



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2022 – 11:02 PM EDT

PDB ID : 7SFR
EMDB ID : EMD-25100
Title : Unmethylated Mtb Ribosome 50S with SEQ-9
Authors : Xing, Z.; Cui, Z.; Zhang, J.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2021-10-04
Resolution : 2.60 Å(reported)
Based on initial model : 7KGB

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:

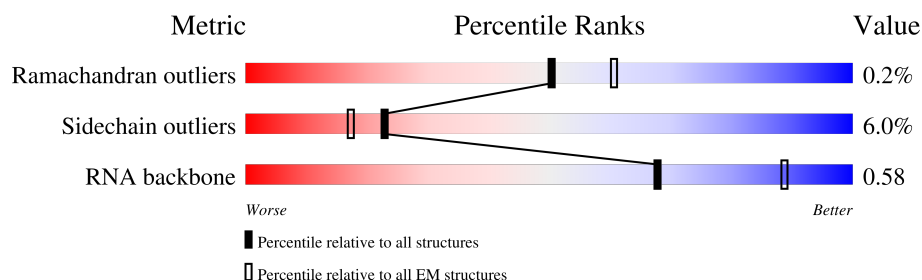
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



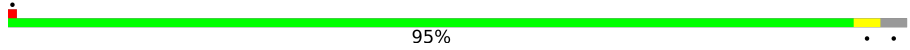
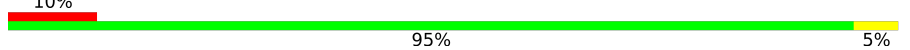
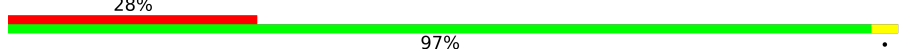

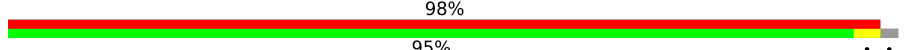

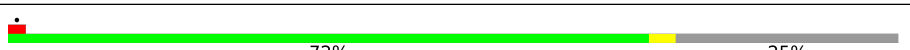
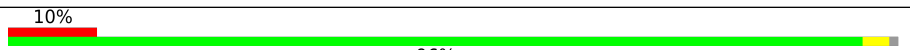
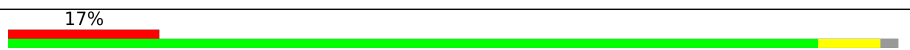
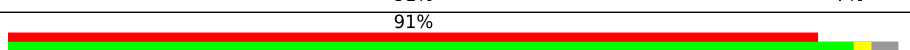
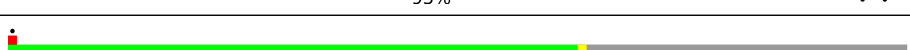

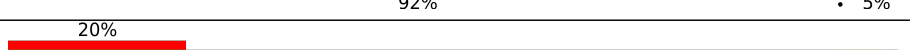
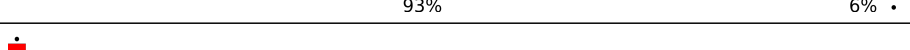
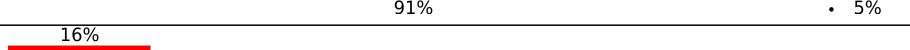
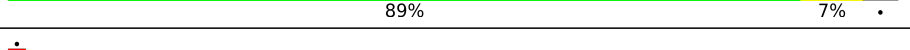

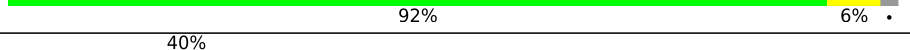



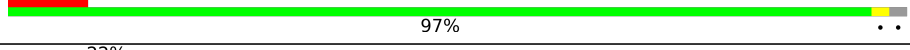
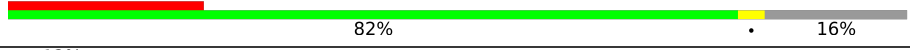


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	57	
2	1	55	
3	2	47	
4	3	64	
5	4	37	
6	6	80	
7	A	3138	
8	B	115	

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Mol	Chain	Length	Quality of chain
9	C	279	
10	D	213	
11	E	207	
12	F	178	
13	G	177	
14	H	152	
15	J	195	
16	K	122	
17	L	146	
18	M	138	
19	N	180	
20	O	122	
21	P	113	
22	Q	129	
23	R	104	
24	S	197	
25	T	100	
26	U	105	
27	V	215	
28	W	86	
29	X	64	
30	Y	77	
31	Z	65	
32	a	1537	
33	c	274	

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Mol	Chain	Length	Quality of chain
34	d	201	
35	e	220	
36	f	96	
37	g	156	
38	h	132	
39	i	151	
40	j	101	
41	k	139	
42	l	124	
43	m	124	
44	n	61	
45	o	89	
46	p	162	
47	q	135	
48	r	84	
49	s	93	
50	t	86	
51	v	22	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 143665 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	54	Total	C	N	O	0	0
			429	266	94	69		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			400	245	84	67	4		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	42	Total	C	N	O	S	0	0
			358	212	94	51	1		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	62	Total	C	N	O	0	0
			494	298	112	84		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			299	182	66	47	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	MET	conflict	UNP A0A3E0V5U0

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	57	Total	C	N	O	S	0	0
			446	277	82	82	5		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	3118	Total	C	N	O	P	0	0
			66961	29850	12340	21653	3118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	115	Total	C	N	O	P	0	0
			2458	1097	456	790	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2088	1277	437	369	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	213	Total	C	N	O	S	0	0
			1590	985	307	292	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	207	Total	C	N	O	S	0	0
			1552	958	303	289	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	178	Total	C	N	O	S	0	0
			1408	885	267	251	5		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	174	Total	C	N	O	S	0	0
			1330	836	249	244	1		

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			350	220	64	65	1		

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	146	Total	C	N	O	S	0	0
			1143	724	217	199	3		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	121	Total	C	N	O	S	0	0
			934	585	179	168	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	VAL	MET	conflict	UNP A0A045HTP7

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	143	Total	C	N	O	S	0	0
			1068	662	216	188	2		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1072	679	215	177	1		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	116	Total	C	N	O	S	0	0
			908	574	175	158	1		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	116	Total	C	N	O		0	0
			886	541	188	157			

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	112	Total	C	N	O	S	0	0
			907	573	174	159	1		

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	122	Total	C	N	O		0	0
			980	608	205	167			

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	100	Total	C	N	O		0	0
			757	482	138	137			

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	113	Total	C	N	O		0	0
			860	533	178	149			

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	98	Total	C	N	O		0	0
			759	480	141	138			

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	90	Total	C	N	O	S	0	0
			699	430	138	129	2		

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	95	Total	C	N	O		0	0
			735	456	152	127			

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	71	Total	C	N	O		0	0
			526	325	108	93			

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	S	0	0
			476	289	101	81	5		

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	65	Total	C	N	O	S	0	0
			541	331	106	103	1		

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	59	Total	C	N	O		0	0
			476	293	101	82			

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1519	Total	C	N	O	P	0	0
			32621	14536	5961	10605	1519		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	207	Total	C	N	O	S	0	0
			1654	1030	322	298	4		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	200	Total	C	N	O	S	0	0
			1650	1036	316	296	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	160	Total	C	N	O	S	0	0
			1149	726	214	206	3		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	95	Total	C	N	O	S	0	0
			757	480	133	141	3		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	152	Total	C	N	O	S	0	0
			1193	742	234	215	2		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			999	627	187	184	1		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	127	Total	C	N	O		0	0
			993	628	195	170			

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	99	Total	C	N	O	S	0	0
			789	496	146	144	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			873	540	175	158			

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			959	594	197	166	2		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	116	Total	C	N	O	S	0	0
			945	578	196	168	3		

- Molecule 44 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			468	294	96	73	5		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	87	Total	C	N	O	S	0	0
			718	449	144	125			

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	91	Total	C	N	O	S	0	0
			728	462	140	126			

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	93	Total	C	N	O	S	0	0
			754	471	149	131	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	63	Total	C	N	O	S	0	0
			497	309	96	89	3		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	83	Total	C	N	O	S	0	0
			672	432	125	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	t	82	Total	C	N	O	0	0
			631	381	137	113		

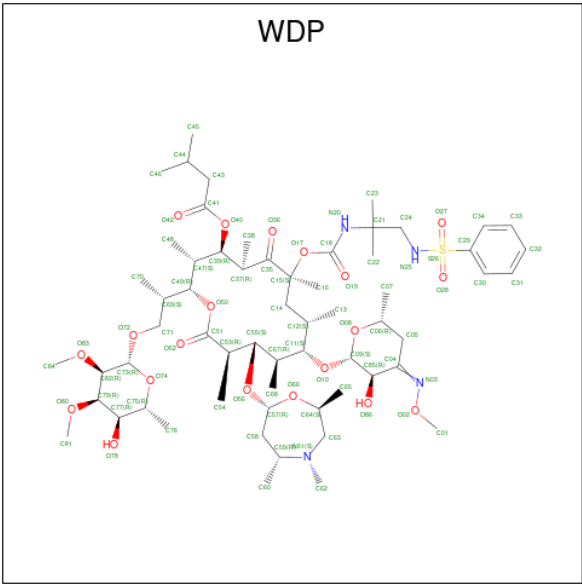
- Molecule 51 is a protein called peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	v	22	Total	C	N	O	0	0
			186	111	47	28		

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	1	1	Total	Zn	0
			1	1	
52	4	1	Total	Zn	0
			1	1	
52	6	1	Total	Zn	0
			1	1	
52	X	1	Total	Zn	0
			1	1	
52	n	1	Total	Zn	0
			1	1	
52	r	1	Total	Zn	0
			1	1	

- Molecule 53 is Sequanamycin 9 (three-letter code: WDP) (formula: C₆₁H₁₀₂N₄O₂₀S) (labeled as "Ligand of Interest" by depositor).



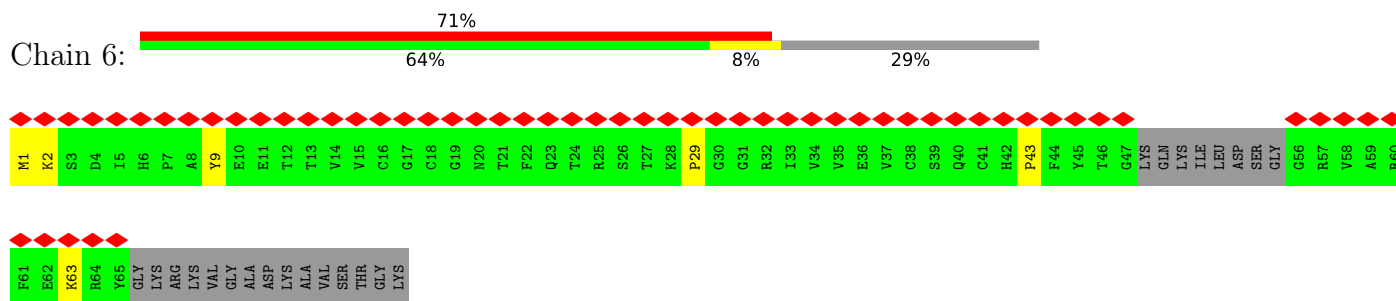
Mol	Chain	Residues	Atoms					AltConf
53	A	1	Total	C	N	O	S	0
			86	61	4	20	1	

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	307	Total	Mg	0
			307	307	
54	B	7	Total	Mg	0
			7	7	
54	C	3	Total	Mg	0
			3	3	
54	D	1	Total	Mg	0
			1	1	
54	L	1	Total	Mg	0
			1	1	
54	M	1	Total	Mg	0
			1	1	
54	a	125	Total	Mg	0
			125	125	
54	e	1	Total	Mg	0
			1	1	
54	t	1	Total	Mg	0
			1	1	

