



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 04:31 AM UTC

PDB ID : 8S8J / pdb_00008s8j
EMDB ID : EMD-19807
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation (model py48S-AUC-eIF5)
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-03-06
Resolution : 4.70 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:

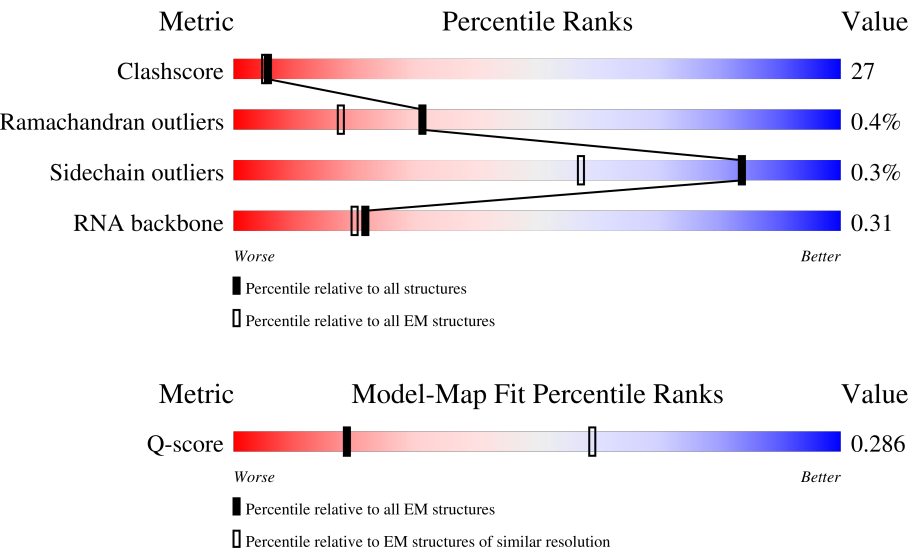
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

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	2	1798	
2	A	254	
3	B	255	

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Mol	Chain	Length	Quality of chain
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q	143	
27	R	136	
28	S	146	

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Mol	Chain	Length	Quality of chain
29	T	144	
30	U	117	
31	Z	108	
32	c	67	
33	d	56	
34	f	150	
35	g	326	
36	i	153	
37	3	49	
38	1	75	
39	j	304	
40	k	527	
41	l	285	
42	m	405	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 87114 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1798	Total	C	N	O	P	0	0
			38190	17073	6722	12597	1798		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	219	Total	C	N	O	S	0	0
			1702	1085	299	316	2		

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	225	Total	C	N	O	S	0	0
			1796	1135	330	328	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	220	Total	C	N	O	S	0	0
			1648	1053	291	300	4		

- Molecule 5 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 6 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	230	Total	C	N	O	S	0	0
			1832	1146	352	330	4		

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 9 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 10 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 11 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	151	Total	C	N	O	S	0	0
			1195	761	224	207	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	129	Total	C	N	O	S	0	0
			955	585	191	176	3		

- Molecule 13 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 15 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 16 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	134	Total	C	N	O	S	0	0
			1061	665	207	189			

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	102	Total	C	N	O	S	0	0
			797	492	168	132	5		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	81	Total	C	N	O	S	0	0
			609	379	112	113	5		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	60	Total	C	N	O	S	0	0
			472	295	96	80	1		

- Molecule 20 is a protein called 40S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	227	Total	C	N	O	S	0	0
			1774	1126	320	323	5		

- Molecule 22 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 23 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	117	Total	C	N	O		0	0
			885	553	161	171			

- Molecule 25 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	117	Total	C	N	O	S	0	0
			923	592	165	161	5		

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	141	Total	C	N	O		0	0
			1105	709	204	192			

- Molecule 27 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	130	Total	C	N	O	S	0	0
			1033	643	194	193	3		

- Molecule 28 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	145	Total	C	N	O	S	0	0
			1189	739	239	209	2		

- Molecule 29 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	143	Total	C	N	O		0	0
			1110	693	210	207			

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	78	Total	C	N	O	S	0	0
			594	376	111	106	1		

- Molecule 32 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	64	Total	C	N	O	S	0	0
			499	308	99	91	1		

- Molecule 33 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	55	Total	C	N	O	S	0	0
			461	289	93	78	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	74	Total	C	N	O	S	0	0
			584	374	111	95	4		

- Molecule 35 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	320	Total	C	N	O	S	0	0
			2469	1561	432	471	5		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	95	Total	C	N	O	S	0	0
			764	474	142	143	5		

- Molecule 37 is a RNA chain called mRNA (5'-R(P*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	26	Total	C	N	O	P	0	0
			536	242	84	184	26		

- Molecule 38 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	267	Total	C	N	O	S	0	0
			2139	1366	355	407	11		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	470	Total	C	N	O	S	0	0
			3596	2279	633	666	18		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	l	23	Total	C	N	O	0	0
			190	124	32	34		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	143	Total	C	N	O	S	0	0
			1113	710	193	203	7		

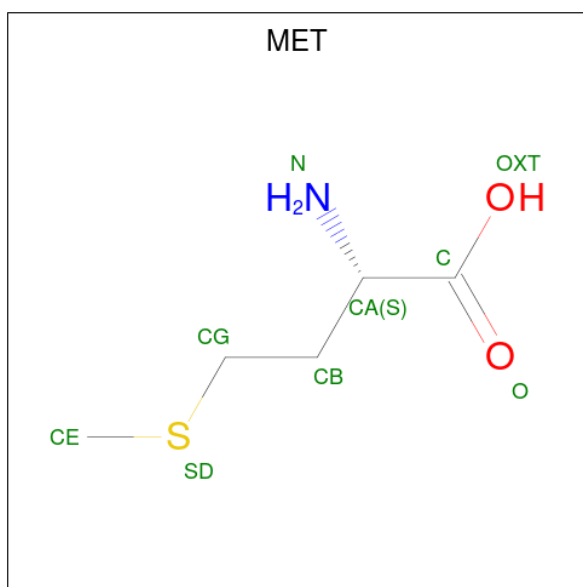
- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
43	2	111	Total	Mg	0
			111	111	
43	Q	1	Total	Mg	0
			1	1	
43	i	1	Total	Mg	0
			1	1	
43	3	1	Total	Mg	0
			1	1	
43	k	1	Total	Mg	0
			1	1	

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

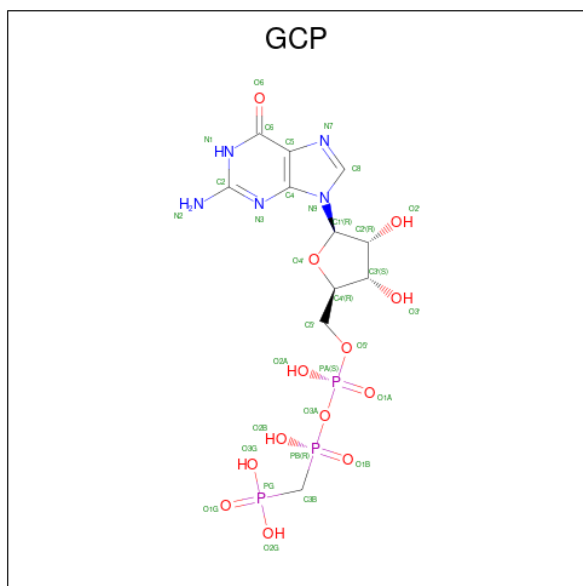
Mol	Chain	Residues	Atoms		AltConf
44	a	1	Total	Zn	0
			1	1	
44	b	1	Total	Zn	0
			1	1	
44	f	1	Total	Zn	0
			1	1	
44	m	1	Total	Zn	0
			1	1	

- Molecule 45 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
45	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 46 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
46	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

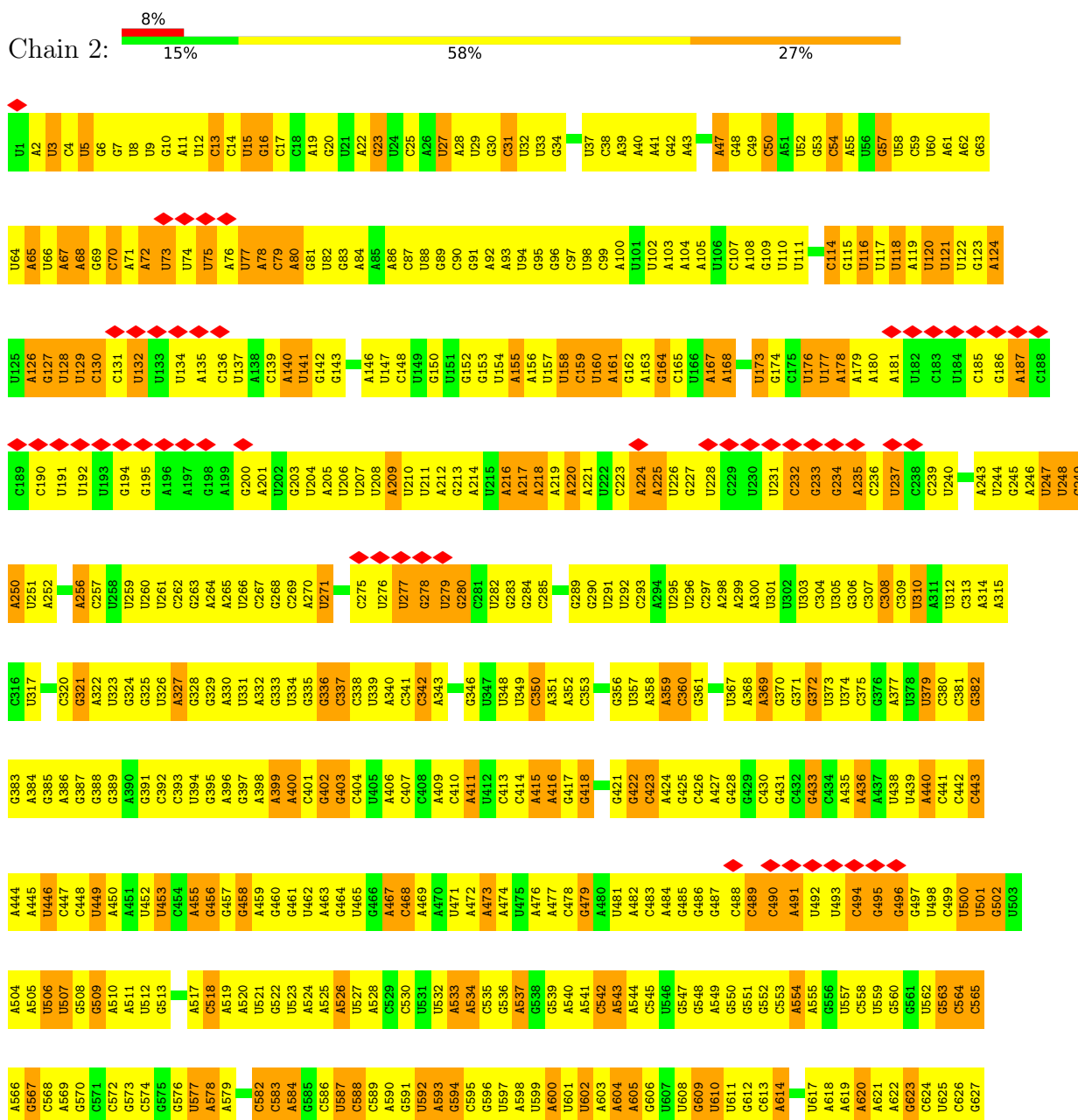
- Molecule 47 is water.

Mol	Chain	Residues	Atoms		AltConf
47	2	3	Total 3	O 3	0

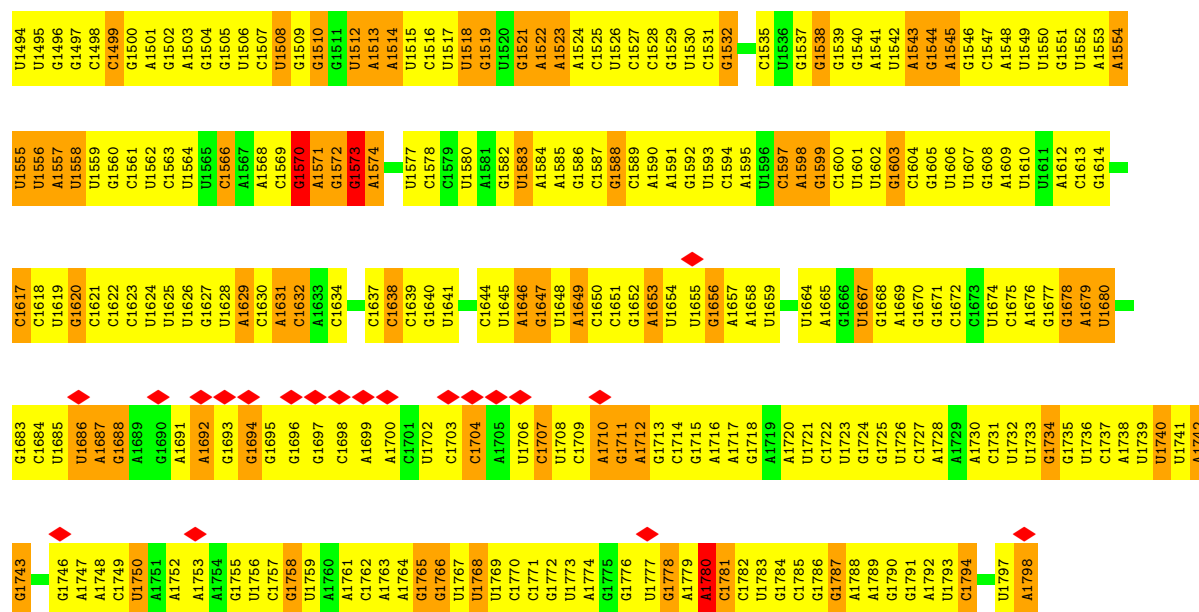
3 Residue-property plots

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.

