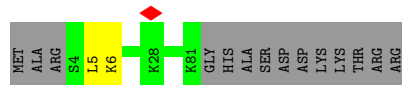
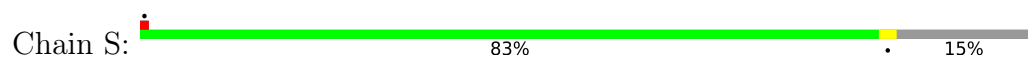
- Molecule 22: 30S ribosomal protein S17



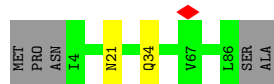
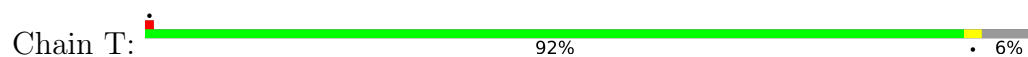
- Molecule 23: 30S ribosomal protein S18

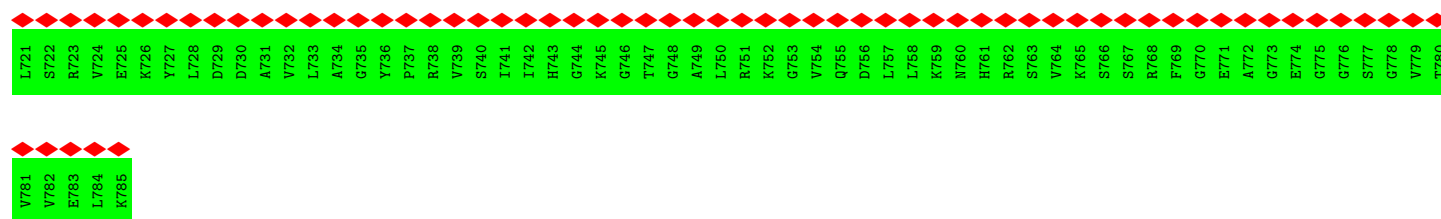


- Molecule 24: 30S ribosomal protein S19



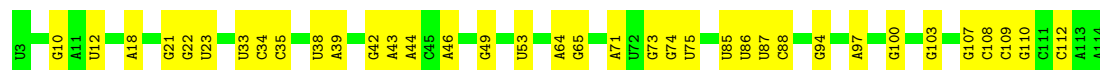
- Molecule 25: 30S ribosomal protein S20





• Molecule 29: 5S rRNA (112-MER)

Chain Y: 68% 32%



• Molecule 30: Large ribosomal subunit protein uL2

Chain Z: 96% ...



• Molecule 31: Large ribosomal subunit protein uL3

Chain a: 96% .



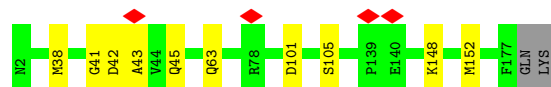
• Molecule 32: Large ribosomal subunit protein uL4

Chain b: 99% .



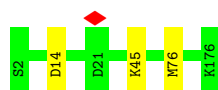
• Molecule 33: Large ribosomal subunit protein uL5

Chain c: 93% 6% .

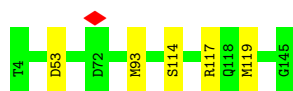


• Molecule 34: Large ribosomal subunit protein uL6

Chain d: 98% .



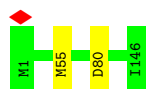
- Molecule 35: Large ribosomal subunit protein uL13



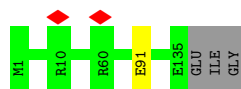
- Molecule 36: 50S ribosomal protein L14



- Molecule 37: 50S ribosomal protein L15



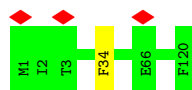
- Molecule 38: Large ribosomal subunit protein uL16



- Molecule 39: Large ribosomal subunit protein bL17

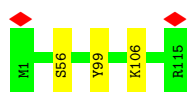


- Molecule 40: 50S ribosomal protein L18



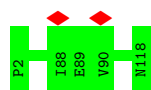
- Molecule 41: 50S ribosomal protein L19

Chain m:  97%



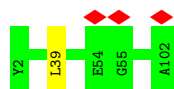
- Molecule 42: Large ribosomal subunit protein bL20

Chain n:  100%



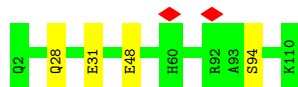
- Molecule 43: Large ribosomal subunit protein bL21

Chain o:  99%



- Molecule 44: Large ribosomal subunit protein uL22

Chain r:  96%



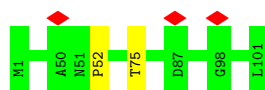
- Molecule 45: Large ribosomal subunit protein uL23

Chain s:  95%



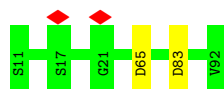
- Molecule 46: Large ribosomal subunit protein uL24

Chain t:  98%

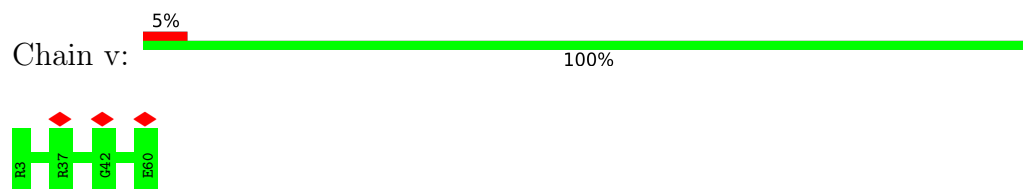


- Molecule 47: Large ribosomal subunit protein bL27

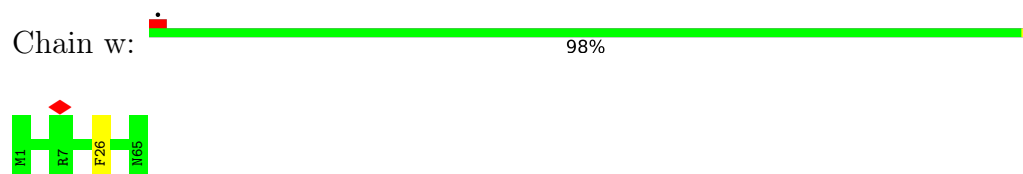
Chain u:  98%



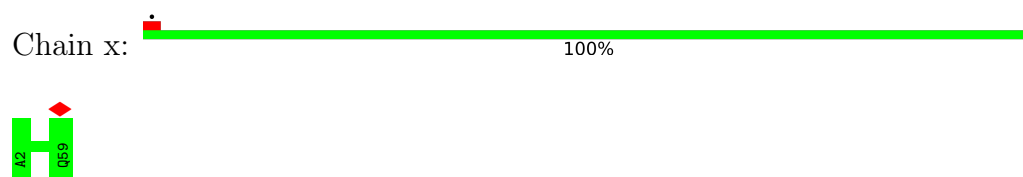
- Molecule 48: Large ribosomal subunit protein bL28