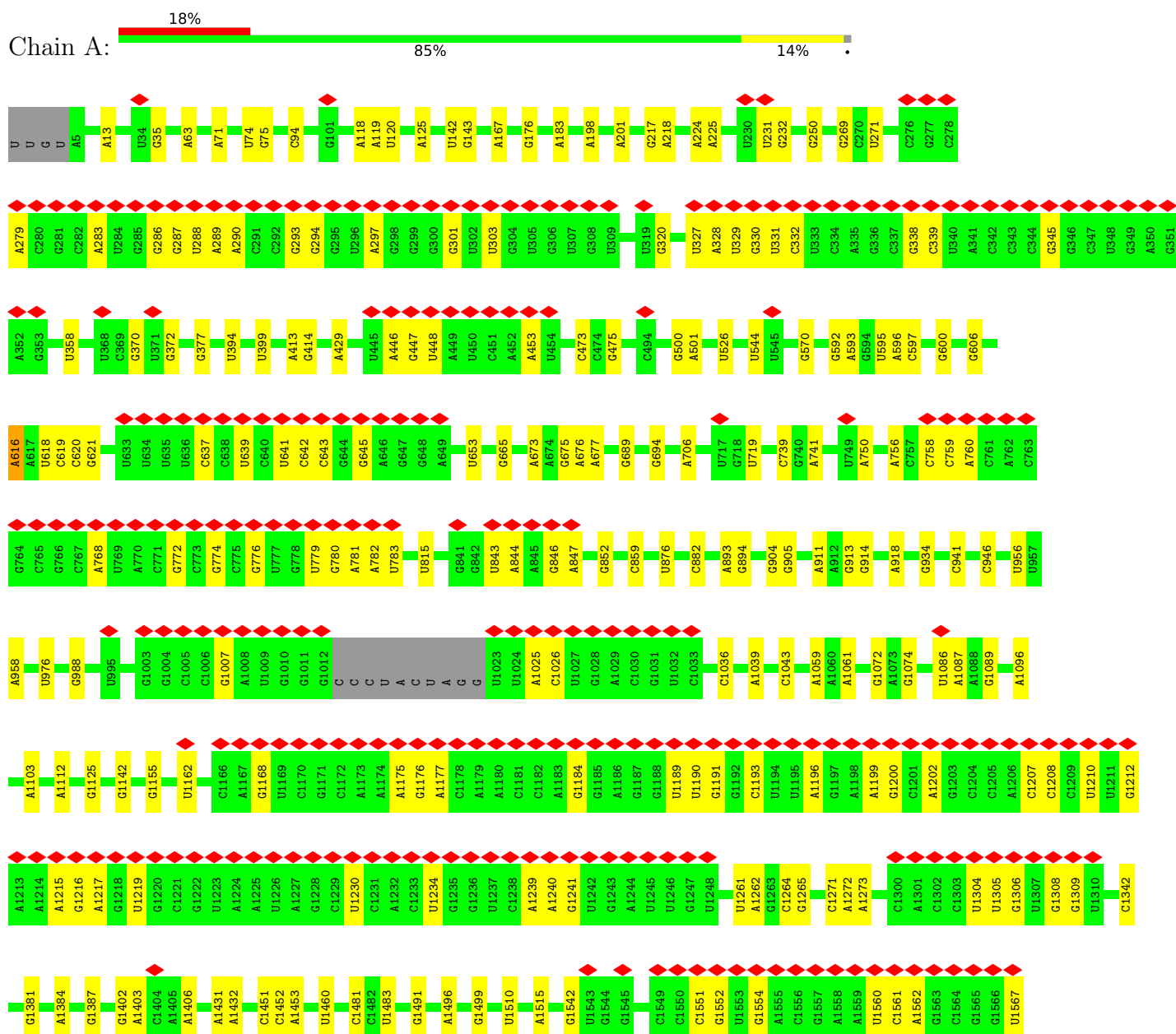
• Molecule 6: 50S ribosomal protein L31

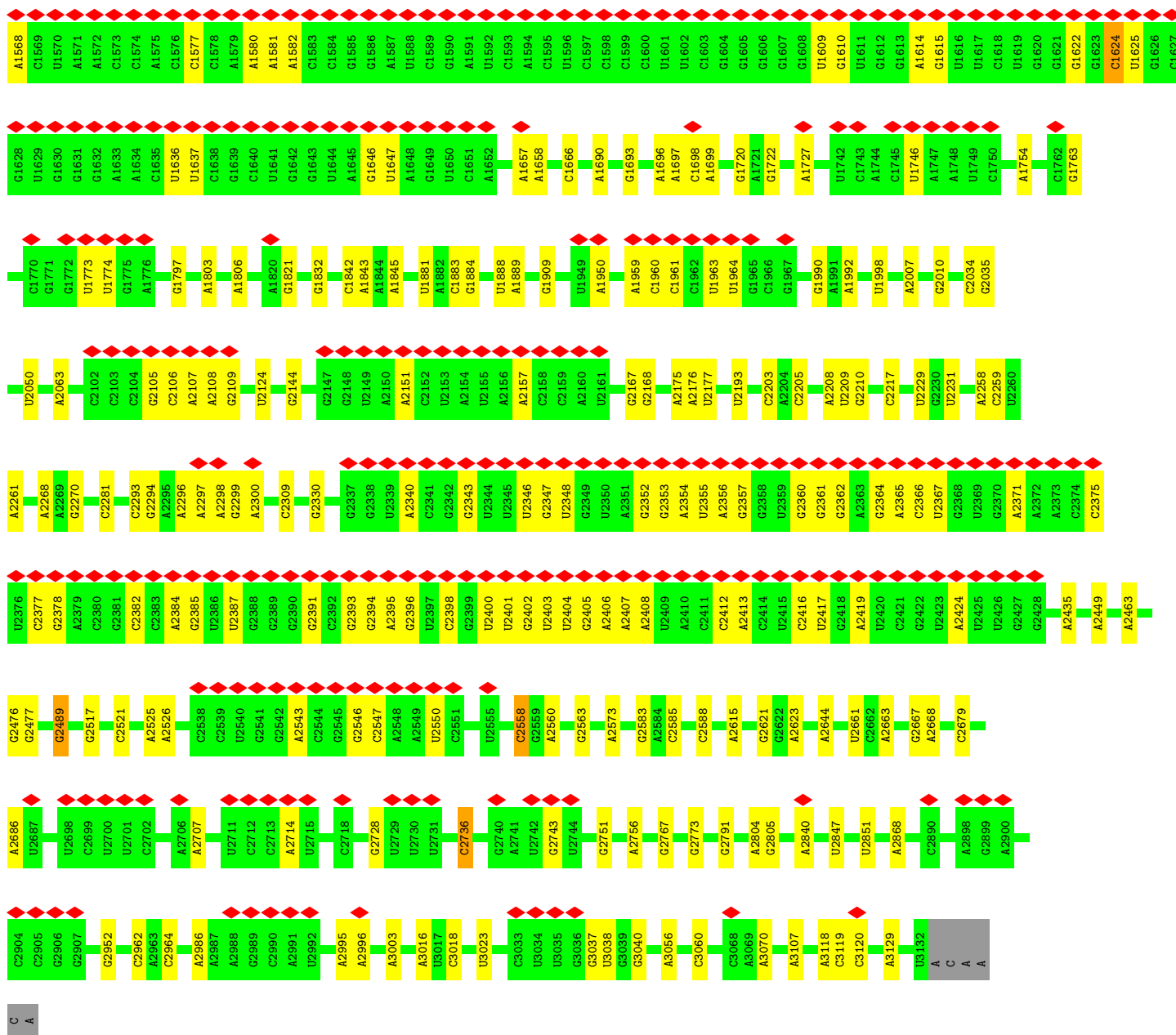
Chain 6:



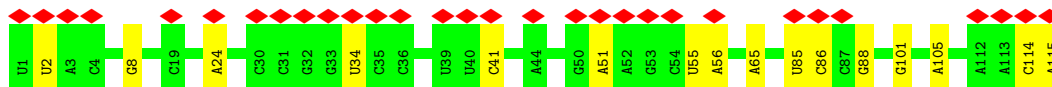
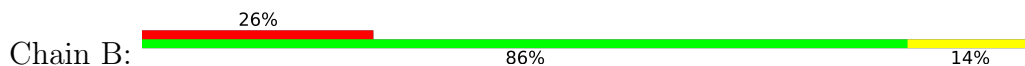
• Molecule 7: 23S rRNA

Chain A:





• Molecule 8: 5S rRNA

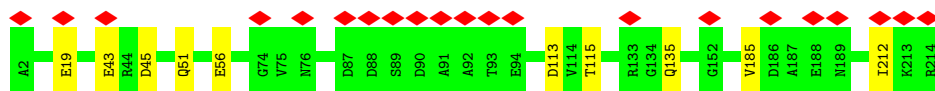


• Molecule 9: 50S ribosomal protein L2

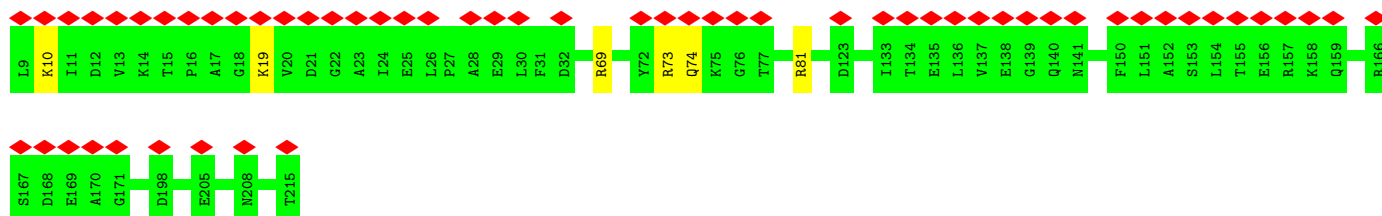




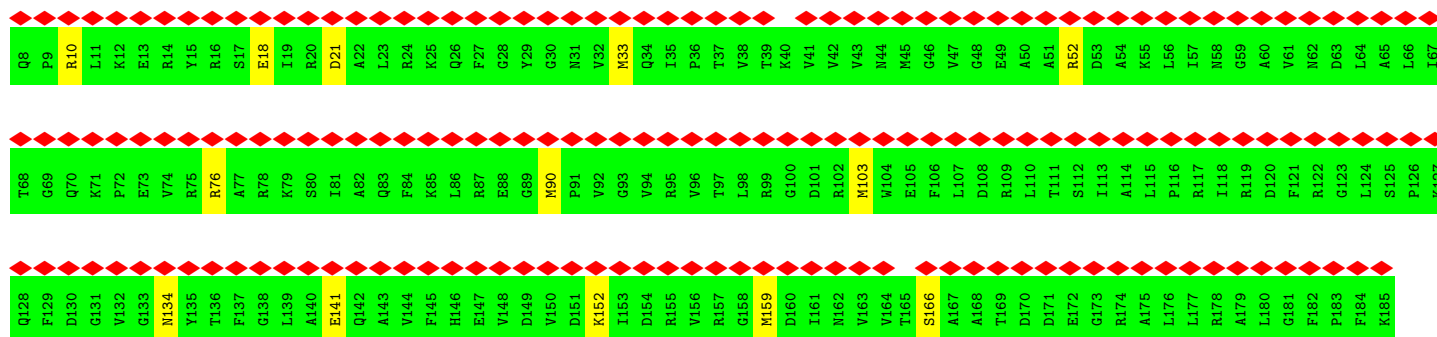
- Molecule 10: 50S ribosomal protein L3



- Molecule 11: 50S ribosomal protein L4

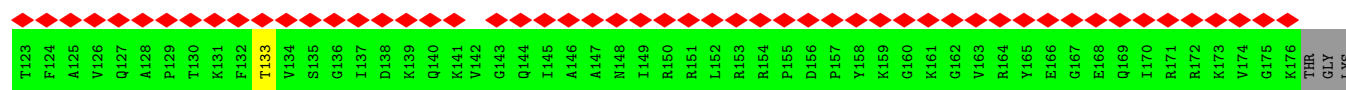


- Molecule 12: 50S ribosomal protein L5

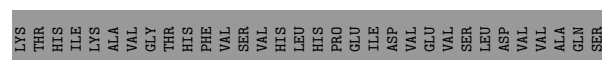
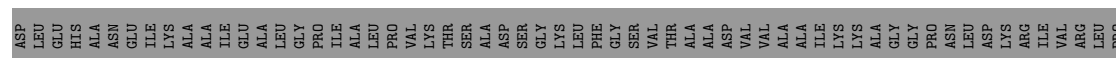
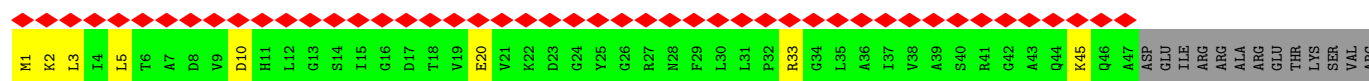


- Molecule 13: 50S ribosomal protein L6

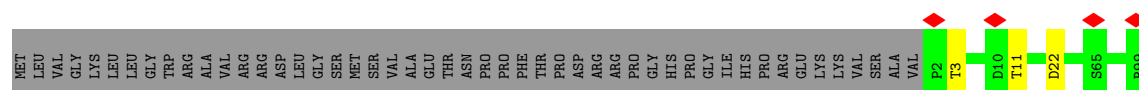




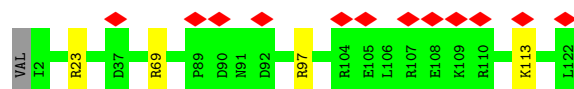
- Molecule 14: 50S ribosomal protein L9



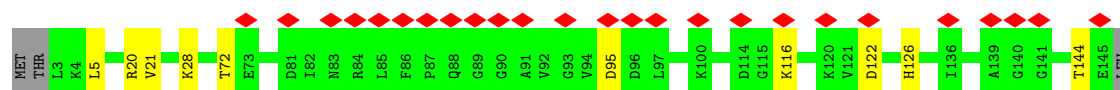
- Molecule 15: 50S ribosomal protein L13



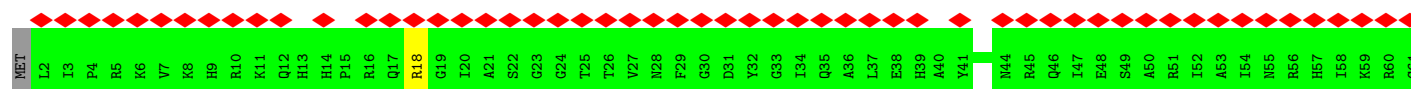
- Molecule 16: 50S ribosomal protein L14



- Molecule 17: 50S ribosomal protein L15

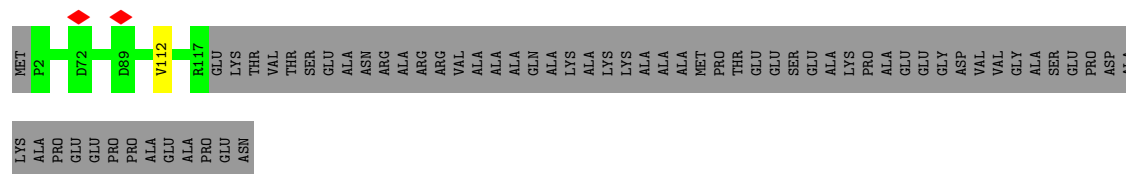


- Molecule 18: 50S ribosomal protein L16

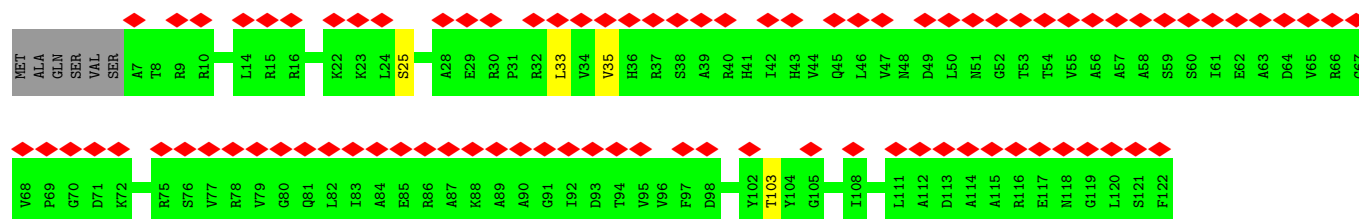
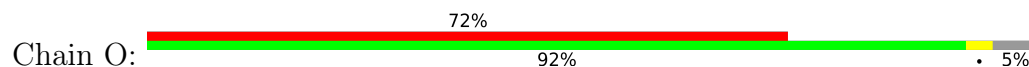




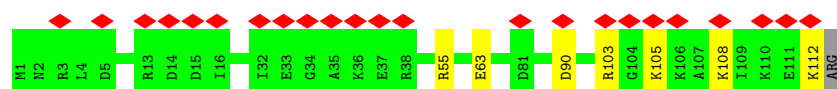
- Molecule 19: 50S ribosomal protein L17



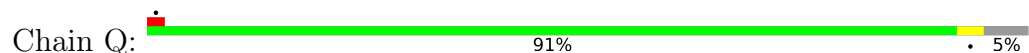
- Molecule 20: 50S ribosomal protein L18



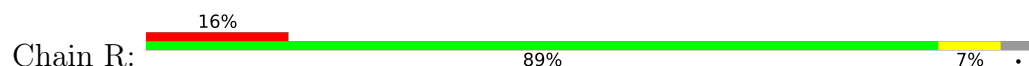
- Molecule 21: 50S ribosomal protein L19

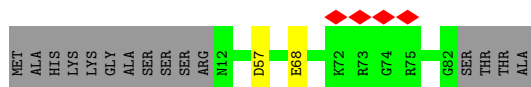
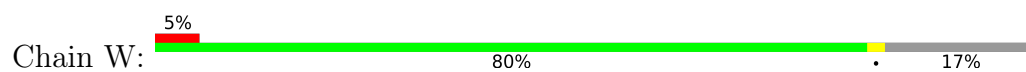