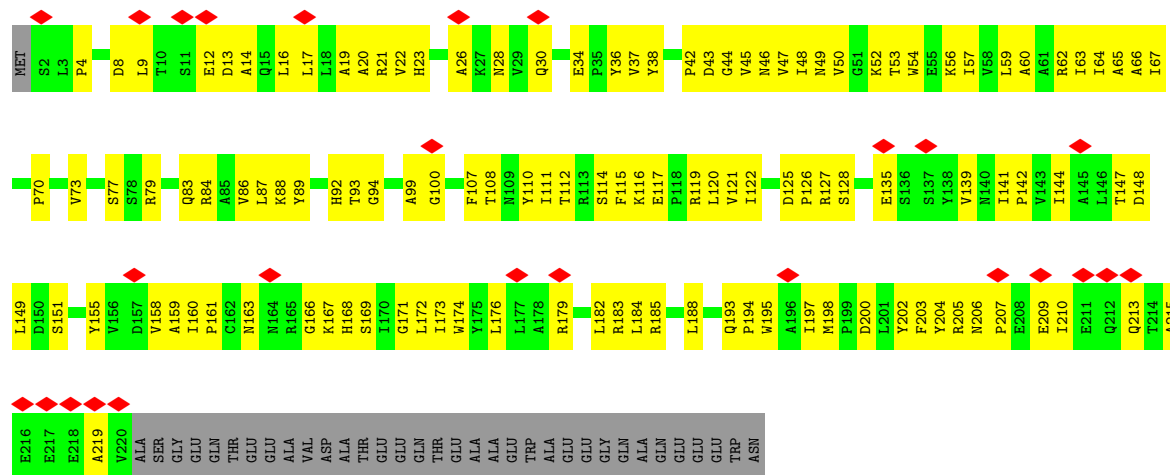
• Molecule 1: 18S ribosomal RNA



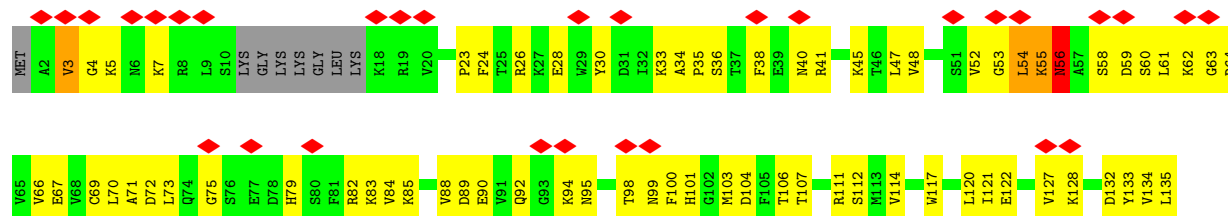
G1433	G1372	G1242	U1181	G1120	U1057	A992	U931	G871	A810	U749	G689	U628
A1434	U1373	A1243	A1182	G1121	C1058	G993	A932	U872	A811	U750	A690	
U1435		G1244	A1183	C1122		G996	C933	C873	A812	G751	U691	U631
G1436	U1376	C1245	U1184	A1123	U1059		U934	G874	A813	A752	C692	U632
C1437	U1377	U1246	U1185	A1124	A1060	U998	G935	G875	G814	A753	U693	G633
C1438	U1378	G1247	U1186	G1125	A1061	U998	C936	G876	G815	A754	U694	A634
C1439	U1379	U1248	G1187	G1126	U1062	C999	G937	G877	A816	A755	U695	A635
U1440	A1380	U1249	A1188	C1127	U1063	A1000	A938	G878	C817	A756	C696	C636
G1381	U1381	U1250	C1189	G1128	G1063	G1001	A939	C879	C818	A757	U697	C637
G1382	A1382	C1251	B8N1190	G1129	A1064		A940	U880	U819	U758	U698	U638
G1383	U1383	U1252		A1130		C1006	G941	U881	U820	U759	U699	G640
A1444	G1384	G1253	A1193	A1131	C1069	G1007	A942	C882	U821	A760	C700	G641
C1445	C1385	G1254	C1194	A1132	U1070	U1008	A943	U883	G822	G761	U701	G642
	A1386	A1255	A1195	G1133	C1071	C1009	U944	G884	G823	A762	G702	
U1448	C1387	U1256	C1196	U1134	G1072	G1010	U945	U885	U824	G763	G703	U643
U1449	U1388	U1257	G1197	U1135		G1011	U946	A886	U825	G764	G704	U644
U1450	U1390	U1258	A1198	A1136	A1075	A1012	G947	U887	C826	G765	U705	U645
G1451	U1391	G1260	G1200	A1137	G1076	G1013	C948	U888	U827	U766	A706	G646
G1452	C1392	U1261	A1201	A1138	C1077	U1014	C949	C889	A828	U767	A707	G647
G1453	G1393	U1262	U1202	G1139	U1078	C1015	A950	A890	U829	C768	A708	U648
C1454	A1394	G1263	A1203	G1140	U1079	U1016	A951	A891	U830	G769	C708	U649
C1455	U1394	A1141	A1080	A1141	U1017	G952	G952	U892	U831	A770	C709	G650
G1456	U1395	G1264	C1081	A1142	A1018	U1017	G953	U893	U832	A771	U710	C652
C1457	U1396	U1265	U1082	U1143	A1019	A954	A954	U894	G833	G772	C653	
C1397	C1397	G1266	G1083	U1144	C1020	C1020	C955	U895	U834	C773	G711	
A1458	A1398	U1267	G1084	G1145	C1021	C1021	G956	C966	U835	A774	G654	
C1459	A1399	U1268	A1085	G1146	A1022	A1022	U957	A897	U836	G775	G655	
G1460	G1400	C1269	A1086	A1147	U1023	U1023	U958	G898	G837	G776	A713	G656
C1461	G1401	G1270	A1209	G1148	A1024	A1024	U959	A899	U838	G777	C714	U657
C1462	C1402	U1271	U1211	G1149	A1025	A1025	U960	G900	U839	G778	U715	
C1463	G1403	G1272	G1212	A1150	C1089	C1027	C961	G901	U840	A779	C716	C658
G1464	G1404	C1273	U1213	A1151	A1090	U1028	A862	U902	C941	A780	C717	G659
C1465	U1405	C1274	C1214	G1152	U1091	U1028	U963	G903	U842	A781	U718	A660
U1466	U1406	U1275	A1215	C1155	A1092	A1029	U964	A904	A843	G782	U719	C661
A1467	G1407	G1276	A1216	C1156	U1093	U1030	U965	A905	G844	C783	C662	
A1469	A1408	G1277	G1217	C1157	U1094	G1031	U966	A906	G845	U784	U663	
C1470	A1409	C1278	C1218	C1158	C1095	C1032	U967	U907	A846	C785	U664	
U1471	U1410	C1279	C1219	C1159	U1096	C1033	C968	U908	C347	G786	U665	
G1472	U1411	G1280	A1220	A1160	U1097	G1034	A969	C909	U850	A787	G722	
A1473	U1412		C1221	C1161	U1098	A1035	A970	U910	C851	A788	G723	U666
G1474	G1413	C1283	A1222	G1162	G1100		A971	G912	C852	U789	G724	G667
G1475	G1414	U1284	U1223	G1163	G1101	A1038	G972	G913	U853	A790	U725	U668
G1476	A1415	U1285	A1224	G1164	U1102	G1039	A973	A914	A854	A792	C727	C669
A1477	G1416	U1286	A1225	A1165	U1103	G1040	C974	U915	U855	G794	G726	
G1478	G1417	G1287	A1226	A1166	G1104	G1041	G975	U917	U856	A795	G727	G670
C1479	C1418	U1288	G1227	G1167	C1104	U1043	A976	U917	A857	G796	A728	C671
C1480	A1419	U1289	G1228	G1168	U1105	U1043	A977	U919	A858	C797	G729	C672
A1481	A1420	C1290	A1229	G1169	G1106	C1044	A978	U920	U859	A798	G730	C673
G1482	U1421	G1291	U1230	G1170	G1107	G1045		U921	U860	U799	C731	A674
C1483	A1422	U1292	U1231	G1171	G1108	G1046	U981	G922	A861	G800	G732	C675
G1484	A1423	G1293	A1232	G1172	G1109	G1047	A862	A922	A862	G801	A733	C676
A1485	C1424	G1294	A1233	C1173	G1110	U1048	G984	A923	G924	A802	A734	U676
G1486	A1425	A1295	C1234	G1174	A1112	G1049	G985	G924	A864	A803	C735	G677
U1487	G1426	G1296	A1235	U1174	G1113	G1050	G986	A925	G926	U804	C736	G678
A1488	G1427	U1297	G1236	G1175	U1114	U1051	A987	C926	G965	A805	A737	U679
U1428	U1428	U1298	G1237	C1176	U1115	G1052	U988	U927	G966		C738	
C1489	C1429	A1299	U1238	G1177	A1116	U1053	U989	A928	G967	G808	A739	U680
A1490	U1430	U1300	U1239	G1178	U1117	U1054	G990	A929	C969	G809	G739	U681
C1491	G1431	U1301	G1240	C1179	G1117	U1055	G991	U929	C930		A740	C682
C1492	U1432	U1302	A1241	U1180	G1118	U1056	A991		G870		C741	A684
C1493					U1119						U742	A685
											U743	A686
											U744	C687
											U745	G688
											A746	
											C747	
											U748	

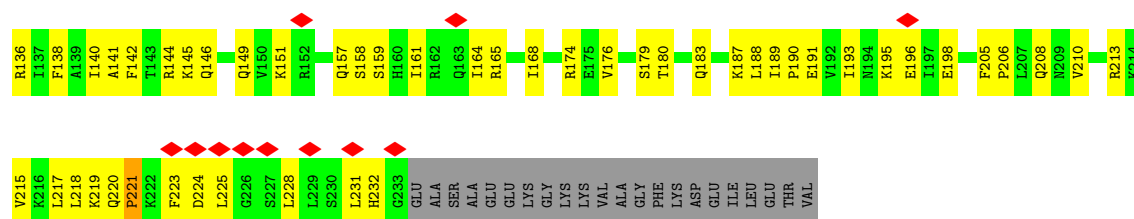


• Molecule 2: Small ribosomal subunit protein uS2

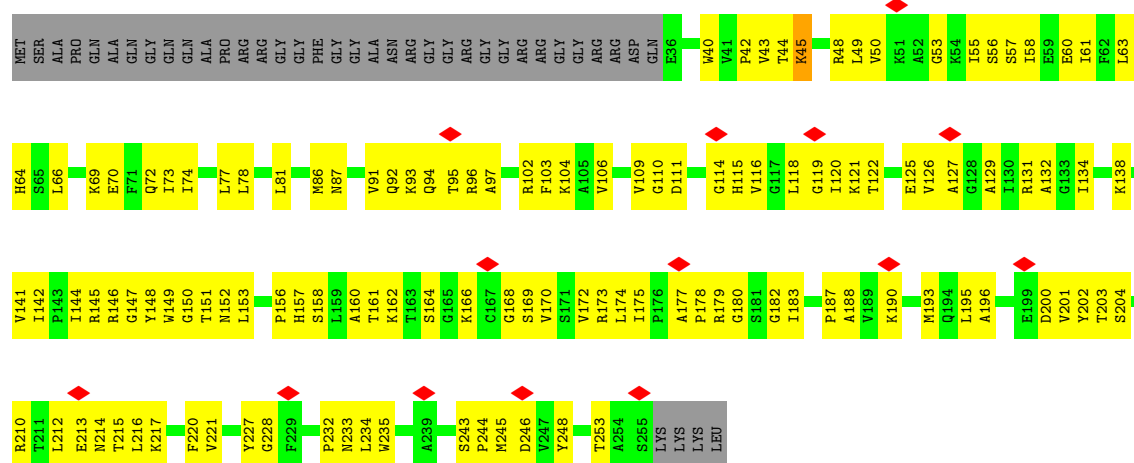


• Molecule 3: Small ribosomal subunit protein eS1

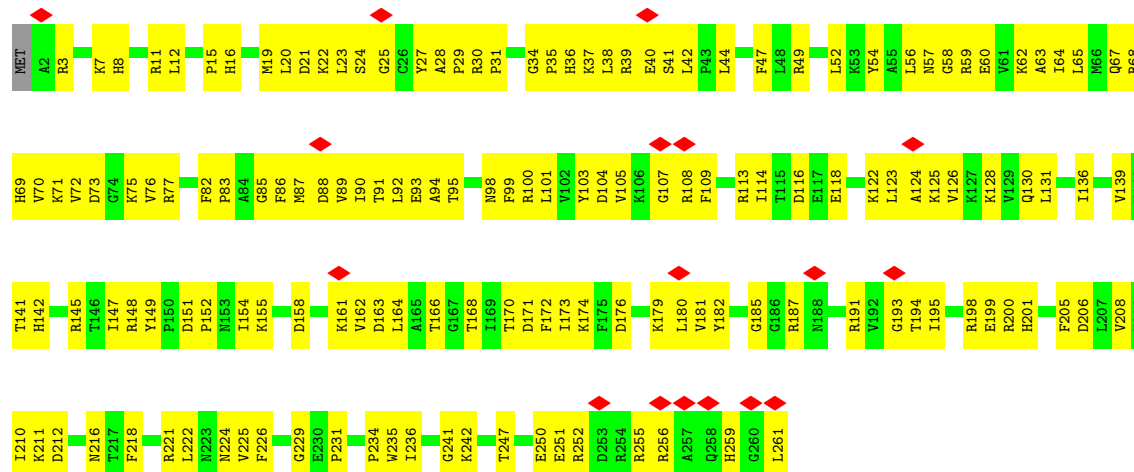




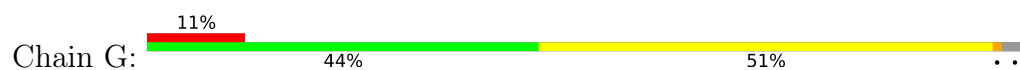
• Molecule 4: Small ribosomal subunit protein uS5

