



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 03:11 PM UTC

PDB ID : 7P48 / pdb_00007p48
EMDB ID : EMD-13191
Title : Staphylococcus aureus ribosome in complex with Sal(B)
Authors : Nicholson, D.; Ranson, N.A.; O'Neill, A.J.
Deposited on : 2021-07-09
Resolution : 2.90 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

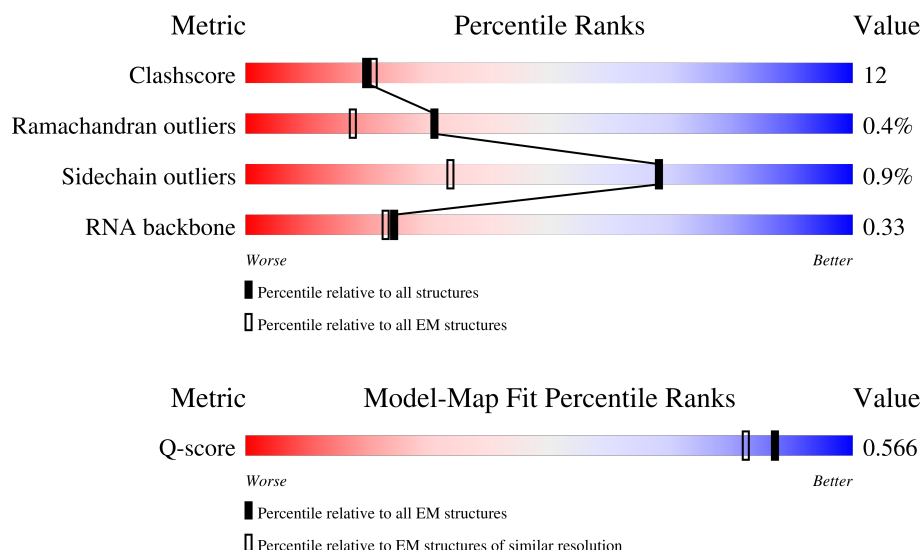
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	1	49	
2	2	45	
3	3	66	

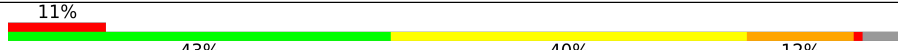
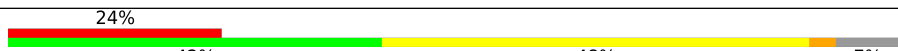
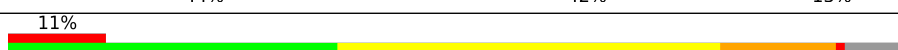
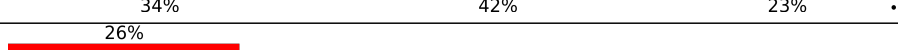
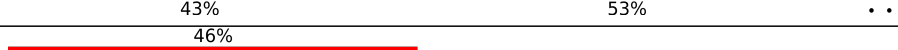
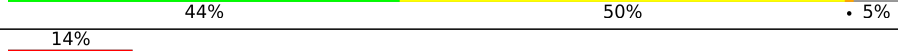
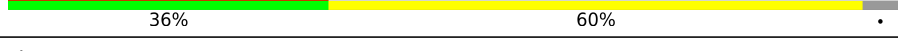
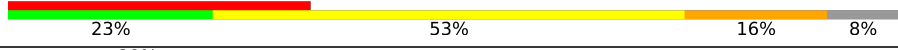
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Mol	Chain	Length	Quality of chain
4	4	37	
5	5	73	
6	6	565	
7	7	3	
8	A	2921	
9	B	115	
10	C	276	
11	D	220	
12	E	207	
13	F	179	
14	G	178	
15	H	145	
16	I	122	
17	J	146	
18	K	144	
19	L	122	
20	M	119	
21	N	116	
22	O	118	
23	P	102	
24	Q	117	
25	R	91	
26	S	105	
27	T	219	
28	U	94	

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Mol	Chain	Length	Quality of chain
29	V	62	
30	W	69	
31	X	59	
32	Y	125	
33	Z	57	
34	a	1548	
35	b	232	
36	c	217	
37	d	200	
38	e	166	
39	f	98	
40	g	156	
41	h	132	
42	i	130	
43	j	102	
44	k	129	
45	l	149	
46	m	121	
47	n	61	
48	o	89	
49	p	91	
50	q	87	
51	r	80	
52	s	108	
53	t	83	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 138850 atoms, of which 24 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 L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	47	Total	C	N	O	S	0	0
			394	240	78	72	4		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

- Molecule 5 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	73	Total	C	N	O	P	0	0
			1560	695	281	511	73		

- Molecule 6 is a protein called ABC-F type ribosomal protection protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	510	Total	C	N	O	S	0	0
			4190	2659	706	808	17		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	33	LEU	ILE	conflict	UNP A0A7D7YNB9
6	39	ILE	VAL	conflict	UNP A0A7D7YNB9
6	66	HIS	TYR	conflict	UNP A0A7D7YNB9
6	84	GLU	GLY	conflict	UNP A0A7D7YNB9
6	156	GLN	GLU	conflict	UNP A0A7D7YNB9
6	253	ARG	SER	conflict	UNP A0A7D7YNB9
6	406	MET	THR	conflict	UNP A0A7D7YNB9
6	456	GLN	GLU	conflict	UNP A0A7D7YNB9
6	464	SER	GLY	conflict	UNP A0A7D7YNB9
6	518	ALA	THR	conflict	UNP A0A7D7YNB9
6	542	GLY	-	expression tag	UNP A0A7D7YNB9
6	543	GLY	-	expression tag	UNP A0A7D7YNB9
6	544	ASP	-	expression tag	UNP A0A7D7YNB9
6	545	TYR	-	expression tag	UNP A0A7D7YNB9
6	546	LYS	-	expression tag	UNP A0A7D7YNB9
6	547	ASP	-	expression tag	UNP A0A7D7YNB9
6	548	HIS	-	expression tag	UNP A0A7D7YNB9
6	549	ASP	-	expression tag	UNP A0A7D7YNB9
6	550	GLY	-	expression tag	UNP A0A7D7YNB9
6	551	ASP	-	expression tag	UNP A0A7D7YNB9
6	552	TYR	-	expression tag	UNP A0A7D7YNB9
6	553	LYS	-	expression tag	UNP A0A7D7YNB9
6	554	ASP	-	expression tag	UNP A0A7D7YNB9
6	555	HIS	-	expression tag	UNP A0A7D7YNB9
6	556	ASP	-	expression tag	UNP A0A7D7YNB9
6	557	ILE	-	expression tag	UNP A0A7D7YNB9
6	558	ASP	-	expression tag	UNP A0A7D7YNB9
6	559	TYR	-	expression tag	UNP A0A7D7YNB9
6	560	LYS	-	expression tag	UNP A0A7D7YNB9
6	561	ASP	-	expression tag	UNP A0A7D7YNB9
6	562	ASP	-	expression tag	UNP A0A7D7YNB9
6	563	ASP	-	expression tag	UNP A0A7D7YNB9
6	564	ASP	-	expression tag	UNP A0A7D7YNB9
6	565	LYS	-	expression tag	UNP A0A7D7YNB9

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	7	3	Total	C	N	O	P	
			65	29	12	21	3	
							0	0

- Molecule 8 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2661	Total	C	N	O	P	0	0
			57062	25475	10455	18471	2661		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	113	Total	C	N	O	P	0	0
			2408	1076	431	788	113		

- Molecule 10 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	215	Total	C	N	O	S	0	0
			1628	1018	299	306	5		

- Molecule 12 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	173	Total	C	N	O		0	0
			853	507	173	173			

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	173	Total	C	N	O	S	0	0
			1180	728	223	227	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	145	Total	C	N	O	S	0	0
			1150	717	211	219	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	146	Total	C	N	O	S	0	0
			1097	680	215	201	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	137	Total	C	N	O	S	0	0
			1096	704	207	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	120	Total	C	N	O	S	0	0
			950	584	182	183	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
20	M	118	Total	C	N	O	0	0
			913	569	173	171		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	N	114	Total	C	N	O	0	0
			921	580	185	156		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	102	Total	C	N	O	S	0	0
			797	506	142	148	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	112	Total	C	N	O	S	0	0
			861	537	164	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	89	Total	C	N	O	S	0	0
			724	457	130	133	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	100	Total	C	N	O	S	0	0
			739	464	137	136	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	94	Total	C	N	O	S	0	0
			735	469	131	134	1		

- Molecule 28 is a protein called LSU ribosomal protein L27P.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	77	Total	C	N	O	0	0
			590	364	115	111		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	58	Total	C	N	O	S	0	0
			458	285	98	74	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	65	Total	C	N	O		0	0
			535	330	101	104			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	58	Total	C	N	O		0	0
			449	280	85	84			

- Molecule 32 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	70	Total	C	N	O		0	0
			390	238	79	73			

- Molecule 33 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	48	Total	C	N	O	S	0	0
			385	235	80	65	5		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1479	Total	C	N	O	P	0	0
			31706	14154	5809	10264	1479		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	224	Total	C	N	O	S	0	0
			1802	1149	314	332	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	202	Total	C	N	O	S	0	0
			1596	1005	300	289	2		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	199	Total	C	N	O	S	0	0
			1616	1020	302	292	2		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	156	Total	C	N	O	S	0	0
			1160	731	212	215	2		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	95	Total	C	N	O	S	0	0
			789	498	138	150	3		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	155	Total	C	N	O	S	0	0
			1242	775	239	224	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	131	Total	C	N	O	S	0	0
			1031	652	183	192	4		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	127	Total	C	N	O	S	0	0
			1007	624	201	181	1		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	97	Total	C	N	O	S	0	0
			773	488	141	143	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	114	Total	C	N	O	S	0	0
			844	520	160	161	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	116	Total	C	N	O	S	0	0
			922	566	183	172	1		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	87	Total	C	N	O	S	0	0
			726	448	149	128	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	87	Total	C	N	O	S	0	0
			688	433	127	127	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			657	416	117	123	1		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	64	Total	C	N	O	S	0	0
			525	336	98	88	3		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			665	427	121	115	2		

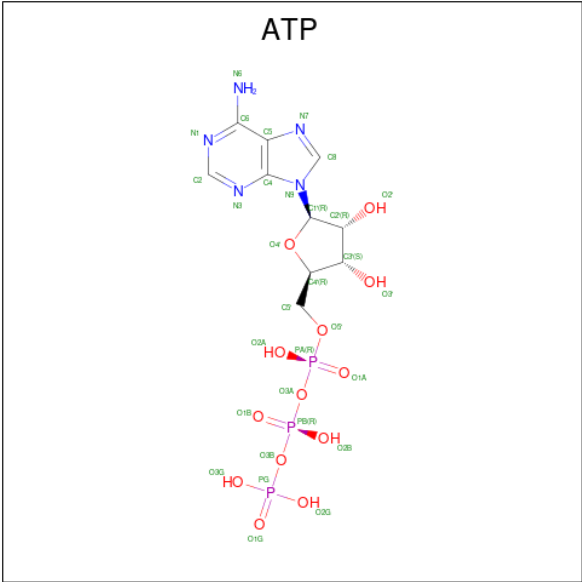
- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	81	Total	C	N	O	S	0	0
			611	370	120	119	2		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	4	1	Total	Zn	0
			1	1	
54	Z	1	Total	Zn	0
			1	1	
54	n	1	Total	Zn	0
			1	1	

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
55	6	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
55	6	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

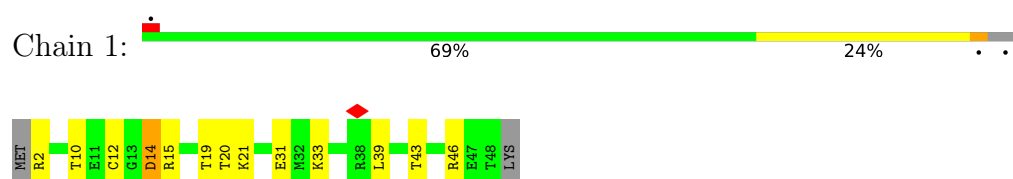
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	6	2	Total	Mg	0
			2	2	

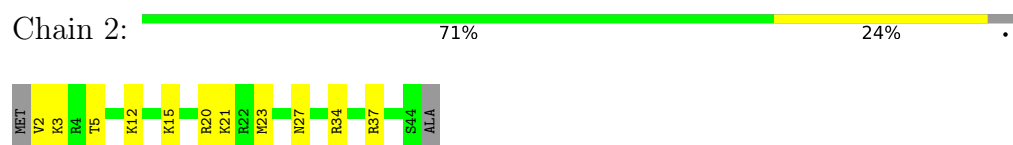
3 Residue-property plots [i](#)

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.