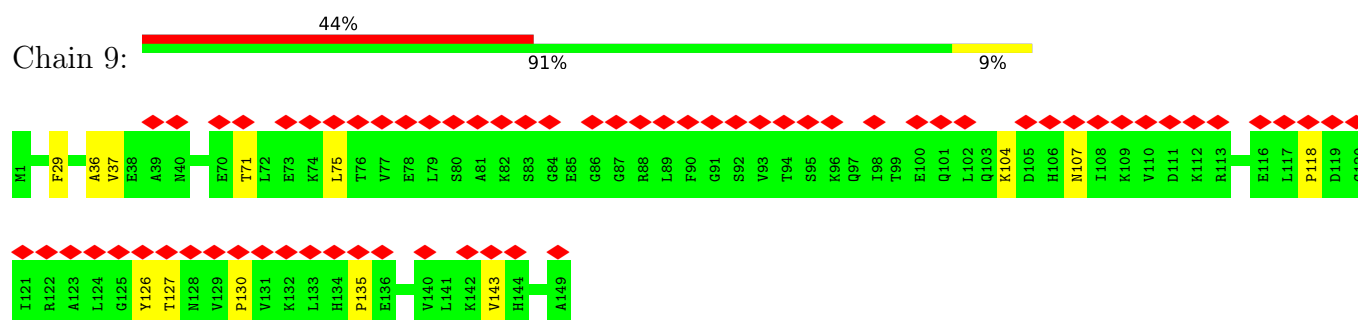
- Molecule 49: Large ribosomal subunit protein uL29



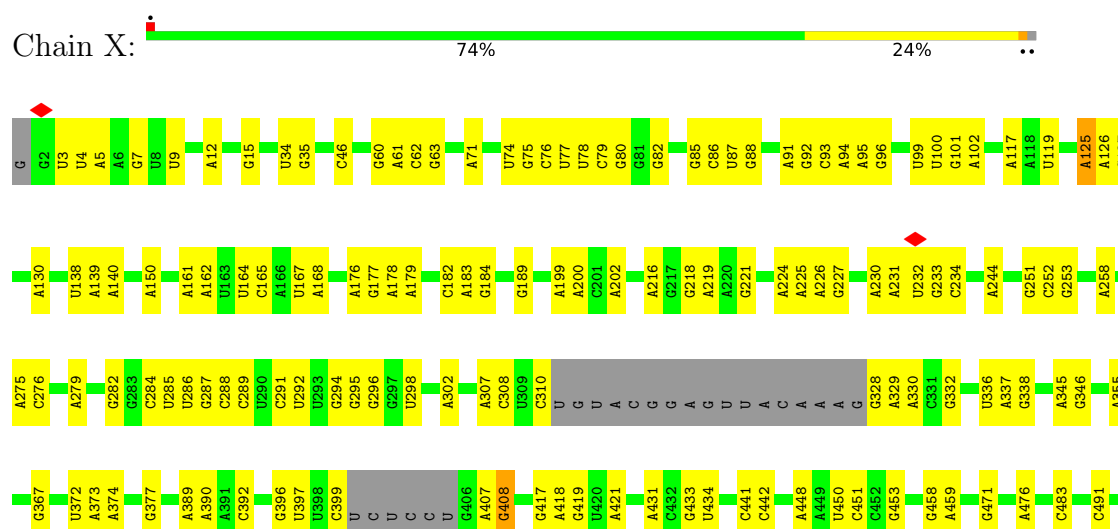
- Molecule 50: Large ribosomal subunit protein uL30



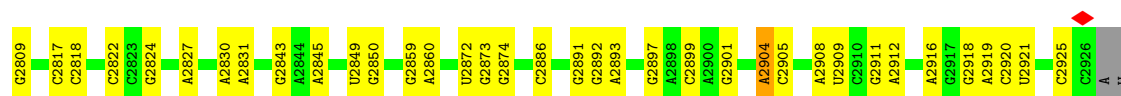
- Molecule 51: 50S ribosomal protein L9



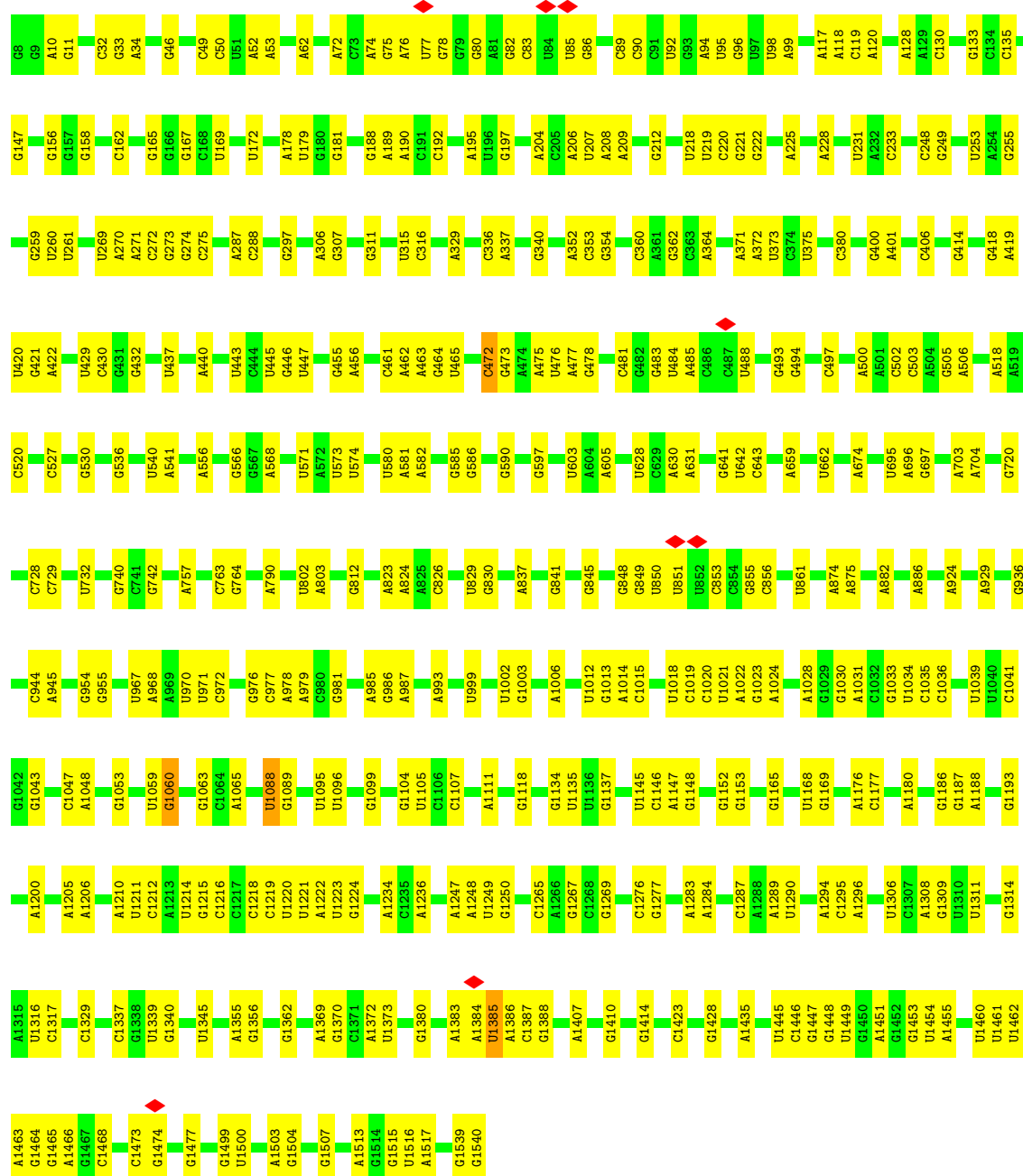
- Molecule 52: 23S ribosomal RNA



U495	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1
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• Molecule 53: 16S rRNA (1533-MER)



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 (\AA)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.045, 1.045, 1.045	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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.