- Molecule 22: 50S ribosomal protein L20

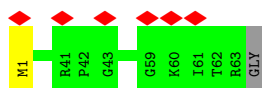


- Molecule 23: 50S ribosomal protein L21

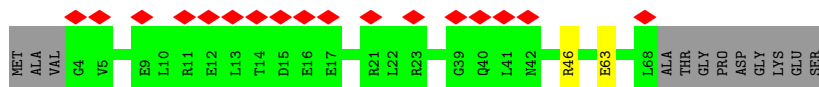
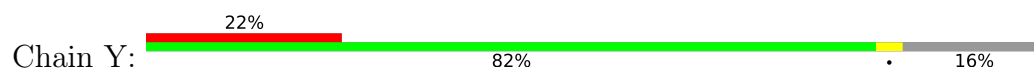




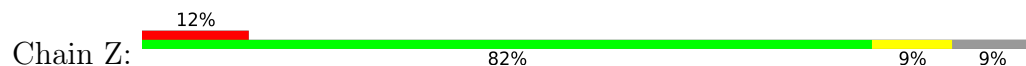
- Molecule 29: 50S ribosomal protein L28



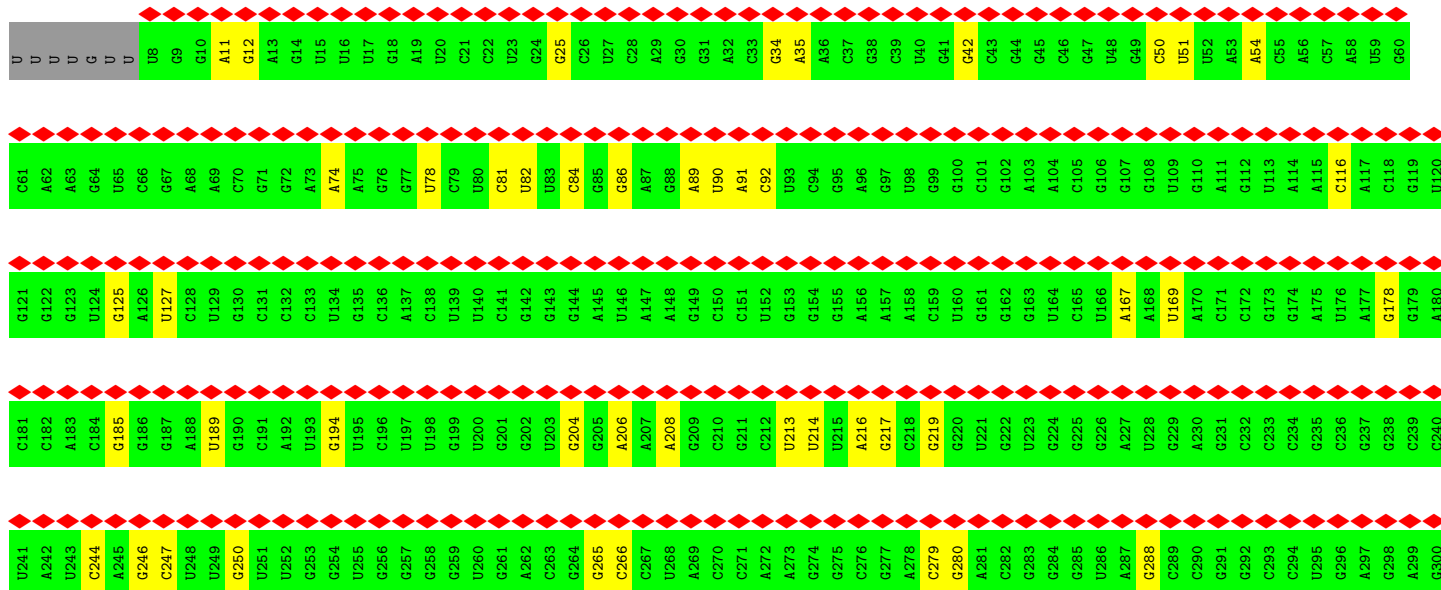
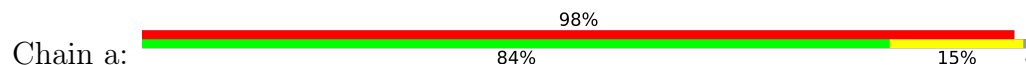
- Molecule 30: 50S ribosomal protein L29



- Molecule 31: 50S ribosomal protein L30



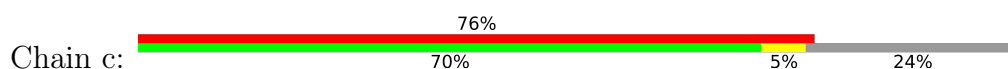
- Molecule 32: 16S rRNA



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U1022	A962	A842	G782	G722	C602	U542	G482	G422	A362	G302
U1023	C963	U843	A783	C723	U603	U543	G483	G423	A363	U303
G1024	G964	C844	U784	G724	C604	G544	A484	G424	U364	G304
U1025	C965	C845	A785	G725	A605	U545	G485	U425	U365	U305
G1026	A966	G846	G786	G726	C606	C546	A486	U426	G366	C306
U1027	A967	U847	C787	U727	G607	C547	A487	G427	U367	C307
C1028	A968	G848	C788	C728	G608	G548	G488	U428	G368	G308
U1029	G969	C849	U789	G729	C609	G549	A489	A429	C369	G309
U1030	A970	C850	G790	C730	U610	A550	A490	A430	A370	C310
G1031	A971	G851	G791	U731	U611	A551	G491	A431	C371	C311
U1032	C972	U852	U792	G732	A612	U552	C492	C432	A372	A312
U1033	C973	A853	A793	G733	A613	U553	A493	C433	A373	C313
U1034	U974	G854	G794	G734	C614	A554	C494	U434	U374	A314
G1035	U975	C855	U795	C735	U615	C555	C495	C435	G375	C315
C1036	A976	U856	C796	G736	G616	U556	G496	U436	G376	U316
U1037	C977	A857	C797	U737	U617	G557	G497	U437	G377	G317
G1038	C978	U858	A798	G738	G618	G558	C498	U438	C378	G318
U1039	U979	C859	C799	A739	A619	G559	C499	C439	G379	G319
U1040	G980	G860	G800	A740	G620	C560	A500	A440	C380	A320
G1041	C981	C861	C801	C741	C621	G561	A501	C441	A381	C321
U1042	A862	C802	C802	U742	G622	U562	C502	C442	A382	U322
U1043	U863	G803	G803	G743	U623	A563	U503	A443	G383	G323
G1044	U864	U804	U804	A744	G624	A564	A504	U444	C384	A324
C1045	A865	A805	A805	C745	C625	A565	C505	G445	C385	G325
A1046	A866	A806	A806	G746	G626	G566	G506	G446	U386	A326
U1047	G867	A807	A807	C747	G627	A567	U507	A447	G387	U327
G1048	U868	C808	C808	U748	G628	G568	G508	C448	A388	A328
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C1050	C870	C810	C810	A750	G630	U570	C510	A450	G390	G330
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C1054	G874	C814	C814	G754	C634	A574	A514	U454	C394	C334
U1055	C875	U815	U815	C755	G635	G575	G515	C455	G395	A335
G1056	C876	A816	A816	G756	G636	G576	C516	C456	A396	G336
U1057	U877	C817	C817	A757	G637	U577	C517	G457	C397	A337
A1058	G878	U818	U818	U758	C638	G578	G518	G458	G398	C338
U1059	C879	A819	A819	A759	A639	G579	C519	G459	C399	U339
C1060	G880	G820	G820	G760	G640	U580	G520	U460	C400	C340
U1061	C881	C821	C821	C761	A641	U581	G521	U461	G401	C341
G1062	U882	U822	U822	G762	C642	G582	U522	C462	C402	U342
U1063	C883	G823	G823	U763	U643	G583	A523	U463	G403	A343
C1064	U884	U824	U824	G764	A644	U584	A524	C464	U404	C344
U1065	A885	G825	G825	G765	G645	C585	U525	U465	G405	G345
G1066	C886	C826	C826	G766	A646	G586	A526	C466	G406	G346
U1067	G887	G827	G827	G767	G647	C587	C527	G467	G407	G347
C1068	U888	U828	U828	A768	U648	G588	G528	G468	G408	A348
U1069	C889	U829	U829	G769	A649	G589	U529	U469	G409	G349
G1070	G890	U830	U830	C770	C650	U590	G530	U470	A410	G350
A1071	C891	C831	C831	G771	U651	G591	G531	U471	U411	C351
G1072	C892	U832	U832	A772	G652	U592	G532	G472	G412	A352
U1073	A893	U833	U833	C773	C653	U593	G533	C473	A413	C353
C1074	U894	U834	U834	G774	A654	C594	U534	G474	C414	G354
G1075	C895	C835	C835	A775	G655	G595	G535	G475	G415	A355
U1076	G896	C836	C836	G776	G656	U596	C536	G476	G416	G356
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G1078	U898	U838	U838	A778	G658	G598	A538	U478	C418	G358
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U1081	U1082	U1083	A1084	G1085	U1086	C1087	C1088	C1089	G1090	C1091	A1092	A1093	C1094	G1095	A1096	G1097	C1098	G1099	G1100	A1101	A1102	C1103	C1104	C1105	U1106	U1107	G1108	U1109	C1110	C1111	C1112	A1113	U1114	G1115	U1116	U1117	G1118	C1119	C1120	A1121	C1122	C1123	A1124	C1125	G1126	U1127	A1128	A1129	U1130	G1131	G1132	U1133	G1134	G1135	G1136	G1137	A1138	C1139	U1140																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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• Molecule 33: 30S ribosomal protein S3



MET	G2	Q3	K4	I5	N6	P7	H8	G9	F10	R11	L12	G13	I14	T15	T16	D17	W18	K19	S20	R21	W22	Y23	A24	D25	K26	Q27	Y28	A29	E30	Y31	V32	K33	E34	D35	G36	Q37	I38	R39	R40	L41	L42	S43	S44	G45	L46	E47	R48	A49	G50	I51	A52	D53	V54	E55	V56	I57	I58	Q117	V119	T59	R60
	D61	R62	V63	R64	V65	D66	I67	H68	T69	A70	R71	P72	G73	I74	V75	I76	G77	R78	R79	G80	T81	E82	A83	D84	R85	I86	R87	A88	D89	L90	E91	K92	L93	T94	G95	K96	Q97	V98	Q99	L100	N101	I102	L103	E104	V105	K106	N107	P108	I109	E110	Q111	A112	Q113	L114	V115	I116	Q117	G118	V119	A120	
E121	Q122	L123	S124	N125	R126	V127	A128	F129	R130	R131	A132	M133	R134	K135	A136	I137	Q138	S139	A140	M141	R142	Q143	P144	N145	V146	K147	G148	I149	R150	V151	Q152	C153	S154	G155	R156	L157	G158	G159	A160	E161	M162	S163	R164	S165	E166	F167	V168	R169	E170	G171	R172	V173	P174	L175	H176	T177	L178	R179	A180		
D181	I182	D183	Y184	G185	L186	Y187	E188	A189	K190	T191	T192	F193	G194	R195	I196	G197	V198	K199	V200	W201	I202	Y203	K204	G205	D206	I207	G208	GLY	GLY	LYS	ARG	GLU	LEU	ALA	ALA	ALA	ALA	ALA	PRO	ALA	ALA	ASP	ARG	PRO	ARG	ARG	GLU	ARG	PRO	SER	GLY	THR	ARG	PRO	ARG	ARG	SER	GLY	ALA		

SER
GLY
THR
THR
ALA
THR
GLY
THR
ASP
ALA
GLY
ARG
ALA
ALA
GLY
GLY
GLU
GLU
ALA
ALA
ALA
PRO
ASP
ALA
ALA
ALA
PRO
VAL
GLU
ALA
GLN
SER
THR
GLU
SER

• Molecule 34: 30S ribosomal protein S4

Chain d: 


ME1
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G6
P7
V8
T9
R10
K11
S12
R13
R14
L15
R16
T17
D18
L19
V20
G21
G22
D23
Q24
A25
F26
E27
K28
R29
F30
Y31
F32
P33
G34
Q35
H36
G37
R38
A39
R40
I41
K42
E43
S44
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Y46
L47
L48
Q49
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E51
E52
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Q54
K55
A56
R57
F58
T59
Y60

G61
V62
M63
E64
K65
G66
F67
R68
S69
Y70
Y71
E72
E73
A74
V75
R76
Q77
F78
G79
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Y98
R99
A100
G101
L102
A103
R104
W105
L106
R107
M108
A109
G110
Q111
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V113
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H117
F118
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V120

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V175
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P181
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Q185
I186
D187
V188
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Y199
S200
K201

• Molecule 35: 30S ribosomal protein S5

Chain e: 

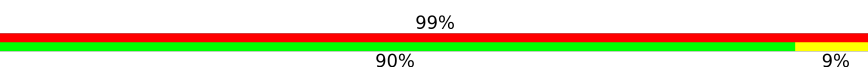
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GLN
THR
THR
ASP
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ASP
ASP
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GLY
GLY
ASP
ARG
GLU
GLY
ARG
ARG
ASP
SER
GLY
ARG
GLY
SER
ARG
GLU
ARG
ASP
GLY
GLU
LYS
SER
N41
Y42
L43
E44
R45
V46
V47
A48
I49
N50
R51
V52
S53
K54
V55
V56
K57
G58
G59
R60

R61
F62
S63
F64
T65
A66
L67
V68
I69
V70
G71
D72
G73
N74
G75
M76
V77
G78
V79
G80
Y81
G82
K83
A84
K85
E86
V87
P88
A89
A90
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A92
K93
G94
V95
E96
E97
R99
K100
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R104
V105
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L107
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G109
G110
T111
I112
T113
H114
P115
V116
Q117
G118
E119
A120

A121
A122
G123
V124
L125
L126
L127
R128
P129
A130
S131
P132
G133
T134
G135
V136
I137
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G140
A141
A142
R143
A144
V145
L146
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G150
V151
H152
D153
I154
L155
A156
K157
S158
L159
G160
S161
D162
N163
A164
I165
N166
V167
V168
H169
A170
T171
V172
A173
H174
L175
K176
L177
Q179
R180

P181
E182
E183
V184
A185
A186
R187
R188
G189
L190
P191
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E193
D194
V195
A196
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A198
G199
M200
L201
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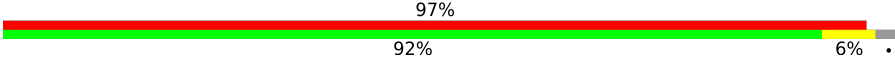
• Molecule 36: 30S ribosomal protein S6