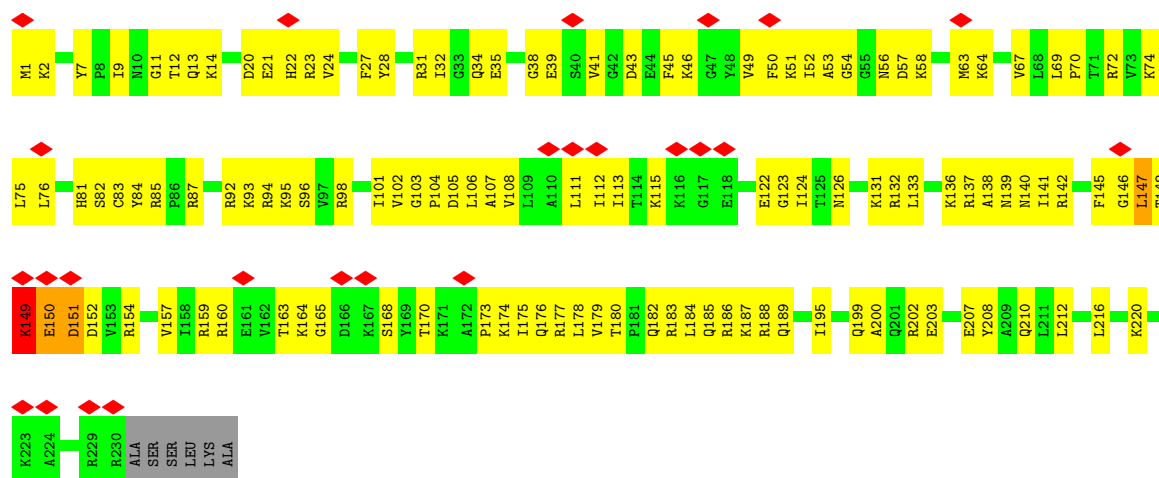


• Molecule 5: 40S ribosomal protein S4

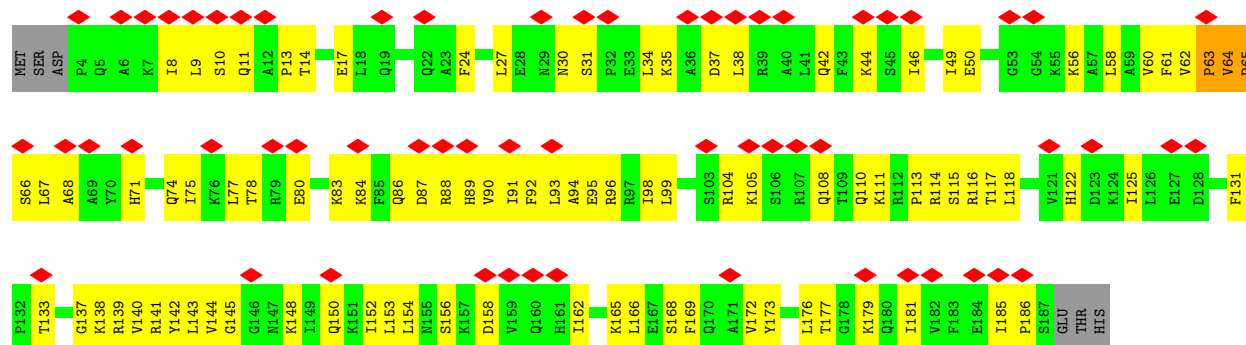


• Molecule 6: Small ribosomal subunit protein eS6

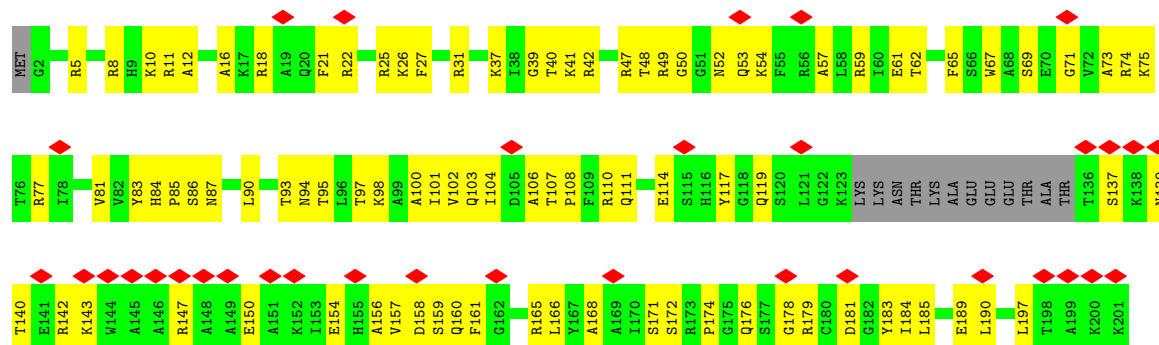




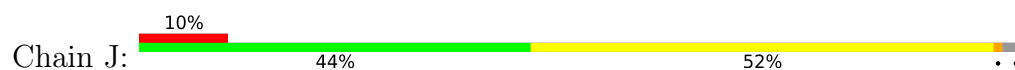
• Molecule 7: 40S ribosomal protein S7

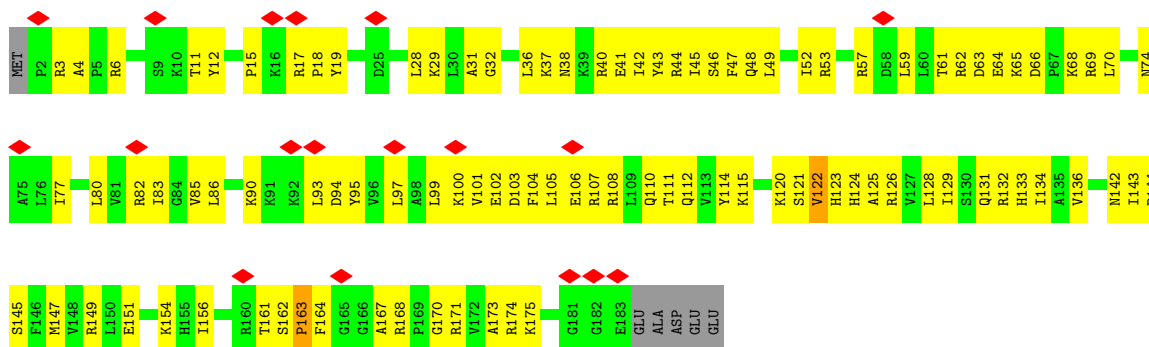


• Molecule 8: 40S ribosomal protein S8

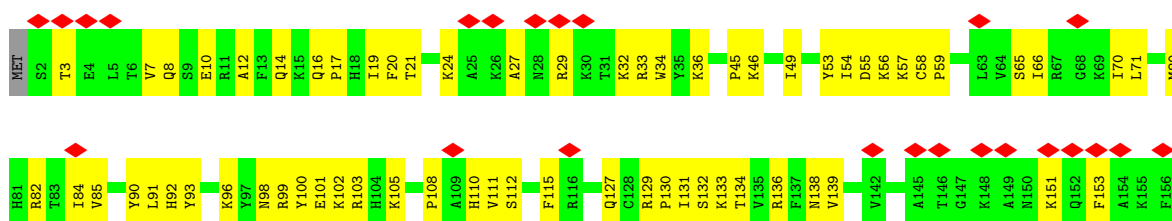


• Molecule 9: KLLA0E23673p

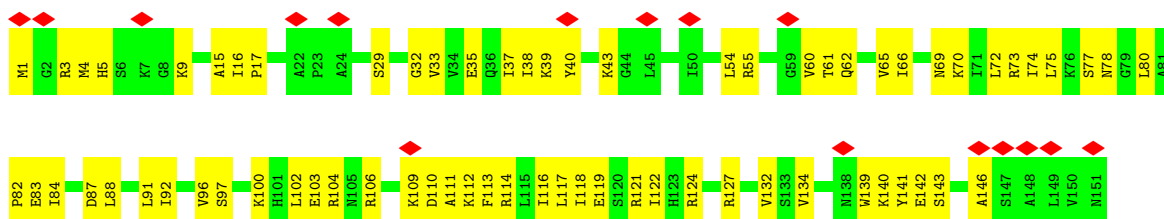




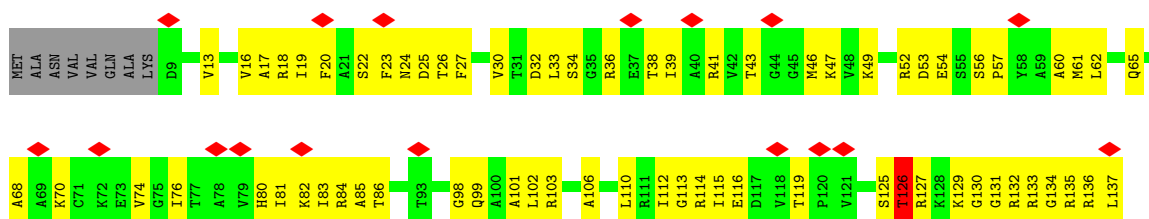
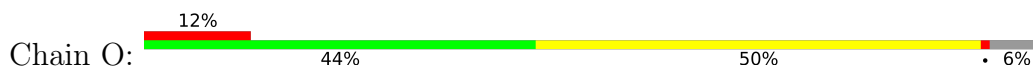
• Molecule 10: KLLA0A10483p



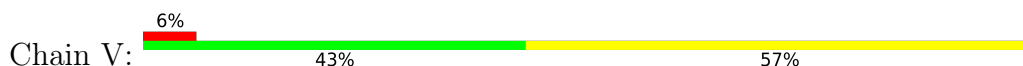
• Molecule 11: KLLA0F18040p

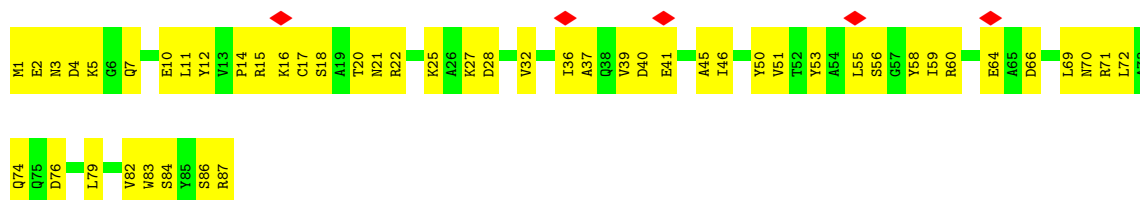


• Molecule 12: Small ribosomal subunit protein uS11

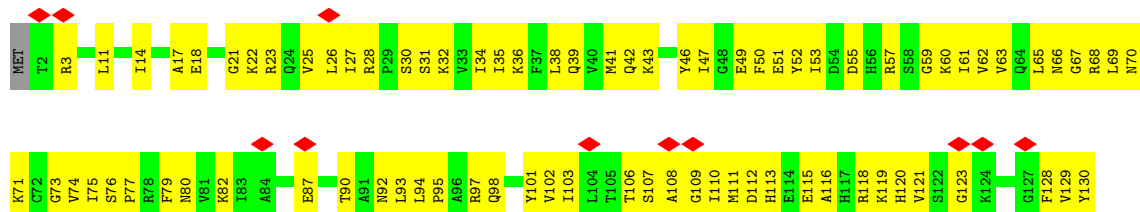


• Molecule 13: 40S ribosomal protein S21

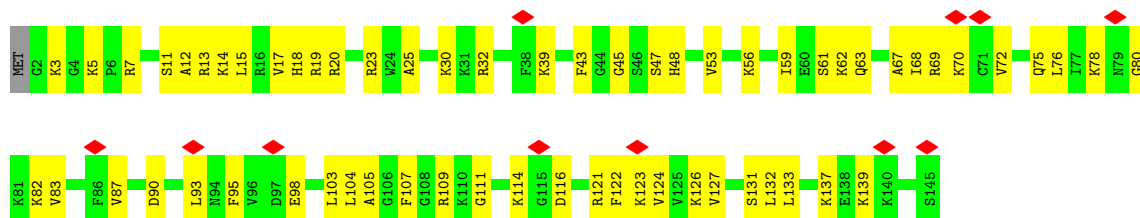




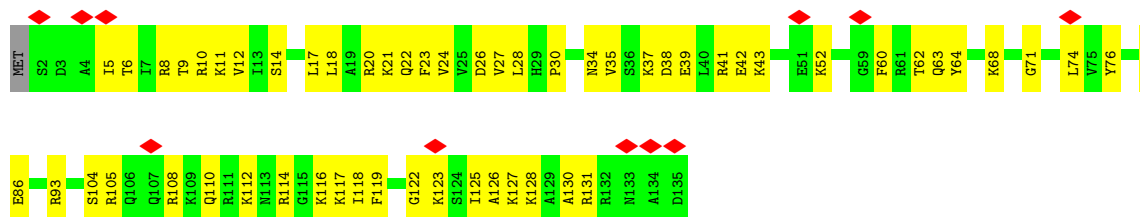
- Molecule 14: Small ribosomal subunit protein uS8