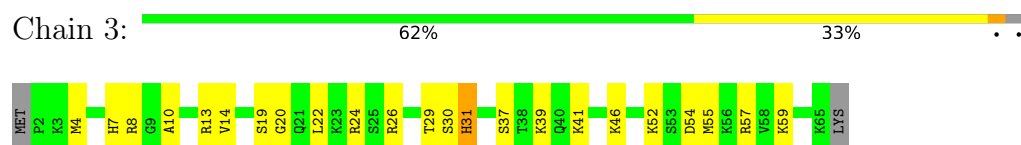
- Molecule 1: 50S ribosomal protein L33



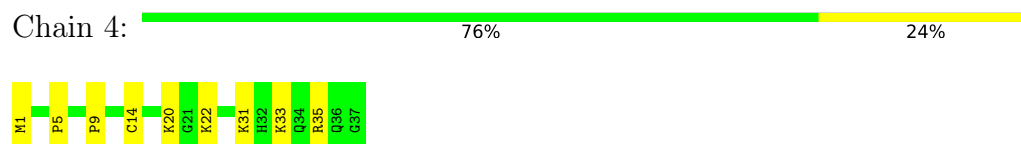
- Molecule 2: 50S ribosomal protein L34



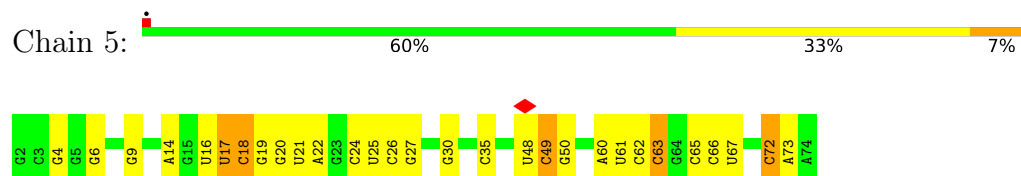
- Molecule 3: 50S ribosomal protein L35



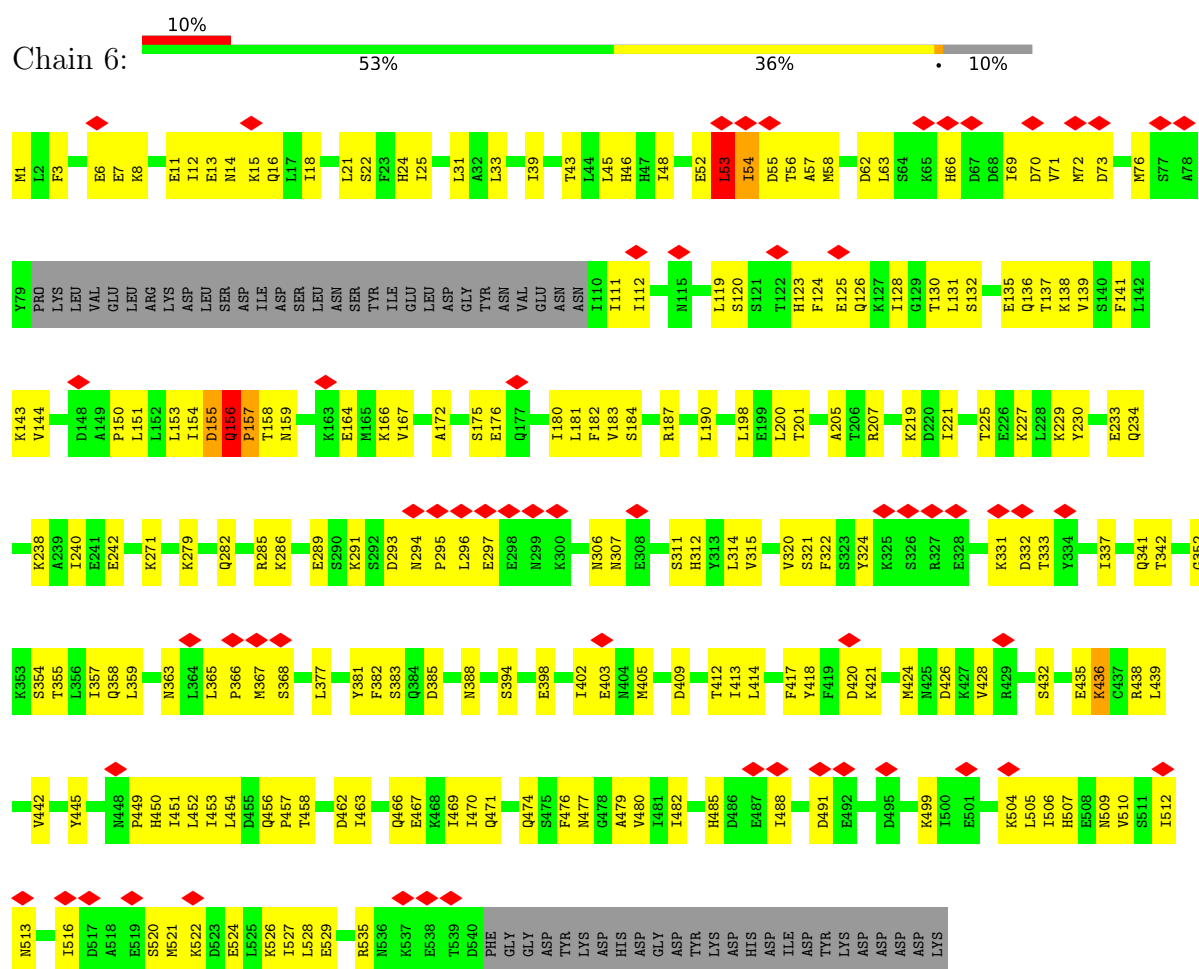
- Molecule 4: 50S ribosomal protein L36



- Molecule 5: P-site tRNA



- Molecule 6: ABC-F type ribosomal protection protein

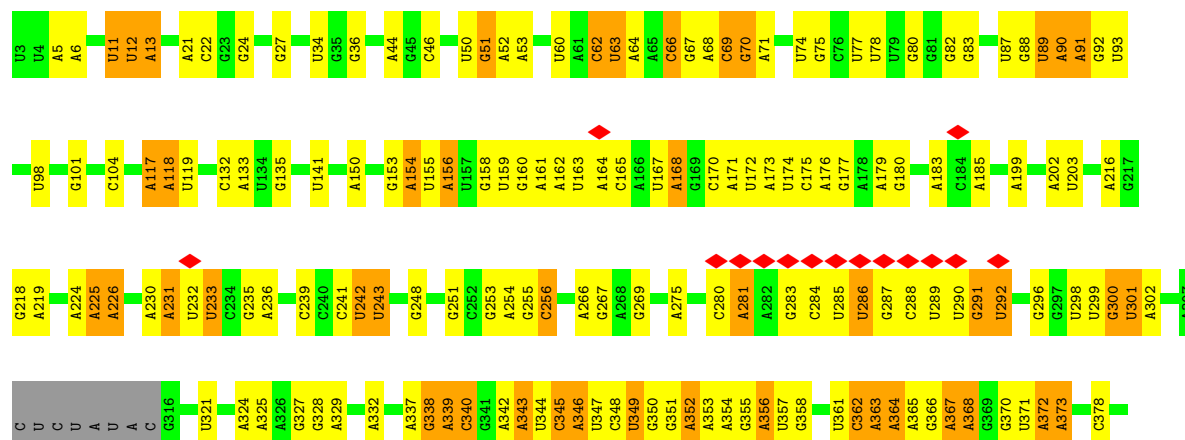


- Molecule 7: mRNA



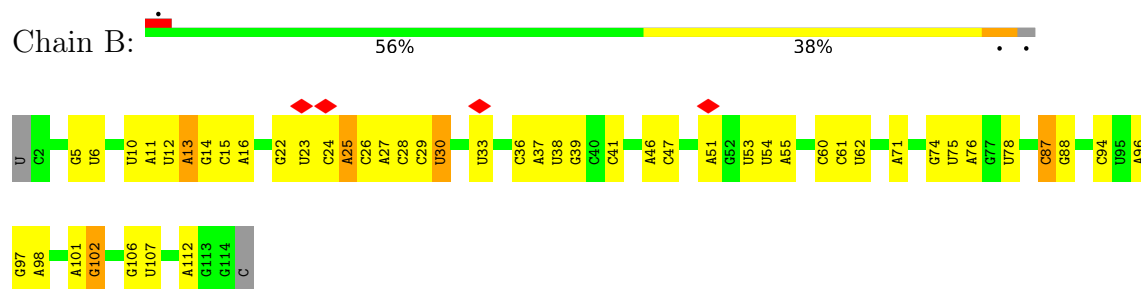
There are no outlier residues recorded for this chain.

- Molecule 8: 23S rRNA

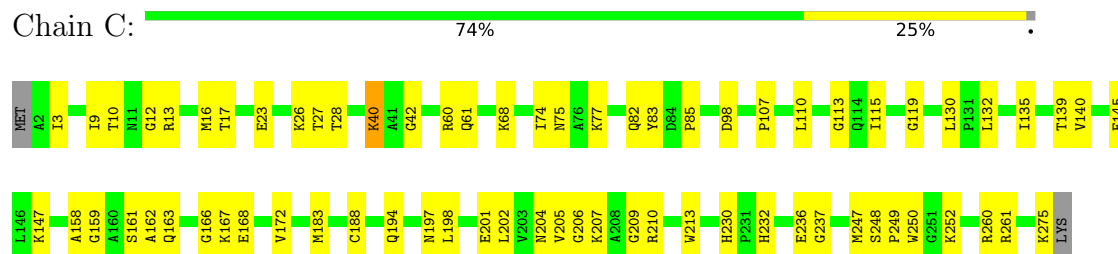


U1548	G1465	U1386	G1253	A1170	G	G1030	A955	U879	G774	A677	U569	A468	G381
C1549	G1468	C1367	A1258	A1171	G	C1031	A956	A880	A775	A678	U570	G471	U352
U1550	G1469	U1372	U1261	U1174	C	A1032	C957	G881	C781	C782	C572	U473	A383
U	G1470	U1373	U1262	U1175	U	C1039	U958	C883	C783	A682	G575	C479	U386
A	G1471	U1374	U1263	U1176	A	C1040	C959	U884	G790	G683	U576	U480	C387
A	G1472	G1376	G1278	A1177	G	C1041	C960	C885	G791	U684	A577	A388	G388
A	G1473	U1377	G1279	C1178	A	C1042	G961	A894	U792	C685	U578	C481	A389
G1555	C1474	U1377	G1280	G1180	A	U1043	A962	U895	G793	A688	C580	U482	A390
G1556	G1475	U1377	A1289	G1181	C	A1044	U964	G900	A794	U689	A583	C483	U394
C1557	G1480	G1382	G1290	G1182	A	A1045	G965	G903	A795	U690	C490	U399	U399
U1558	G1481	G1383	G1291	G1183	C	G1046	A969	U904	A796	A691	U589	C400	C400
A1559	G1482	C1388	U1293	C1184	C	G1047	U970	G905	A797	U692	U590	U401	U401
G1560	G1483	G1389	A1294	A1185	A	C1048	U971	U906	G798	U693	G498	A402	A402
U1564	C1490	U1388	U1295	U1186	C	C1049	A972	G909	A809	A700	A591	A500	U403
U1565	G1491	U1389	C1296	A1187	U	C1050	A973	C910	A810	G701	A592	A501	U403
G1566	U1492	U1390	G1297	A1188	C	A1051	U974	G911	G817	U702	U593	C501	U
A1567	G1493	G1391	U1298	U1191	A	A1052	U975	A912	U706	A703	G594	A503	A
U1568	C1494	U1392	U1299	A1192	U	A1053	U976	G913	G820	G707	U597	G513	U
G1495	G1495	G1395	U1300	C1197	U	A1054	A977	U914	G821	U711	G601	A517	G
A1497	U1497	C1400	G1309	U1197	U	A1057	A978	U915	G822	G712	U605	A518	A
U1498	G1498	G1401	A1310	G1198	A	U1058	G979	G916	A827	G713	G606	G519	U412
U1499	G1499	A1402	A1311	A1199	A	A1059	U980	U917	U828	G714	A615	A523	G428
G1500	G1500	G1403	A1312	A1200	G	U1060	U981	U918	U829	A715	A616	A524	C429
U1504	U1504	G1405	G1313	G1201	A	G1061	G984	G919	C831	A720	A617	A525	A430
G1505	G1505	U1409	A1314	C1202	G	G1066	G985	U920	A834	G727	A618	A526	C431
C1506	C1506	A1410	G1320	U1205	U	A1070	A989	C	U835	A730	U619	C528	U433
A1507	A1507	G1411	A1321	G1206	C	A1071	U990	G	U836	C732	G620	A536	A435
C1508	C1508	U1415	G1322	G1207	G	A1072	A991	G	G850	G745	G628	A537	A436
U1509	U1509	U1416	C1326	G1211	U	A1073	A992	G	C851	U748	U631	G538	U437
C1511	C1511	A1421	U1329	C1214	A	U1077	U995	C	U857	G749	U632	G539	U438
U1512	U1512	A1422	U1330	U1218	G	G1082	G996	C	C858	U753	A633	G545	C440
A1513	A1513	U1439	A1333	U1219	C	U	U1002	C	U859	U754	A646	A547	G446
C1516	C1516	U1443	G1336	G1226	U	U	G1005	C	C863	C755	A651	A548	A447
G1517	G1517	C1444	U1337	A1220	C	U	C1008	C	G864	A756	A652	U549	C450
U1518	U1518	U1448	U1338	C1221	C	U	U1013	C	A865	G757	A552	A550	G456
U1519	U1519	A	A1344	G1227	A	A	U1014	C	U868	U758	A553	C554	G457
C1520	C1520	U	G1347	A1228	G	A	C1015	C	A869	A760	A554	C561	C460
A1521	A1521	C	U1350	G1234	C	A	G1016	C	G870	C762	A555	C562	A461
G1522	G1522	G	U1351	U1238	C	A	A1017	C	U871	A763	A556	G563	U462
G1523	G1523	A	C1352	C1239	U	A	A1018	C	U872	C764	A557	U564	C463
C1524	C1524	U	U1238	A1241	U	A	G1021	C	U873	U765	A558	G565	U464
U1525	U1525	U	G1242	G1244	G	A	G1022	C	A874	A767	A559	U566	C465
G1526	G1526	C	U1248	U1248	U	U	A1023	C	G877	C878	A560	G567	C466
U1527	U1527	U	U1249	U1249	C	A	A1024	C	U947	U773	A561	U467	U467
A1528	A1528	U	G1250	G1250	A	A	C1025	C	U948	U774	A562	C468	C468
U1529	U1529	U	U1251	U1251	U	A	A1026	C	C949	A775	A563	U469	U469
A1530	A1530	U	G1252	G1252	U	A	A1027	C	A952	U776	A564	C470	C470
U1531	U1531	U	U1253	U1253	U	U	A1028	C	U953	U777	A565	C471	C471
U1532	U1532	A	U1254	U1254	C	U	A1029	C	U954	U778	A566	C472	C472
A1533	A1533	U1459	G1357	G1255	C	A	C1030	C	U955	U779	A567	C473	C473
G1534	G1534	U1460	U1358	G1256	A	A	C1031	C	U956	U780	A568	C474	C474
C1535	C1535	C1461	A1359	G1257	U	U	A1032	C	U957	U781	A569	C475	C475
G1536	G1536	G1462	U1360	G1258	G	U	A1033	C	U958	U782	A570	C476	C476
U1537	U1537	A1463	U1361	U1259	U	U	A1034	C	U959	U783	A571	C477	C477
A1538	A1538	U1464	C1362	U1260	U	U	C1035	C	U960	U784	A572	C478	C478

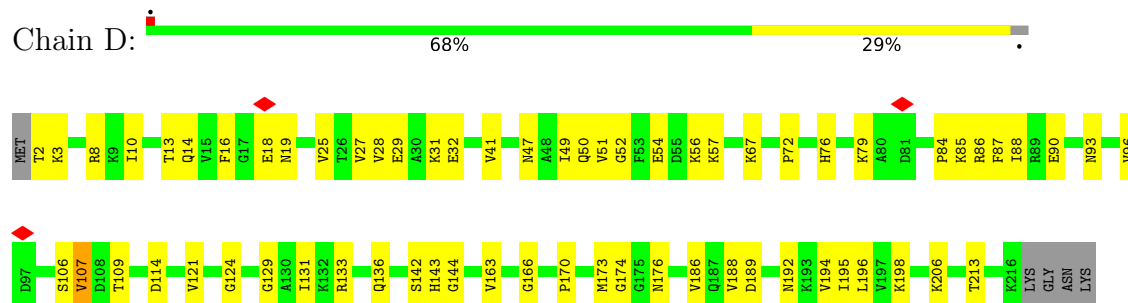




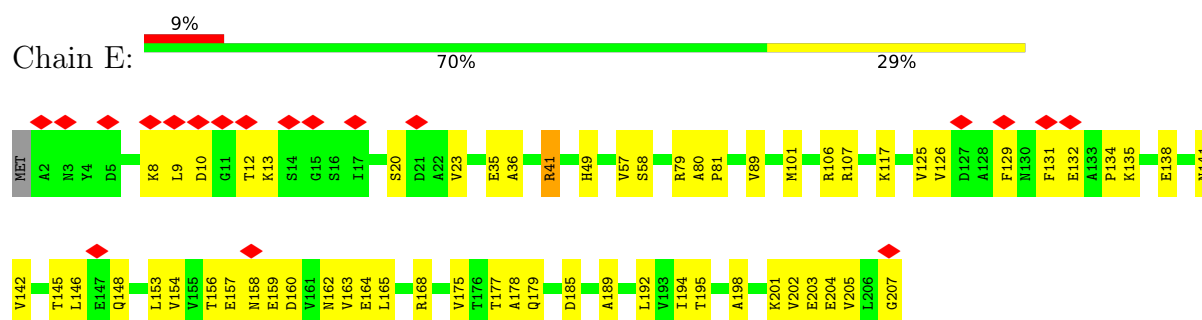
- Molecule 10: 50S ribosomal protein L2



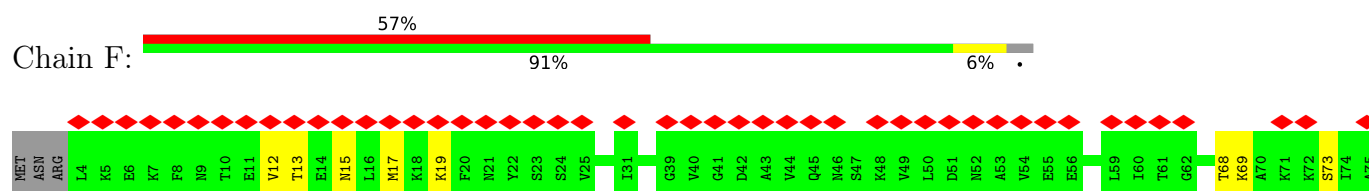
- Molecule 11: 50S ribosomal protein L3

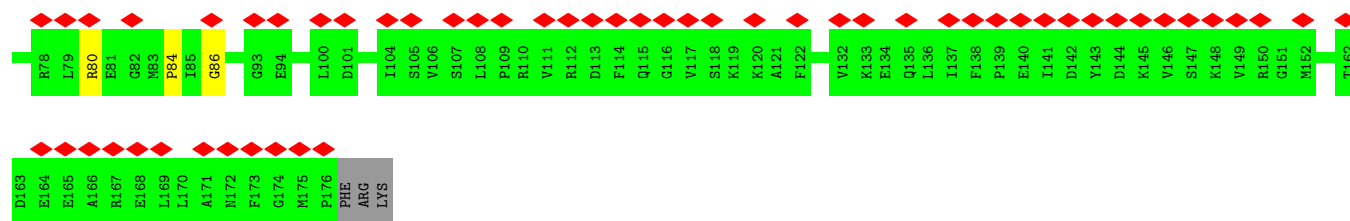


- Molecule 12: 50S ribosomal protein L4

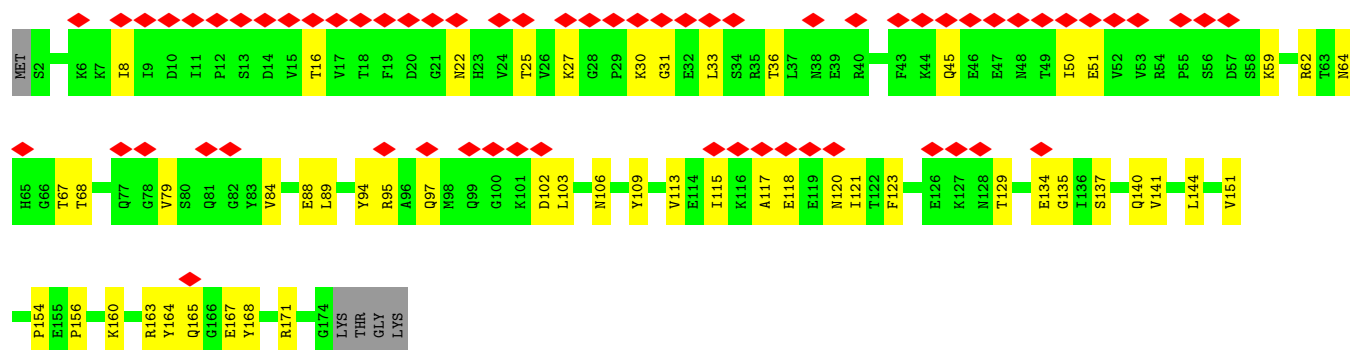


- Molecule 13: 50S ribosomal protein L5

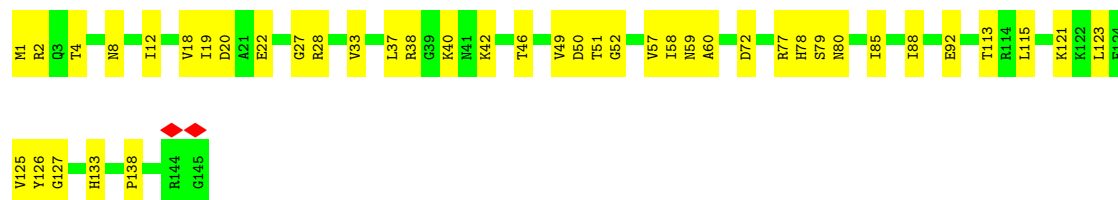




• Molecule 14: 50S ribosomal protein L6



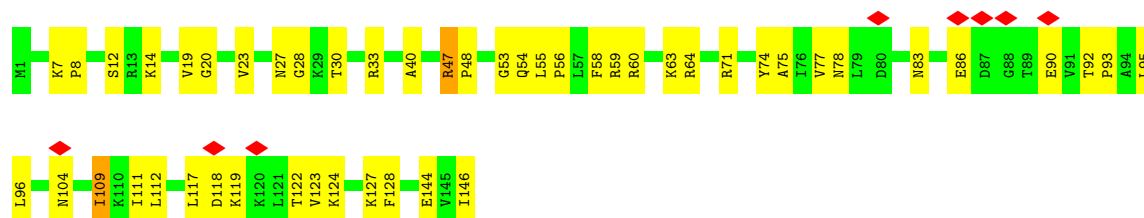
• Molecule 15: 50S ribosomal protein L13