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

5 of 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

5.3.2 Protein sidechains ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	l	34	PHE
43	o	39	LEU
14	I	127	PHE
14	I	113	ARG
44	r	31	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
35	e	8	ASN
40	l	43	GLN
39	k	72	ASN
43	o	50	ASN
11	F	33	ASN

5.3.3 RNA [i](#)

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%)

5 of 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

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	X	2192	U
53	A	1369	A
52	X	2469	C
53	A	1316	U

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Mol	Chain	Res	Type
53	A	1022	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

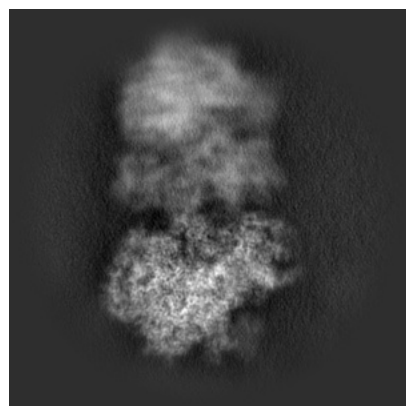
6 Map visualisation [i](#)

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.

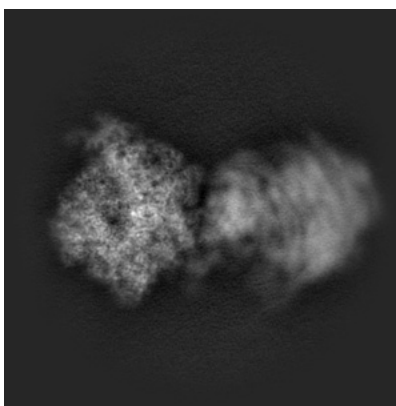
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

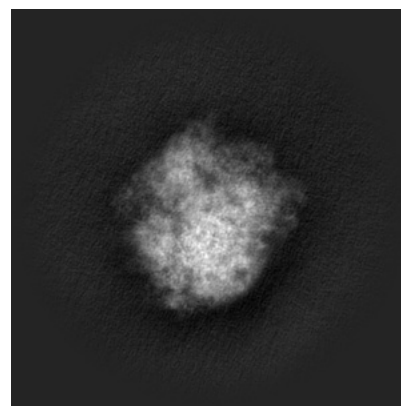
6.1.1 Primary map



X

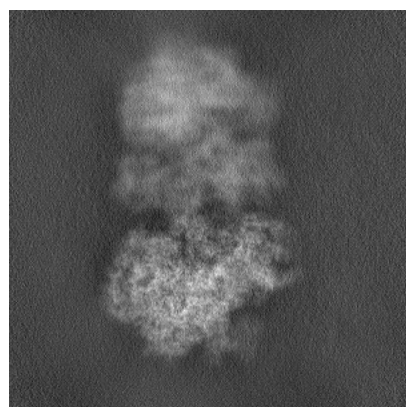


Y

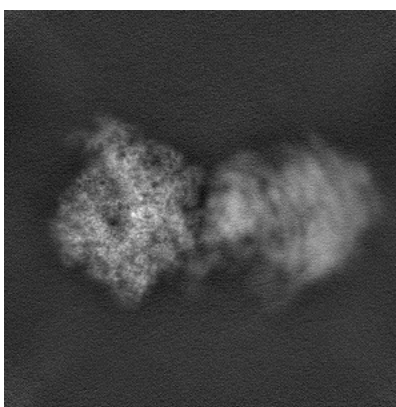


Z

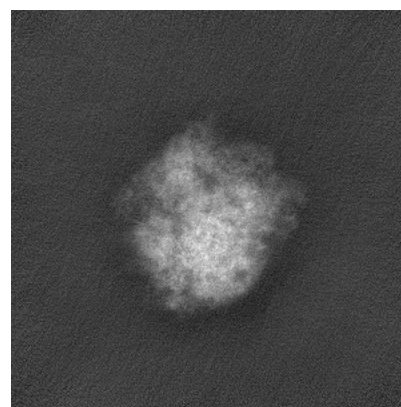
6.1.2 Raw map



X



Y

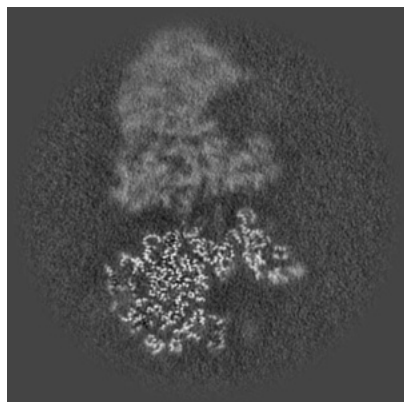


Z

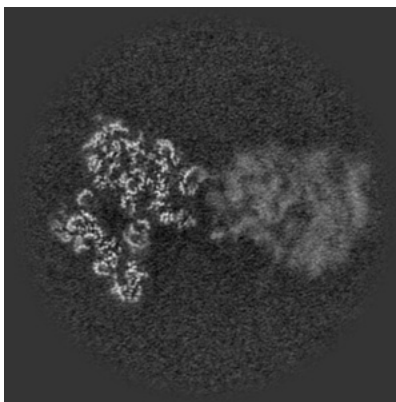
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