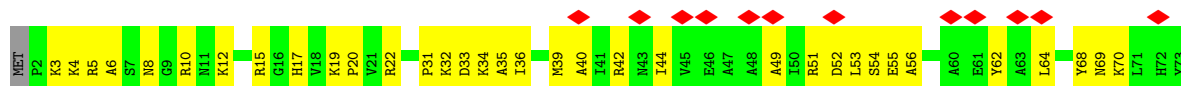
- Molecule 15: KLLA0B11231p

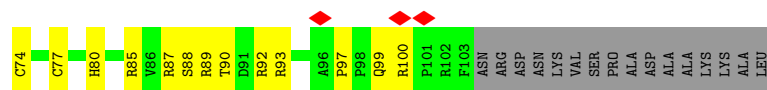


- Molecule 16: 40S ribosomal protein S24

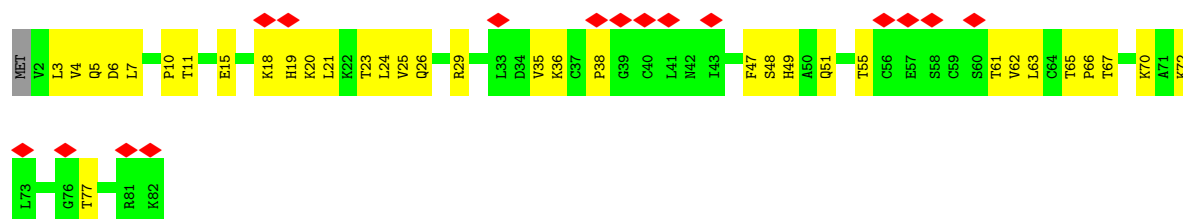


- Molecule 17: 40S ribosomal protein S26

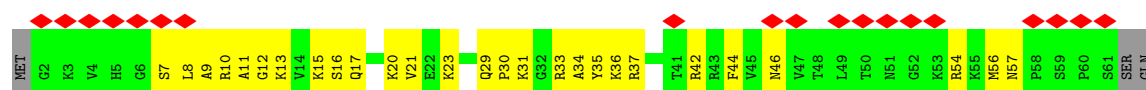




- Molecule 18: 40S ribosomal protein S27



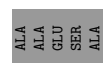
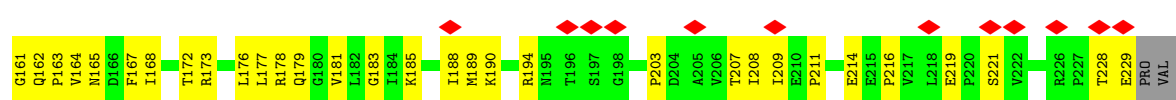
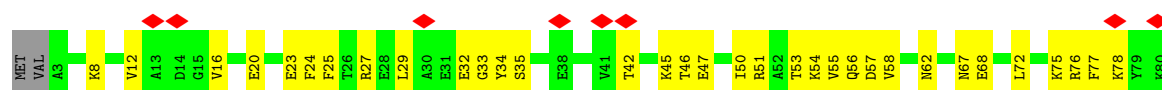
- Molecule 19: 40S ribosomal protein S30



- Molecule 20: 40S ribosomal protein L41-A



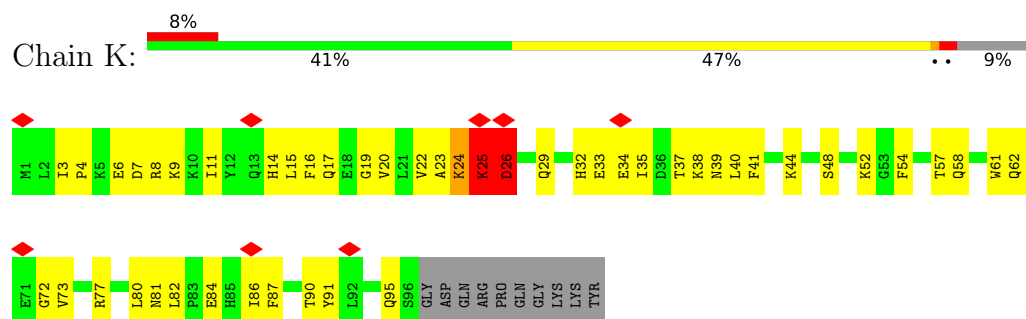
- Molecule 21: 40S ribosomal protein S3



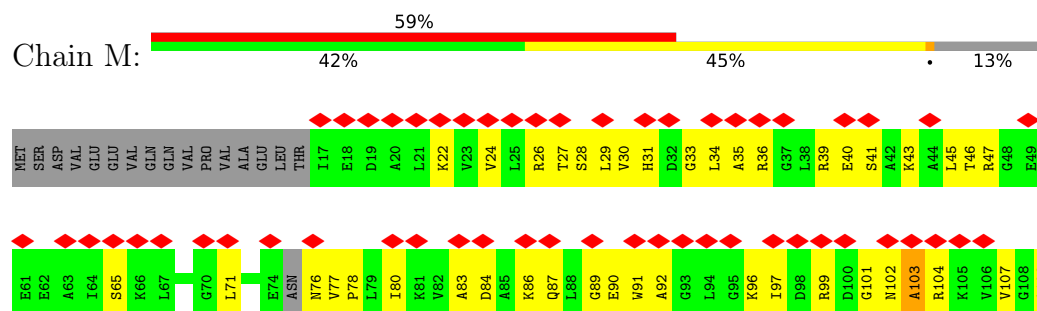
- Molecule 22: KLLA0D10659p



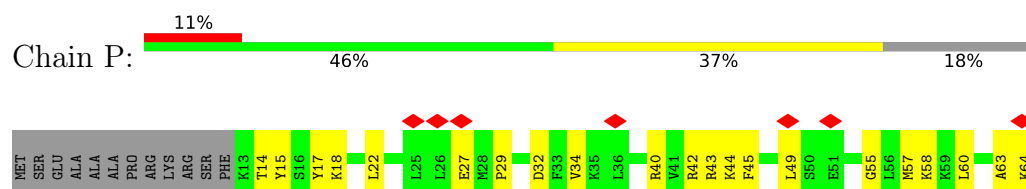
- Molecule 23: KLLA0B08173p

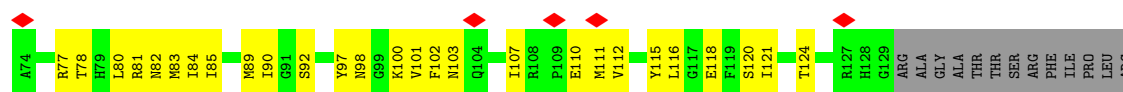


- Molecule 24: 40S ribosomal protein S12



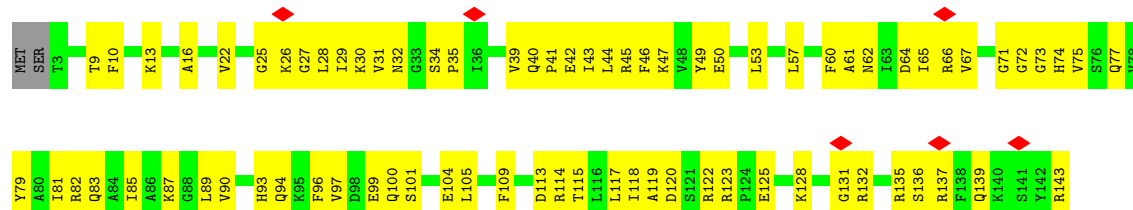
- Molecule 25: KLLA0F07843p





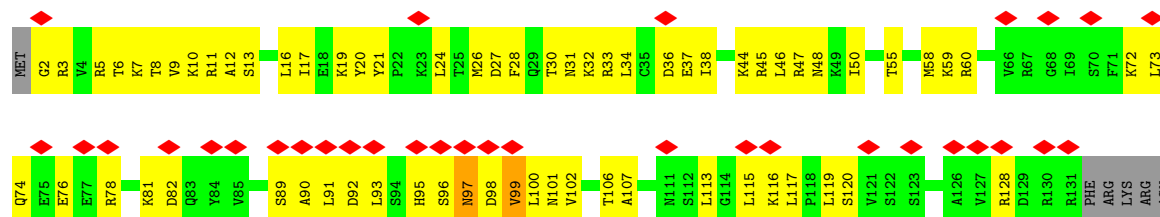
- Molecule 26: Small ribosomal subunit protein uS9

Chain Q: 45% 54%



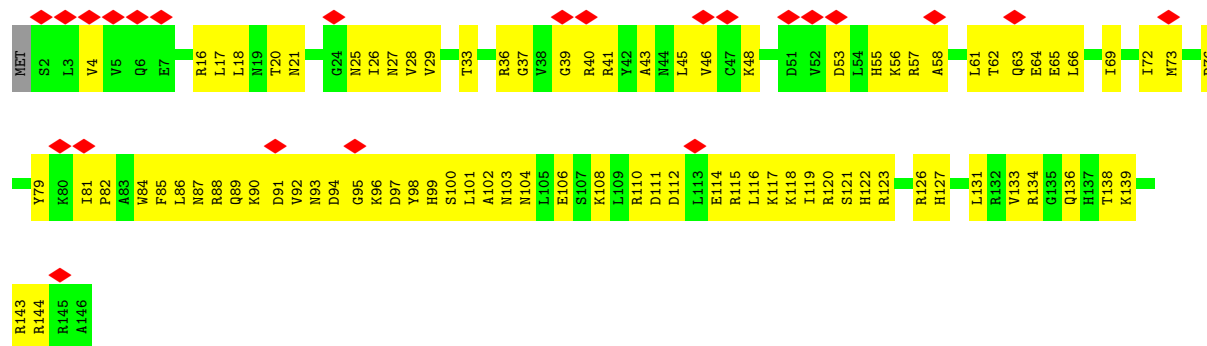
- Molecule 27: KLLA0B01474p

Chain R: 24% 46% 48%



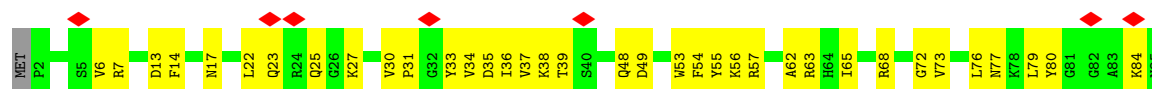
- Molecule 28: KLLA0B01562p

Chain S: 16% 41% 58%



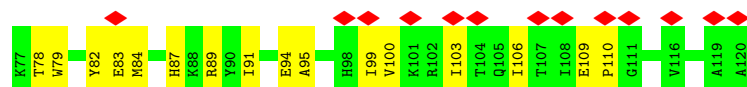
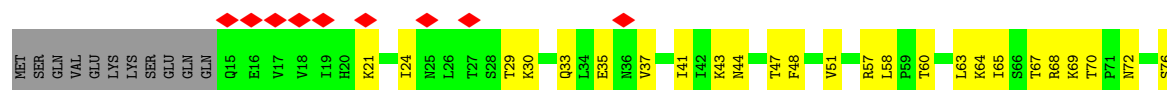
- Molecule 29: KLLA0A07194p

Chain T: 8% 58% 41%

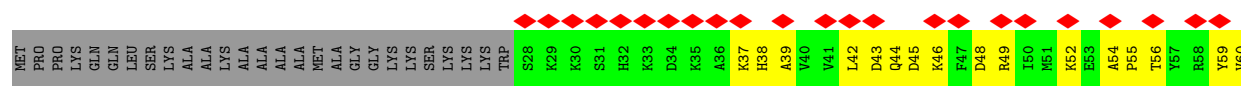




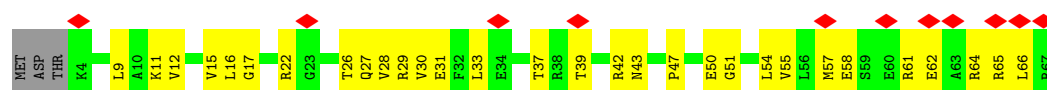
- Molecule 30: Small ribosomal subunit protein uS10



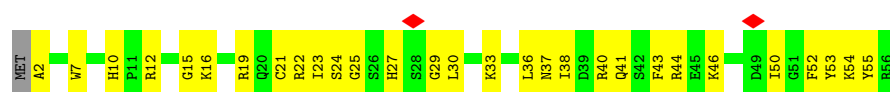
- Molecule 31: 40S ribosomal protein S25



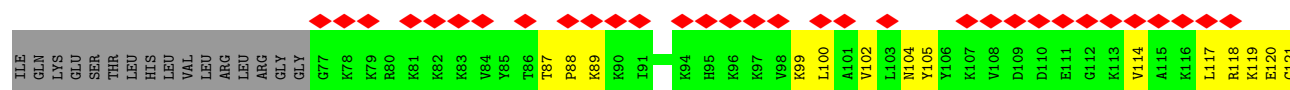
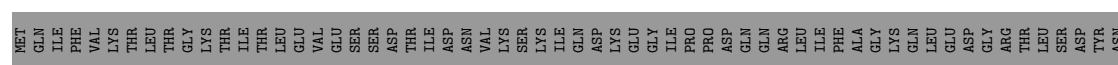
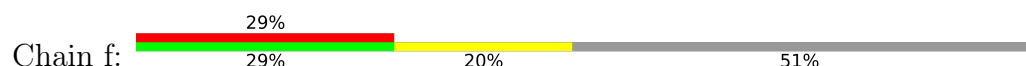
- Molecule 32: Small ribosomal subunit protein eS28