• Molecule 16: 50S ribosomal protein L14

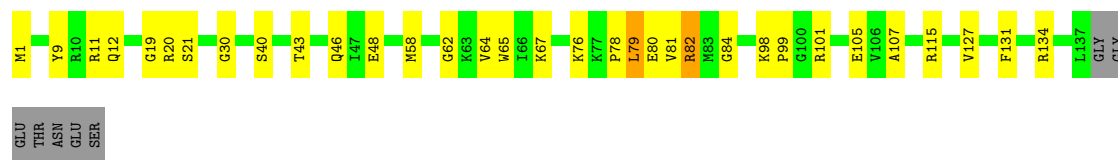


• Molecule 17: 50S ribosomal protein L15



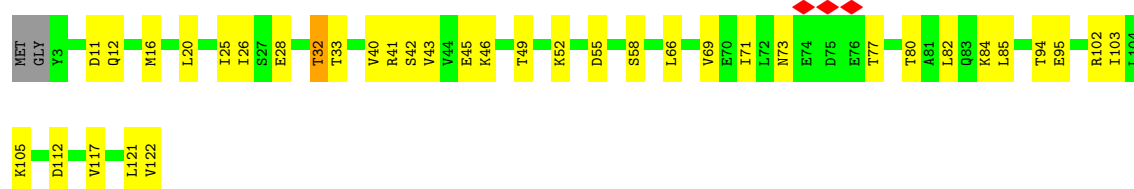
- Molecule 18: 50S ribosomal protein L16

Chain K:  72% 22% 5%



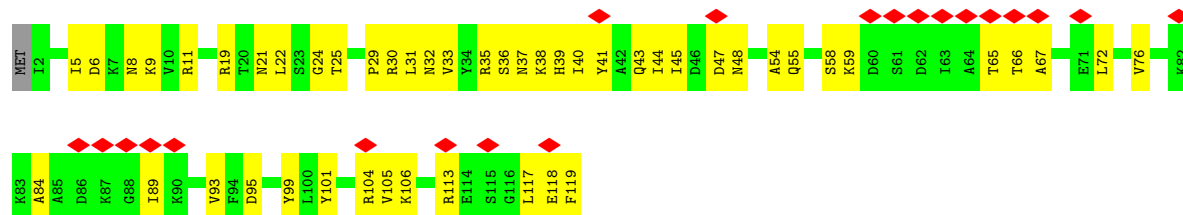
- Molecule 19: 50S ribosomal protein L17

Chain L:  68% 30% 2%



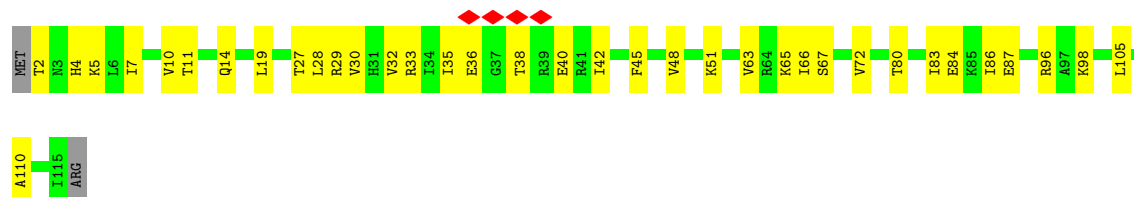
- Molecule 20: 50S ribosomal protein L18

Chain M:  18% 58% 41%



- Molecule 21: 50S ribosomal protein L19

Chain N:  67% 31% 2%

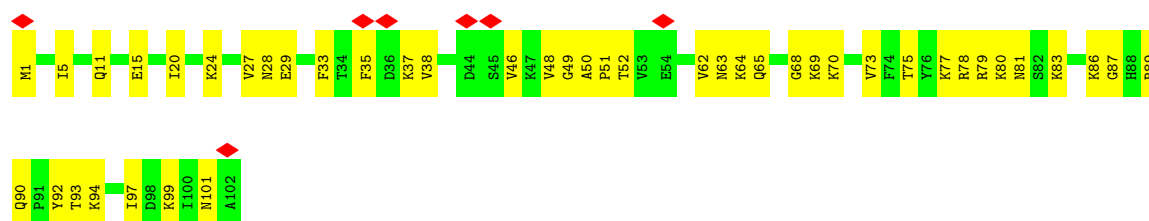


- Molecule 22: 50S ribosomal protein L20

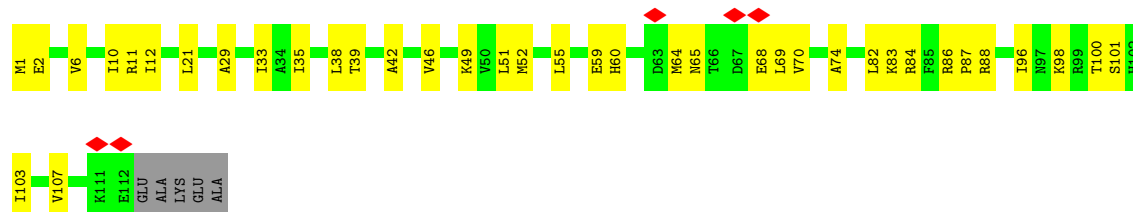
Chain O:  76% 22% 2%



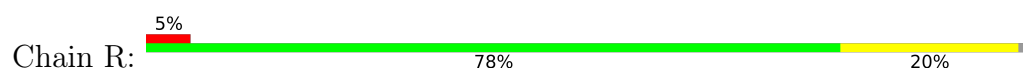
- Molecule 23: 50S ribosomal protein L21



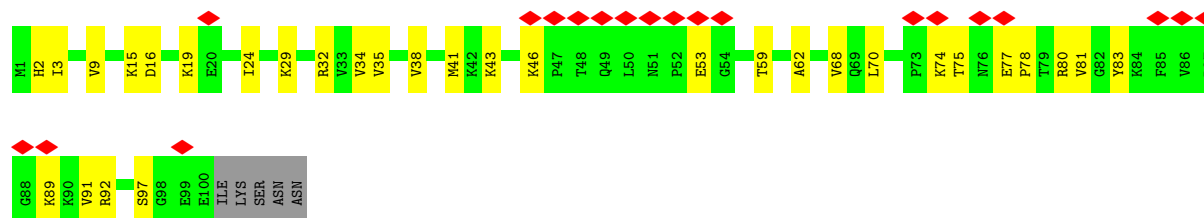
- Molecule 24: 50S ribosomal protein L22



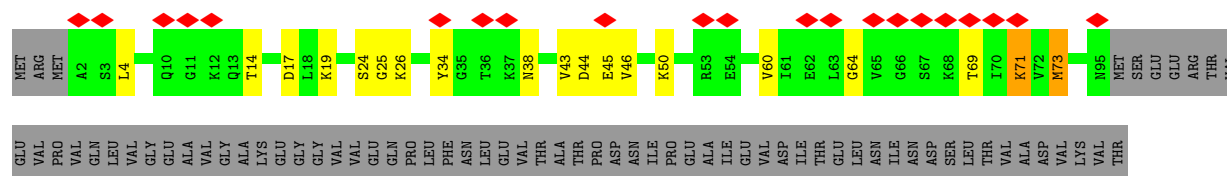
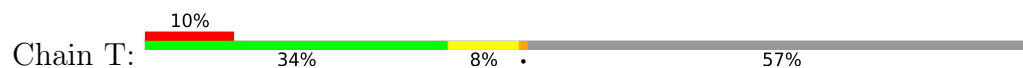
- Molecule 25: 50S ribosomal protein L23



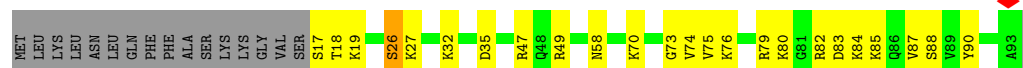
- Molecule 26: 50S ribosomal protein L24



- Molecule 27: 50S ribosomal protein L25



- Molecule 28: LSU ribosomal protein L27P



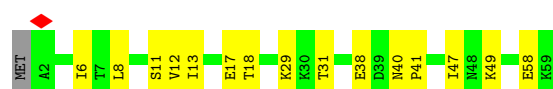
- Molecule 29: 50S ribosomal protein L28



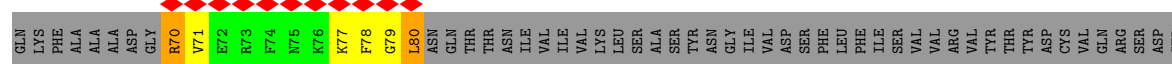
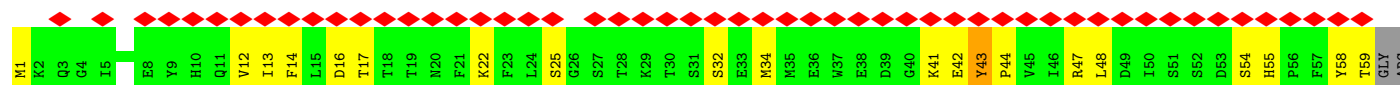
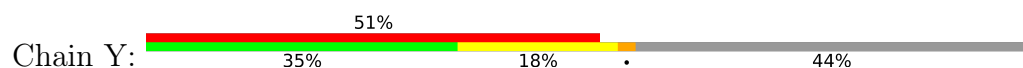
- Molecule 30: 50S ribosomal protein L29



- Molecule 31: 50S ribosomal protein L30



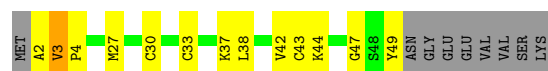
- Molecule 32: 50S ribosomal protein L31 type B



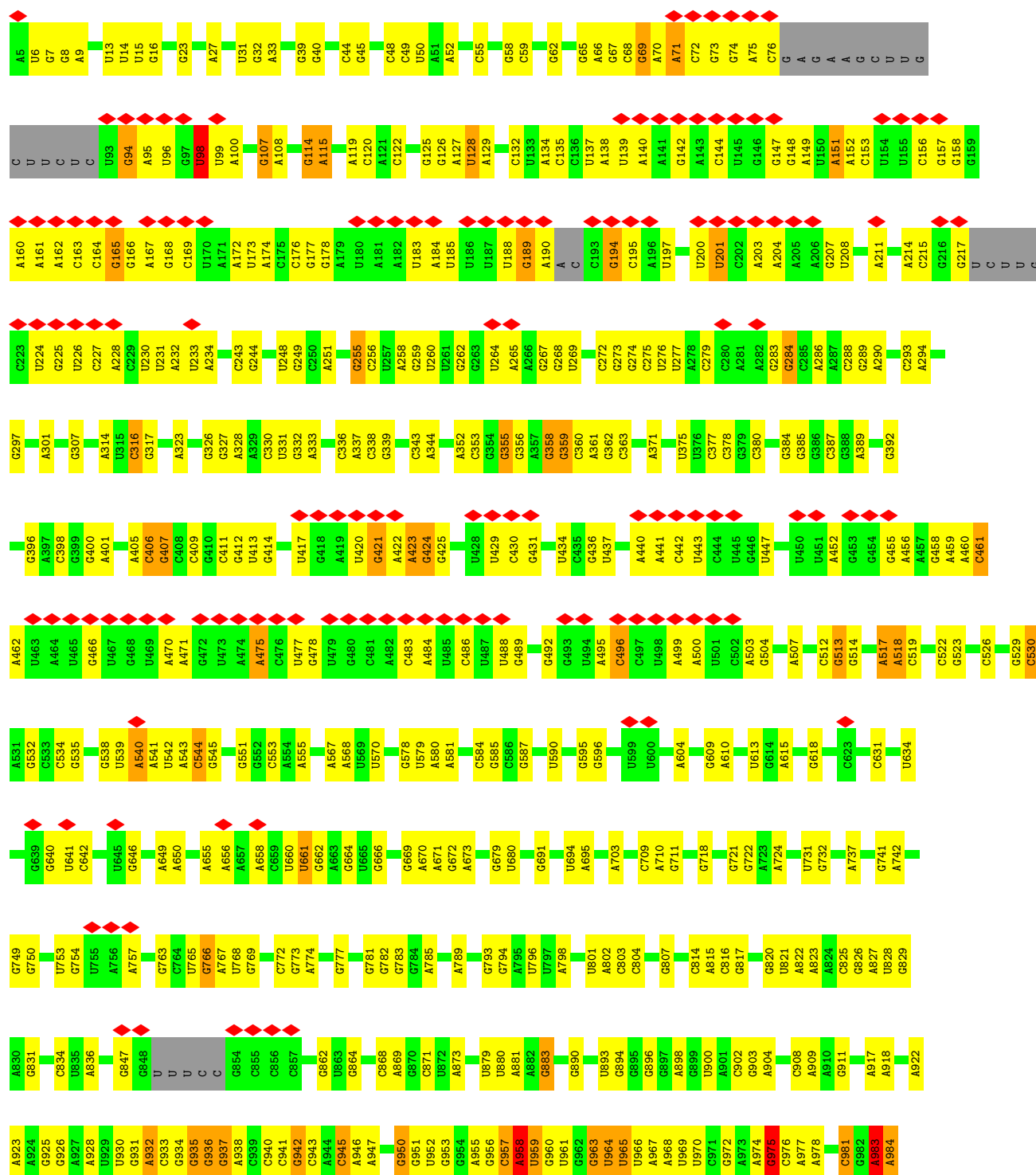
ILE
PRO
CYS
CYS

- Molecule 33: 50S ribosomal protein L32



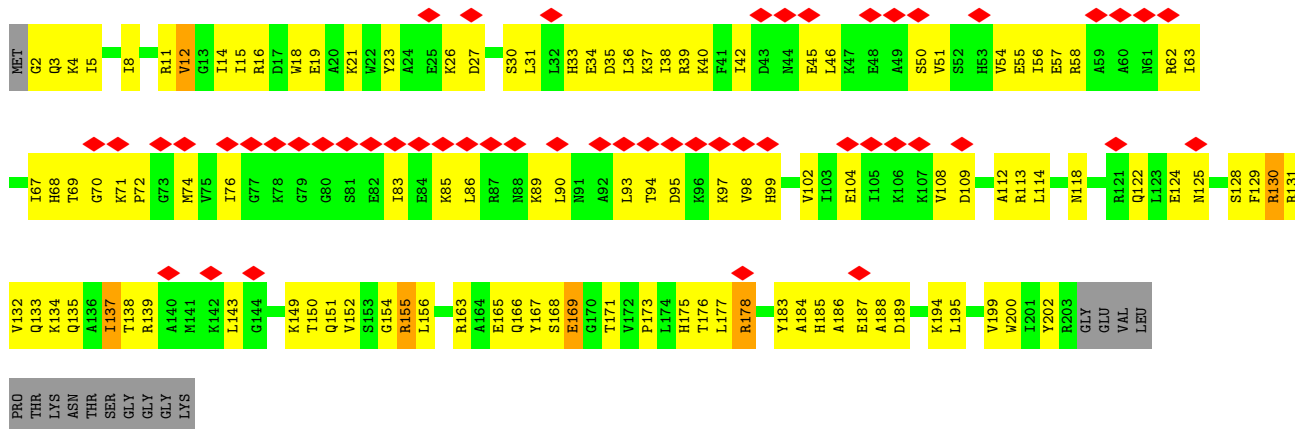
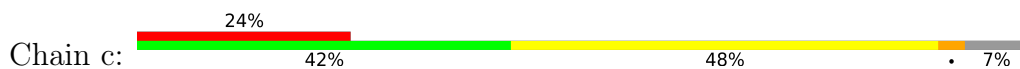


• Molecule 34: 16S rRNA

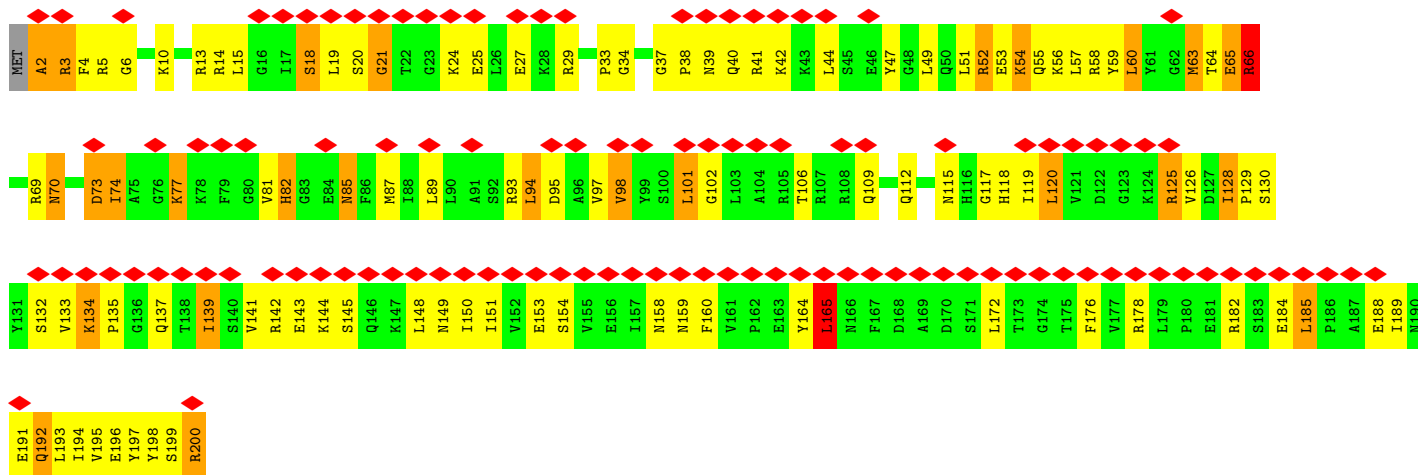
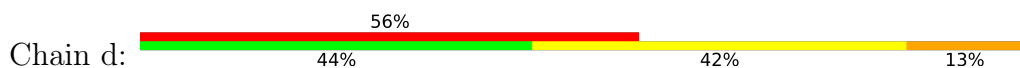