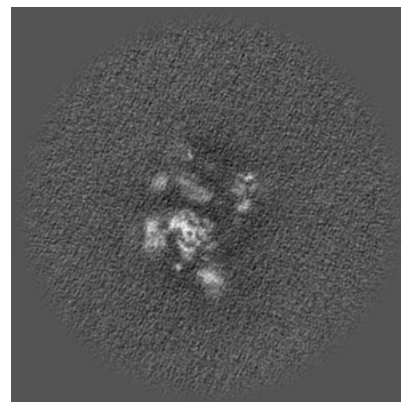
6.2.1 Primary map



X Index: 250

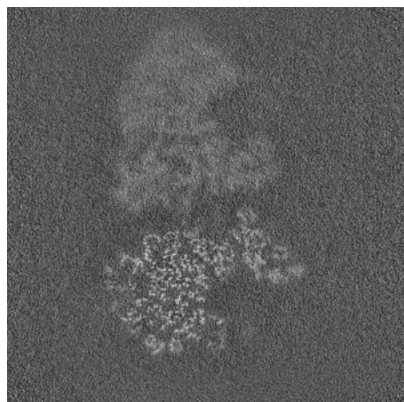


Y Index: 250

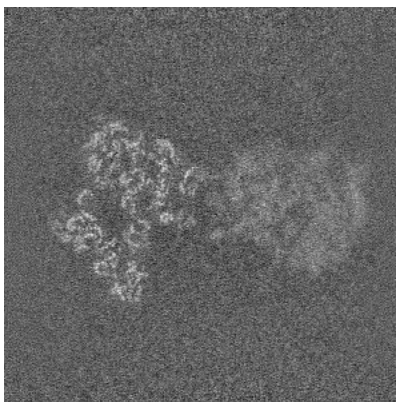


Z Index: 250

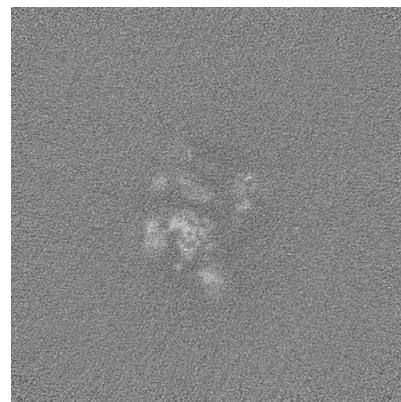
6.2.2 Raw map



X Index: 250



Y Index: 250

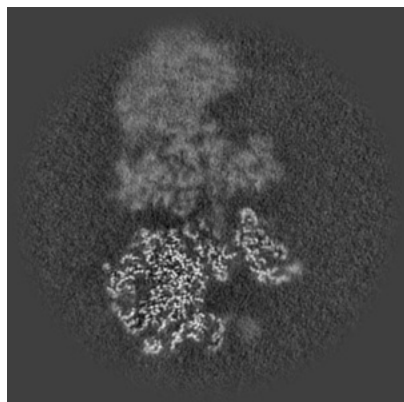


Z Index: 250

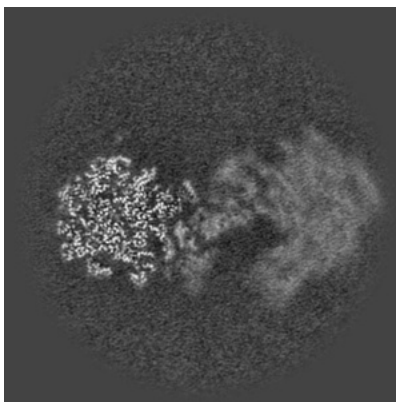
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

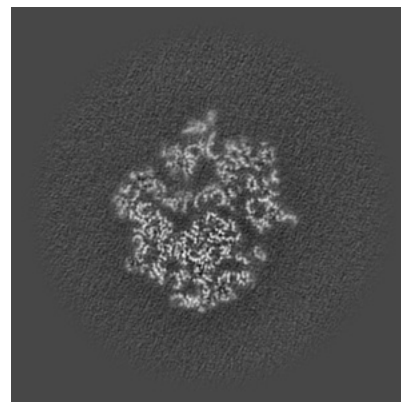
6.3.1 Primary map



X Index: 246

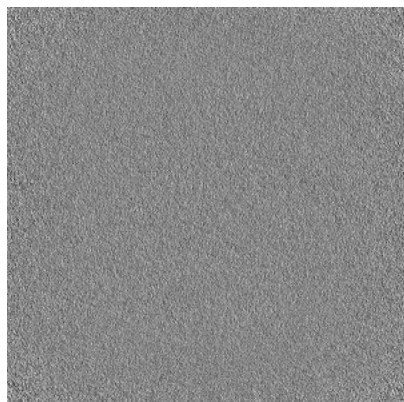


Y Index: 210

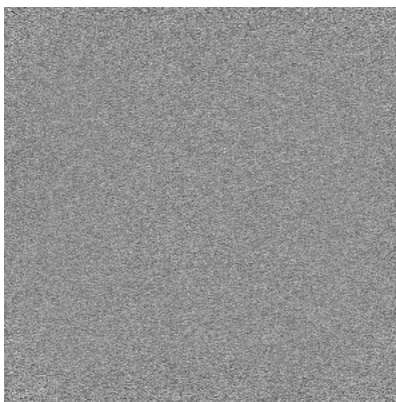


Z Index: 167

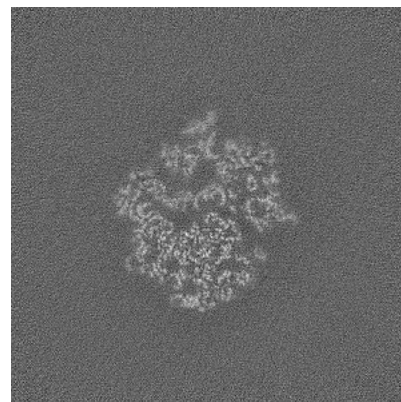
6.3.2 Raw map



X Index: 0



Y Index: 0

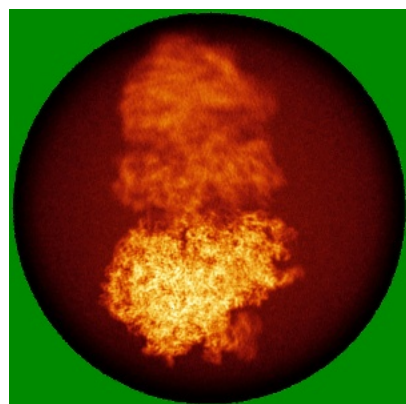


Z Index: 168

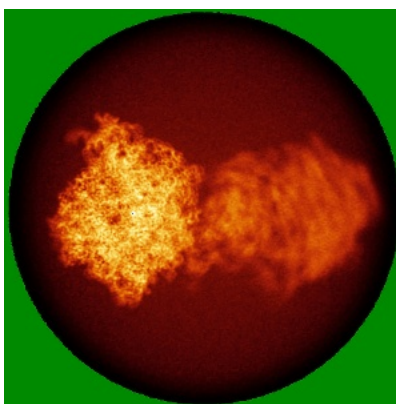
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