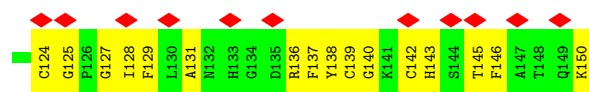


- Molecule 33: Small ribosomal subunit protein uS14

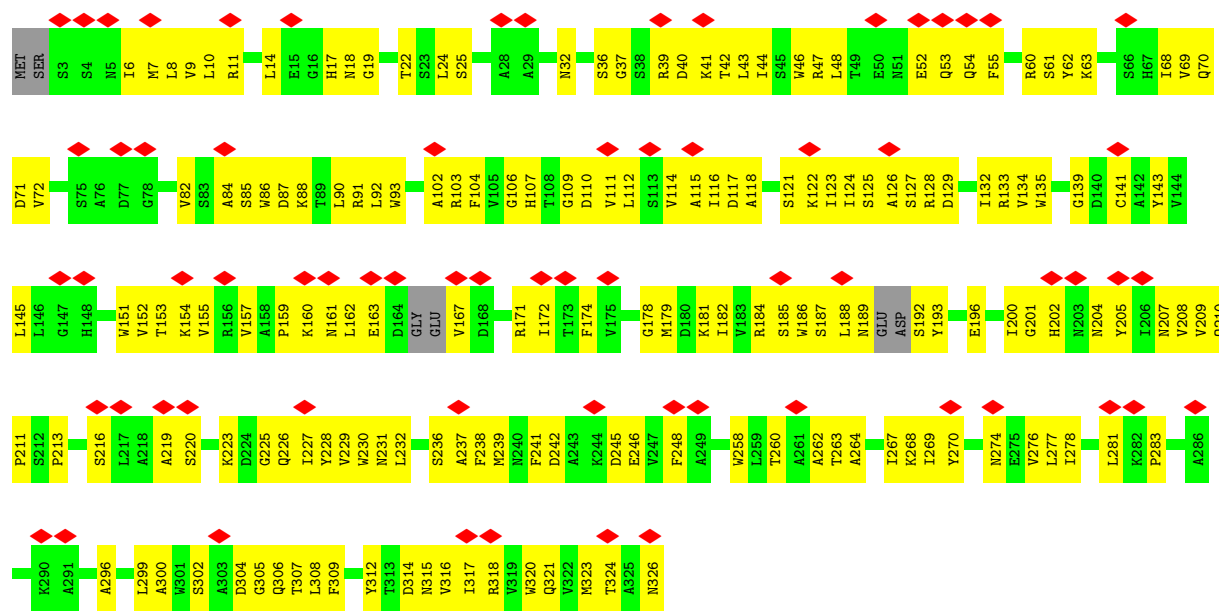


- Molecule 34: Small ribosomal subunit protein eS31

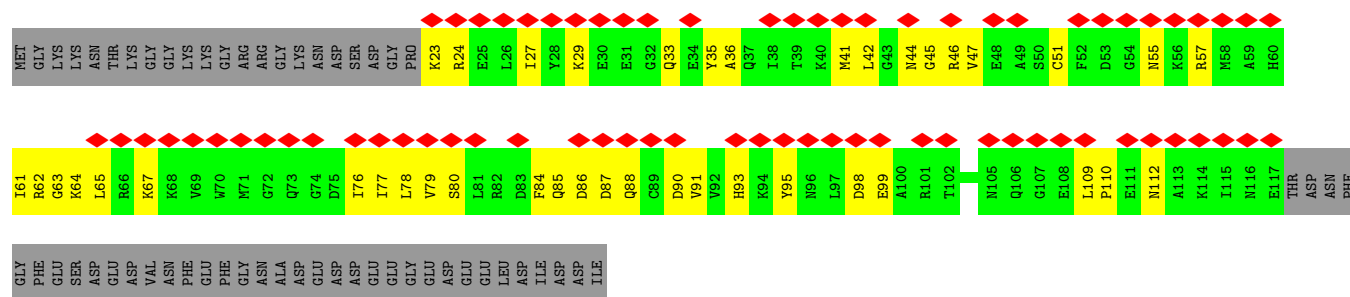




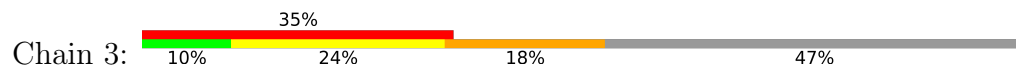
• Molecule 35: KLLA0E12277p



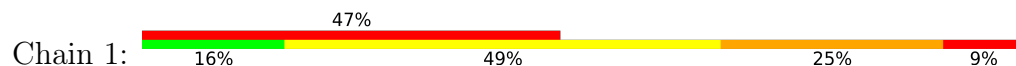
• Molecule 36: Eukaryotic translation initiation factor 1A

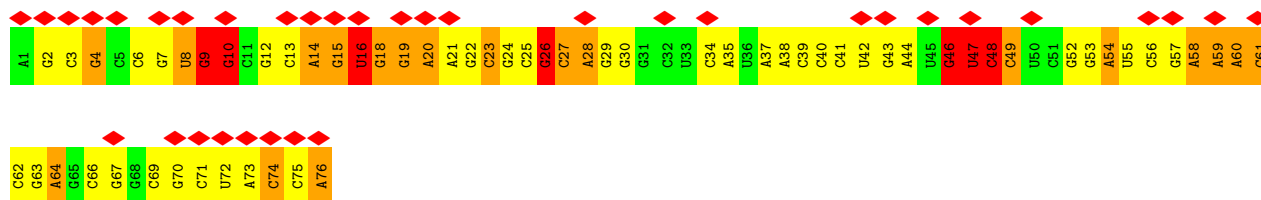


• Molecule 37: mRNA (5'-R(P*AP*AP*U)-3')

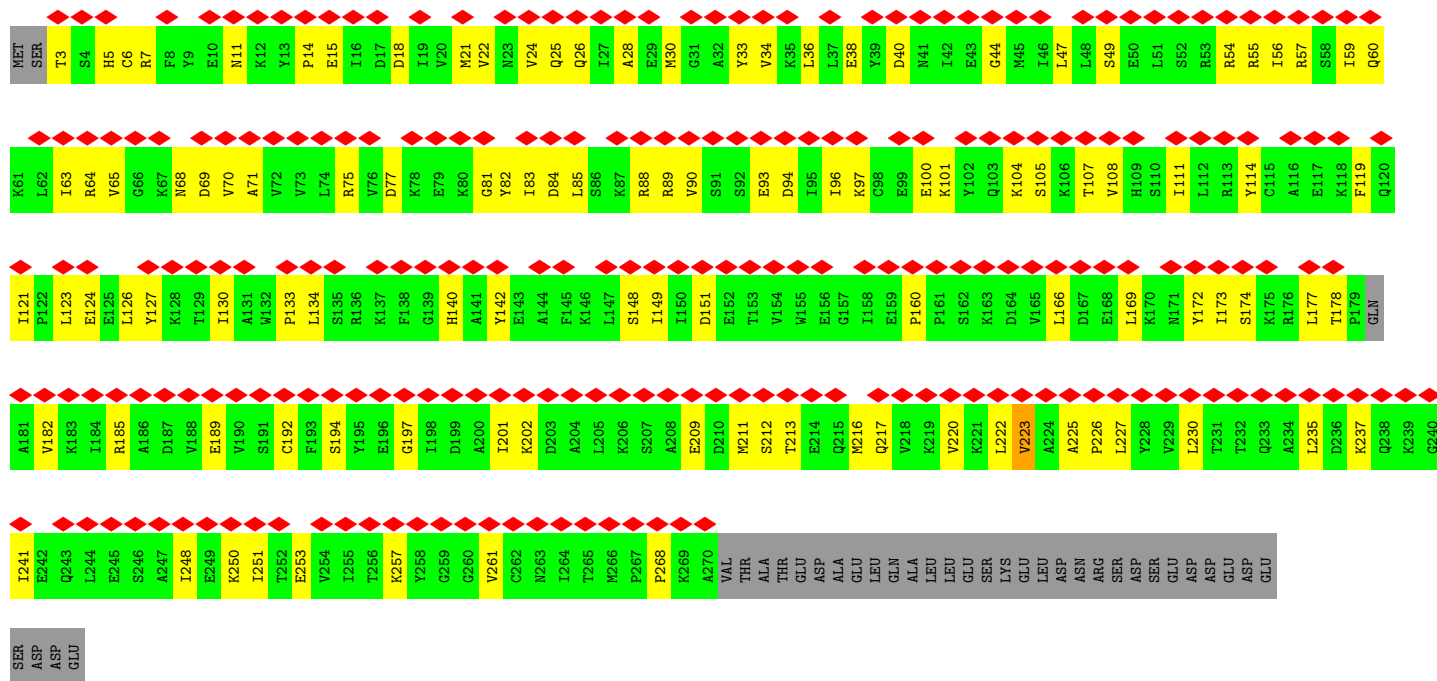
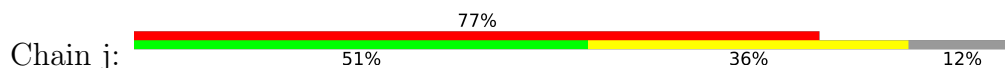


• Molecule 38: Met-tRNAⁱ

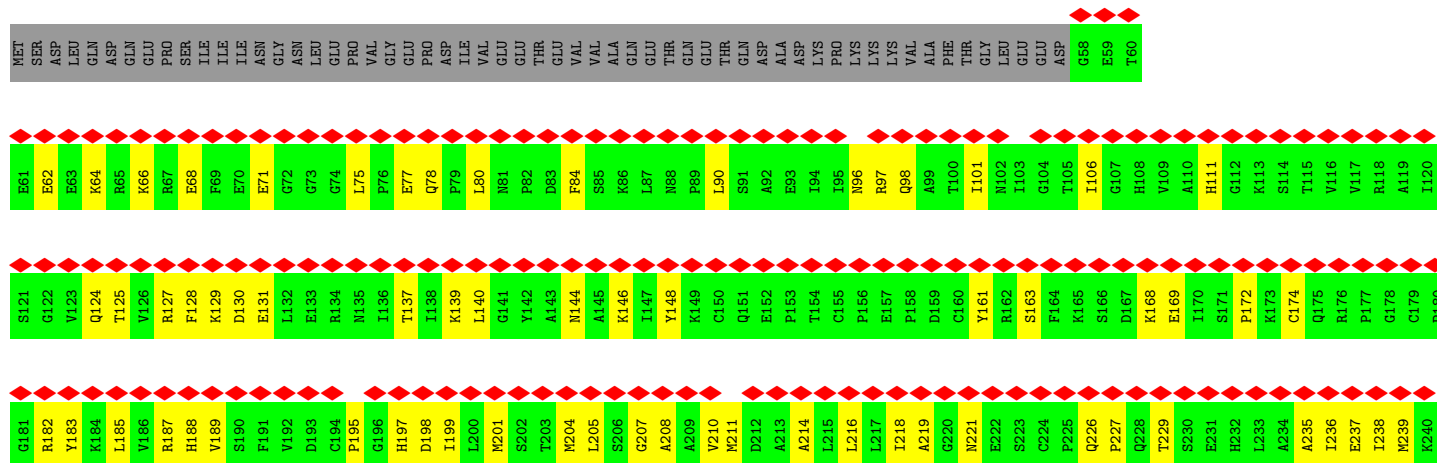
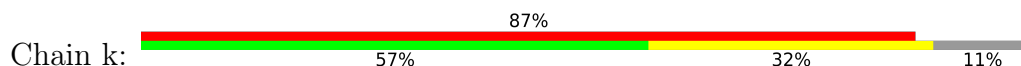




• Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha



• Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13862	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.399	Depositor
Minimum map value	-0.191	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, 2MG, RIA, H2U, 1MG, ZN, MA6, 1MA, MG, M2G, 5MC, T6A, GCP, PSU, 7MG

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	2	0.20	0/42410	0.35	0/66079
2	A	0.21	0/1742	0.46	0/2383
3	B	0.24	0/1820	0.52	0/2448
4	C	0.22	0/1678	0.49	0/2277
5	E	0.19	0/2122	0.46	0/2861
6	G	0.20	0/1855	0.42	0/2479
7	H	0.24	0/1507	0.52	0/2028
8	I	0.19	0/1515	0.47	0/2029
9	J	0.23	0/1495	0.57	0/2001
10	L	0.22	0/1276	0.45	0/1718
11	N	0.21	0/1218	0.42	0/1638
12	O	0.23	0/966	0.52	1/1297 (0.1%)
13	V	0.23	0/696	0.47	0/938
14	W	0.24	0/1039	0.52	0/1399
15	X	0.22	0/1137	0.49	0/1516
16	Y	0.17	0/1075	0.42	0/1433
17	a	0.26	0/810	0.49	0/1087
18	b	0.19	0/619	0.52	0/837
19	e	0.24	0/480	0.55	0/640
20	h	0.14	0/234	0.38	0/300
21	D	0.19	0/1800	0.47	2/2421 (0.1%)
22	F	0.27	0/1628	0.53	0/2198
23	K	0.27	0/831	0.50	0/1123
24	M	0.16	0/891	0.57	0/1201
25	P	0.21	0/942	0.55	0/1269
26	Q	0.22	0/1125	0.51	0/1510
27	R	0.29	0/1044	0.59	0/1402
28	S	0.18	0/1208	0.51	0/1624
29	T	0.19	0/1129	0.44	0/1520
30	U	0.24	0/857	0.46	0/1158
31	Z	0.17	0/603	0.45	0/814
32	c	0.20	0/501	0.43	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.22	0/473	0.48	0/629
34	f	0.13	0/597	0.43	0/795
35	g	0.20	0/2523	0.46	0/3434
36	i	0.18	0/773	0.53	0/1031
37	3	0.14	0/595	0.29	0/920
38	1	0.18	0/1529	0.33	0/2376
39	j	0.18	0/2171	0.48	1/2924 (0.0%)
40	k	0.19	0/3657	0.48	0/4946
41	l	0.16	0/194	0.41	0/263
42	m	0.18	0/1136	0.45	0/1537
All	All	0.20	0/91901	0.42	4/133156 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	j	223	VAL	N-CA-C	-6.31	107.71	113.71
21	D	209	ILE	CA-C-N	5.79	131.95	120.94
21	D	209	ILE	C-N-CA	5.79	131.95	120.94
12	O	126	THR	CB-CA-C	-5.74	109.97	116.63

There are no chirality outliers.