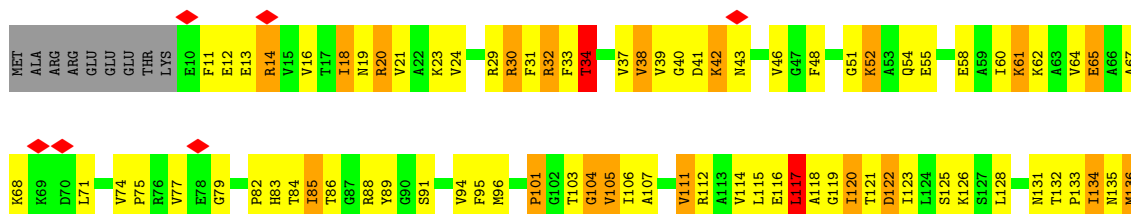
• Molecule 36: 30S ribosomal protein S3

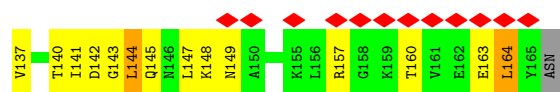


• Molecule 37: 30S ribosomal protein S4

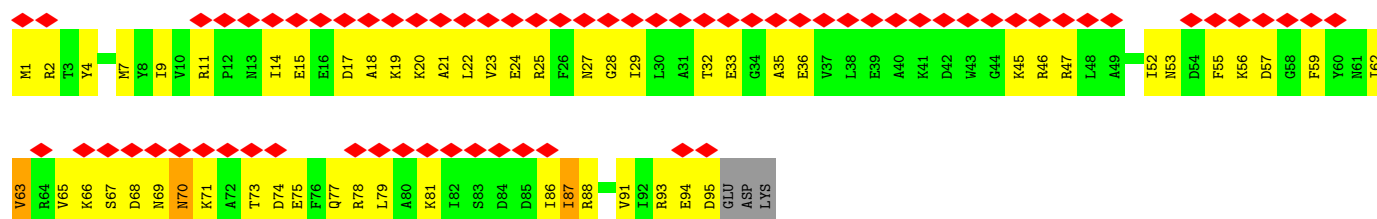


• Molecule 38: 30S ribosomal protein S5

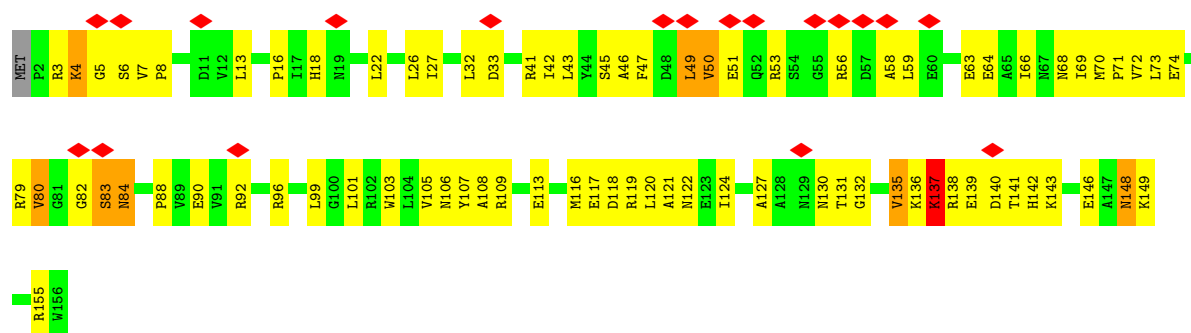




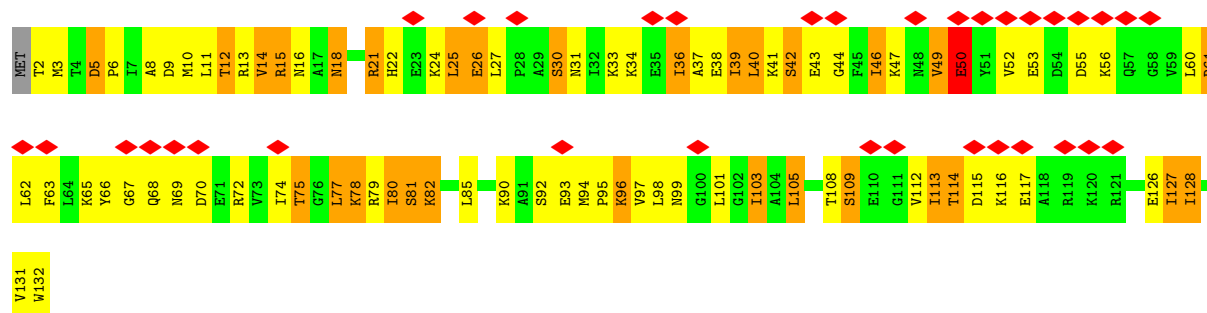
- Molecule 39: 30S ribosomal protein S6



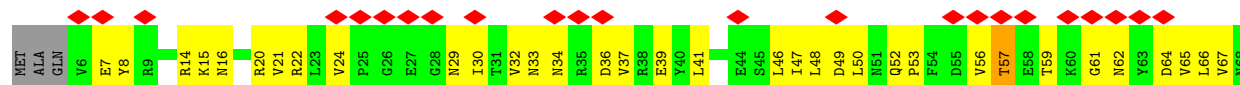
- Molecule 40: 30S ribosomal protein S7

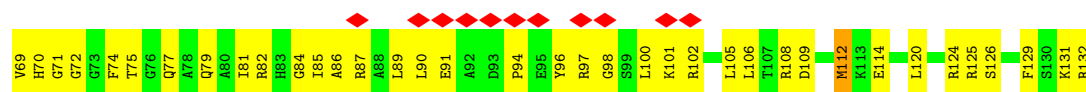


- Molecule 41: 30S ribosomal protein S8

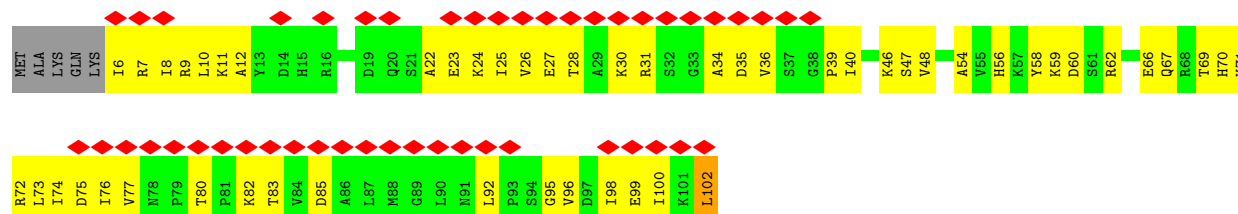
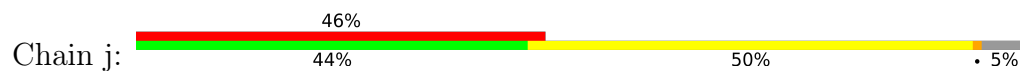


- Molecule 42: 30S ribosomal protein S9

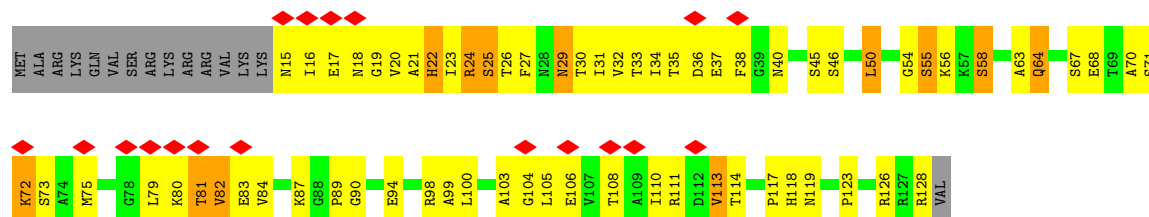




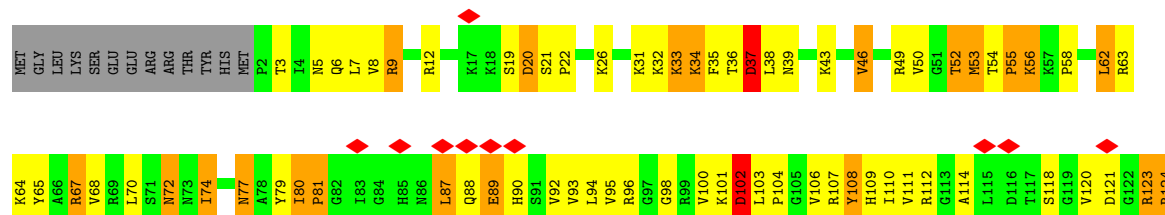
• Molecule 43: 30S ribosomal protein S10



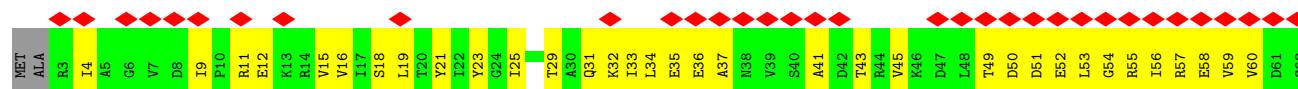
• Molecule 44: 30S ribosomal protein S11

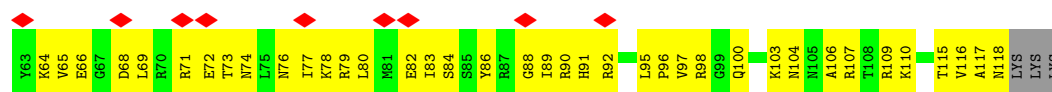


• Molecule 45: 30S ribosomal protein S12



• Molecule 46: 30S ribosomal protein S13

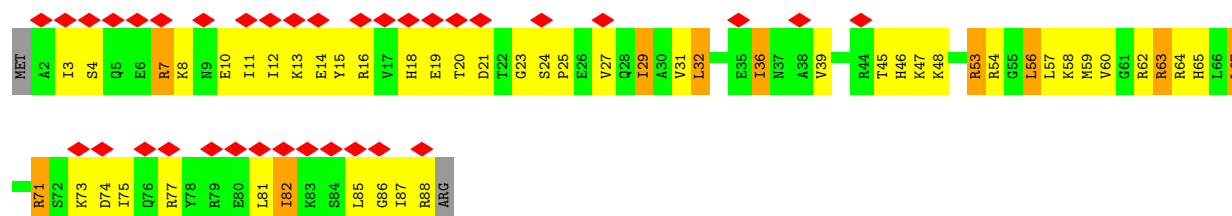




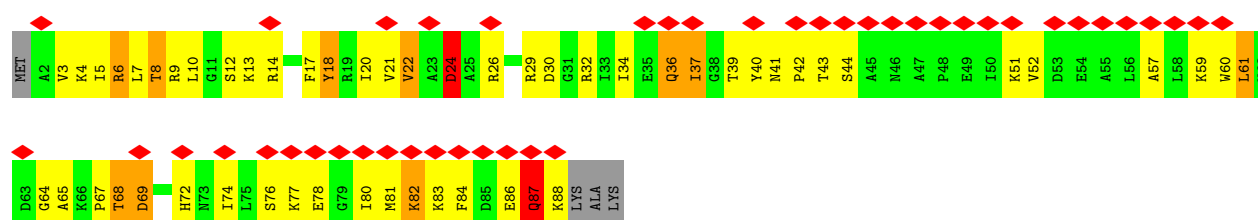
- Molecule 47: 30S ribosomal protein S14 type Z



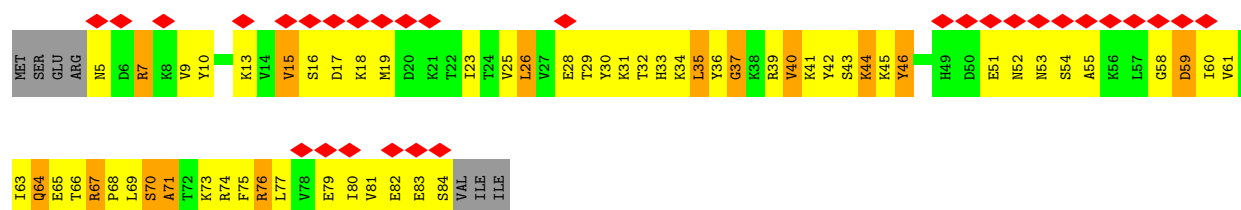
- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16

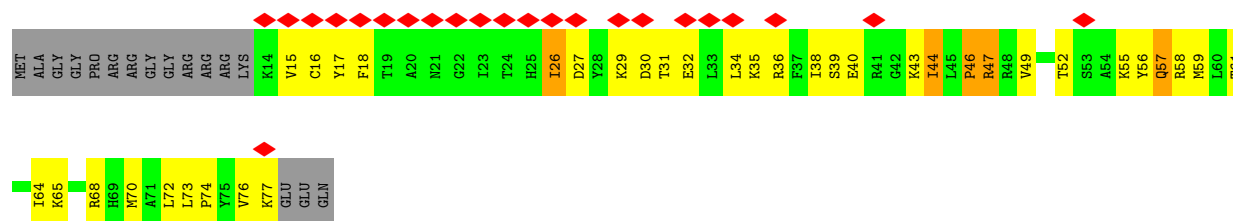


- Molecule 50: 30S ribosomal protein S17

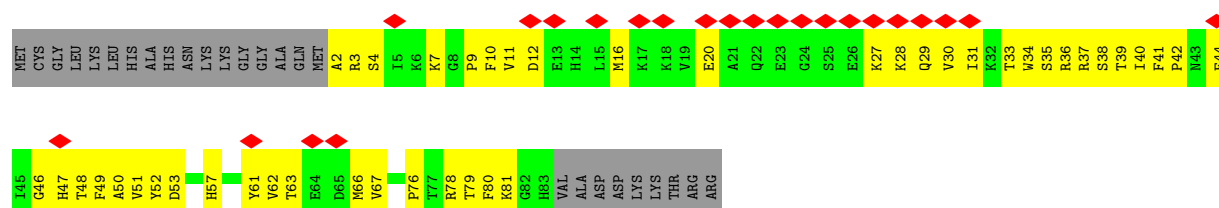


- Molecule 51: 30S ribosomal protein S18

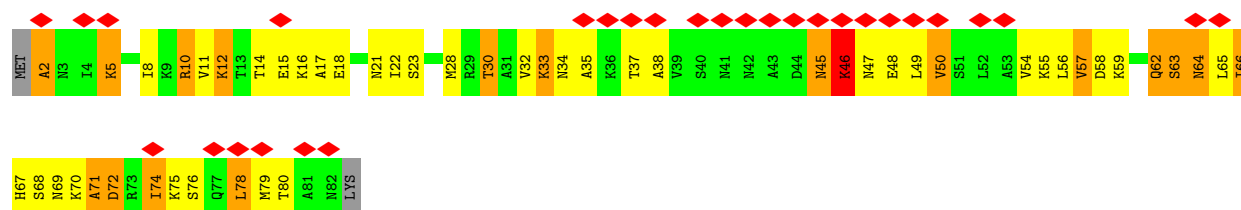




• Molecule 52: 30S ribosomal protein S19



• Molecule 53: 30S ribosomal protein S20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59889	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 ($e^-/\text{\AA}^2$)	60	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	0.935	Depositor
Minimum map value	-0.478	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.065	Depositor
Map size ($\text{\AA}$)	445.12003, 445.12003, 445.12003	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.32	0/399	0.59	0/535
2	2	0.50	0/371	0.70	0/484
3	3	0.44	0/526	0.66	0/690
4	4	0.39	0/298	0.45	0/392
5	5	0.30	0/1743	0.27	0/2716
6	6	0.28	0/4264	0.51	2/5725 (0.0%)
7	7	0.45	0/72	0.30	0/110
8	A	0.50	0/63900	0.47	3/99638 (0.0%)
9	B	0.28	0/2692	0.26	0/4193
10	C	0.39	0/2129	0.53	0/2858
11	D	0.39	0/1652	0.59	0/2216
12	E	0.37	0/1595	0.57	0/2154
13	F	0.12	0/852	0.35	0/1184
14	G	0.20	0/1192	0.44	0/1617
15	H	0.39	0/1172	0.52	0/1578
16	I	0.34	0/925	0.51	0/1242
17	J	0.41	0/1111	0.57	0/1480
18	K	0.41	0/1120	0.58	0/1502
19	L	0.38	0/954	0.53	0/1276
20	M	0.26	0/922	0.52	0/1234
21	N	0.34	0/933	0.50	0/1247
22	O	0.43	0/955	0.59	0/1265
23	P	0.42	0/807	0.59	0/1079
24	Q	0.38	0/869	0.56	0/1170
25	R	0.38	0/732	0.55	0/977
26	S	0.26	0/746	0.43	0/997
27	T	0.38	0/743	0.55	0/997
28	U	0.39	0/596	0.54	0/792
29	V	0.34	0/464	0.53	0/619
30	W	0.27	0/536	0.46	0/713
31	X	0.34	0/451	0.48	0/606
32	Y	0.55	1/390 (0.3%)	0.61	0/532