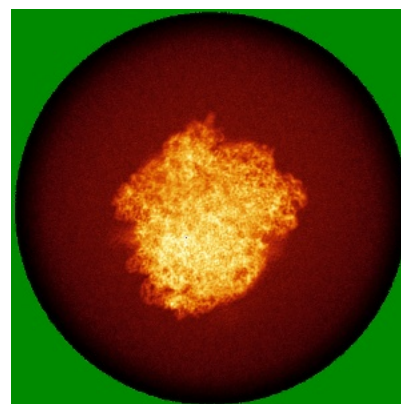
6.4.1 Primary map



X

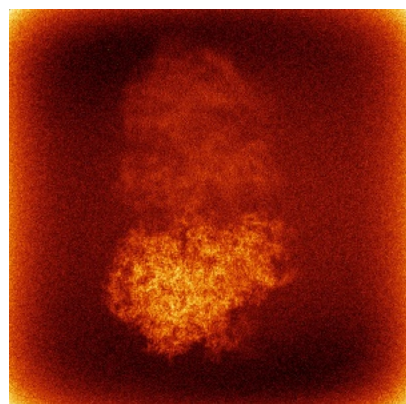


Y

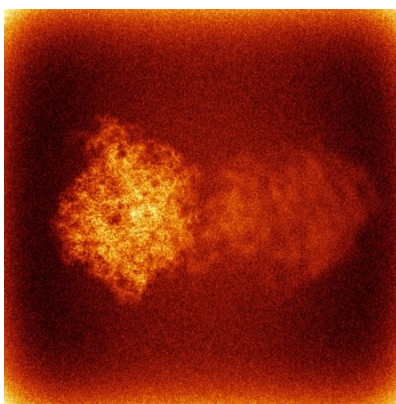


Z

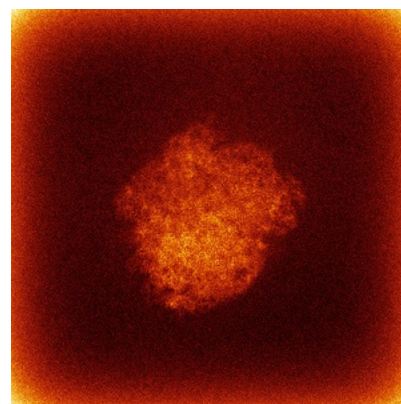
6.4.2 Raw map



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.

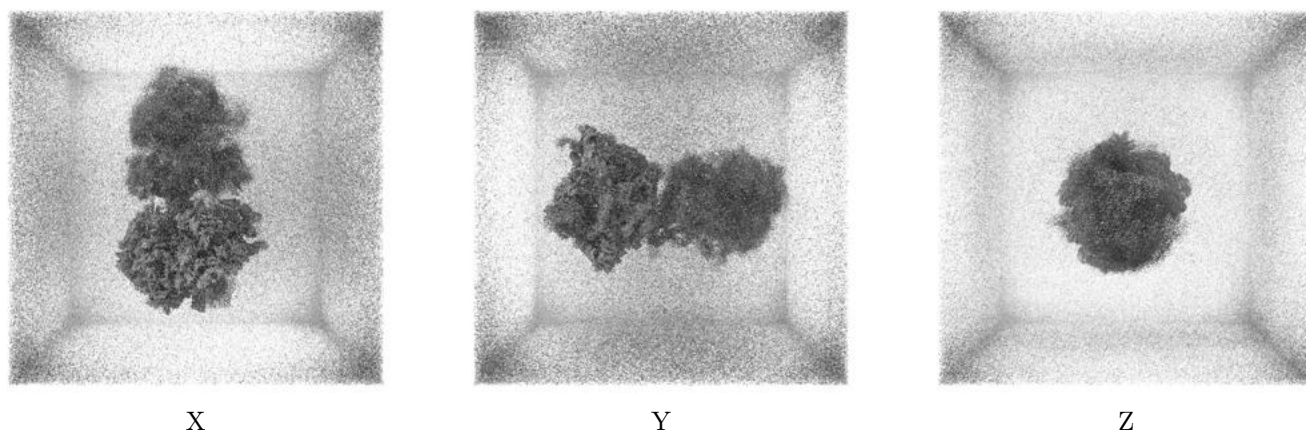
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

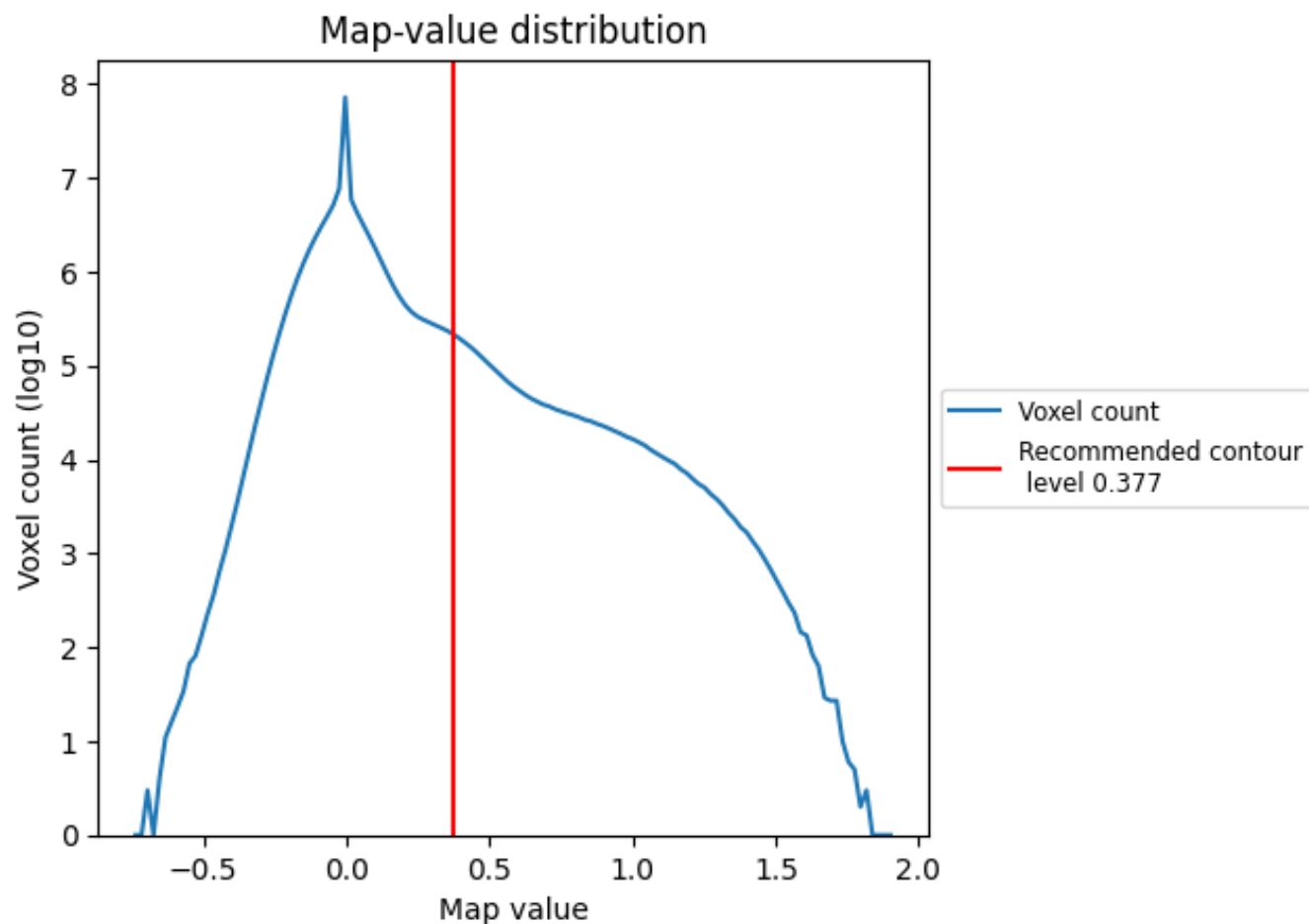
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