There are no planarity outliers.

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	2	38190	0	19208	1809	0
2	A	1702	0	1695	117	0
3	B	1796	0	1874	126	0
4	C	1648	0	1727	128	0
5	E	2078	0	2157	153	0
6	G	1832	0	1919	132	0
7	H	1483	0	1579	99	0
8	I	1489	0	1504	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	1471	0	1554	128	0
10	L	1248	0	1311	85	0
11	N	1195	0	1263	72	0
12	O	955	0	987	81	0
13	V	687	0	682	55	0
14	W	1021	0	1056	107	0
15	X	1119	0	1198	84	0
16	Y	1061	0	1111	64	0
17	a	797	0	835	54	0
18	b	609	0	627	34	0
19	e	472	0	508	45	0
20	h	233	0	284	11	0
21	D	1774	0	1855	95	0
22	F	1609	0	1679	155	0
23	K	809	0	810	65	0
24	M	885	0	917	53	0
25	P	923	0	960	55	0
26	Q	1105	0	1170	85	0
27	R	1033	0	1082	76	0
28	S	1189	0	1211	87	0
29	T	1110	0	1124	73	0
30	U	845	0	913	49	0
31	Z	594	0	590	38	0
32	c	499	0	536	31	0
33	d	461	0	448	41	0
34	f	584	0	601	34	0
35	g	2469	0	2403	165	0
36	i	764	0	763	44	0
37	3	536	0	277	22	0
38	1	1639	0	852	62	0
39	j	2139	0	2205	94	0
40	k	3596	0	3713	122	0
41	l	190	0	191	3	0
42	m	1113	0	1113	69	0
43	2	111	0	0	0	0
43	3	1	0	0	0	0
43	Q	1	0	0	0	0
43	i	1	0	0	0	0
43	k	1	0	0	0	0
44	a	1	0	0	0	0
44	b	1	0	0	0	0
44	f	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	m	1	0	0	0	0
45	k	8	0	8	0	0
46	k	32	0	13	0	0
47	2	3	0	0	1	0
All	All	87114	0	68513	4217	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 27.

The worst 5 of 4217 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)
22:F:101:MET:N	22:F:105:ASN:HB2	1.50	1.26
22:F:107:GLY:O	22:F:108:LYS:HG3	1.17	1.25
1:2:1585:A:O2'	22:F:103:GLY:HA3	1.41	1.19
22:F:104:ARG:O	22:F:108:LYS:HE2	1.43	1.16
22:F:107:GLY:O	22:F:108:LYS:CG	1.95	1.15

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	217/254 (85%)	192 (88%)	25 (12%)	0	100	100
3	B	221/255 (87%)	193 (87%)	25 (11%)	3 (1%)	9	39
4	C	218/259 (84%)	194 (89%)	23 (11%)	1 (0%)	24	63
5	E	258/261 (99%)	233 (90%)	25 (10%)	0	100	100
6	G	228/236 (97%)	216 (95%)	9 (4%)	3 (1%)	9	41
7	H	182/190 (96%)	154 (85%)	26 (14%)	2 (1%)	11	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	184/201 (92%)	161 (88%)	23 (12%)	0	100	100
9	J	180/188 (96%)	146 (81%)	30 (17%)	4 (2%)	5	28
10	L	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
11	N	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
12	O	127/137 (93%)	108 (85%)	19 (15%)	0	100	100
13	V	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
14	W	127/130 (98%)	112 (88%)	15 (12%)	0	100	100
15	X	142/145 (98%)	117 (82%)	25 (18%)	0	100	100
16	Y	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
17	a	100/119 (84%)	80 (80%)	20 (20%)	0	100	100
18	b	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
19	e	58/63 (92%)	48 (83%)	10 (17%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	214 (95%)	11 (5%)	0	100	100
22	F	204/227 (90%)	177 (87%)	23 (11%)	4 (2%)	6	31
23	K	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	5	29
24	M	113/134 (84%)	94 (83%)	18 (16%)	1 (1%)	14	49
25	P	115/142 (81%)	97 (84%)	18 (16%)	0	100	100
26	Q	139/143 (97%)	121 (87%)	18 (13%)	0	100	100
27	R	128/136 (94%)	104 (81%)	21 (16%)	3 (2%)	5	28
28	S	143/146 (98%)	124 (87%)	19 (13%)	0	100	100
29	T	141/144 (98%)	128 (91%)	13 (9%)	0	100	100
30	U	104/117 (89%)	93 (89%)	11 (11%)	0	100	100
31	Z	76/108 (70%)	65 (86%)	11 (14%)	0	100	100
32	c	62/67 (92%)	56 (90%)	6 (10%)	0	100	100
33	d	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
34	f	72/150 (48%)	56 (78%)	16 (22%)	0	100	100
35	g	314/326 (96%)	276 (88%)	38 (12%)	0	100	100
36	i	93/153 (61%)	83 (89%)	10 (11%)	0	100	100
39	j	263/304 (86%)	242 (92%)	21 (8%)	0	100	100
40	k	468/527 (89%)	423 (90%)	43 (9%)	2 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	l	21/285 (7%)	20 (95%)	1 (5%)	0	100	100
42	m	139/405 (34%)	119 (86%)	20 (14%)	0	100	100
All	All	5830/6987 (83%)	5144 (88%)	661 (11%)	25 (0%)	31	67

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	65	PRO
22	F	108	LYS
24	M	103	ALA
27	R	92	ASP
27	R	98	ASP

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	
2	A	180/211 (85%)	180 (100%)	0	100	100
3	B	202/228 (89%)	199 (98%)	3 (2%)	57	71
4	C	177/203 (87%)	177 (100%)	0	100	100
5	E	223/224 (100%)	223 (100%)	0	100	100
6	G	192/200 (96%)	189 (98%)	3 (2%)	55	69
7	H	164/170 (96%)	163 (99%)	1 (1%)	78	81
8	I	147/159 (92%)	147 (100%)	0	100	100
9	J	153/158 (97%)	153 (100%)	0	100	100
10	L	136/137 (99%)	136 (100%)	0	100	100
11	N	128/128 (100%)	128 (100%)	0	100	100
12	O	97/104 (93%)	96 (99%)	1 (1%)	68	76
13	V	73/73 (100%)	73 (100%)	0	100	100
14	W	110/111 (99%)	110 (100%)	0	100	100
15	X	119/120 (99%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Y	108/109 (99%)	108 (100%)	0	100	100
17	a	83/100 (83%)	83 (100%)	0	100	100
18	b	71/72 (99%)	71 (100%)	0	100	100
19	e	51/55 (93%)	51 (100%)	0	100	100
20	h	23/23 (100%)	23 (100%)	0	100	100
21	D	188/196 (96%)	188 (100%)	0	100	100
22	F	174/194 (90%)	171 (98%)	3 (2%)	53	68
23	K	88/96 (92%)	85 (97%)	3 (3%)	32	55
24	M	93/109 (85%)	93 (100%)	0	100	100
25	P	99/119 (83%)	99 (100%)	0	100	100
26	Q	117/119 (98%)	117 (100%)	0	100	100
27	R	116/124 (94%)	114 (98%)	2 (2%)	53	68
28	S	127/129 (98%)	127 (100%)	0	100	100
29	T	117/118 (99%)	117 (100%)	0	100	100
30	U	96/107 (90%)	96 (100%)	0	100	100
31	Z	59/88 (67%)	59 (100%)	0	100	100
32	c	55/59 (93%)	55 (100%)	0	100	100
33	d	47/48 (98%)	47 (100%)	0	100	100
34	f	60/133 (45%)	60 (100%)	0	100	100
35	g	264/272 (97%)	264 (100%)	0	100	100
36	i	80/130 (62%)	80 (100%)	0	100	100
39	j	239/274 (87%)	239 (100%)	0	100	100
40	k	393/449 (88%)	393 (100%)	0	100	100
41	l	22/246 (9%)	22 (100%)	0	100	100
42	m	123/352 (35%)	123 (100%)	0	100	100
All	All	4994/5947 (84%)	4978 (100%)	16 (0%)	84	84

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	R	97	ASN
23	K	26	ASP
22	F	37	GLN

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Mol	Chain	Res	Type
23	K	25	LYS
12	O	126	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
21	D	159	HIS
40	k	228	GLN
23	K	32	HIS
40	k	144	ASN
42	m	134	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	676 (37%)	26 (1%)
37	3	25/49 (51%)	16 (64%)	1 (4%)
38	1	72/75 (96%)	30 (41%)	1 (1%)
All	All	1894/1922 (98%)	722 (38%)	28 (1%)

5 of 722 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	5	U
1	2	13	C

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	828	A
38	1	47	H2U
1	2	1320	A
1	2	1765	G
1	2	1206	C

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

23 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$
38	RIA	1	64	38	35,38,39	4.61	14 (40%)	50,57,60	2.12	13 (26%)
38	1MG	1	9	38	23,26,27	3.33	7 (30%)	33,39,42	2.33	8 (24%)
1	5MC	2	1006	1	19,22,23	3.68	8 (42%)	26,32,35	1.02	2 (7%)
1	PSU	2	465	1,43	18,21,22	4.36	7 (38%)	21,30,33	1.75	4 (19%)
38	H2U	1	16	38	18,21,22	3.15	4 (22%)	19,30,33	1.46	4 (21%)
38	5MC	1	48	38	19,22,23	3.87	8 (42%)	26,32,35	1.02	1 (3%)
38	1MA	1	58	38	21,25,26	3.14	6 (28%)	30,37,40	2.38	8 (26%)
38	H2U	1	47	38	18,21,22	3.20	4 (22%)	19,30,33	1.38	4 (21%)
1	5MC	2	1637	1	19,22,23	3.78	8 (42%)	26,32,35	1.10	3 (11%)
38	7MG	1	46	38	23,26,27	3.57	10 (43%)	27,39,42	2.16	9 (33%)
1	PSU	2	766	1	18,21,22	4.42	8 (44%)	21,30,33	2.02	6 (28%)
38	5MC	1	49	38	19,22,23	3.89	8 (42%)	26,32,35	1.33	4 (15%)
38	T6A	1	37	38	31,34,35	1.76	7 (22%)	43,49,52	2.09	11 (25%)
38	M2G	1	26	38	24,27,28	2.71	8 (33%)	33,40,43	1.78	8 (24%)
1	PSU	2	120	1	18,21,22	4.38	7 (38%)	21,30,33	2.04	5 (23%)
1	7MG	2	1573	1	23,26,27	3.52	10 (43%)	27,39,42	2.25	9 (33%)
1	PSU	2	998	1	18,21,22	4.36	8 (44%)	21,30,33	2.02	5 (23%)
1	2MG	2	1570	1	23,26,27	2.89	8 (34%)	33,38,41	2.21	11 (33%)
1	PSU	2	1289	1	18,21,22	4.45	8 (44%)	21,30,33	1.78	4 (19%)
1	MA6	2	1780	1	23,26,27	1.37	4 (17%)	33,38,41	3.29	12 (36%)
38	2MG	1	10	38	23,26,27	2.93	8 (34%)	33,38,41	2.30	10 (30%)
1	B8N	2	1190	1	25,29,30	3.35	9 (36%)	28,42,45	2.06	9 (32%)
1	2MG	2	1426	1,43	23,26,27	2.81	9 (39%)	33,38,41	2.17	11 (33%)

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
38	RIA	1	64	38	-	8/17/51/52	0/4/4/4
38	1MG	1	9	38	-	2/7/25/26	0/3/3/3
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
1	PSU	2	465	1,43	-	4/7/25/26	0/2/2/2
38	H2U	1	16	38	-	5/7/38/39	0/2/2/2
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2
38	1MA	1	58	38	-	0/7/25/26	0/3/3/3
38	H2U	1	47	38	-	4/7/38/39	0/2/2/2
1	5MC	2	1637	1	-	2/7/25/26	0/2/2/2
38	7MG	1	46	38	-	1/7/37/38	0/3/3/3
1	PSU	2	766	1	-	0/7/25/26	0/2/2/2
38	5MC	1	49	38	-	5/7/25/26	0/2/2/2
38	T6A	1	37	38	-	7/23/41/42	0/3/3/3
38	M2G	1	26	38	-	2/11/29/30	0/3/3/3
1	PSU	2	120	1	-	0/7/25/26	0/2/2/2
1	7MG	2	1573	1	-	3/7/37/38	0/3/3/3
1	PSU	2	998	1	-	3/7/25/26	0/2/2/2
1	2MG	2	1570	1	-	2/9/27/28	0/3/3/3
1	PSU	2	1289	1	-	4/7/25/26	0/2/2/2
1	MA6	2	1780	1	-	2/11/29/30	0/3/3/3
38	2MG	1	10	38	-	3/9/27/28	0/3/3/3
1	B8N	2	1190	1	-	4/16/34/35	0/2/2/2
1	2MG	2	1426	1,43	-	1/9/27/28	0/3/3/3

The worst 5 of 178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	64	RIA	C1'-C2'	-16.01	1.32	1.52
1	2	1289	PSU	C6-C5	11.93	1.48	1.35
1	2	465	PSU	C6-C5	11.64	1.48	1.35
1	2	766	PSU	C6-C5	11.57	1.48	1.35
1	2	120	PSU	C6-C5	11.53	1.48	1.35

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	N1-C6-N6	-12.09	102.13	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	C5-C6-N6	7.78	137.65	125.33
38	1	10	2MG	C2-N3-C4	6.98	120.73	112.00
38	1	58	1MA	C1'-N9-C8	-6.70	107.70	126.73
38	1	9	1MG	C1'-N9-C4	-6.67	106.78	126.49

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	465	PSU	C2'-C1'-C5-C4
1	2	465	PSU	O4'-C4'-C5'-O5'
1	2	998	PSU	O4'-C4'-C5'-O5'
1	2	1190	B8N	O4'-C4'-C5'-O5'
1	2	1289	PSU	C2'-C1'-C5-C4

There are no ring outliers.