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.42	0/392	0.60	0/521
34	a	0.88	202/35498 (0.6%)	0.80	87/55345 (0.2%)
35	b	1.58	12/1829 (0.7%)	1.41	12/2455 (0.5%)
36	c	1.03	2/1618 (0.1%)	1.17	5/2173 (0.2%)
37	d	2.31	46/1646 (2.8%)	1.77	36/2211 (1.6%)
38	e	2.56	72/1174 (6.1%)	1.90	34/1584 (2.1%)
39	f	1.97	10/800 (1.2%)	1.62	9/1073 (0.8%)
40	g	0.96	1/1262 (0.1%)	1.14	3/1698 (0.2%)
41	h	2.62	59/1043 (5.7%)	1.85	40/1401 (2.9%)
42	i	0.76	1/1023 (0.1%)	1.07	2/1374 (0.1%)
43	j	0.64	0/785	0.94	0/1060
44	k	1.91	16/859 (1.9%)	1.72	22/1161 (1.9%)
45	l	2.55	60/1075 (5.6%)	2.25	47/1439 (3.3%)
46	m	0.54	0/929	0.93	2/1246 (0.2%)
47	n	0.99	2/511 (0.4%)	1.30	3/678 (0.4%)
48	o	2.37	27/735 (3.7%)	1.68	10/982 (1.0%)
49	p	2.54	36/699 (5.2%)	2.01	29/942 (3.1%)
50	q	2.24	21/665 (3.2%)	1.79	13/889 (1.5%)
51	r	2.56	26/534 (4.9%)	1.80	9/715 (1.3%)
52	s	0.51	0/683	0.85	0/916
53	t	2.46	26/611 (4.3%)	2.04	24/817 (2.9%)
All	All	0.86	620/150482 (0.4%)	0.76	392/224498 (0.2%)

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
1	1	0	1
6	6	0	3
10	C	0	1
16	I	0	1
17	J	0	1
22	O	0	1
28	U	0	1
32	Y	0	1
34	a	0	1
35	b	0	2
36	c	0	4
37	d	0	5
38	e	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	g	0	4
41	h	0	2
43	j	0	1
44	k	0	2
45	l	0	5
47	n	0	2
48	o	0	1
49	p	0	2
50	q	0	2
52	s	0	1
53	t	0	3
All	All	0	50

The worst 5 of 620 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	t	46	LYS	CB-CG	-12.04	1.16	1.52
45	l	102	ASP	CB-CG	-11.71	1.22	1.52
45	l	124	ARG	CG-CD	-11.13	1.19	1.52
37	d	65	GLU	CB-CG	-10.86	1.19	1.52
44	k	22	HIS	CA-CB	-9.83	1.27	1.53

The worst 5 of 392 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	t	46	LYS	CB-CG-CD	18.33	153.46	111.30
34	a	1095	G	OP1-P-OP2	-18.32	64.65	119.60
45	l	114	ALA	CA-C-N	-15.69	103.76	122.44
45	l	114	ALA	C-N-CA	-15.69	103.76	122.44
34	a	930	U	O5'-P-OP1	-14.04	65.89	108.00

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	14	ASP	Peptide
6	6	156	GLN	Peptide
6	6	436	LYS	Peptide
6	6	53	LEU	Peptide
10	C	40	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	394	0	398	16	0
2	2	367	0	415	15	0
3	3	521	0	586	24	0
4	4	295	0	339	9	0
5	5	1560	0	790	19	0
6	6	4190	0	4184	186	0
7	7	65	0	33	0	0
8	A	57062	0	28694	575	0
9	B	2408	0	1218	26	0
10	C	2094	0	2205	68	0
11	D	1628	0	1667	58	0
12	E	1572	0	1619	54	0
13	F	853	0	378	6	0
14	G	1180	0	1027	39	0
15	H	1150	0	1145	34	0
16	I	918	0	981	27	0
17	J	1097	0	1142	53	0
18	K	1096	0	1166	22	0
19	L	950	0	999	28	0
20	M	913	0	956	53	0
21	N	921	0	994	29	0
22	O	943	0	1014	28	0
23	P	797	0	836	45	0
24	Q	861	0	920	35	0
25	R	724	0	761	23	0
26	S	739	0	763	20	0
27	T	735	0	783	16	0
28	U	590	0	602	25	0
29	V	458	0	498	24	0
30	W	535	0	567	22	0
31	X	449	0	491	12	0
32	Y	390	0	224	25	0
33	Z	385	0	399	14	0
34	a	31706	0	15808	322	0
35	b	1802	0	1866	155	0
36	c	1596	0	1659	107	0
37	d	1616	0	1646	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	e	1160	0	1223	44	0
39	f	789	0	788	50	0
40	g	1242	0	1276	79	0
41	h	1031	0	1082	55	0
42	i	1007	0	1031	77	0
43	j	773	0	812	56	0
44	k	844	0	851	65	0
45	l	1058	0	1130	37	0
46	m	922	0	970	80	0
47	n	501	0	525	26	0
48	o	726	0	756	33	0
49	p	688	0	713	25	0
50	q	657	0	694	46	0
51	r	525	0	561	23	0
52	s	665	0	668	52	0
53	t	611	0	655	32	0
54	4	1	0	0	0	0
54	Z	1	0	0	0	0
54	n	1	0	0	0	0
55	6	62	24	24	3	0
56	6	2	0	0	0	0
All	All	138826	24	93532	2815	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 2815 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:m:50:ASP:HA	46:m:53:LEU:HB2	1.37	1.06
43:j:9:ARG:HB2	43:j:99:GLU:HB2	1.39	1.05
41:h:114:THR:HG22	41:h:117:GLU:HG2	1.40	1.04
8:A:2346:U:H4'	8:A:2347:A:H5'	1.41	1.02
35:b:117:ILE:HA	35:b:120:MET:HE2	1.41	1.00

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1	45/49 (92%)	39 (87%)	6 (13%)	0	100	100
2	2	41/45 (91%)	39 (95%)	2 (5%)	0	100	100
3	3	62/66 (94%)	55 (89%)	7 (11%)	0	100	100
4	4	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
6	6	506/565 (90%)	422 (83%)	80 (16%)	4 (1%)	16	44
10	C	272/276 (99%)	253 (93%)	19 (7%)	0	100	100
11	D	213/220 (97%)	186 (87%)	27 (13%)	0	100	100
12	E	204/207 (99%)	185 (91%)	19 (9%)	0	100	100
13	F	171/179 (96%)	137 (80%)	34 (20%)	0	100	100
14	G	171/178 (96%)	149 (87%)	22 (13%)	0	100	100
15	H	143/145 (99%)	130 (91%)	13 (9%)	0	100	100
16	I	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
17	J	144/146 (99%)	130 (90%)	14 (10%)	0	100	100
18	K	135/144 (94%)	124 (92%)	10 (7%)	1 (1%)	18	48
19	L	118/122 (97%)	108 (92%)	10 (8%)	0	100	100
20	M	116/119 (98%)	105 (90%)	11 (10%)	0	100	100
21	N	112/116 (97%)	100 (89%)	12 (11%)	0	100	100
22	O	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
23	P	100/102 (98%)	88 (88%)	12 (12%)	0	100	100
24	Q	110/117 (94%)	108 (98%)	2 (2%)	0	100	100
25	R	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
26	S	98/105 (93%)	85 (87%)	13 (13%)	0	100	100
27	T	92/219 (42%)	83 (90%)	9 (10%)	0	100	100
28	U	75/94 (80%)	71 (95%)	4 (5%)	0	100	100
29	V	56/62 (90%)	51 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	W	63/69 (91%)	57 (90%)	6 (10%)	0	100	100
31	X	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
32	Y	66/125 (53%)	48 (73%)	16 (24%)	2 (3%)	3	14
33	Z	46/57 (81%)	39 (85%)	7 (15%)	0	100	100
35	b	222/232 (96%)	180 (81%)	39 (18%)	3 (1%)	9	30
36	c	200/217 (92%)	169 (84%)	30 (15%)	1 (0%)	24	54
37	d	197/200 (98%)	157 (80%)	40 (20%)	0	100	100
38	e	154/166 (93%)	134 (87%)	19 (12%)	1 (1%)	21	51
39	f	93/98 (95%)	64 (69%)	29 (31%)	0	100	100
40	g	153/156 (98%)	125 (82%)	28 (18%)	0	100	100
41	h	129/132 (98%)	115 (89%)	14 (11%)	0	100	100
42	i	125/130 (96%)	109 (87%)	16 (13%)	0	100	100
43	j	95/102 (93%)	80 (84%)	15 (16%)	0	100	100
44	k	112/129 (87%)	82 (73%)	30 (27%)	0	100	100
45	l	133/149 (89%)	104 (78%)	27 (20%)	2 (2%)	8	28
46	m	114/121 (94%)	95 (83%)	19 (17%)	0	100	100
47	n	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	26
48	o	85/89 (96%)	72 (85%)	13 (15%)	0	100	100
49	p	85/91 (93%)	68 (80%)	16 (19%)	1 (1%)	10	34
50	q	78/87 (90%)	57 (73%)	19 (24%)	2 (3%)	4	17
51	r	62/80 (78%)	57 (92%)	5 (8%)	0	100	100
52	s	80/108 (74%)	65 (81%)	14 (18%)	1 (1%)	9	32
53	t	79/83 (95%)	64 (81%)	12 (15%)	3 (4%)	2	10
All	All	5825/6385 (91%)	5019 (86%)	784 (14%)	22 (0%)	31	59

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	6	156	GLN
36	c	155	ARG
49	p	87	GLN
32	Y	44	PRO
38	e	101	PRO

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	1	45/47 (96%)	45 (100%)	0	100	100
2	2	39/40 (98%)	39 (100%)	0	100	100
3	3	55/57 (96%)	54 (98%)	1 (2%)	51	80
4	4	35/35 (100%)	35 (100%)	0	100	100
6	6	473/524 (90%)	472 (100%)	1 (0%)	87	96
10	C	221/223 (99%)	221 (100%)	0	100	100
11	D	173/177 (98%)	172 (99%)	1 (1%)	78	93
12	E	168/169 (99%)	167 (99%)	1 (1%)	78	93
14	G	96/155 (62%)	96 (100%)	0	100	100
15	H	123/123 (100%)	122 (99%)	1 (1%)	73	90
16	I	100/100 (100%)	99 (99%)	1 (1%)	68	89
17	J	112/112 (100%)	111 (99%)	1 (1%)	70	90
18	K	114/119 (96%)	110 (96%)	4 (4%)	32	66
19	L	101/102 (99%)	100 (99%)	1 (1%)	68	89
20	M	94/95 (99%)	94 (100%)	0	100	100
21	N	100/102 (98%)	100 (100%)	0	100	100
22	O	96/98 (98%)	96 (100%)	0	100	100
23	P	86/86 (100%)	85 (99%)	1 (1%)	63	86
24	Q	91/94 (97%)	91 (100%)	0	100	100
25	R	80/82 (98%)	79 (99%)	1 (1%)	61	86
26	S	75/90 (83%)	75 (100%)	0	100	100
27	T	82/192 (43%)	79 (96%)	3 (4%)	30	64
28	U	60/75 (80%)	60 (100%)	0	100	100
29	V	49/52 (94%)	49 (100%)	0	100	100
30	W	59/62 (95%)	59 (100%)	0	100	100
31	X	52/53 (98%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y	10/114 (9%)	9 (90%)	1 (10%)	7	24
33	Z	44/52 (85%)	43 (98%)	1 (2%)	44	76
35	b	194/201 (96%)	186 (96%)	8 (4%)	27	61
36	c	164/175 (94%)	163 (99%)	1 (1%)	78	93
37	d	174/175 (99%)	171 (98%)	3 (2%)	53	82
38	e	122/131 (93%)	118 (97%)	4 (3%)	33	67
39	f	83/86 (96%)	83 (100%)	0	100	100
40	g	131/132 (99%)	128 (98%)	3 (2%)	44	76
41	h	112/113 (99%)	111 (99%)	1 (1%)	70	90
42	i	105/107 (98%)	104 (99%)	1 (1%)	68	89
43	j	87/91 (96%)	86 (99%)	1 (1%)	65	88
44	k	90/104 (86%)	90 (100%)	0	100	100
45	l	117/130 (90%)	116 (99%)	1 (1%)	70	90
46	m	100/104 (96%)	100 (100%)	0	100	100
47	n	52/53 (98%)	51 (98%)	1 (2%)	50	79
48	o	79/81 (98%)	79 (100%)	0	100	100
49	p	74/77 (96%)	74 (100%)	0	100	100
50	q	75/82 (92%)	75 (100%)	0	100	100
51	r	57/68 (84%)	57 (100%)	0	100	100
52	s	71/91 (78%)	71 (100%)	0	100	100
53	t	67/69 (97%)	66 (98%)	1 (2%)	57	84
All	All	4787/5300 (90%)	4743 (99%)	44 (1%)	68	90

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	d	27	GLU
40	g	49	LEU
37	d	29	ARG
38	e	38	VAL
40	g	80	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
36	c	175	HIS
45	l	39	ASN
37	d	118	HIS
40	g	106	ASN
45	l	125	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1470/1548 (94%)	593 (40%)	0
5	5	72/73 (98%)	14 (19%)	0
7	7	2/3 (66%)	0	0
8	A	2648/2921 (90%)	673 (25%)	44 (1%)
9	B	112/115 (97%)	17 (15%)	1 (0%)
All	All	4304/4660 (92%)	1297 (30%)	45 (1%)

5 of 1297 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	5	4	G
5	5	6	G
5	5	9	G
5	5	14	A
5	5	16	U

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1178	C
8	A	1519	U
8	A	1186	A
8	A	1383	G
8	A	1605	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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
55	ATP	6	602	56	32,33,33	1.29	5 (15%)	48,52,52	1.76	11 (22%)
55	ATP	6	601	56	32,33,33	1.26	4 (12%)	48,52,52	1.87	11 (22%)

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
55	ATP	6	602	56	-	0/22/38/38	0/3/3/3
55	ATP	6	601	56	-	5/22/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	6	602	ATP	C5-C4	4.20	1.46	1.39
55	6	601	ATP	C5-C4	3.97	1.46	1.39
55	6	602	ATP	C5-N7	-2.54	1.34	1.39
55	6	601	ATP	C5-C6	2.46	1.47	1.41
55	6	601	ATP	C8-N7	2.35	1.36	1.31

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	6	601	ATP	C5-C4-N3	-5.78	118.75	126.72
55	6	602	ATP	C5-C4-N3	-5.38	119.31	126.72
55	6	601	ATP	N3-C4-N9	4.55	134.90	127.17
55	6	602	ATP	N3-C4-N9	4.41	134.66	127.17
55	6	601	ATP	C2-N3-C4	3.94	121.44	111.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	6	601	ATP	C5'-O5'-PA-O1A
55	6	601	ATP	C5'-O5'-PA-O3A
55	6	601	ATP	PG-O3B-PB-O2B
55	6	601	ATP	O4'-C4'-C5'-O5'
55	6	601	ATP	PA-O3A-PB-O1B

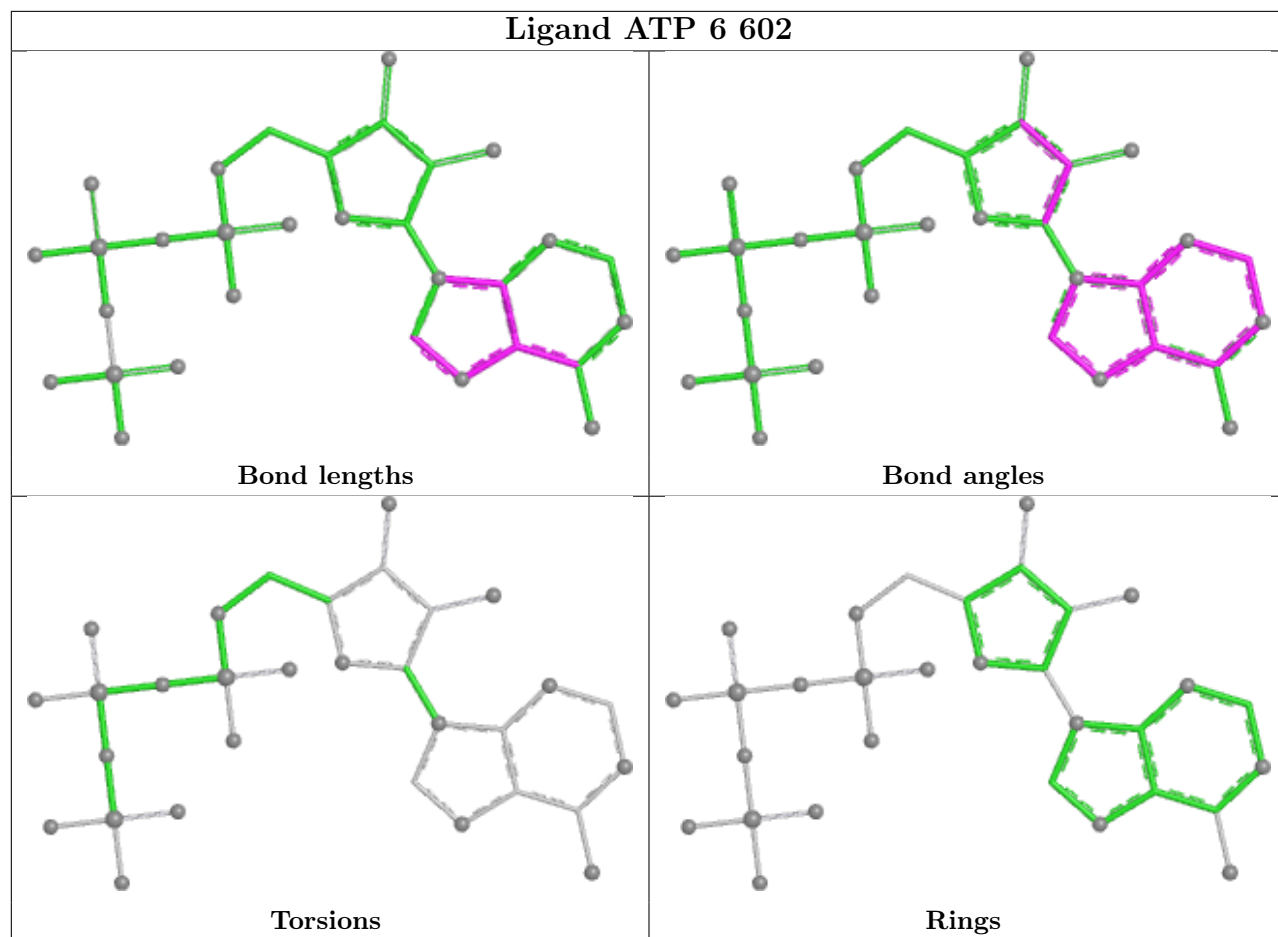
There are no ring outliers.