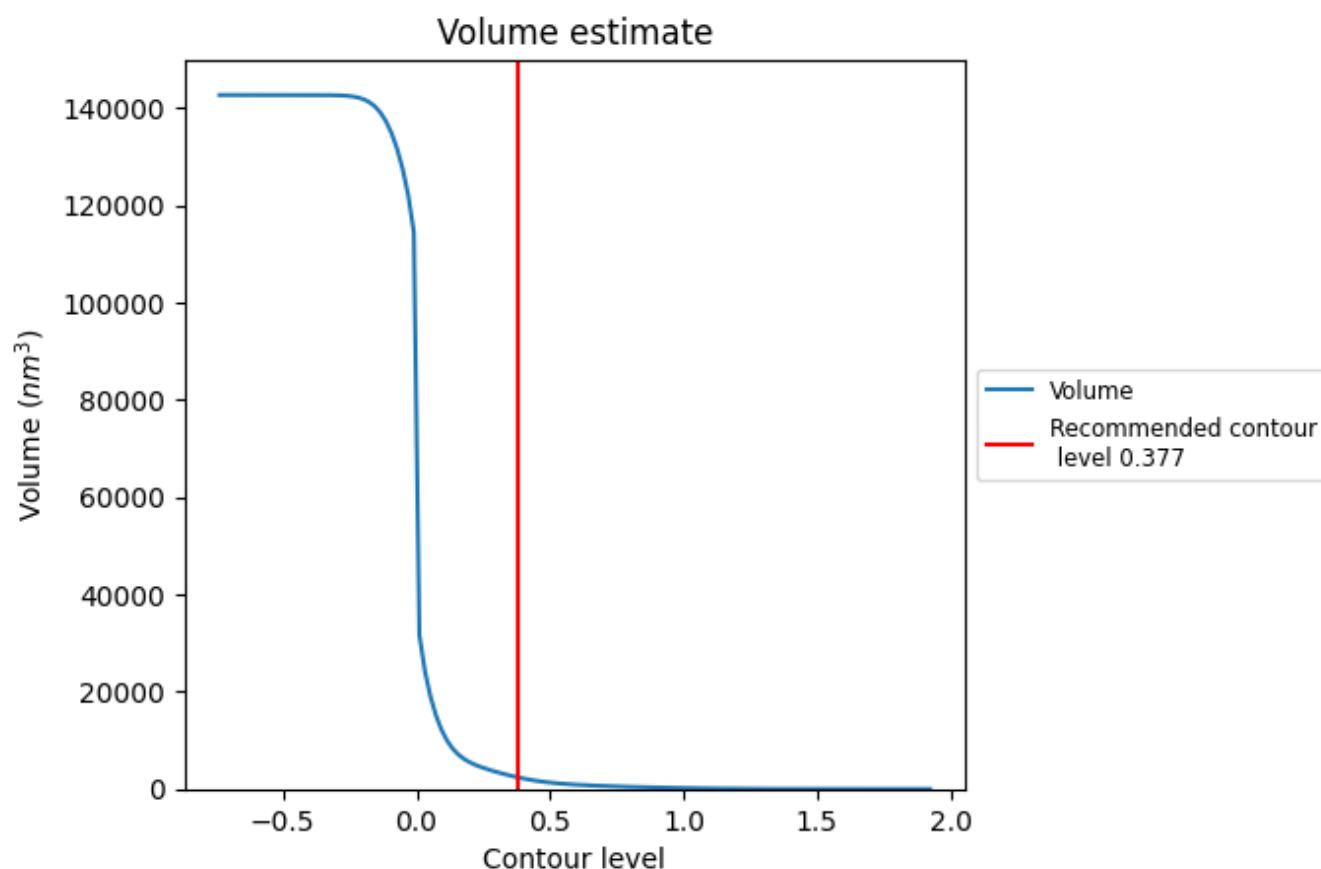
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

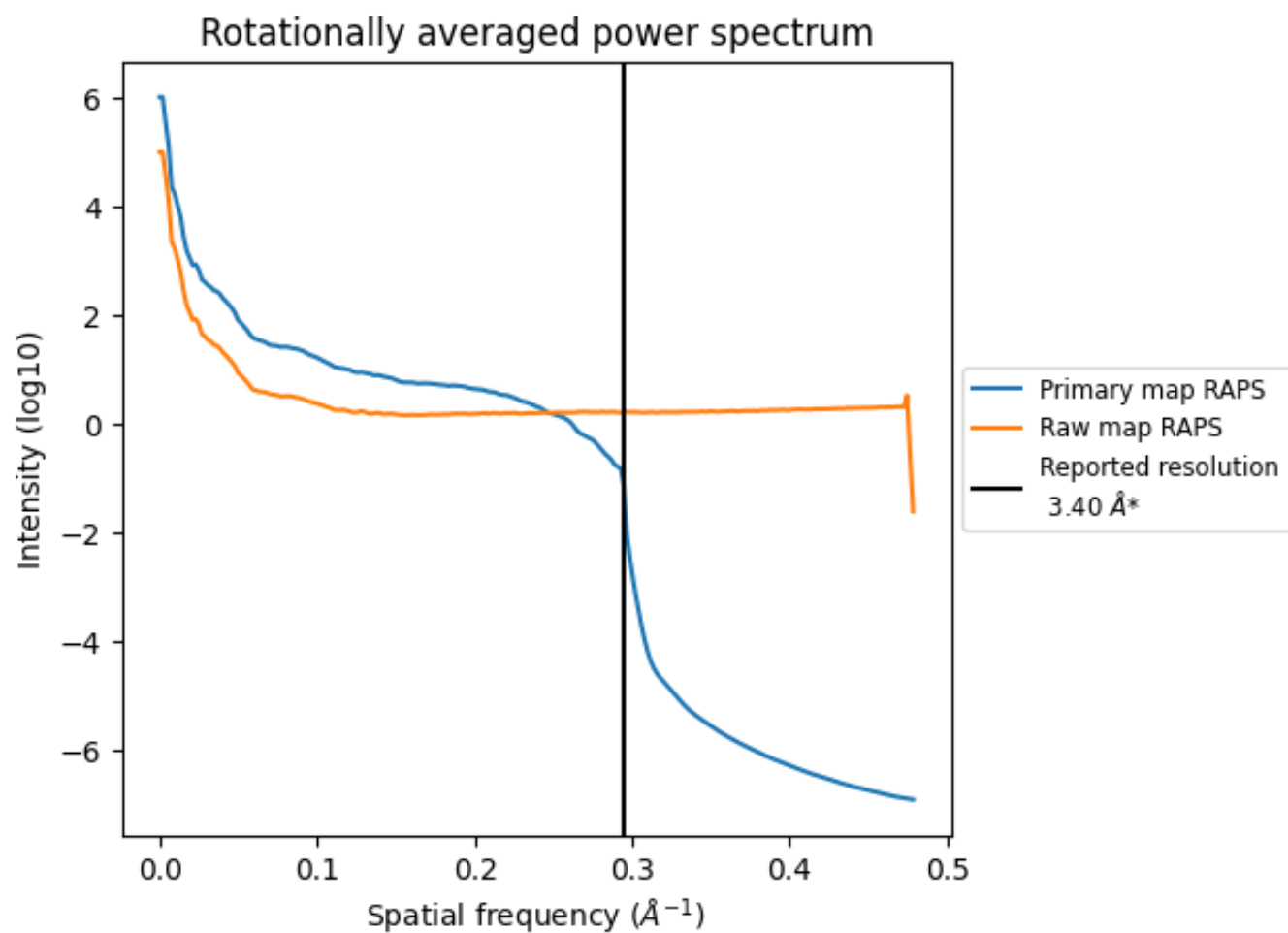
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2415 nm³; 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 ⓘ