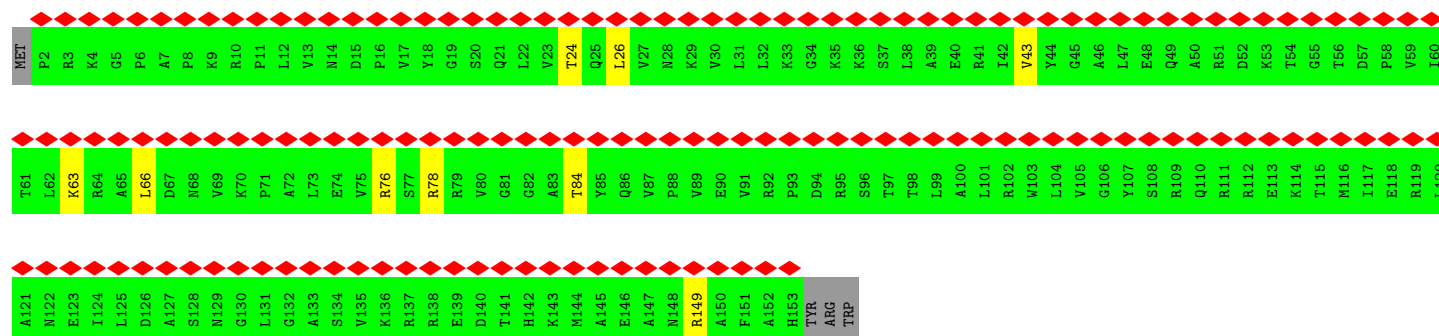
Chain f: 

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Y4
E5
I6
M7
V8
I9
L10
D11
P12
T13
L14
D15
E16
R17
T18
V19
A20
P21
S22
L23
E24
T25
F26
L27
N28
V29
Q30
R31
K32
D33
G34
G35
K36
V37
E38
K39
V40
D41
L42
W43
G44
K45
R46
R47
L48
A49
Y50
E51
T52
A53
K54
H55
A56
E57
G58
I59
Y60

V61
V62
I63
D64
V65
K66
A67
A68
P69
A70
T71
V72
S73
E74
L75
D76
R77
Q78
L79
S80
L81
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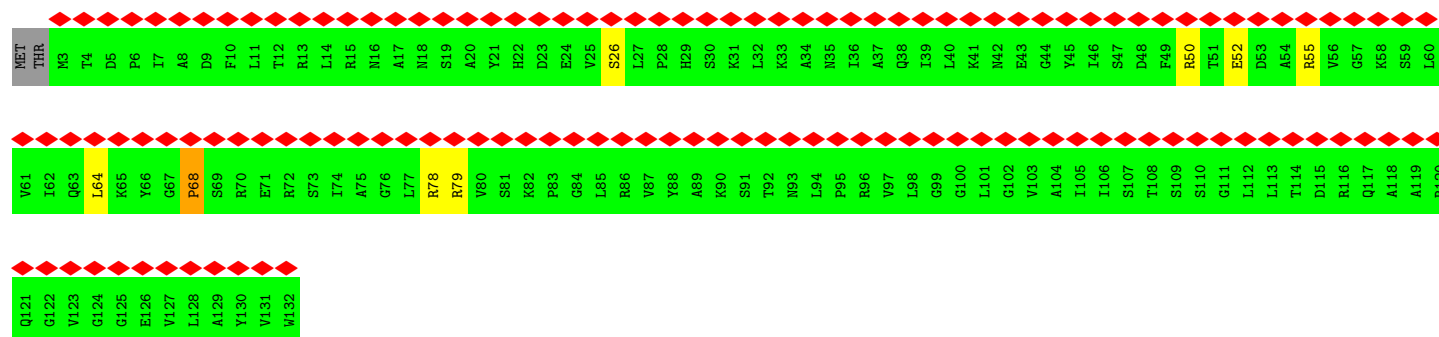
• Molecule 37: 30S ribosomal protein S7

Chain g: 




• Molecule 38: 30S ribosomal protein S8

Chain h: 

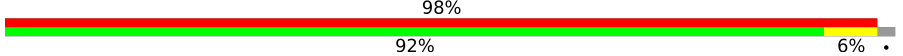


• Molecule 39: 30S ribosomal protein S9

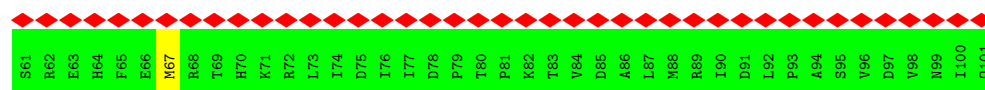
Chain i: 



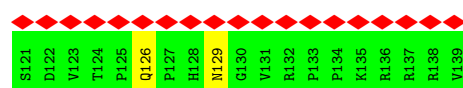
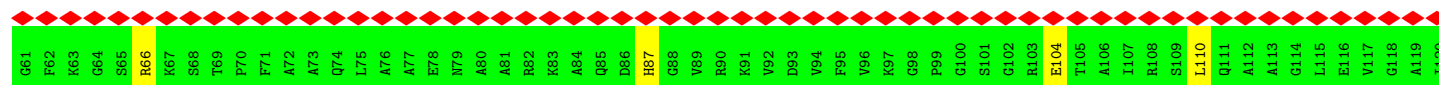
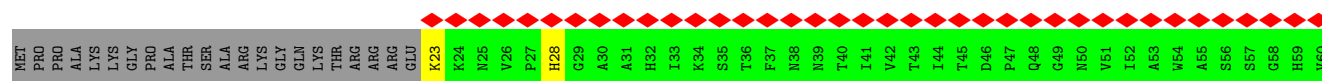
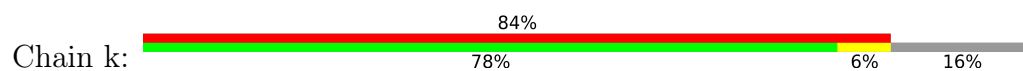
• Molecule 40: 30S ribosomal protein S10

Chain j: 

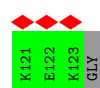
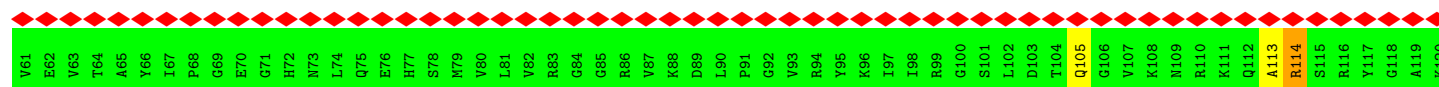
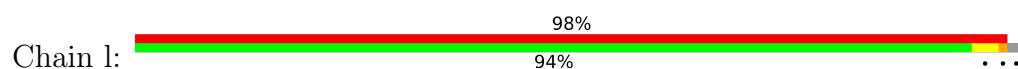




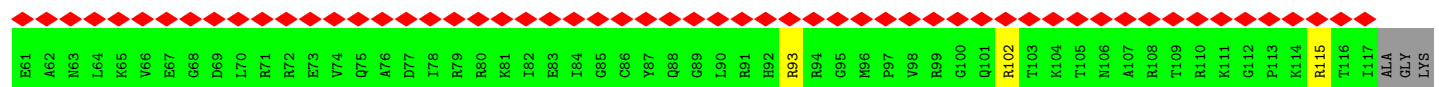
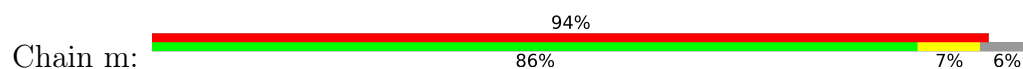
• Molecule 41: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S12

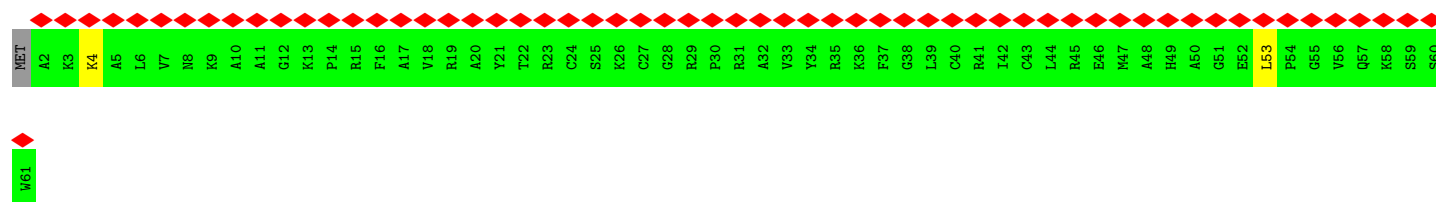


• Molecule 43: 30S ribosomal protein S13



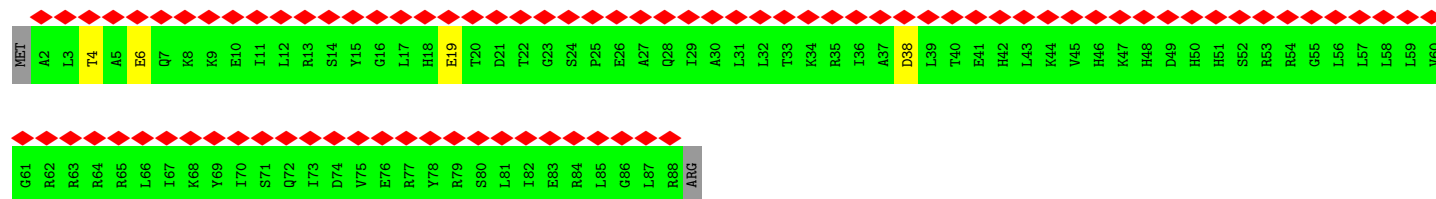
• Molecule 44: 30S ribosomal protein S14 type Z





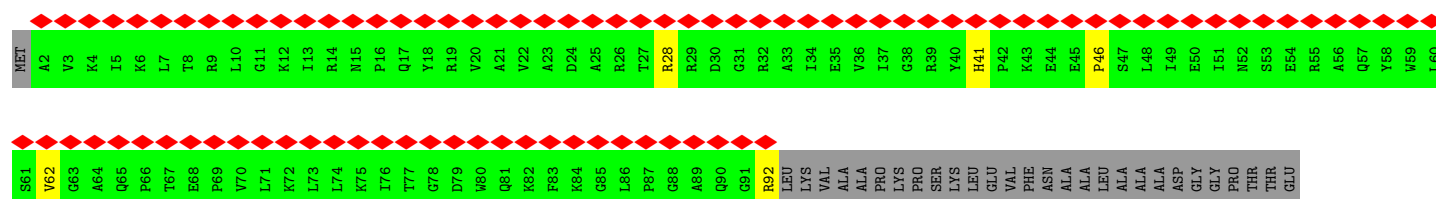
- Molecule 45: 30S ribosomal protein S15

Chain o: 98%
93%



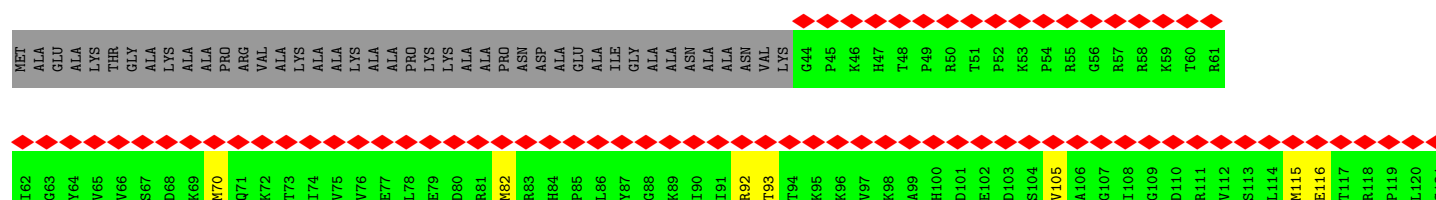
- Molecule 46: 30S ribosomal protein S16

Chain p: 56%
53% 44%



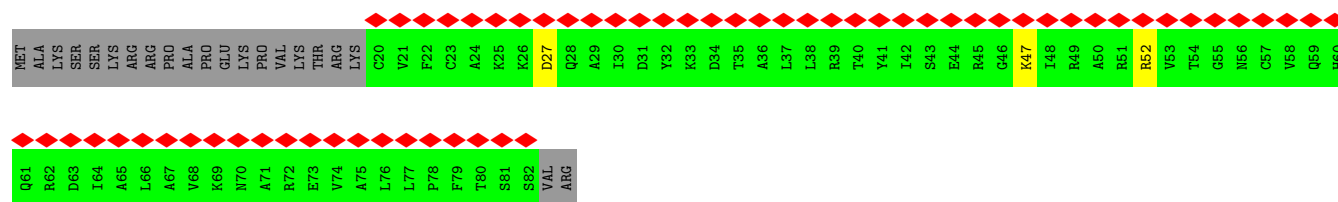
- Molecule 47: 30S ribosomal protein S17

Chain q: 69%
64% 5% 31%

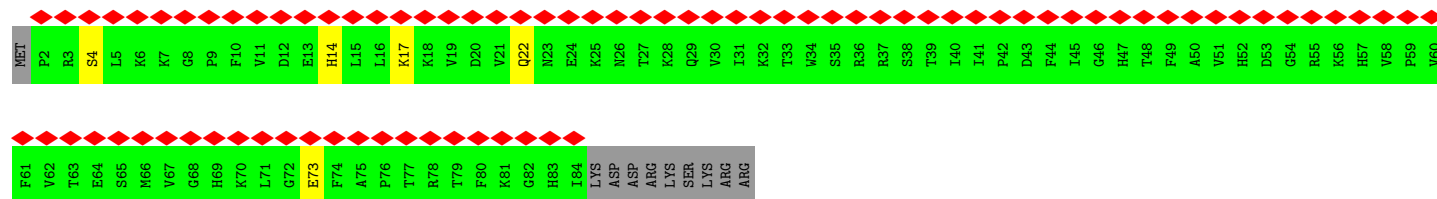
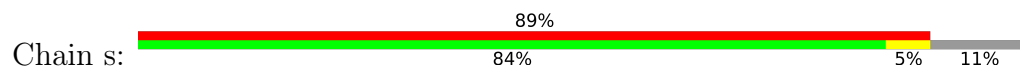


- Molecule 48: 30S ribosomal protein S18

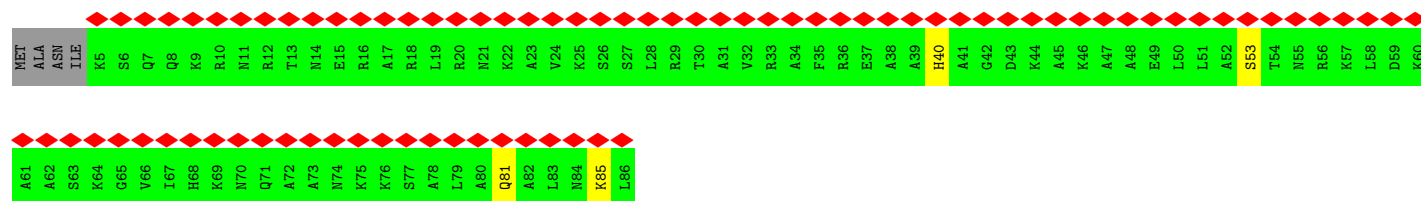
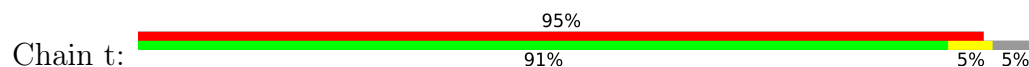
Chain r: 75%
71% 25%