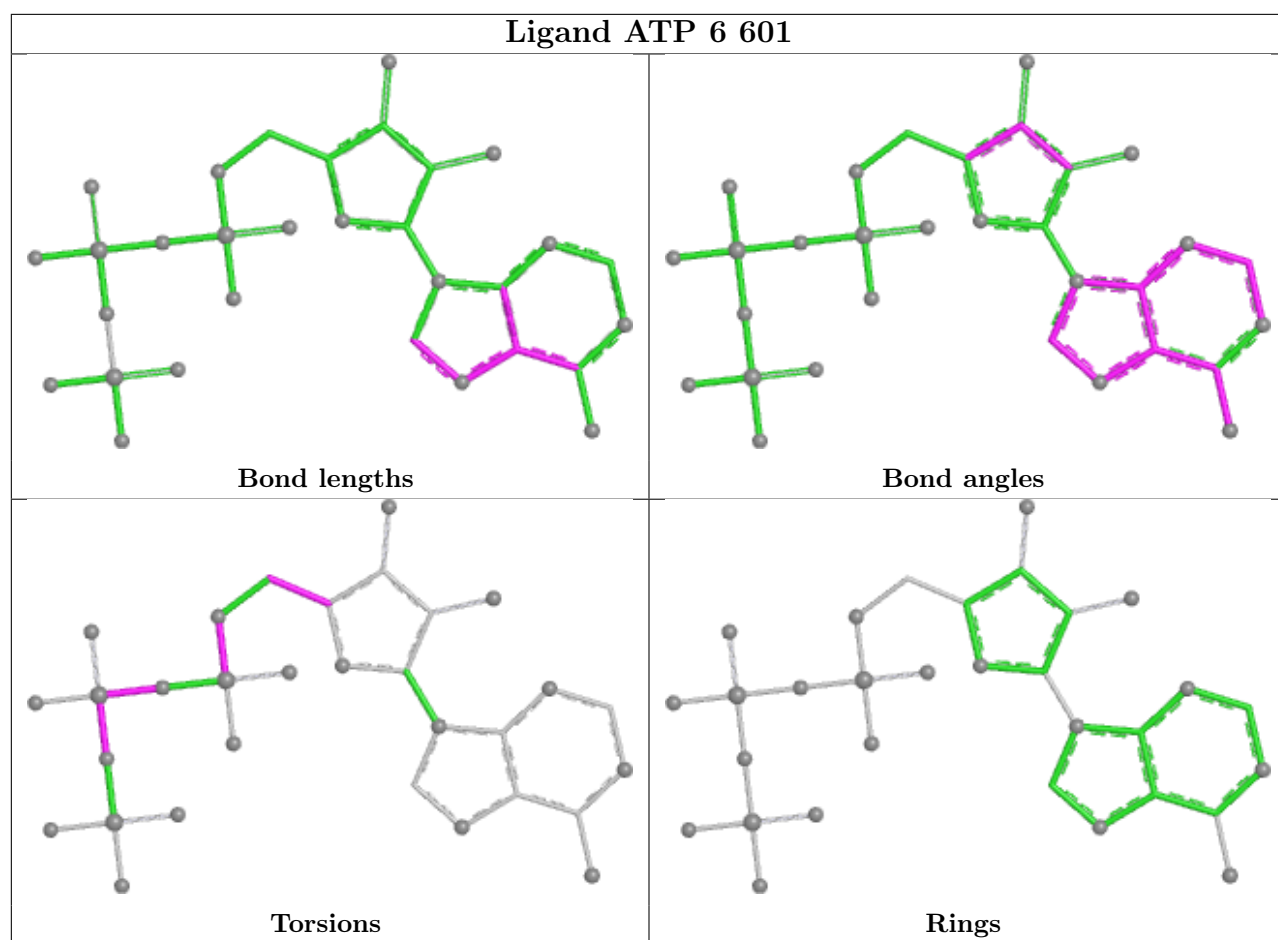
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	6	602	ATP	1	0
55	6	601	ATP	2	0

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.

Ligand ATP 6 602





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.

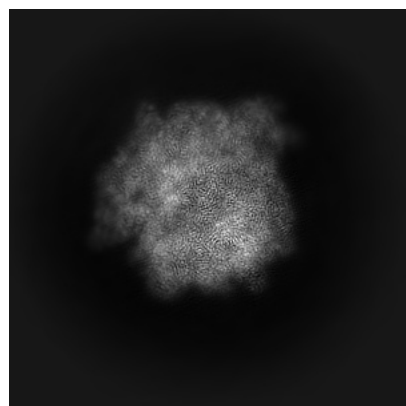
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13191. These allow visual inspection of the internal detail of the map and identification of artifacts.

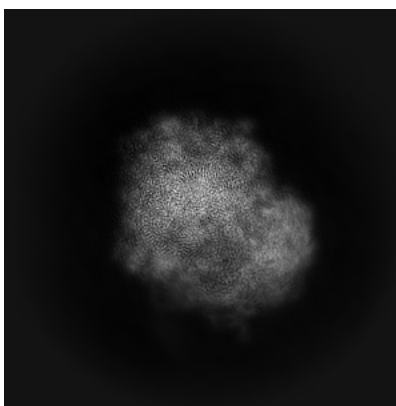
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

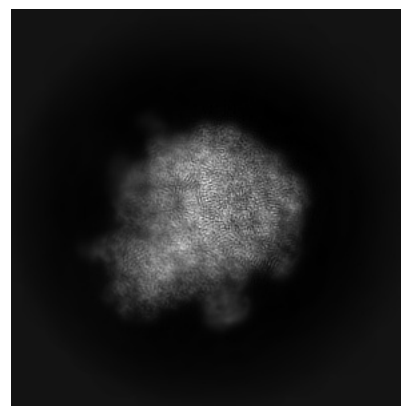
6.1.1 Primary map



X

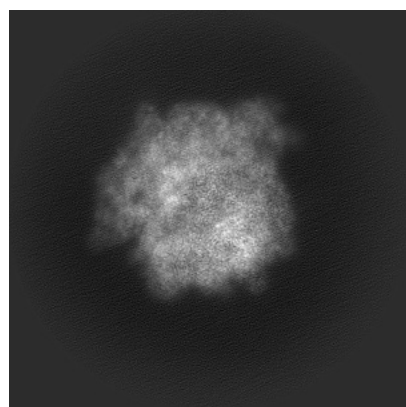


Y

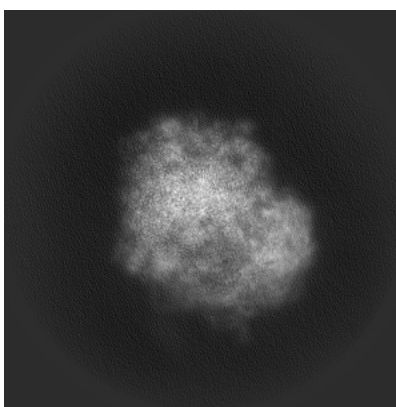


Z

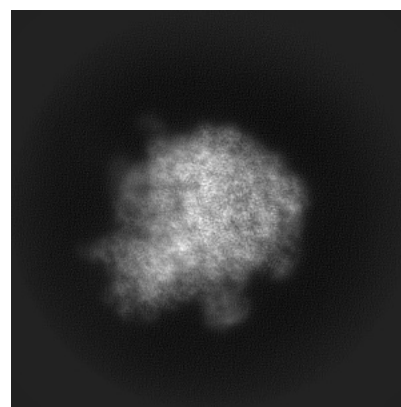
6.1.2 Raw map



X



Y

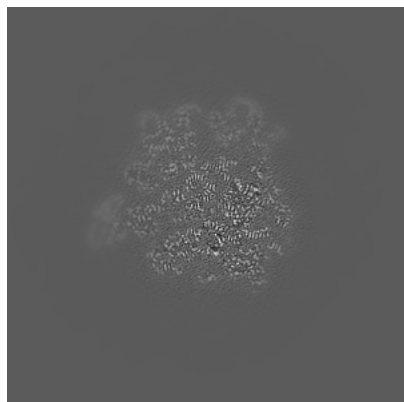


Z

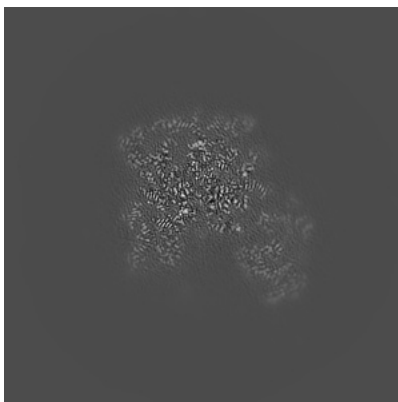
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

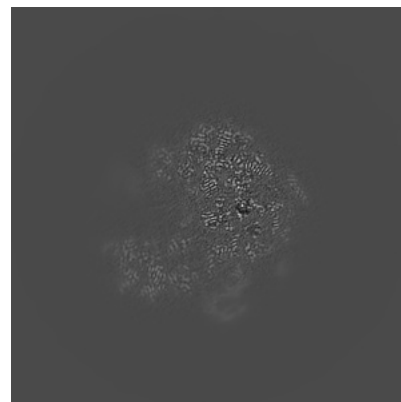
6.2.1 Primary map



X Index: 208

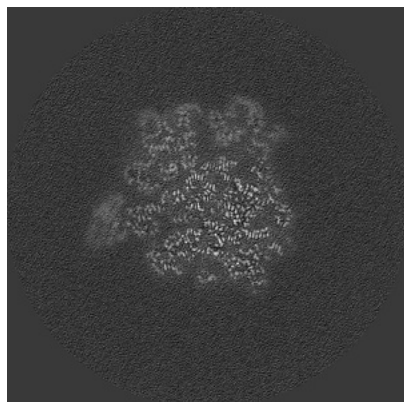


Y Index: 208

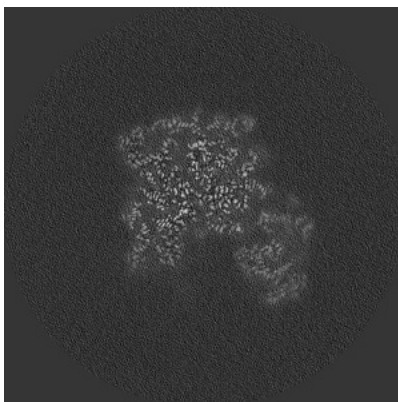


Z Index: 208

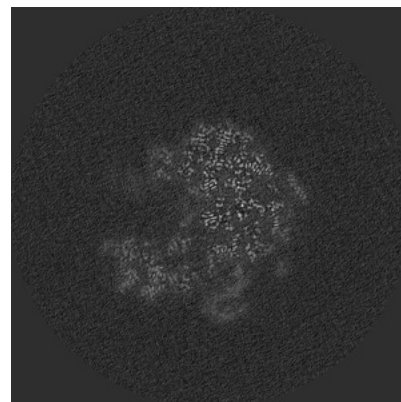
6.2.2 Raw map



X Index: 208



Y Index: 208

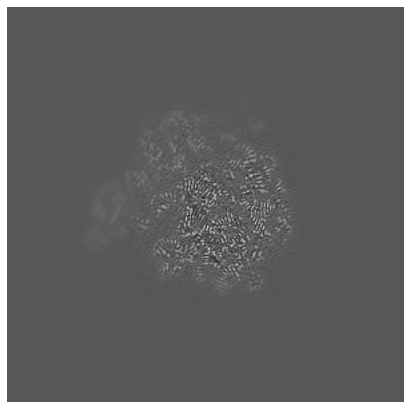


Z Index: 208

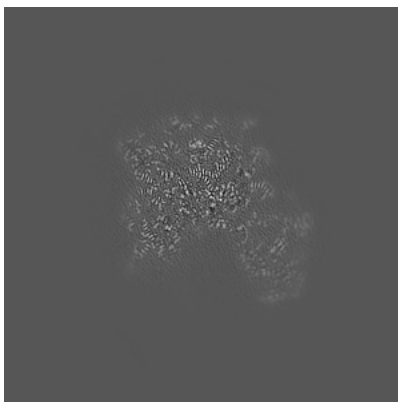
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

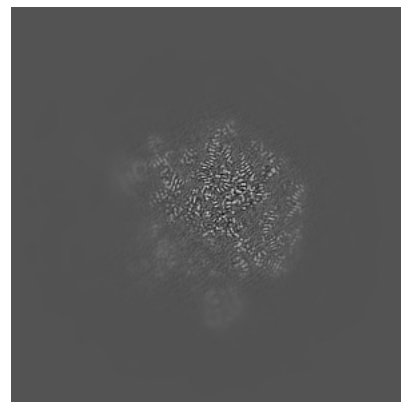
6.3.1 Primary map



X Index: 219

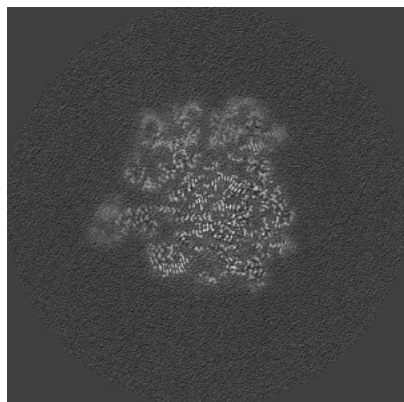


Y Index: 204

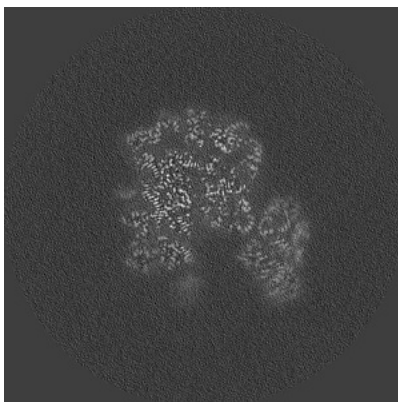


Z Index: 177

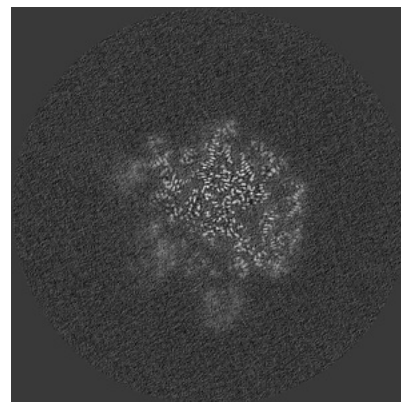
6.3.2 Raw map



X Index: 204



Y Index: 218

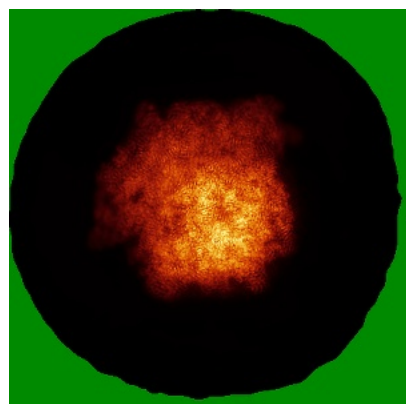


Z Index: 177

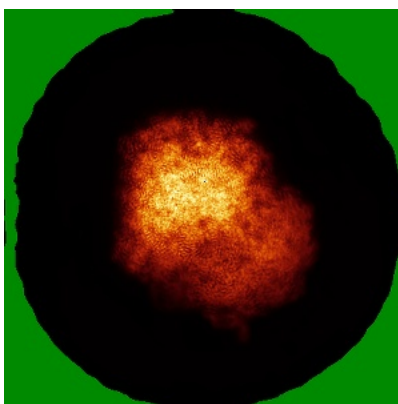
The images above show the largest variance slices of the map in three orthogonal directions.