18 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	1	64	RIA	3	0
38	1	9	1MG	2	0
1	2	1006	5MC	4	0
38	1	16	H2U	1	0
38	1	48	5MC	2	0
38	1	58	1MA	2	0
38	1	47	H2U	1	0
38	1	46	7MG	2	0
38	1	26	M2G	3	0
1	2	120	PSU	4	0
1	2	1573	7MG	2	0
1	2	998	PSU	3	0
1	2	1570	2MG	1	0
1	2	1289	PSU	1	0
1	2	1780	MA6	1	0
38	1	10	2MG	1	0
1	2	1190	B8N	1	0
1	2	1426	2MG	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 121 ligands modelled in this entry, 119 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
46	GCP	k	602	-	32,34,34	3.19	12 (37%)	49,54,54	1.67	9 (18%)
45	MET	k	601	-	6,7,8	0.48	0	2,7,9	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GCP	k	602	-	-	0/19/38/38	0/3/3/3
45	MET	k	601	-	-	1/5/6/8	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	k	602	GCP	O4'-C1'	8.68	1.62	1.42
46	k	602	GCP	C2'-C1'	-7.17	1.30	1.53
46	k	602	GCP	O4'-C4'	-6.32	1.30	1.45
46	k	602	GCP	PB-O3A	6.18	1.65	1.58
46	k	602	GCP	PA-O3A	5.33	1.65	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	k	602	GCP	C5-C4-N3	-5.28	119.99	128.39
46	k	602	GCP	C2-N3-C4	4.56	120.15	112.30
46	k	602	GCP	N9-C4-N3	3.00	131.95	125.95
46	k	602	GCP	N9-C8-N7	-2.99	107.86	113.40
46	k	602	GCP	C2-N1-C6	-2.88	119.88	125.11

There are no chirality outliers.

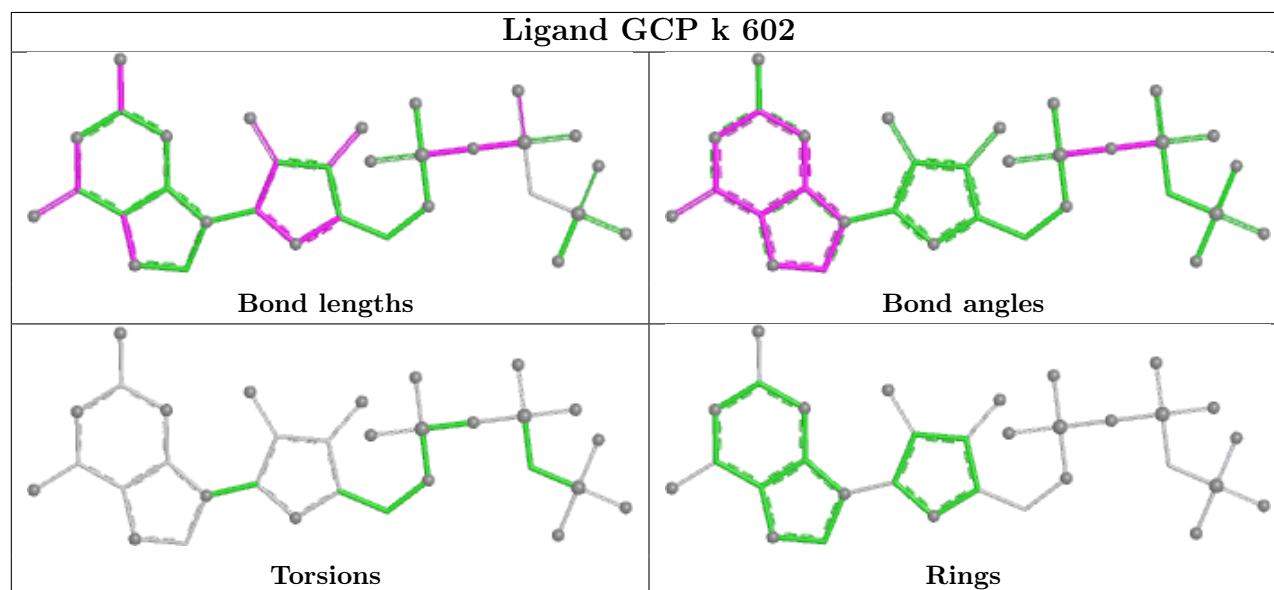
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	k	601	MET	CA-CB-CG-SD

There are no ring outliers.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	64:RIA	O3'	65:G	P	9.98
1	1	63:G	O3'	64:RIA	P	4.41
1	1	16:H2U	O3'	18:G	P	3.33

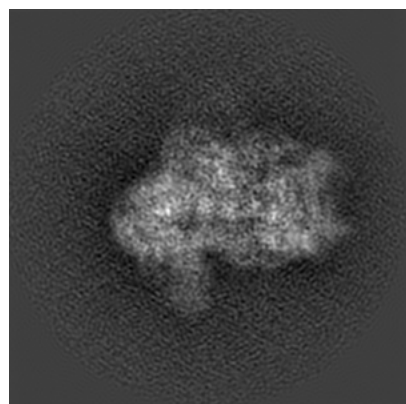
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19807. These allow visual inspection of the internal detail of the map and identification of artifacts.

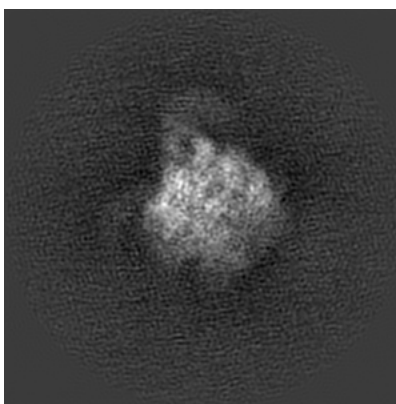
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

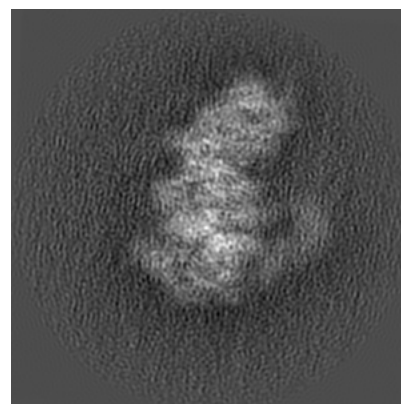
6.1.1 Primary map



X

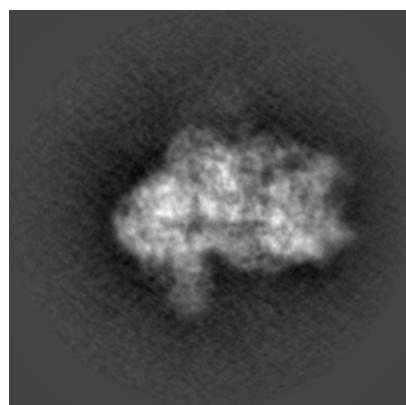


Y

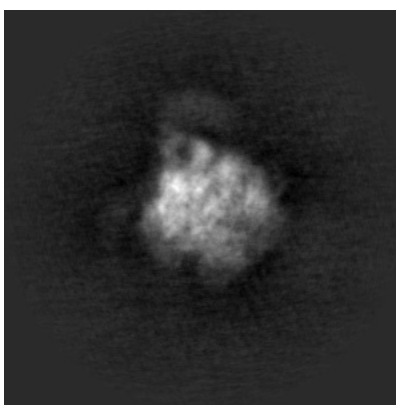


Z

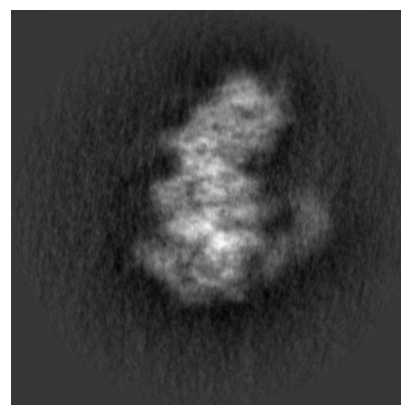
6.1.2 Raw map



X



Y

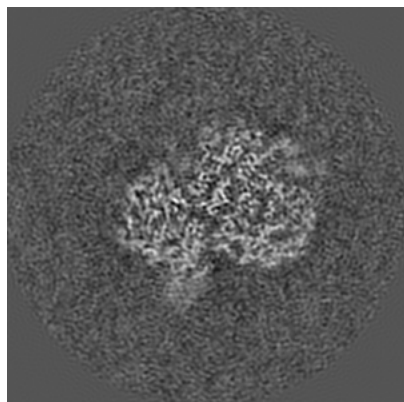


Z

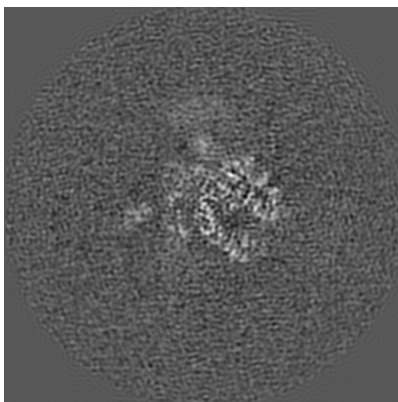
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

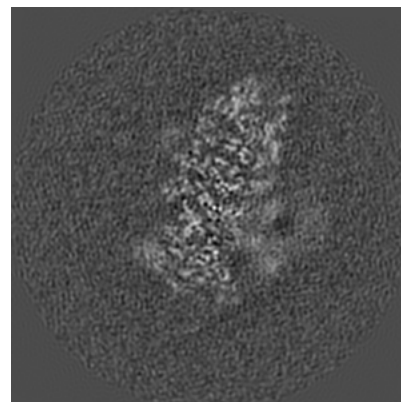
6.2.1 Primary map



X Index: 150

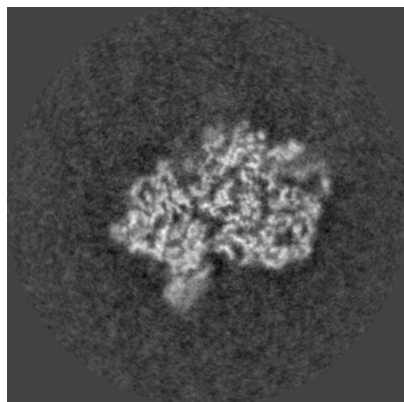


Y Index: 150

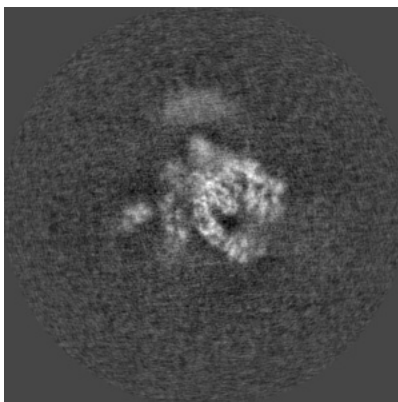


Z Index: 150

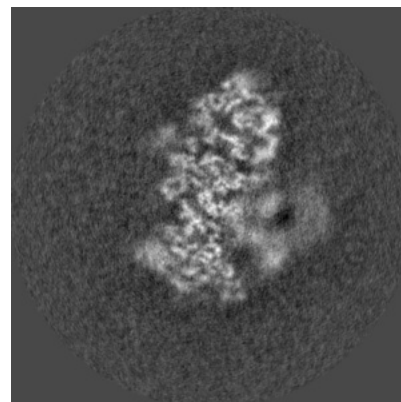
6.2.2 Raw map



X Index: 150



Y Index: 150

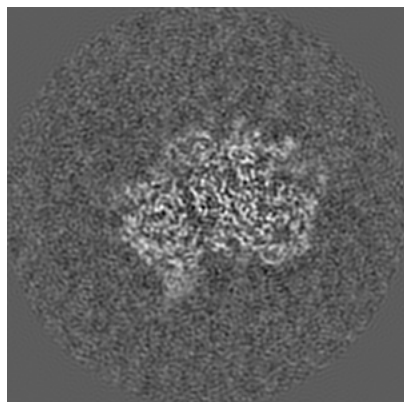


Z Index: 150

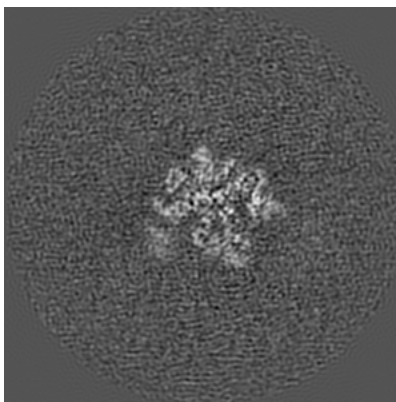
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