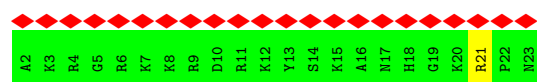
• Molecule 49: 30S ribosomal protein S19



• Molecule 50: 30S ribosomal protein S20



• Molecule 51: peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	719250	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.618	Depositor
Minimum map value	-0.335	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	348.6, 348.6, 348.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, G7M, ZN, 2MG, OMC, WDP, MG, 5MC, MA6, UR3, OMG, 6MZ, 5MU

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	0.27	0/435	0.58	0/581
2	1	0.30	0/407	0.57	0/543
3	2	0.39	0/361	0.75	0/473
4	3	0.28	0/499	0.61	0/664
5	4	0.27	0/303	0.60	0/402
6	6	0.53	1/455 (0.2%)	0.81	3/611 (0.5%)
7	A	0.68	4/74851 (0.0%)	0.81	28/116786 (0.0%)
8	B	0.36	0/2749	0.76	0/4284
9	C	0.37	0/2129	0.59	0/2861
10	D	0.38	0/1613	0.59	0/2174
11	E	0.36	0/1575	0.59	0/2129
12	F	0.27	0/1429	0.59	0/1921
13	G	0.28	0/1351	0.57	0/1824
14	H	0.25	0/353	0.55	0/474
15	J	0.40	0/1170	0.55	0/1584
16	K	0.37	0/944	0.60	0/1268
17	L	0.33	0/1081	0.62	0/1443
18	M	0.27	0/1098	0.54	0/1481
19	N	0.38	0/925	0.54	0/1242
20	O	0.27	0/895	0.64	0/1202
21	P	0.38	0/922	0.59	0/1236
22	Q	0.41	0/992	0.63	1/1329 (0.1%)
23	R	0.39	0/766	0.59	0/1030
24	S	0.37	0/874	0.60	0/1186
25	T	0.35	0/770	0.57	0/1038
26	U	0.33	0/705	0.67	2/941 (0.2%)
27	V	0.26	0/747	0.60	0/1010
28	W	0.34	0/531	0.59	0/707
29	X	0.37	0/484	0.62	0/648
30	Y	0.32	0/544	0.59	0/727
31	Z	0.34	0/480	0.66	0/645
32	a	0.22	0/36305	0.76	6/56645 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.24	0/1678	0.55	0/2254
34	d	0.24	0/1683	0.54	0/2269
35	e	0.50	2/1165 (0.2%)	0.79	4/1578 (0.3%)
36	f	0.25	0/767	0.55	0/1036
37	g	0.24	0/1210	0.58	2/1631 (0.1%)
38	h	0.28	0/1014	0.63	1/1369 (0.1%)
39	i	0.25	0/1011	0.59	0/1356
40	j	0.22	0/803	0.52	0/1086
41	k	0.26	0/891	0.55	0/1204
42	l	0.24	0/970	0.58	0/1295
43	m	0.24	0/953	0.64	0/1274
44	n	0.25	0/477	0.55	0/634
45	o	0.23	0/727	0.55	0/973
46	p	0.25	0/742	0.55	0/1000
47	q	0.25	0/766	0.62	0/1024
48	r	0.26	0/502	0.52	0/674
49	s	0.25	0/690	0.54	0/928
50	t	0.26	0/633	0.60	0/838
51	v	0.24	0/188	0.64	0/243
All	All	0.51	7/155613 (0.0%)	0.75	47/233755 (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
17	L	0	2
23	R	0	1
26	U	0	2
42	l	0	1
All	All	0	6

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2296	A	C6-N6	15.53	1.46	1.33
35	e	191	PRO	CG-CD	-13.69	1.05	1.50
6	6	43	PRO	CG-CD	-8.61	1.22	1.50
7	A	2296	A	N7-C5	-7.68	1.34	1.39
7	A	2296	A	N9-C8	-6.59	1.32	1.37

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2296	A	C2-N3-C4	18.90	120.05	110.60
35	e	191	PRO	N-CD-CG	-15.42	80.07	103.20
7	A	2296	A	N1-C2-N3	-13.61	122.50	129.30
7	A	2296	A	N3-C4-C5	-10.82	119.22	126.80
6	6	43	PRO	N-CD-CG	-10.72	87.12	103.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	L	20	ARG	Peptide
17	L	28	LYS	Peptide
23	R	50	THR	Peptide
26	U	90	GLU	Peptide
26	U	91	THR	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	52/57 (91%)	52 (100%)	0	0	100	100
2	1	46/55 (84%)	45 (98%)	1 (2%)	0	100	100
3	2	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
4	3	60/64 (94%)	60 (100%)	0	0	100	100
5	4	35/37 (95%)	35 (100%)	0	0	100	100
6	6	53/80 (66%)	46 (87%)	7 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	C	270/279 (97%)	259 (96%)	11 (4%)	0	100	100
10	D	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
11	E	205/207 (99%)	201 (98%)	4 (2%)	0	100	100
12	F	176/178 (99%)	162 (92%)	14 (8%)	0	100	100
13	G	172/177 (97%)	167 (97%)	5 (3%)	0	100	100
14	H	45/152 (30%)	38 (84%)	7 (16%)	0	100	100
15	J	144/195 (74%)	141 (98%)	3 (2%)	0	100	100
16	K	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
17	L	141/146 (97%)	128 (91%)	12 (8%)	1 (1%)	22	43
18	M	132/138 (96%)	122 (92%)	10 (8%)	0	100	100
19	N	114/180 (63%)	110 (96%)	4 (4%)	0	100	100
20	O	114/122 (93%)	107 (94%)	7 (6%)	0	100	100
21	P	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
22	Q	120/129 (93%)	117 (98%)	3 (2%)	0	100	100
23	R	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	15	32
24	S	111/197 (56%)	108 (97%)	3 (3%)	0	100	100
25	T	96/100 (96%)	88 (92%)	8 (8%)	0	100	100
26	U	86/105 (82%)	73 (85%)	12 (14%)	1 (1%)	13	27
27	V	93/215 (43%)	90 (97%)	3 (3%)	0	100	100
28	W	69/86 (80%)	64 (93%)	5 (7%)	0	100	100
29	X	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
30	Y	63/77 (82%)	60 (95%)	3 (5%)	0	100	100
31	Z	57/65 (88%)	56 (98%)	1 (2%)	0	100	100
33	c	205/274 (75%)	191 (93%)	14 (7%)	0	100	100
34	d	198/201 (98%)	188 (95%)	10 (5%)	0	100	100
35	e	158/220 (72%)	145 (92%)	12 (8%)	1 (1%)	25	47
36	f	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
37	g	150/156 (96%)	146 (97%)	4 (3%)	0	100	100
38	h	128/132 (97%)	123 (96%)	4 (3%)	1 (1%)	19	39
39	i	125/151 (83%)	107 (86%)	18 (14%)	0	100	100
40	j	97/101 (96%)	86 (89%)	11 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	k	115/139 (83%)	108 (94%)	7 (6%)	0	100	100
42	l	120/124 (97%)	95 (79%)	24 (20%)	1 (1%)	19	39
43	m	114/124 (92%)	105 (92%)	9 (8%)	0	100	100
44	n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	o	85/89 (96%)	79 (93%)	5 (6%)	1 (1%)	13	27
46	p	89/162 (55%)	81 (91%)	7 (8%)	1 (1%)	14	30
47	q	91/135 (67%)	82 (90%)	9 (10%)	0	100	100
48	r	61/84 (73%)	58 (95%)	3 (5%)	0	100	100
49	s	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
50	t	80/86 (93%)	80 (100%)	0	0	100	100
51	v	20/22 (91%)	20 (100%)	0	0	100	100
All	All	5161/6154 (84%)	4843 (94%)	310 (6%)	8 (0%)	50	71

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	R	51	THR
42	l	114	ARG
17	L	5	LEU
45	o	19	GLU
26	U	91	THR

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	44/47 (94%)	41 (93%)	3 (7%)	16	32
2	1	45/51 (88%)	42 (93%)	3 (7%)	16	33
3	2	36/40 (90%)	34 (94%)	2 (6%)	21	42
4	3	53/54 (98%)	51 (96%)	2 (4%)	33	59
5	4	35/35 (100%)	34 (97%)	1 (3%)	42	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	49/66 (74%)	44 (90%)	5 (10%)	7	14
9	C	212/218 (97%)	205 (97%)	7 (3%)	38	64
10	D	163/163 (100%)	153 (94%)	10 (6%)	18	38
11	E	159/159 (100%)	153 (96%)	6 (4%)	33	59
12	F	147/147 (100%)	134 (91%)	13 (9%)	10	19
13	G	143/145 (99%)	137 (96%)	6 (4%)	30	55
14	H	36/121 (30%)	28 (78%)	8 (22%)	1	1
15	J	120/161 (74%)	115 (96%)	5 (4%)	30	55
16	K	100/101 (99%)	96 (96%)	4 (4%)	31	57
17	L	107/110 (97%)	100 (94%)	7 (6%)	17	34
18	M	110/114 (96%)	107 (97%)	3 (3%)	44	71
19	N	94/139 (68%)	93 (99%)	1 (1%)	73	88
20	O	88/93 (95%)	84 (96%)	4 (4%)	27	52
21	P	98/99 (99%)	91 (93%)	7 (7%)	14	29
22	Q	95/99 (96%)	92 (97%)	3 (3%)	39	65
23	R	81/83 (98%)	76 (94%)	5 (6%)	18	37
24	S	87/140 (62%)	84 (97%)	3 (3%)	37	63
25	T	82/83 (99%)	76 (93%)	6 (7%)	14	28
26	U	77/88 (88%)	69 (90%)	8 (10%)	7	13
27	V	75/164 (46%)	68 (91%)	7 (9%)	9	17
28	W	51/62 (82%)	49 (96%)	2 (4%)	32	58
29	X	52/52 (100%)	51 (98%)	1 (2%)	57	79
30	Y	58/66 (88%)	56 (97%)	2 (3%)	37	63
31	Z	51/55 (93%)	45 (88%)	6 (12%)	5	9
33	c	170/210 (81%)	155 (91%)	15 (9%)	10	19
34	d	176/177 (99%)	167 (95%)	9 (5%)	24	46
35	e	114/159 (72%)	108 (95%)	6 (5%)	22	45
36	f	84/85 (99%)	75 (89%)	9 (11%)	6	12
37	g	127/131 (97%)	120 (94%)	7 (6%)	21	43
38	h	106/108 (98%)	99 (93%)	7 (7%)	16	33
39	i	102/120 (85%)	95 (93%)	7 (7%)	15	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	89/90 (99%)	83 (93%)	6 (7%)	16	33
41	k	90/107 (84%)	82 (91%)	8 (9%)	9	19
42	l	104/105 (99%)	100 (96%)	4 (4%)	33	59
43	m	99/104 (95%)	90 (91%)	9 (9%)	9	18
44	n	46/47 (98%)	44 (96%)	2 (4%)	29	54
45	o	77/79 (98%)	74 (96%)	3 (4%)	32	58
46	p	75/125 (60%)	71 (95%)	4 (5%)	22	45
47	q	83/105 (79%)	76 (92%)	7 (8%)	11	21
48	r	53/72 (74%)	50 (94%)	3 (6%)	20	41
49	s	75/85 (88%)	70 (93%)	5 (7%)	16	33
50	t	62/65 (95%)	58 (94%)	4 (6%)	17	34
51	v	18/18 (100%)	17 (94%)	1 (6%)	21	42
All	All	4298/4947 (87%)	4042 (94%)	256 (6%)	23	39

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	o	38	ASP
47	q	92	ARG
22	Q	53	ARG
21	P	105	LYS
48	r	27	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
34	d	24	GLN
34	d	167	GLN
43	m	55	HIS
18	M	110	ASN
27	V	38	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1515/1537 (98%)	224 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	3115/3138 (99%)	423 (13%)	2 (0%)
8	B	114/115 (99%)	16 (14%)	0
All	All	4744/4790 (99%)	663 (13%)	2 (0%)

5 of 663 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	13	A
7	A	35	G
7	A	63	A
7	A	71	A
7	A	74	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	338	G
7	A	913	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	OMG	A	2791	7	18,26,27	2.68	6 (33%)	19,38,41	1.49	4 (21%)
32	5MC	a	960	32	18,22,23	1.89	6 (33%)	26,32,35	1.17	1 (3%)
32	UR3	a	1491	32	19,22,23	2.78	4 (21%)	26,32,35	1.21	2 (7%)
32	2MG	a	1509	32	18,26,27	2.96	4 (22%)	16,38,41	1.17	2 (12%)
32	2MG	a	959	32	18,26,27	2.96	4 (22%)	16,38,41	1.25	2 (12%)
7	OMC	A	2736	7,54	19,22,23	1.62	2 (10%)	26,31,34	1.05	1 (3%)
32	MA6	a	1511	32	19,26,27	0.79	0	18,38,41	1.51	2 (11%)
32	G7M	a	518	32	20,26,27	2.58	4 (20%)	17,39,42	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	a	1512	32	19,26,27	0.77	0	18,38,41	1.51	2 (11%)
7	OMG	A	2489	7	18,26,27	2.67	5 (27%)	19,38,41	1.46	4 (21%)
7	6MZ	A	2268	7	18,25,26	1.70	1 (5%)	16,36,39	2.54	3 (18%)
32	4OC	a	1395	32	20,23,24	2.56	4 (20%)	26,32,35	0.90	1 (3%)
7	5MU	A	2177	7	19,22,23	2.28	8 (42%)	28,32,35	2.40	6 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OMG	A	2791	7	-	0/5/27/28	0/3/3/3
32	5MC	a	960	32	-	0/7/25/26	0/2/2/2
32	UR3	a	1491	32	-	1/7/25/26	0/2/2/2
32	2MG	a	1509	32	-	0/5/27/28	0/3/3/3
32	2MG	a	959	32	-	3/5/27/28	0/3/3/3
7	OMC	A	2736	7,54	-	0/9/27/28	0/2/2/2
32	MA6	a	1511	32	-	0/7/29/30	0/3/3/3
32	G7M	a	518	32	-	0/3/25/26	0/3/3/3
32	MA6	a	1512	32	-	2/7/29/30	0/3/3/3
7	OMG	A	2489	7	-	3/5/27/28	0/3/3/3
7	6MZ	A	2268	7	-	2/5/27/28	0/3/3/3
32	4OC	a	1395	32	-	0/9/29/30	0/2/2/2
7	5MU	A	2177	7	-	0/7/25/26	0/2/2/2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1491	UR3	O4-C4	10.14	1.45	1.23
32	a	518	G7M	O6-C6	9.96	1.43	1.23
32	a	959	2MG	O6-C6	9.16	1.41	1.23
32	a	1509	2MG	O6-C6	9.03	1.41	1.23
32	a	1395	4OC	O2-C2	9.00	1.40	1.23