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

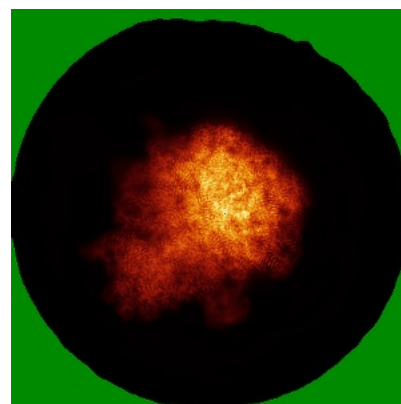
6.4.1 Primary map



X

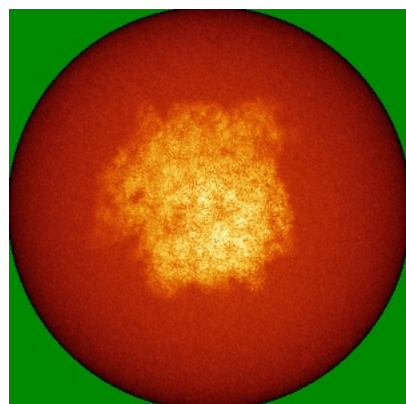


Y

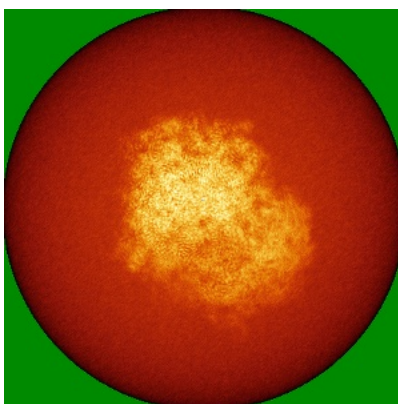


Z

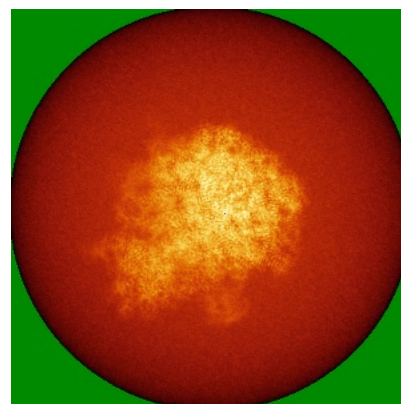
6.4.2 Raw map



X



Y

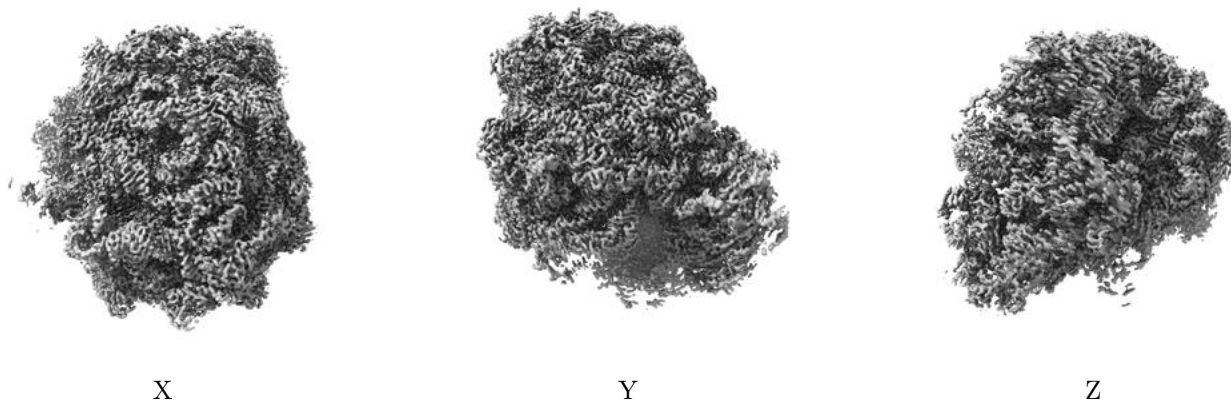


Z

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.

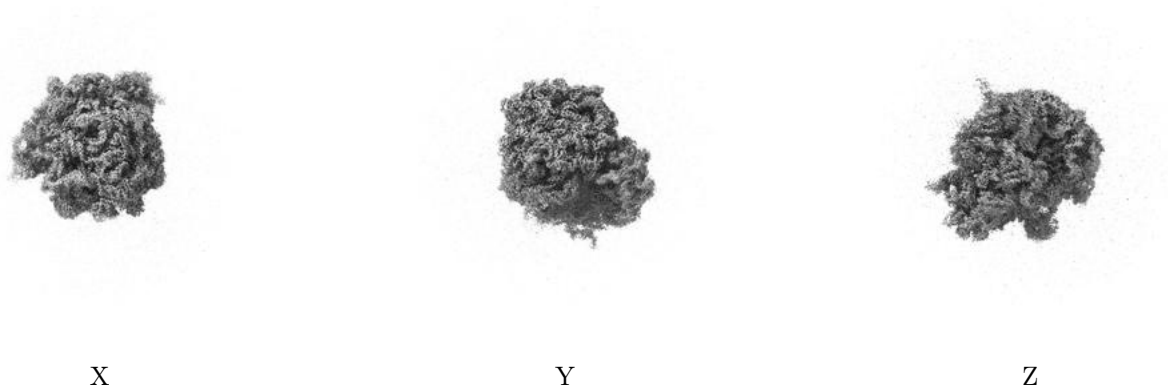
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. 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.

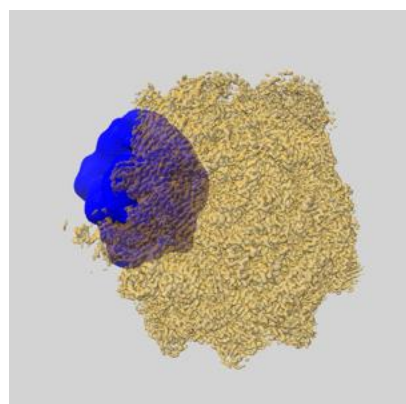
6.6 Mask visualisation [i](#)

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

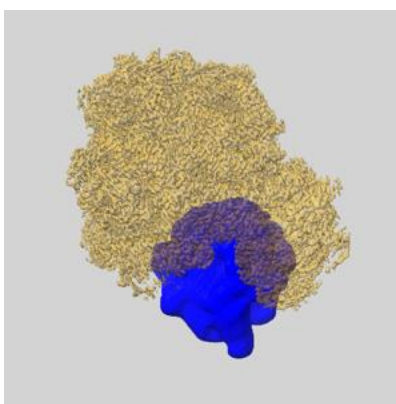
A mask typically either:

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

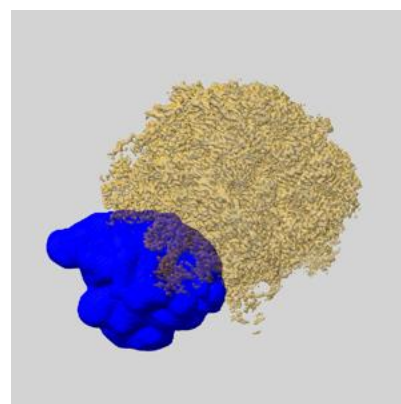
6.6.1 emd_13191_msk_1.map [i](#)



X

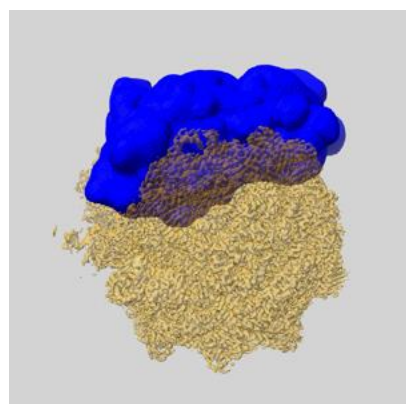


Y

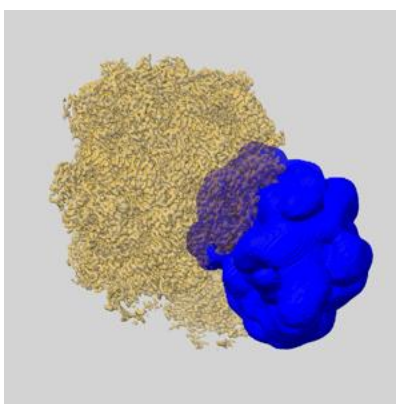


Z

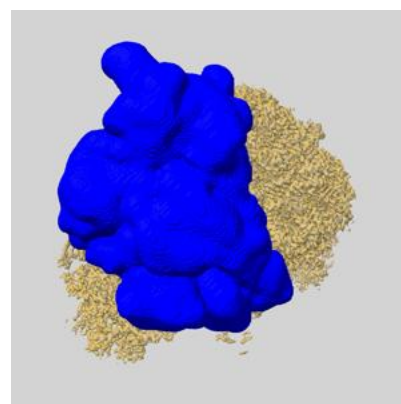
6.6.2 emd_13191_msk_2.map [i](#)



X



Y

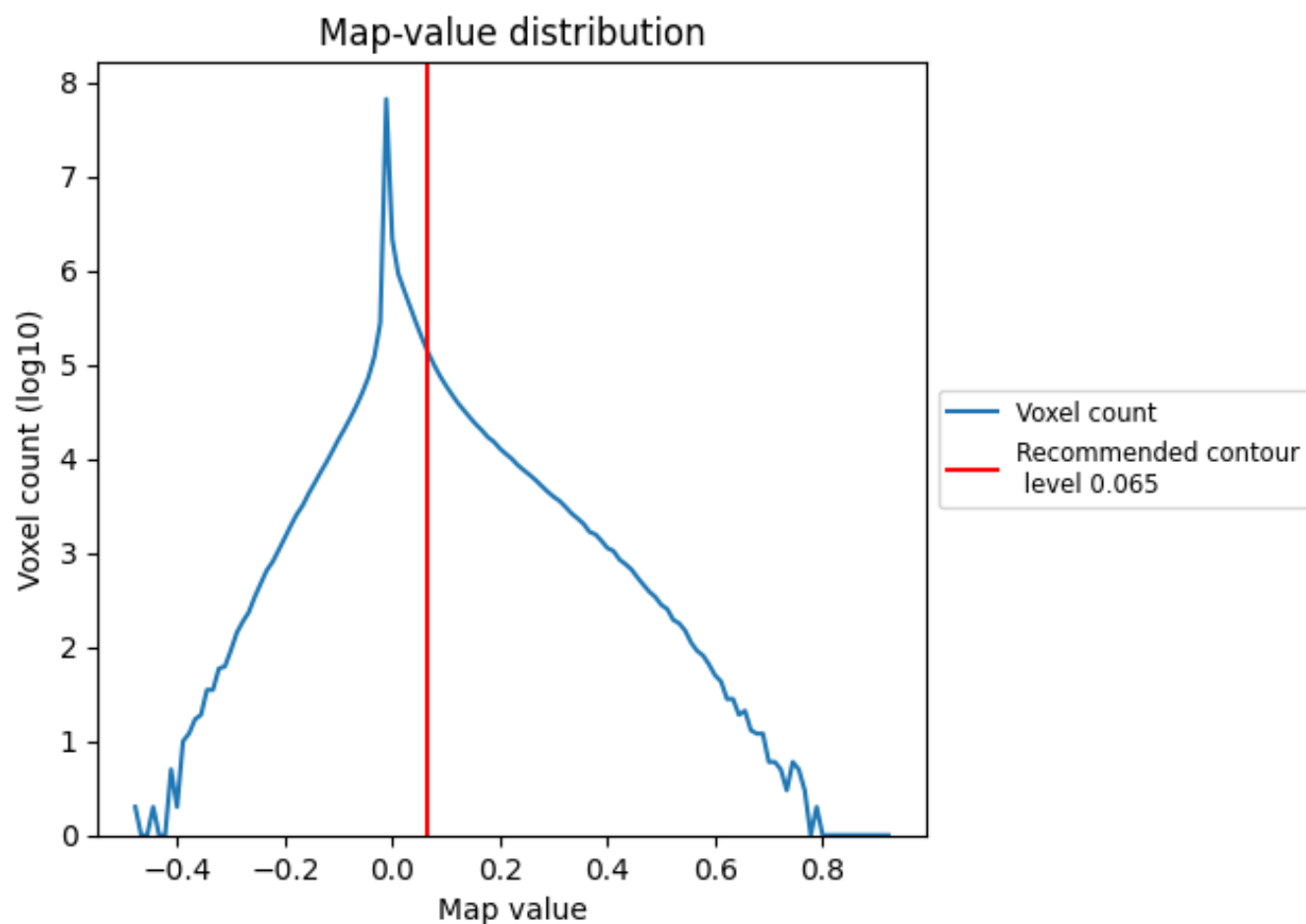


Z

7 Map analysis [i](#)

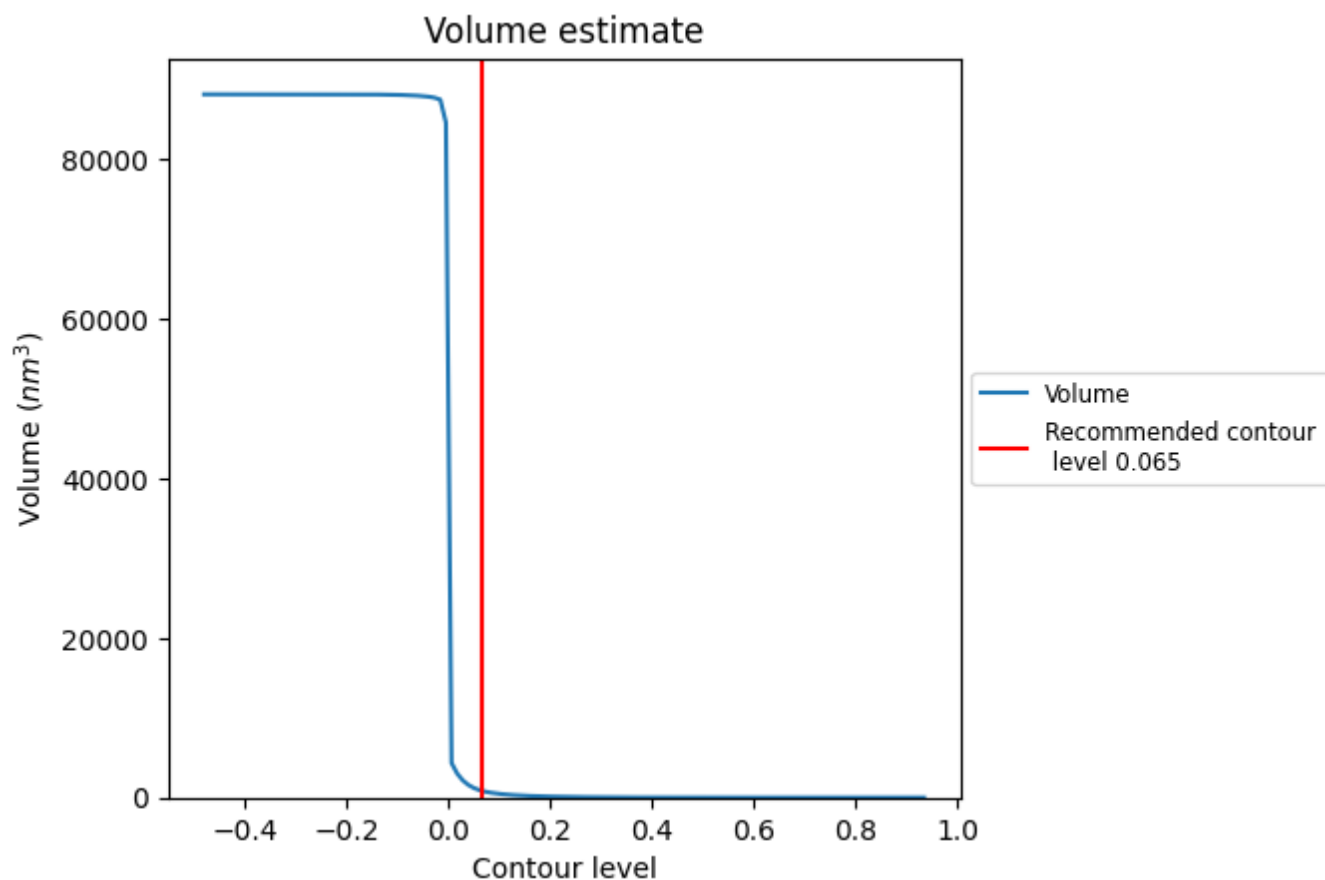
This section contains the results of statistical analysis of the map.

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.