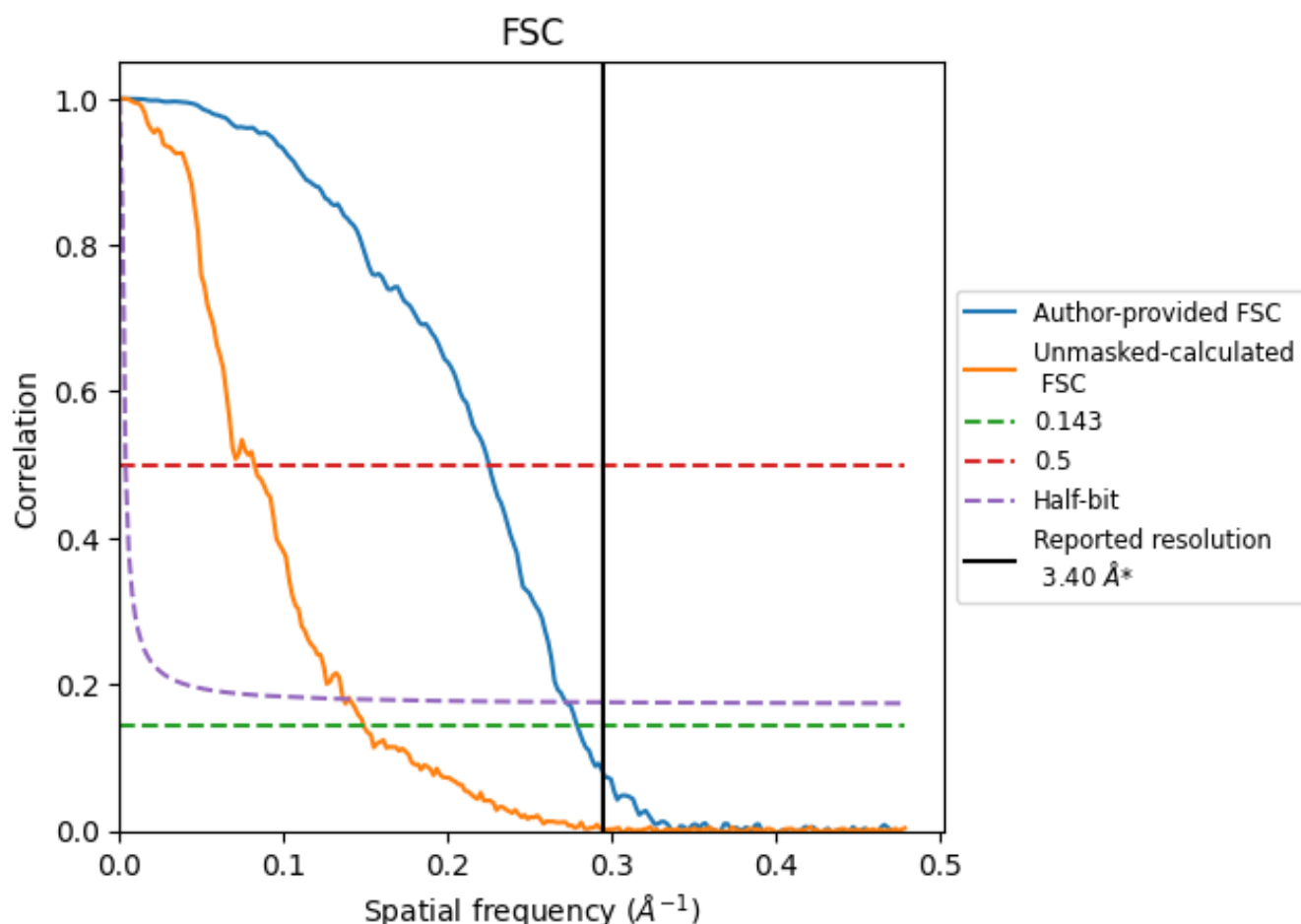


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

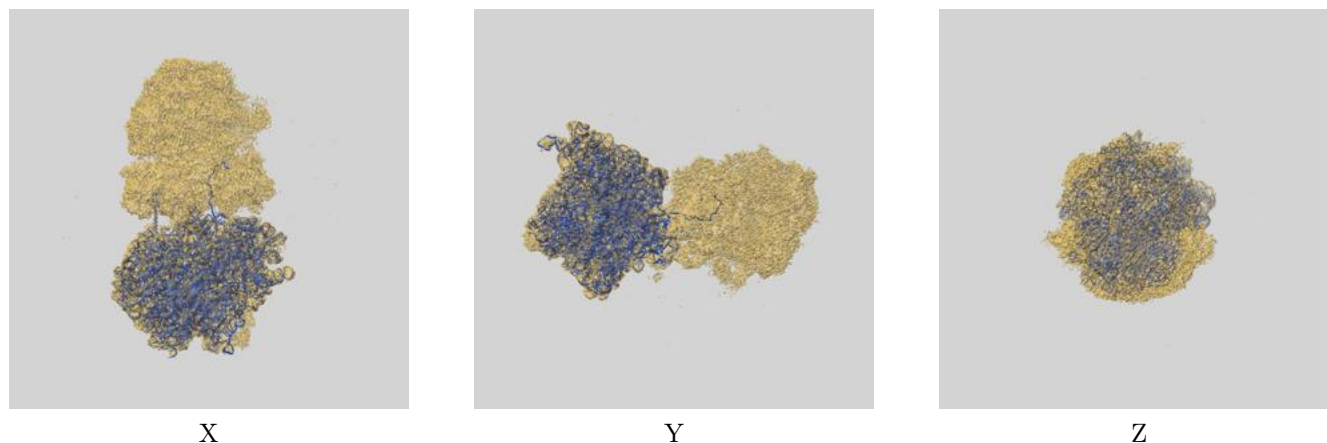
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.59	4.44	3.68
Unmasked-calculated*	6.72	12.17	7.33

*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 [i](#)