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2268	6MZ	C9-N6-C6	-7.06	116.79	122.87
7	A	2177	5MU	C5-C6-N1	-5.86	117.31	123.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2177	5MU	C4-N3-C2	-5.85	119.78	127.35
7	A	2177	5MU	N3-C2-N1	5.46	122.14	114.89
7	A	2268	6MZ	C2-N1-C6	5.10	120.97	116.59

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2489	OMG	O4'-C4'-C5'-O5'
7	A	2489	OMG	C1'-C2'-O2'-CM2
32	a	959	2MG	N1-C2-N2-CM2
32	a	959	2MG	N3-C2-N2-CM2
7	A	2268	6MZ	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 454 ligands modelled in this entry, 453 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	WDP	A	3201	-	83,90,90	2.45	21 (25%)	102,132,132	2.26	18 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	WDP	A	3201	-	-	37/103/158/158	1/4/5/5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3201	WDP	C18-N20	8.92	1.50	1.35
53	A	3201	WDP	S26-N25	7.37	1.73	1.61
53	A	3201	WDP	C62-N61	-6.42	1.33	1.46
53	A	3201	WDP	O17-C18	5.99	1.46	1.34
53	A	3201	WDP	O50-C51	5.82	1.47	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	3201	WDP	O28-S26-O27	-14.94	101.18	119.55
53	A	3201	WDP	O17-C18-N20	7.55	119.98	109.92
53	A	3201	WDP	C05-C04-N03	-5.83	120.13	126.93
53	A	3201	WDP	O02-N03-C04	5.35	119.95	110.97
53	A	3201	WDP	O40-C41-C43	4.61	119.94	111.46

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	A	3201	WDP	C22-C21-C24-N25
53	A	3201	WDP	C23-C21-C24-N25
53	A	3201	WDP	N20-C21-C24-N25
53	A	3201	WDP	C22-C21-N20-C18
53	A	3201	WDP	C24-C21-N20-C18

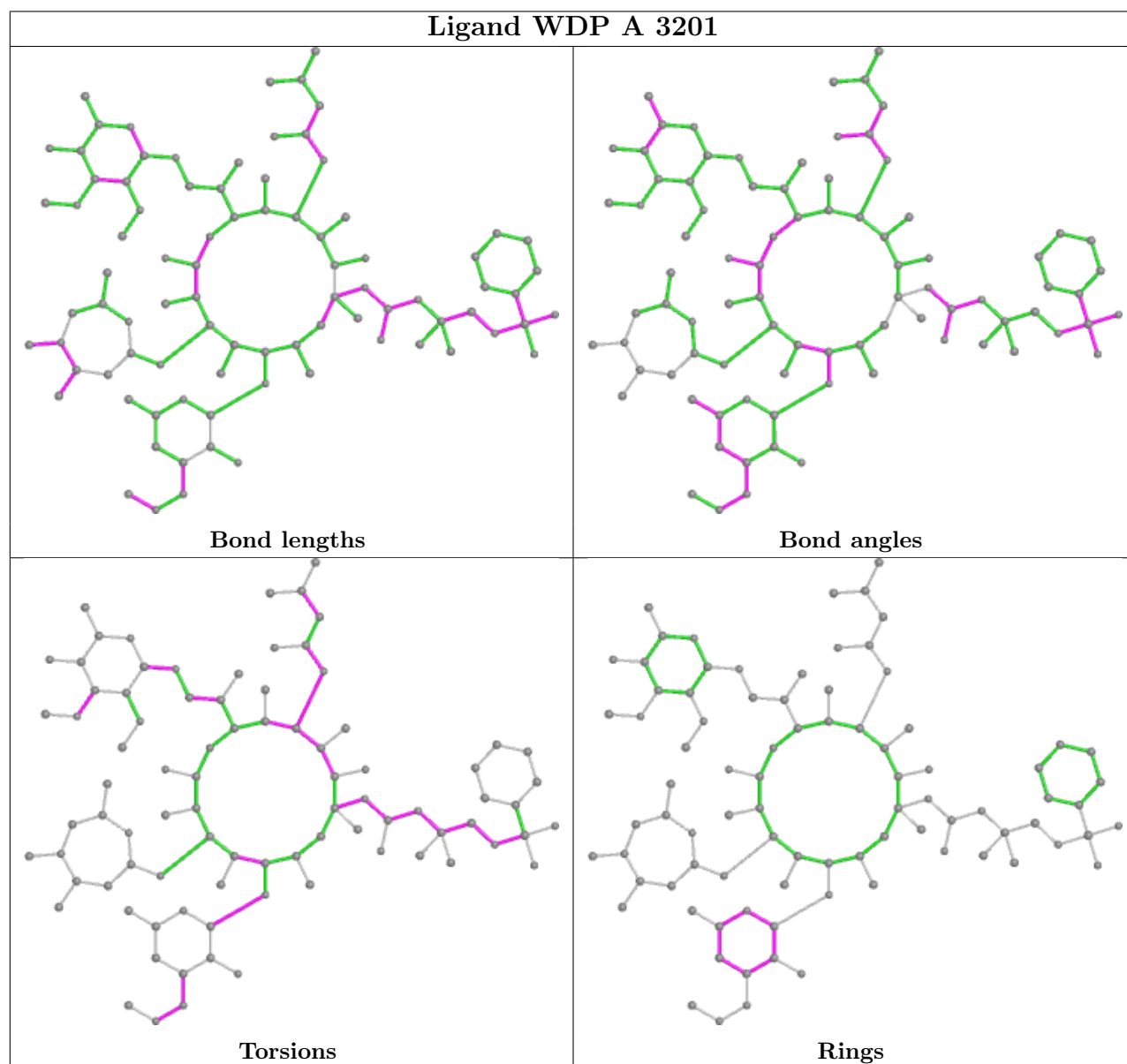
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	A	3201	WDP	C04-C05-C06-C09-C85-O08

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

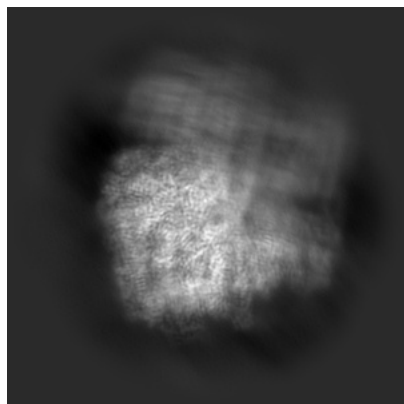
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25100. These allow visual inspection of the internal detail of the map and identification of artifacts.

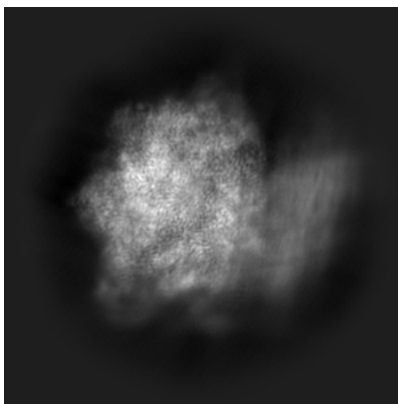
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

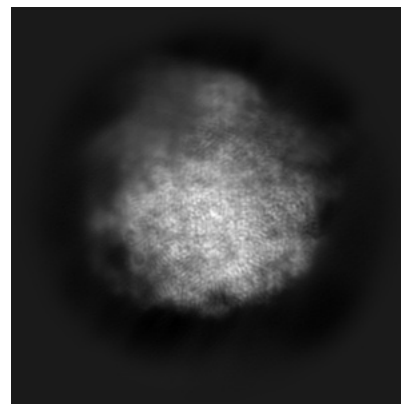
6.1.1 Primary map



X

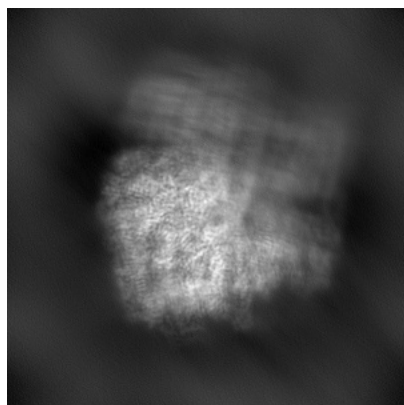


Y

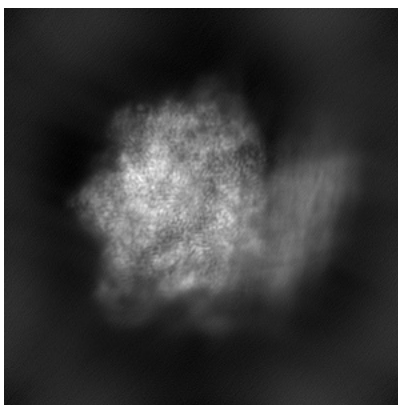


Z

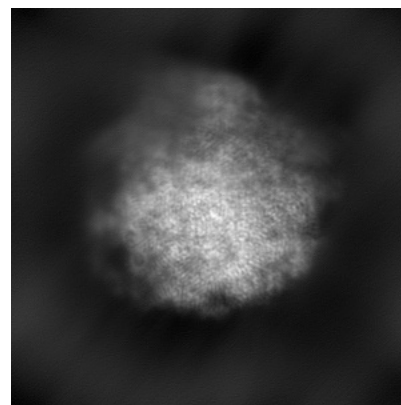
6.1.2 Raw map



X



Y

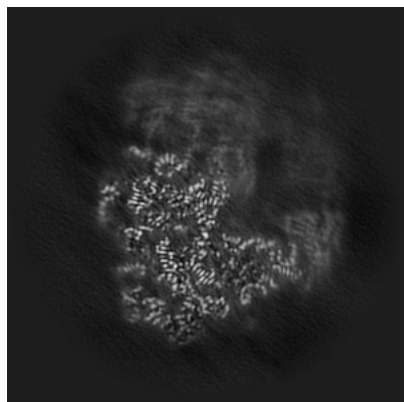


Z

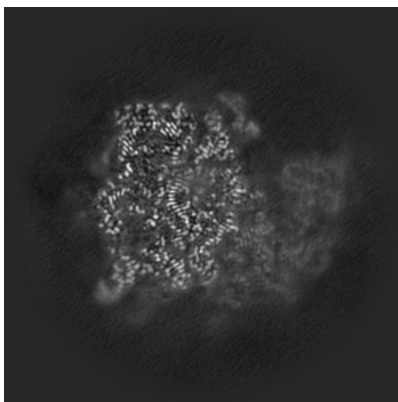
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

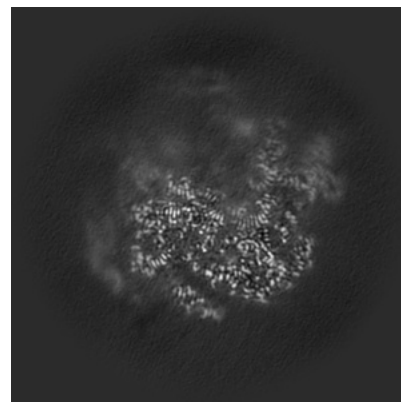
6.2.1 Primary map



X Index: 210

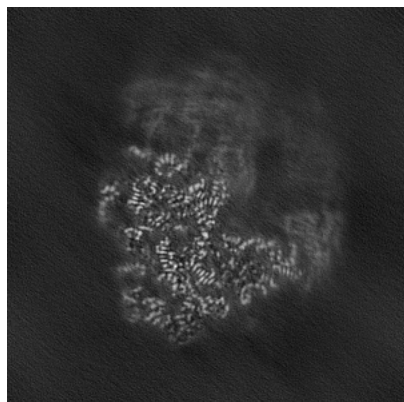


Y Index: 210

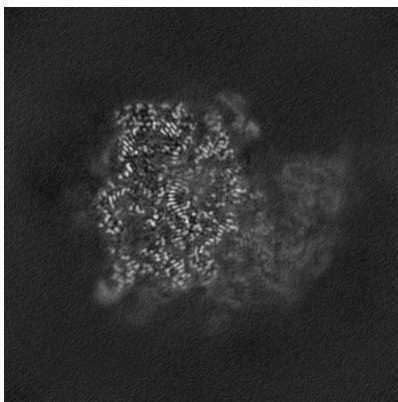


Z Index: 210

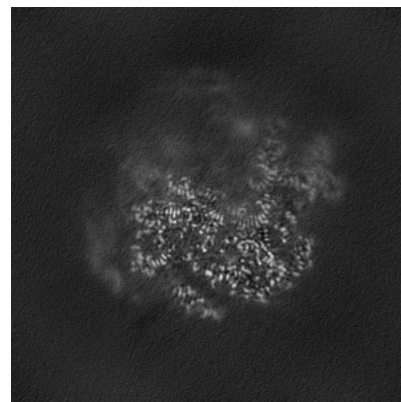
6.2.2 Raw map



X Index: 210



Y Index: 210

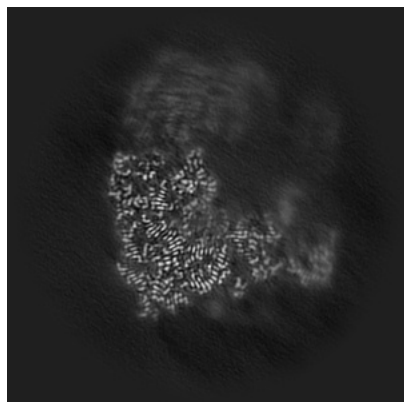


Z Index: 210

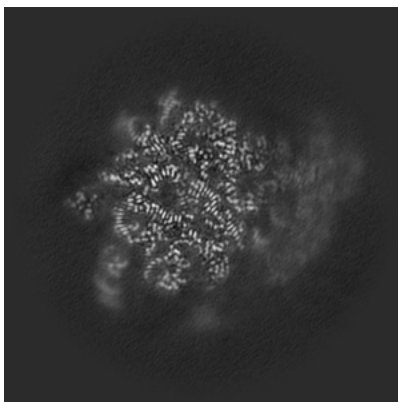
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