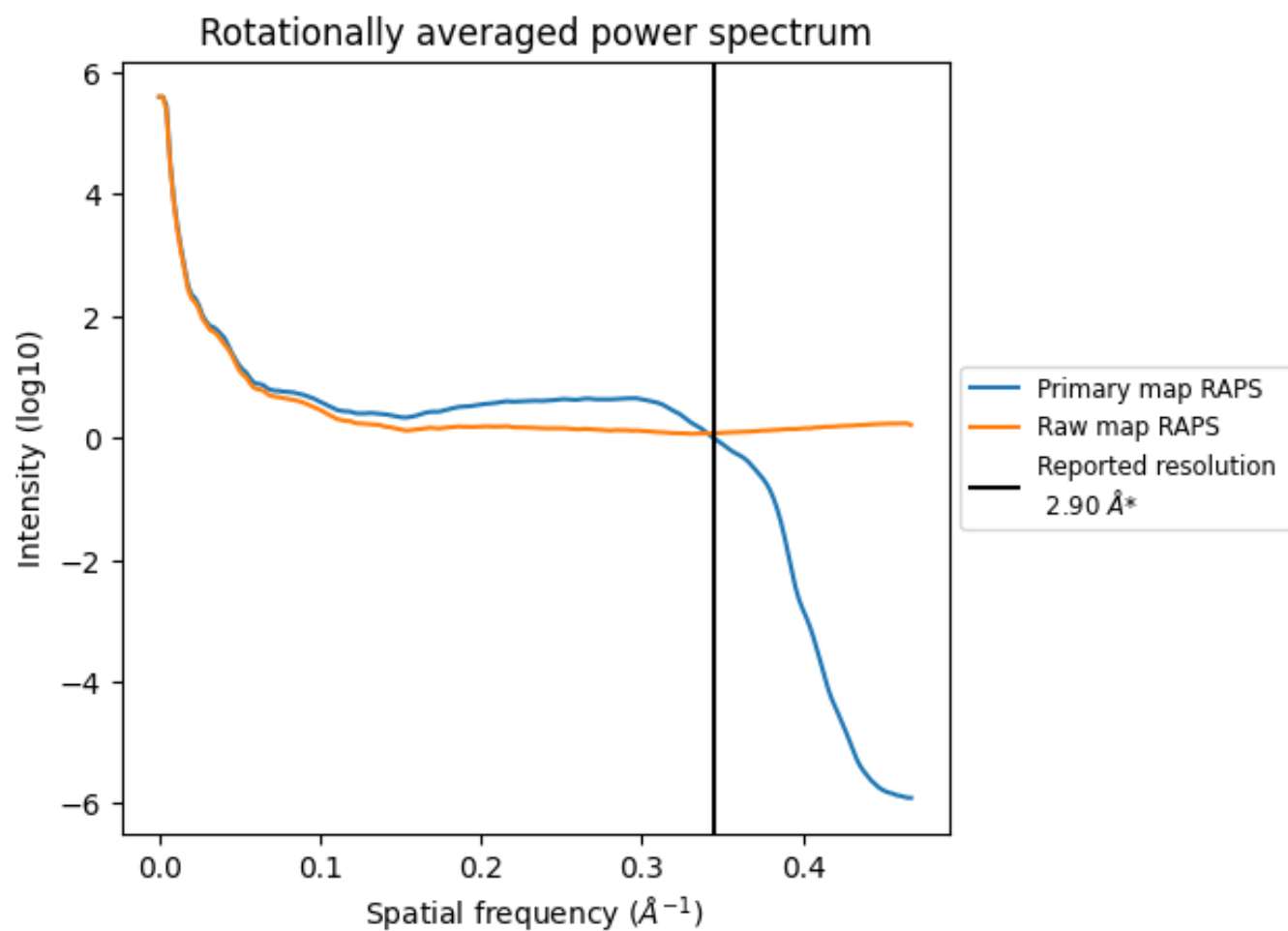
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 884 nm³; this corresponds to an approximate mass of 799 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 ⓘ

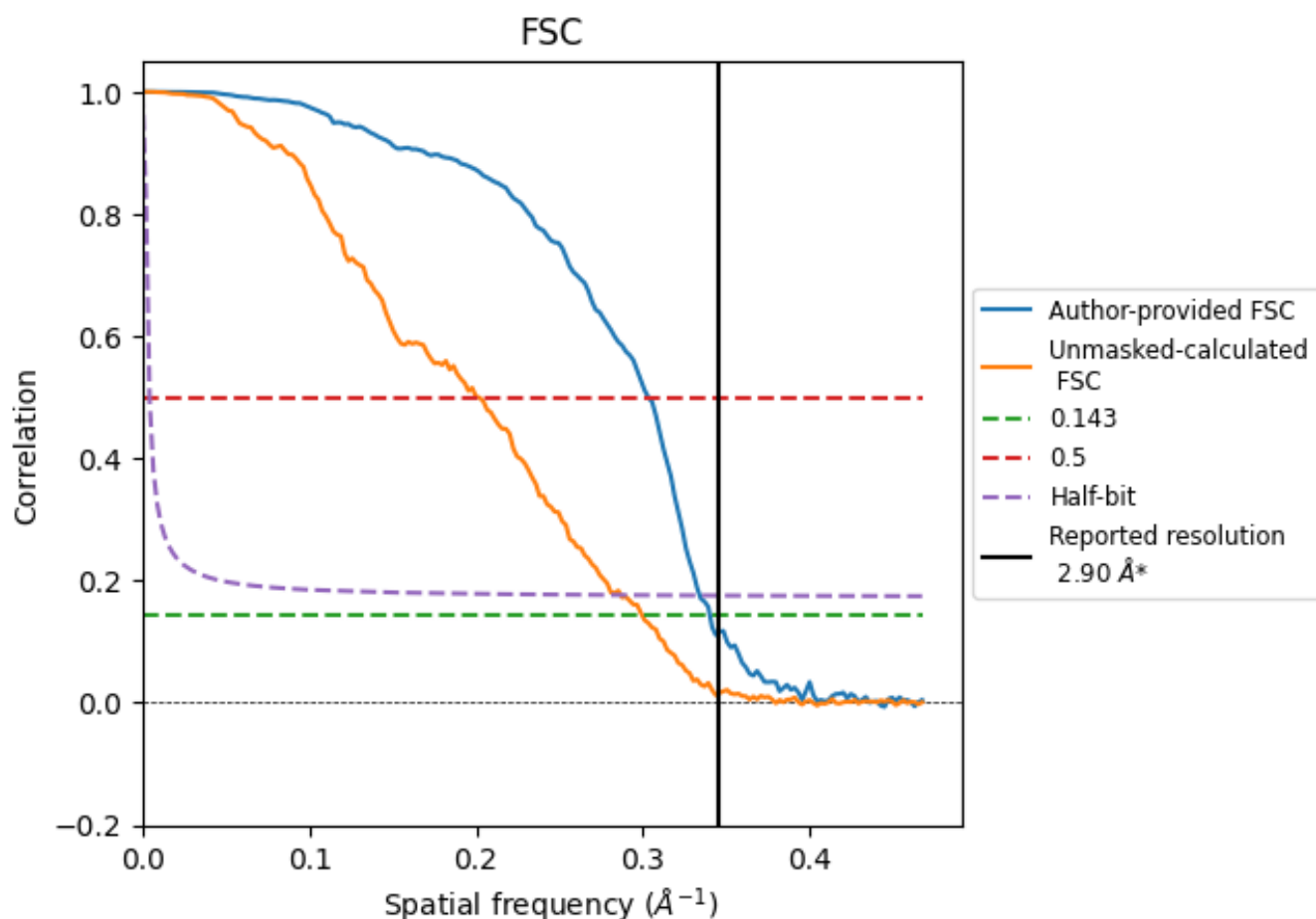


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

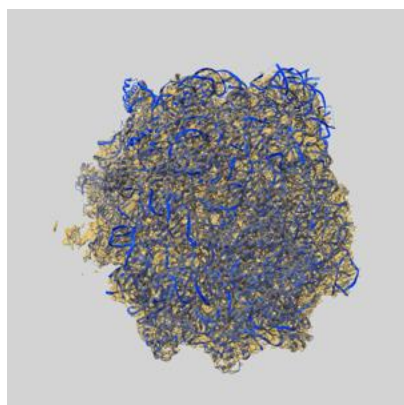
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.30	2.99
Unmasked-calculated*	3.34	4.97	3.49

*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 3.34 differs from the reported value 2.9 by more than 10 %

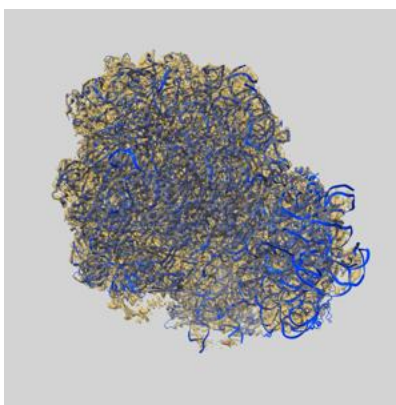
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13191 and PDB model 7P48. Per-residue inclusion information can be found in section 3 on page 15.

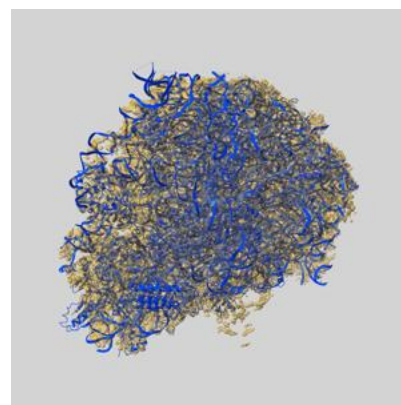
9.1 Map-model overlay [i](#)



X



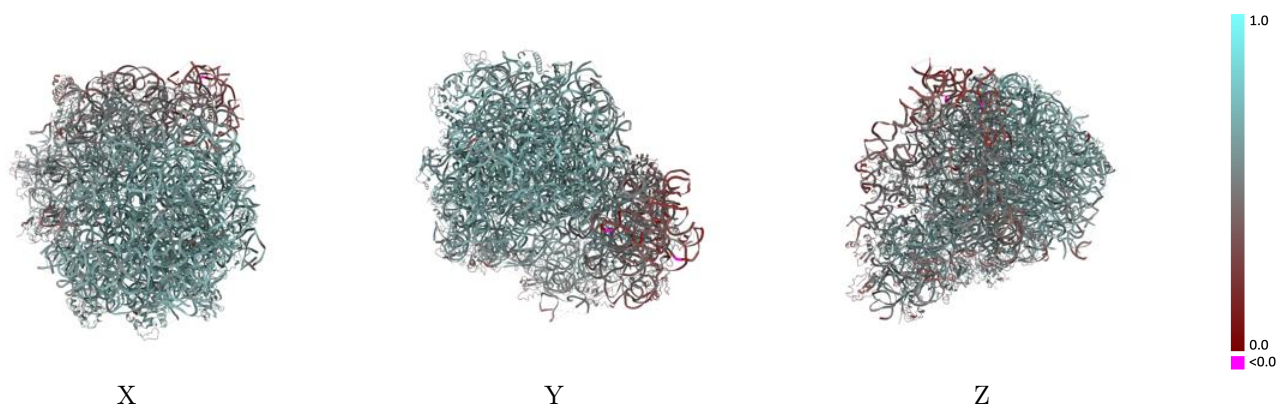
Y



Z

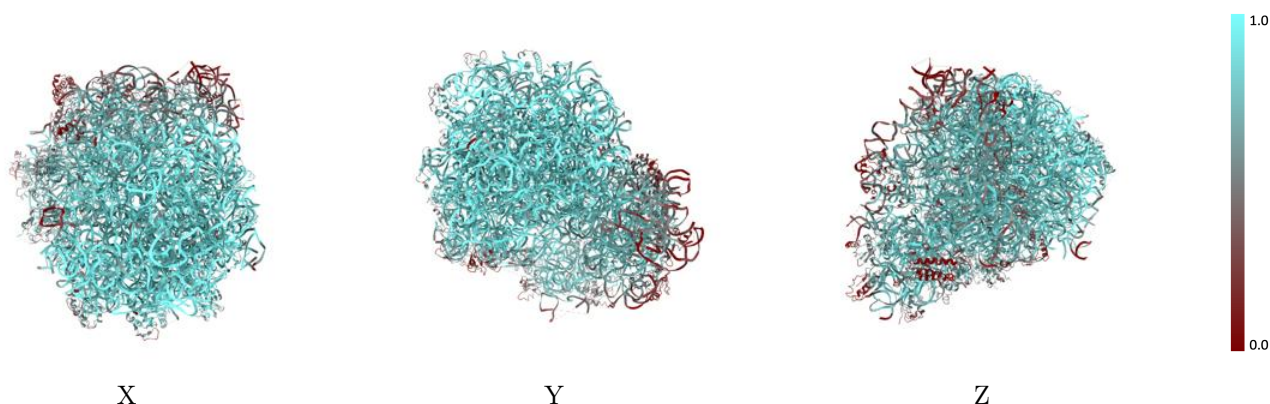
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



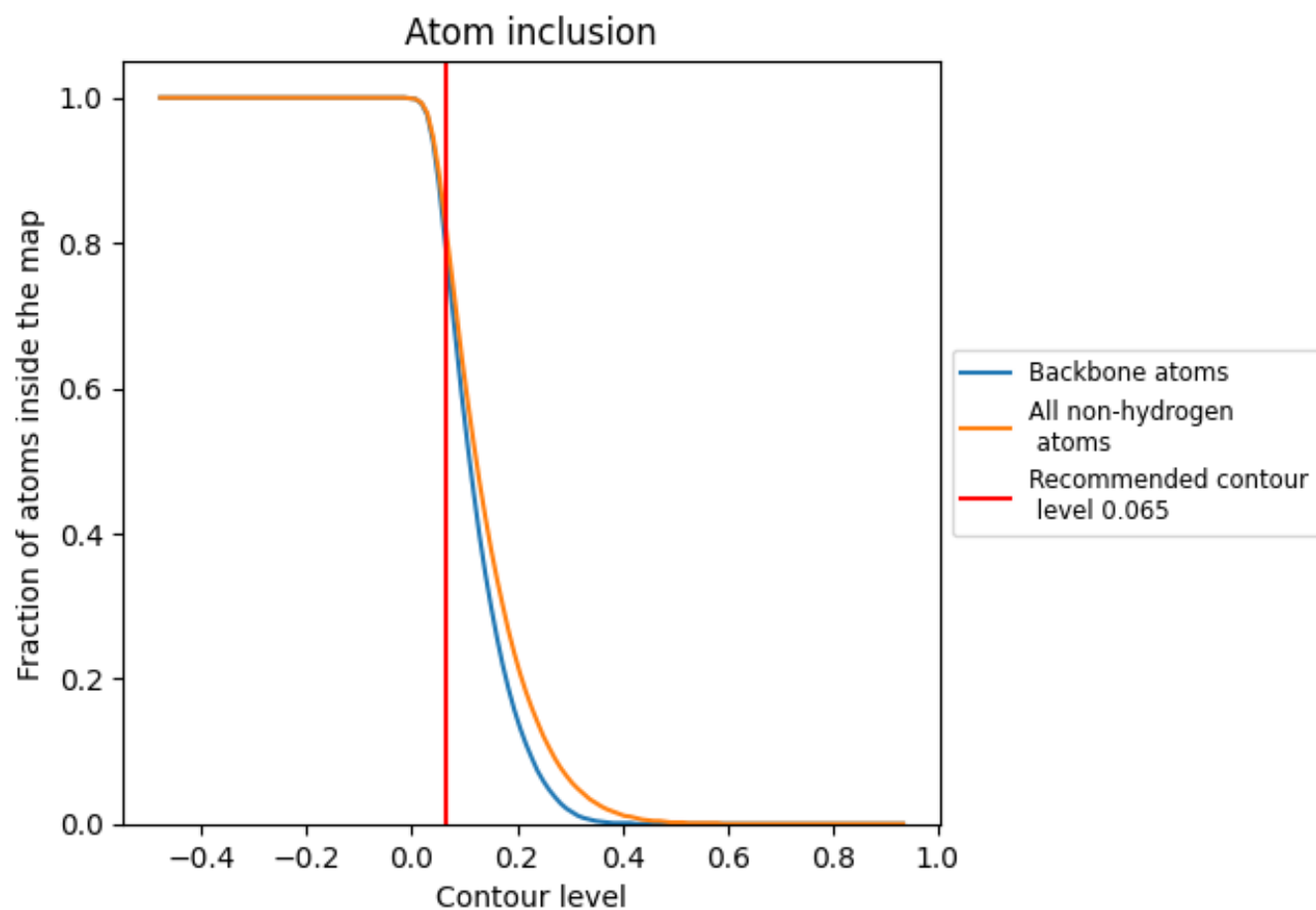
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 82% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5660
1	 0.8340	 0.5770
2	 0.9680	 0.6590
3	 0.9720	 0.6530
4	 0.9310	 0.6210
5	 0.8940	 0.5850
6	 0.7160	 0.5560
7	 1.0000	 0.6410
A	 0.9550	 0.6310
B	 0.8400	 0.5650
C	 0.9260	 0.6370
D	 0.8980	 0.6300
E	 0.7890	 0.5870
F	 0.4030	 0.4500
G	 0.5300	 0.5100
H	 0.9120	 0.6190
I	 0.9270	 0.6280
J	 0.8150	 0.5950
K	 0.8900	 0.6040
L	 0.8870	 0.6210
M	 0.6220	 0.5230
N	 0.8580	 0.6100
O	 0.9220	 0.6370
P	 0.7830	 0.5800
Q	 0.9140	 0.6370
R	 0.8360	 0.5850
S	 0.6750	 0.5470
T	 0.6370	 0.5440
U	 0.9090	 0.6050
V	 0.8690	 0.6030
W	 0.7360	 0.5620
X	 0.8710	 0.5970
Y	 0.1090	 0.3180
Z	 0.9270	 0.6330
a	 0.7660	 0.4840



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.2580	 0.4340
c	 0.5960	 0.4840
d	 0.3810	 0.4380
e	 0.7020	 0.5230
f	 0.2810	 0.4340
g	 0.6650	 0.4980
h	 0.5470	 0.5010
i	 0.6090	 0.4890
j	 0.4600	 0.4220
k	 0.6820	 0.5270
l	 0.7070	 0.5200
m	 0.5300	 0.4340
n	 0.7900	 0.5200
o	 0.5260	 0.4850
p	 0.4410	 0.4200
q	 0.5080	 0.4690
r	 0.5310	 0.5040
s	 0.5060	 0.4610
t	 0.4740	 0.4360