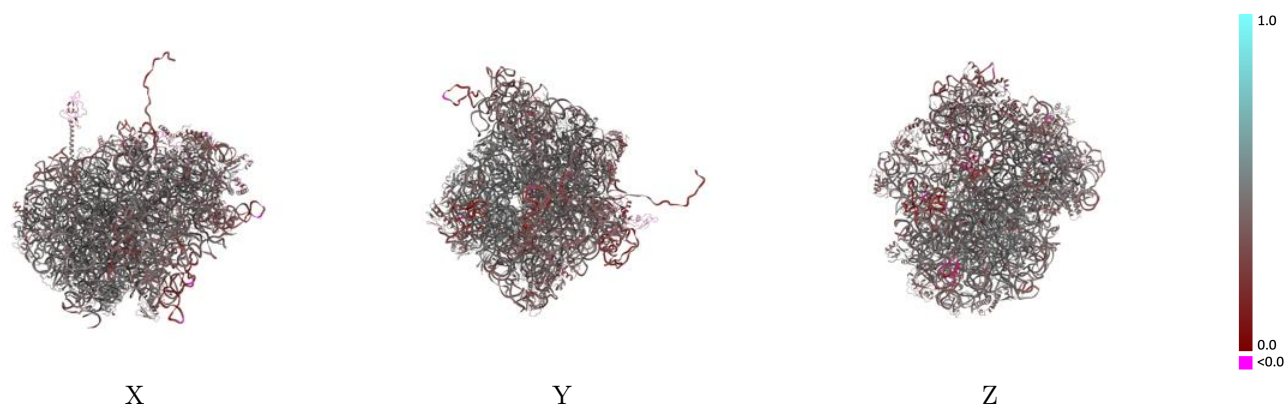
This section contains information regarding the fit between EMDB map EMD-18558 and PDB model 8QPP. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



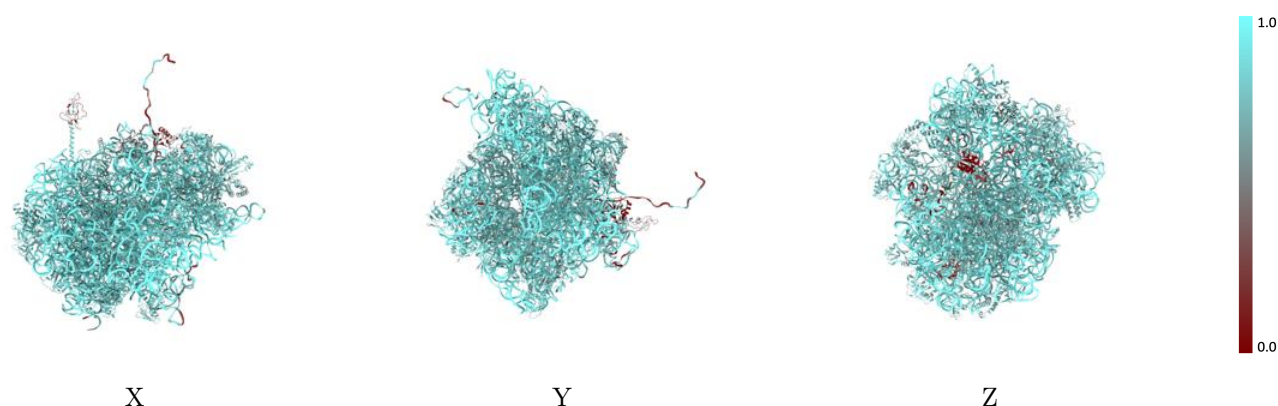
The images above show the 3D surface view of the map at the recommended contour level 0.377 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



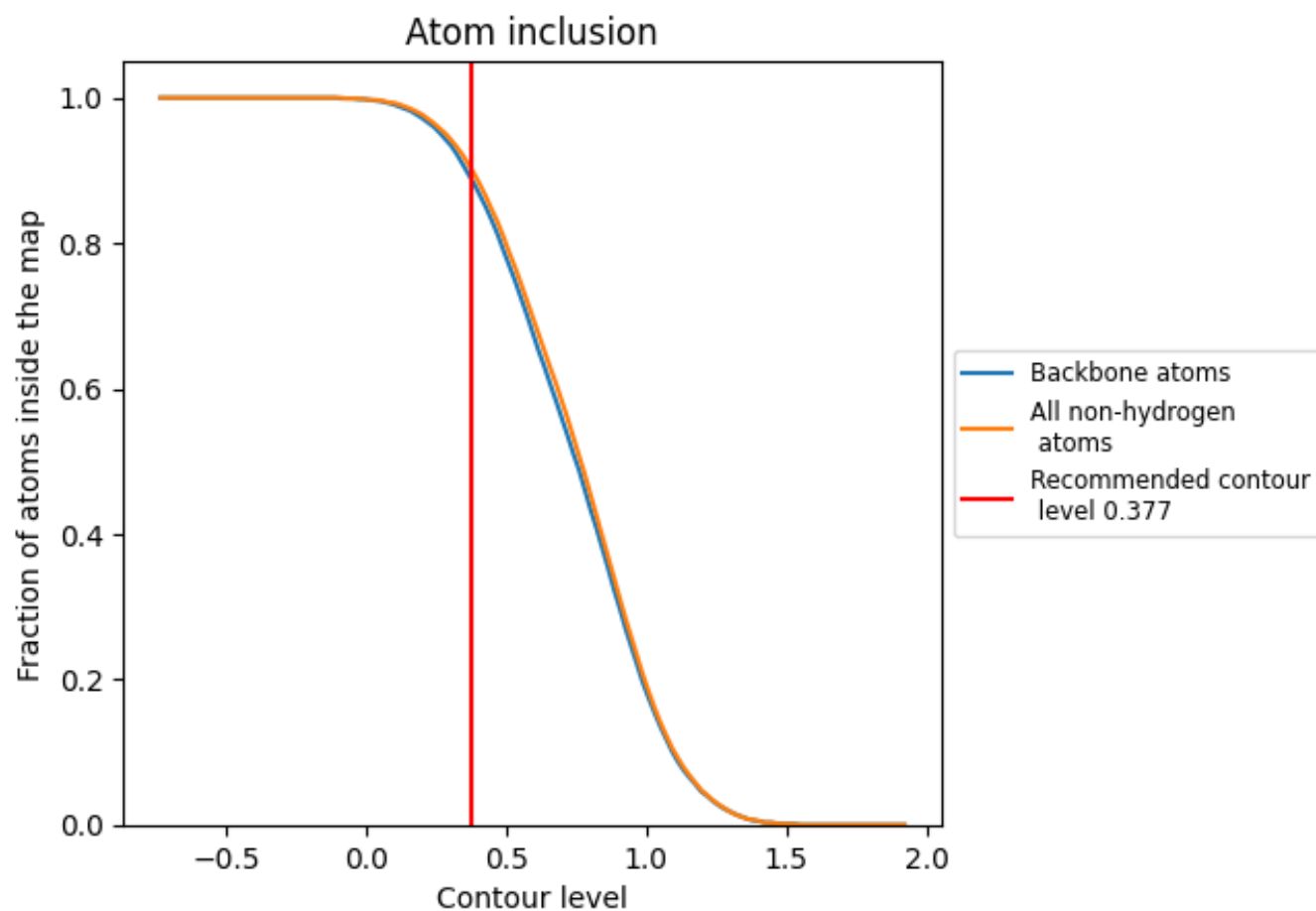
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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