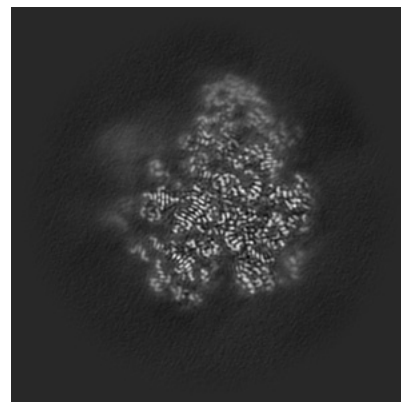
6.3.1 Primary map



X Index: 244

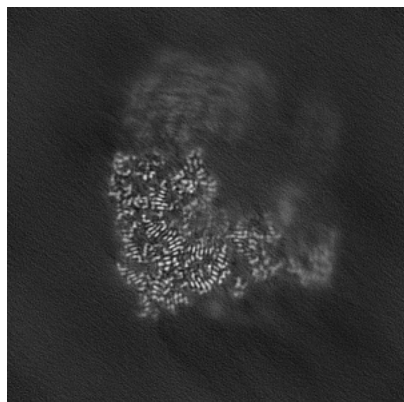


Y Index: 172

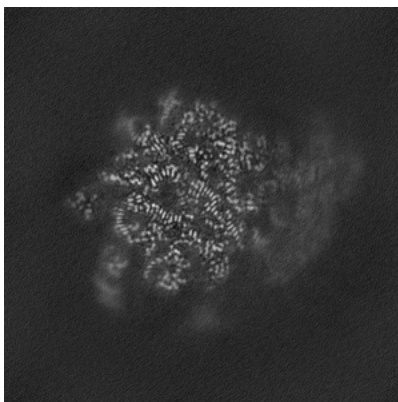


Z Index: 158

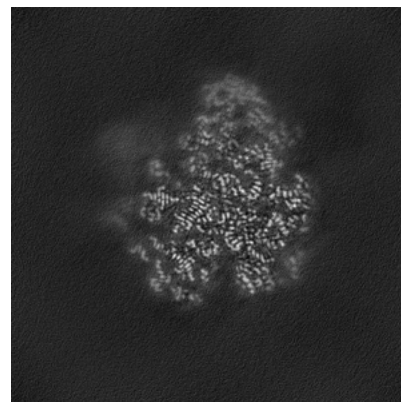
6.3.2 Raw map



X Index: 244



Y Index: 172



Z Index: 158

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

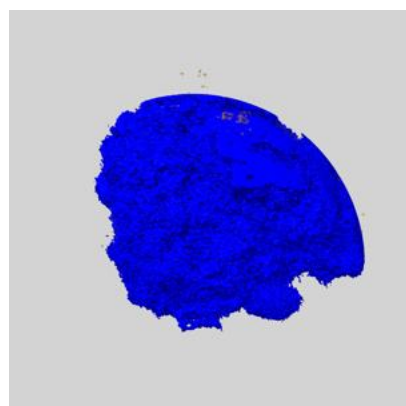
6.5 Mask visualisation [i](#)

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

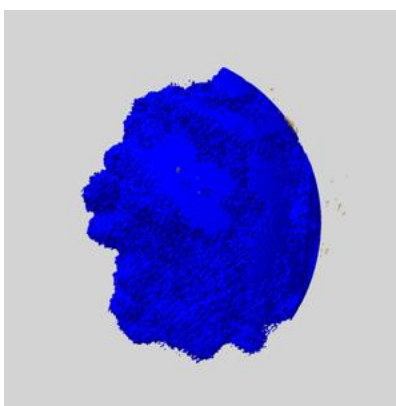
A mask typically either:

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

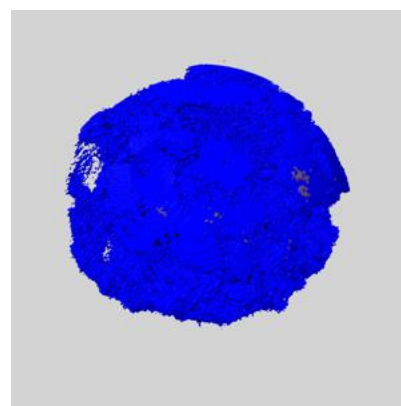
6.5.1 emd_25100_msk_1.map [i](#)



X



Y

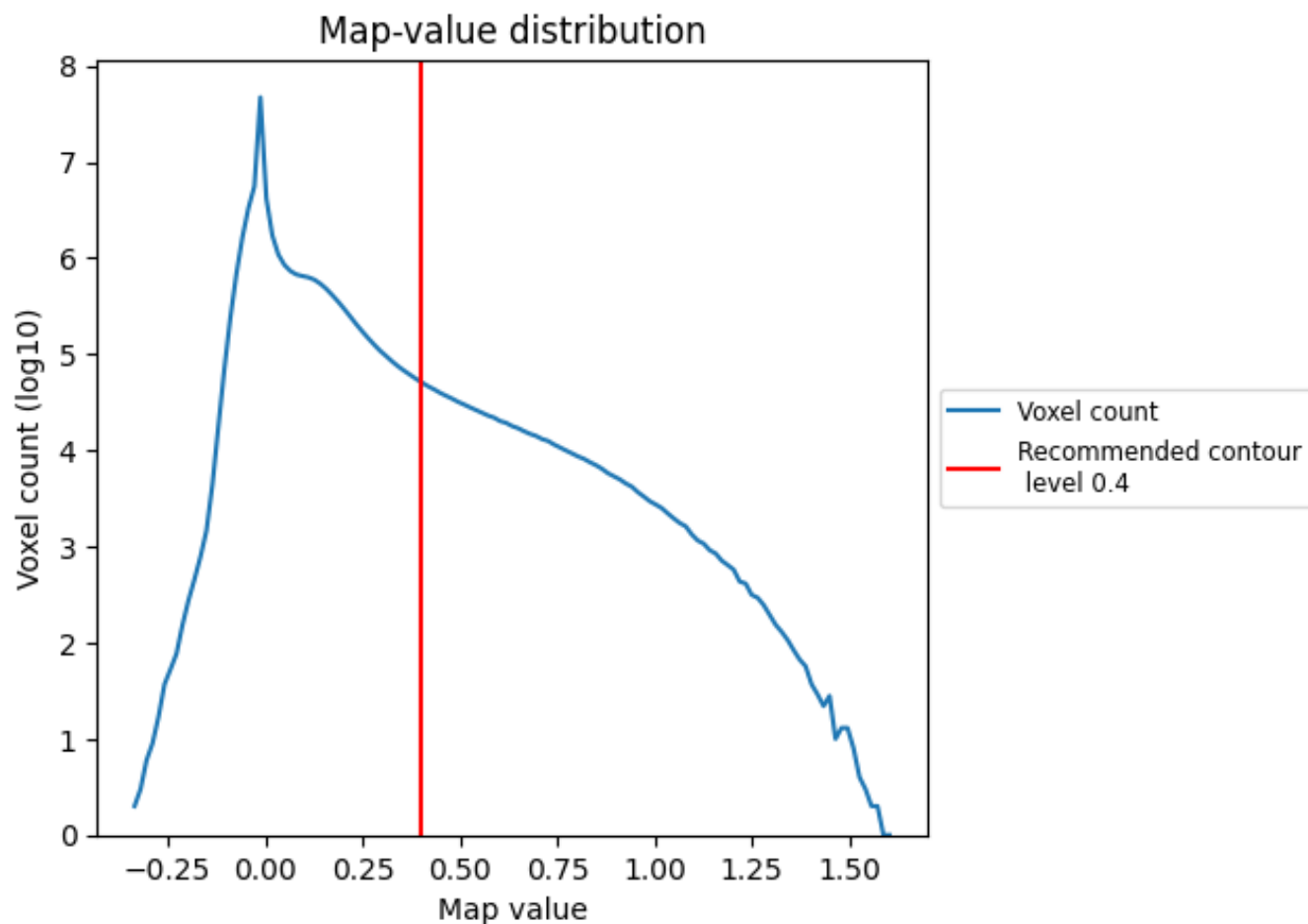


Z

7 Map analysis [i](#)

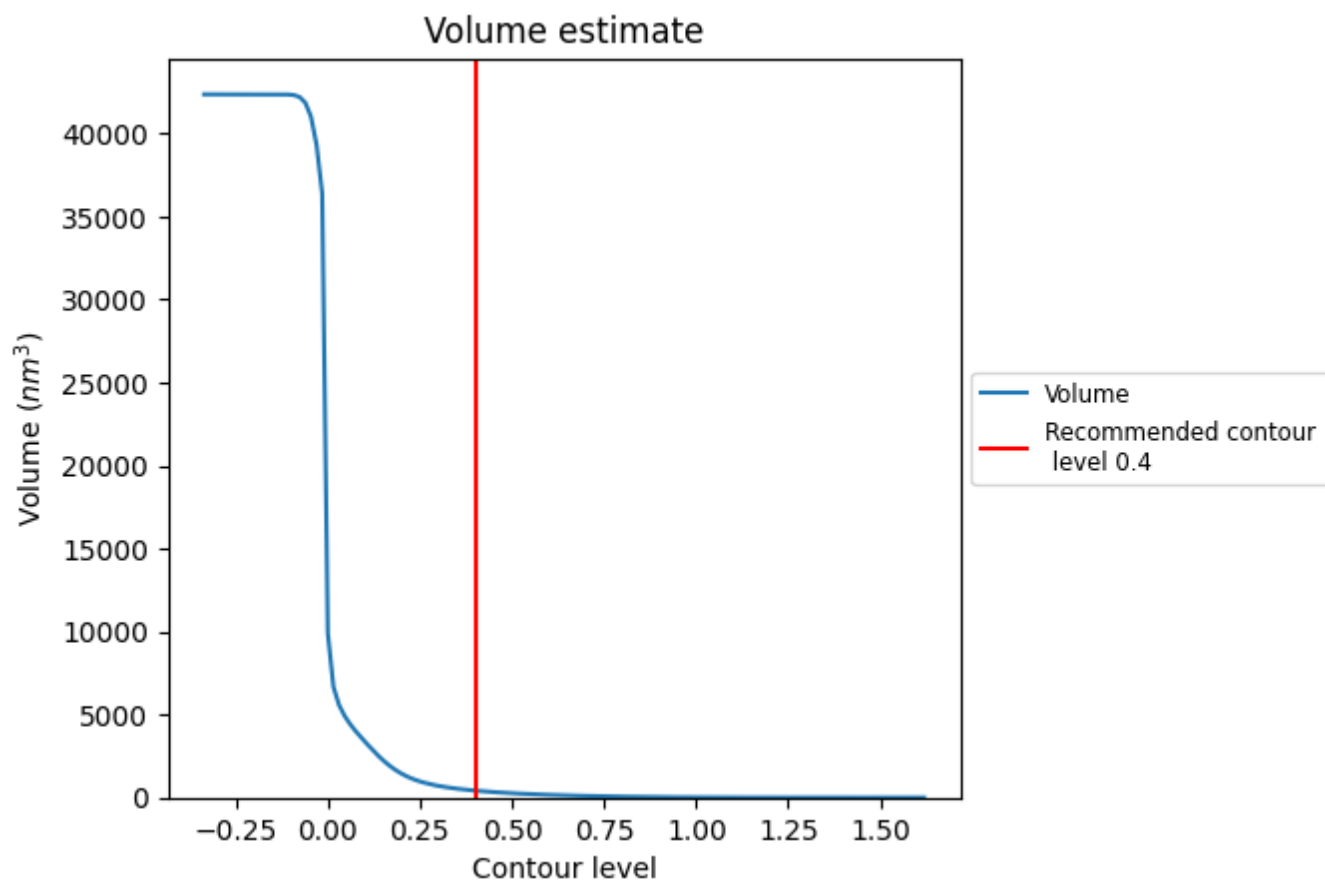
This section contains the results of statistical analysis of the map.

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.

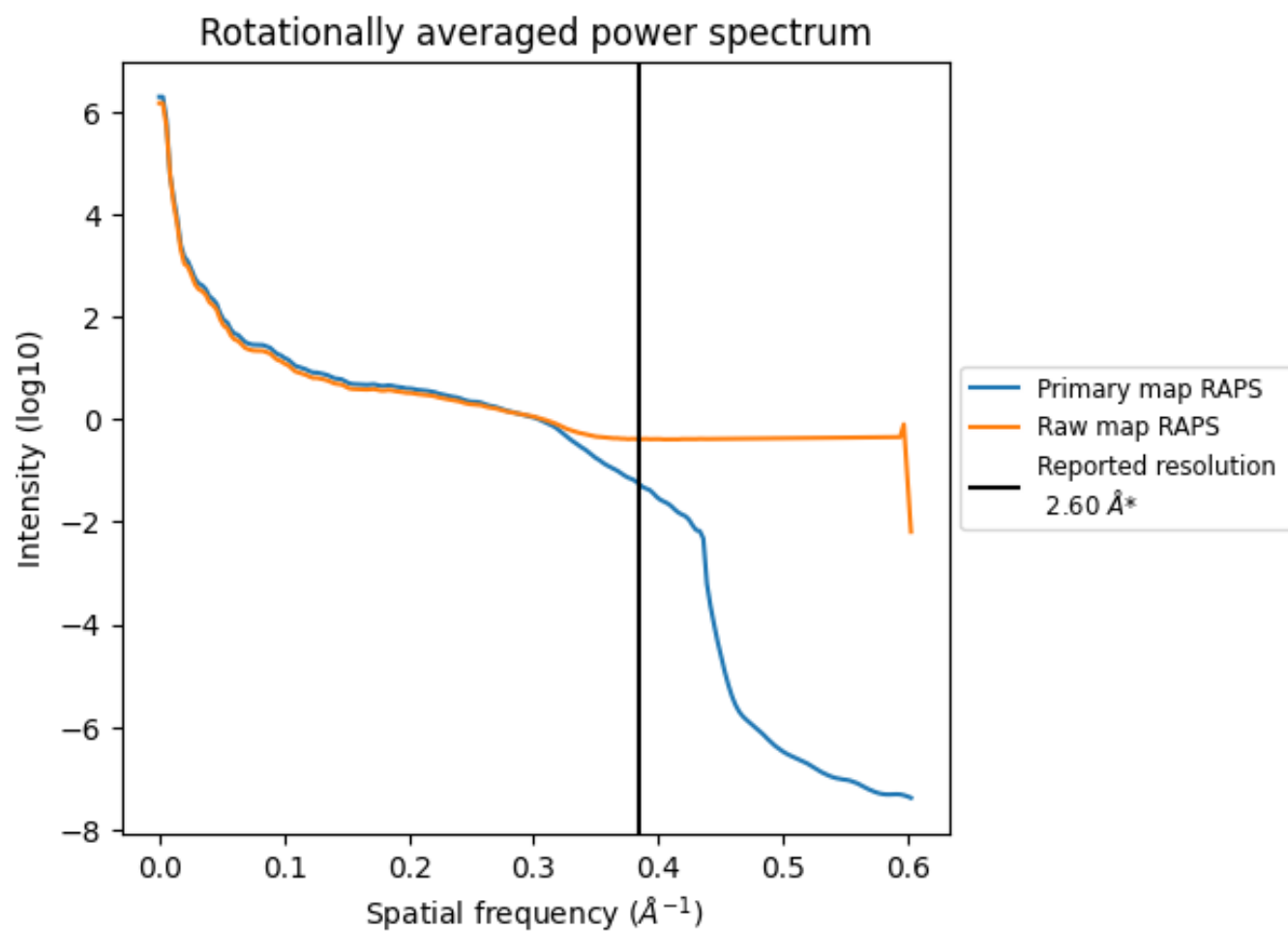
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 418 nm³; this corresponds to an approximate mass of 377 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 ⓘ

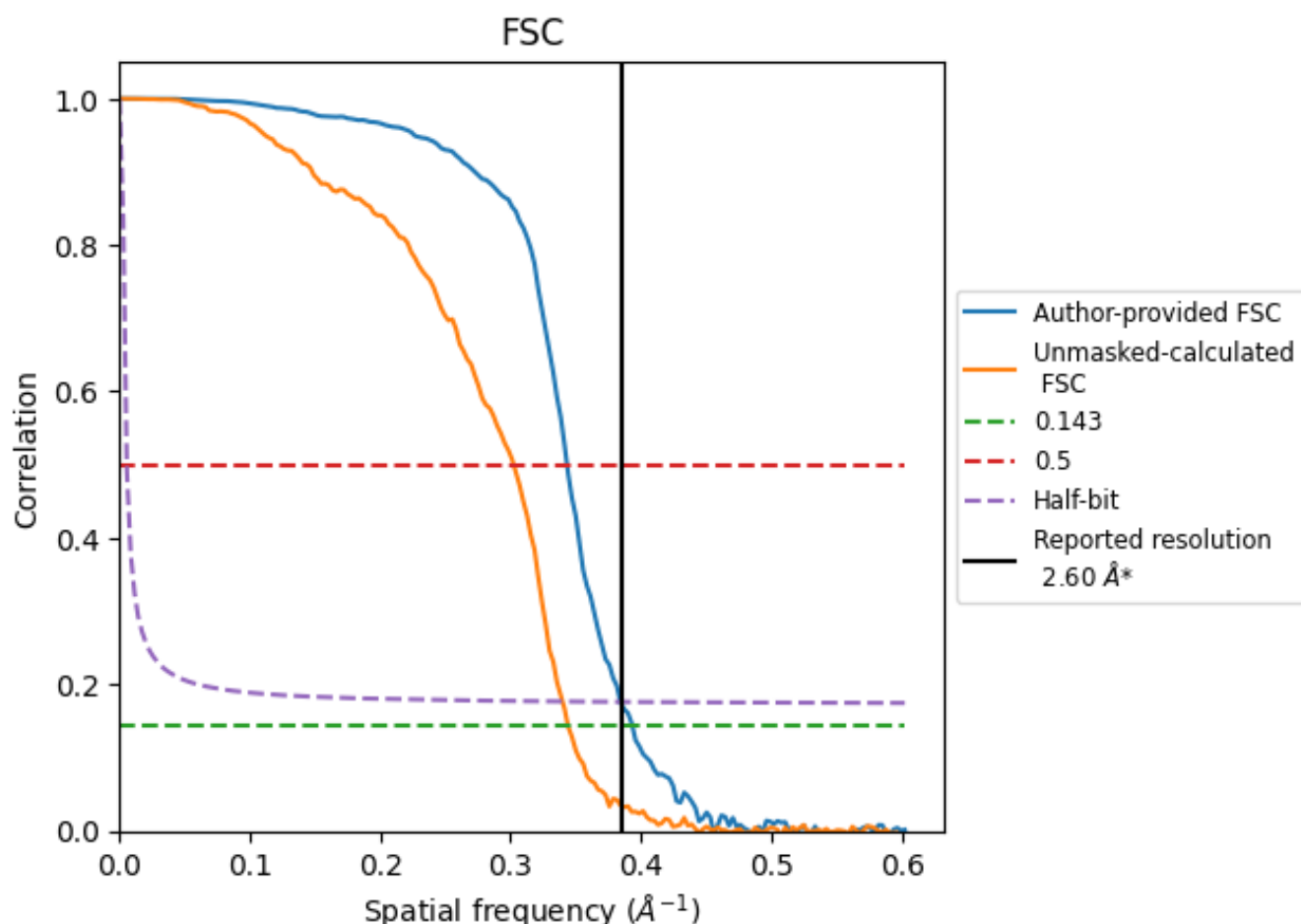


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

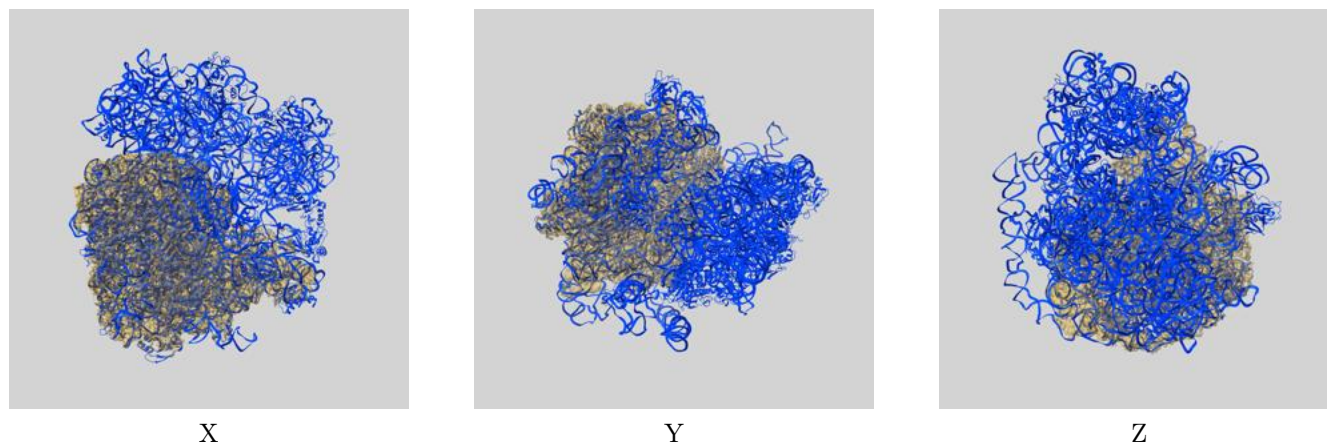
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.54	2.91	2.60
Unmasked-calculated*	2.91	3.31	2.94

*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 2.91 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

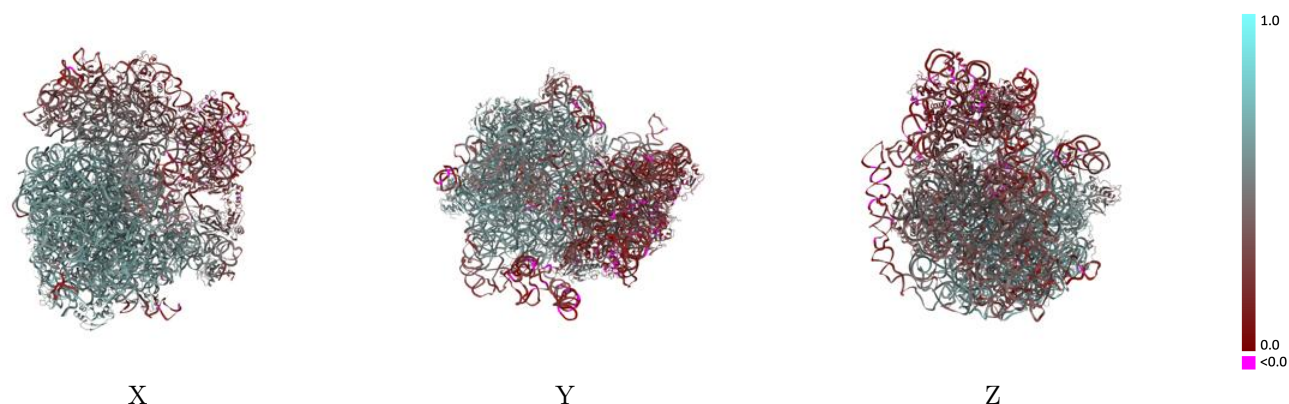
This section contains information regarding the fit between EMDB map EMD-25100 and PDB model 7SFR. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



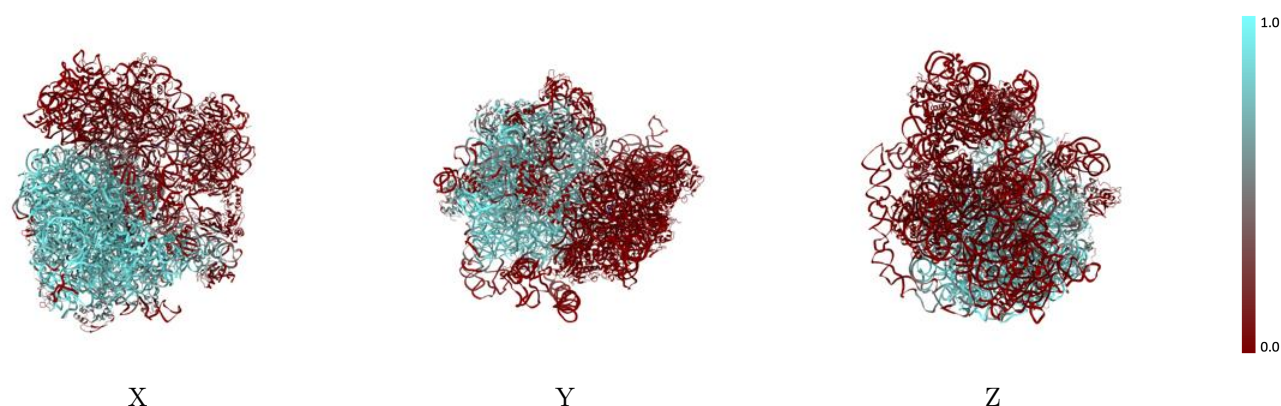
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



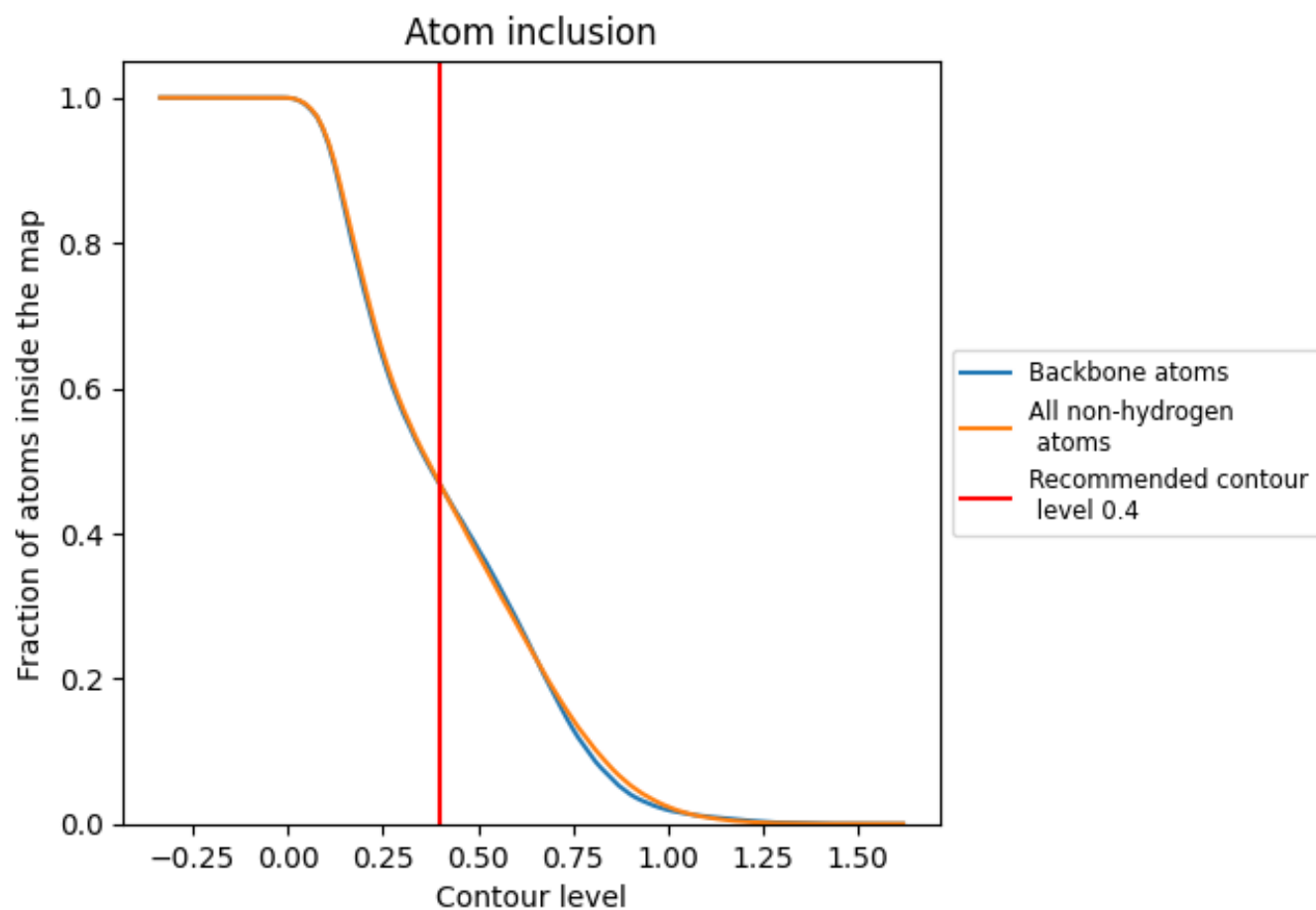
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 47% of all backbone atoms, 47% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4681	 0.4680
0	 0.4537	 0.6090
1	 0.6701	 0.5810
2	 0.9573	 0.6490
3	 0.7055	 0.6210
4	 0.1910	 0.5570
6	 0.0000	 0.2530
A	 0.7685	 0.5450
B	 0.5465	 0.4700
C	 0.8569	 0.6210
D	 0.7294	 0.6040
E	 0.6066	 0.5910
F	 0.0140	 0.3610
G	 0.0402	 0.4250
H	 0.0262	 0.3940
J	 0.8133	 0.6090
K	 0.6925	 0.6030
L	 0.6590	 0.5850
M	 0.1205	 0.5530
N	 0.8348	 0.6250
O	 0.2182	 0.4590
P	 0.6230	 0.5890
Q	 0.8515	 0.6190
R	 0.6471	 0.6010
S	 0.8141	 0.6220
T	 0.6409	 0.5780
U	 0.4141	 0.5220
V	 0.0436	 0.4840
W	 0.7623	 0.5990
X	 0.7662	 0.6190
Y	 0.5869	 0.5510
Z	 0.6989	 0.5880
a	 0.0181	 0.3330
c	 0.0000	 0.2250
d	 0.0000	 0.2260



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Chain	Atom inclusion	Q-score
e	 0.0000	 0.3140
f	 0.0000	 0.4430
g	 0.0000	 0.2290
h	 0.0000	 0.3360
i	 0.0000	 0.1610
j	 0.0000	 0.1700
k	 0.0000	 0.4060
l	 0.0000	 0.3460
m	 0.0000	 0.2100
n	 0.0000	 0.2030
o	 0.0000	 0.4150
p	 0.0000	 0.3030
q	 0.0000	 0.3330
r	 0.0000	 0.4080
s	 0.0000	 0.1790
t	 0.0000	 0.3420
v	 0.0171	 0.5040