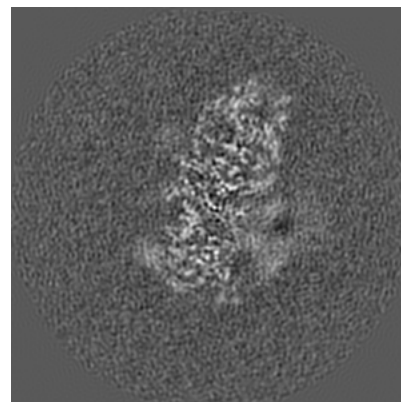
6.3.1 Primary map



X Index: 154

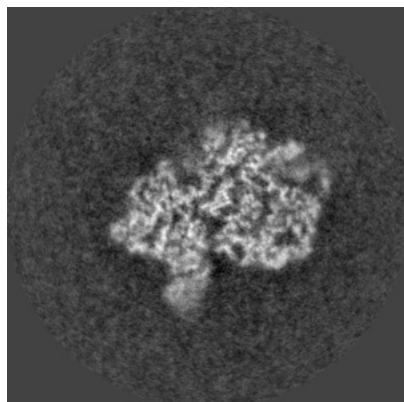


Y Index: 167

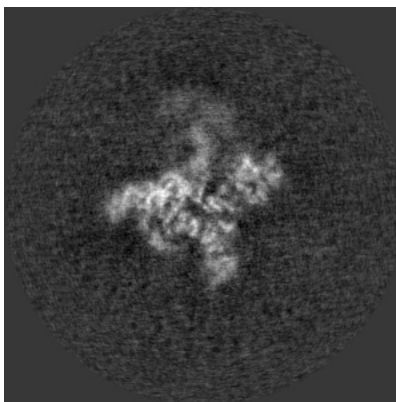


Z Index: 149

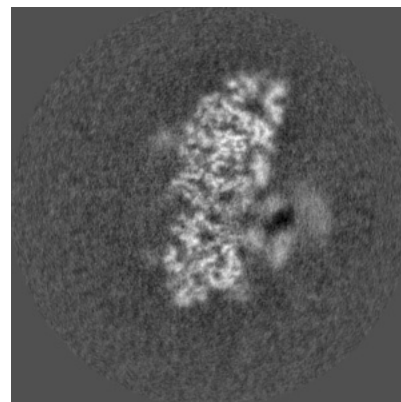
6.3.2 Raw map



X Index: 149



Y Index: 125

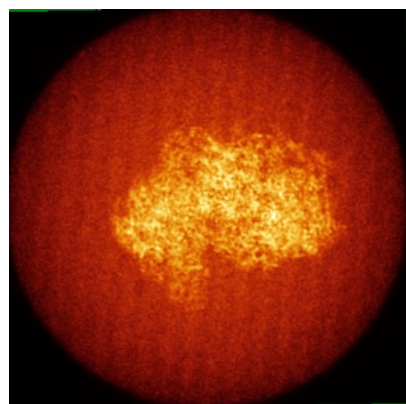


Z Index: 143

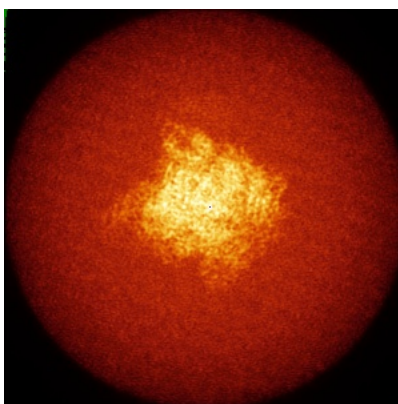
The images above show the largest variance slices of the map in three orthogonal directions.

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

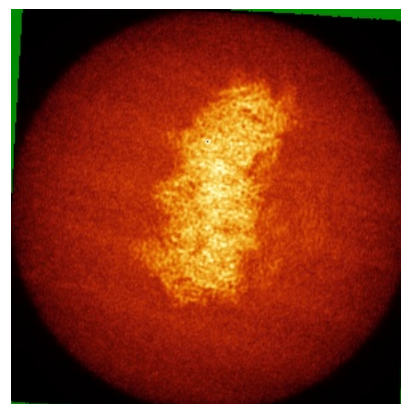
6.4.1 Primary map



X

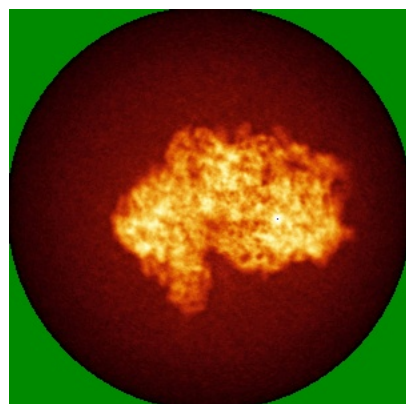


Y

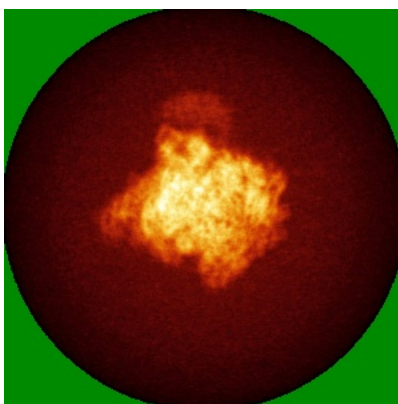


Z

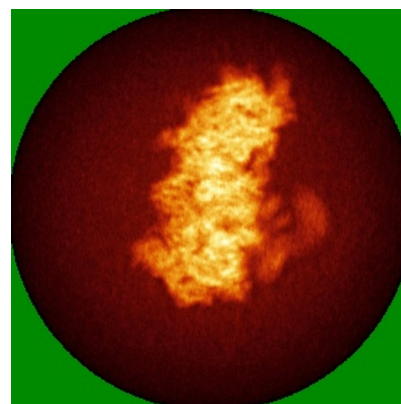
6.4.2 Raw map



X



Y

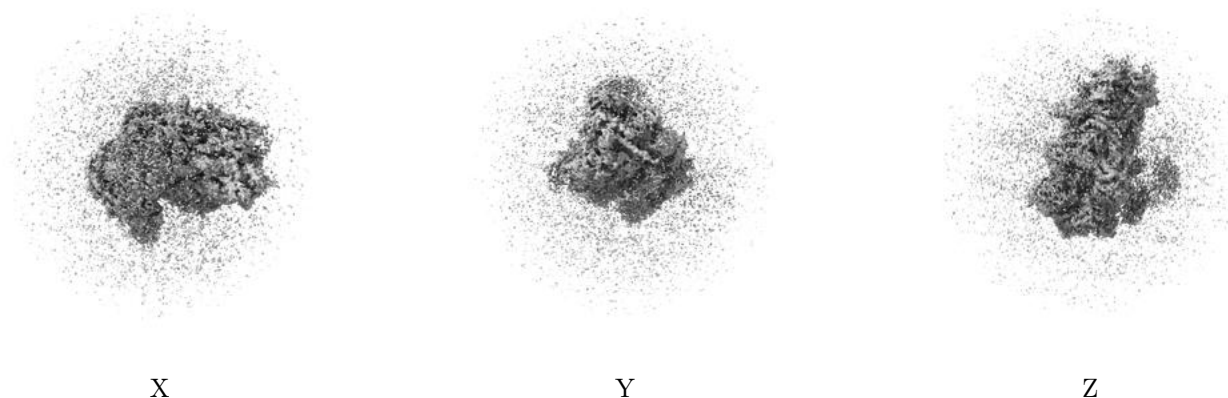


Z

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 0.07. 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.

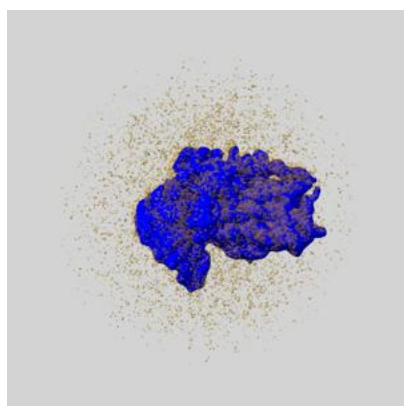
6.6 Mask visualisation [i](#)

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

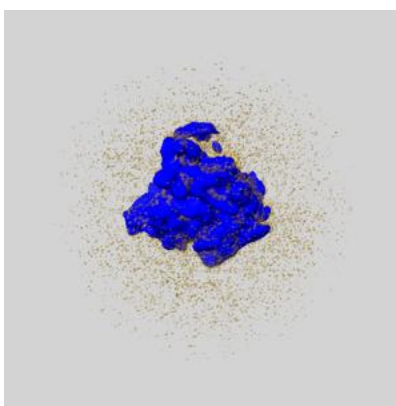
A mask typically either:

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

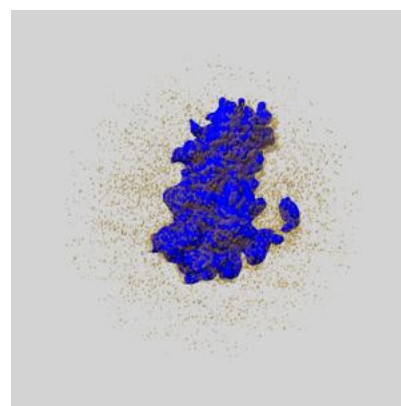
6.6.1 emd_19807_msk_1.map [i](#)



X



Y

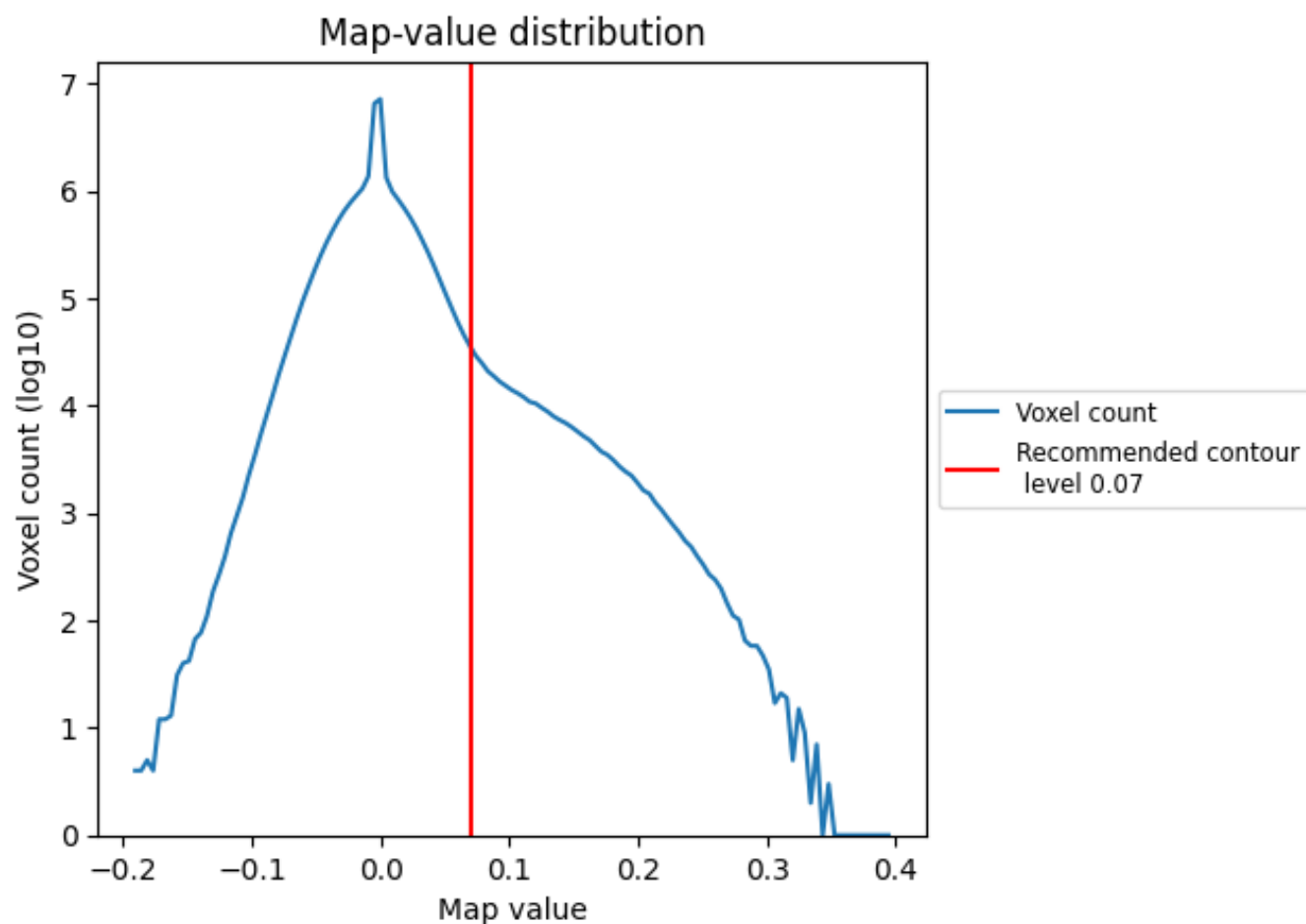


Z

7 Map analysis [i](#)

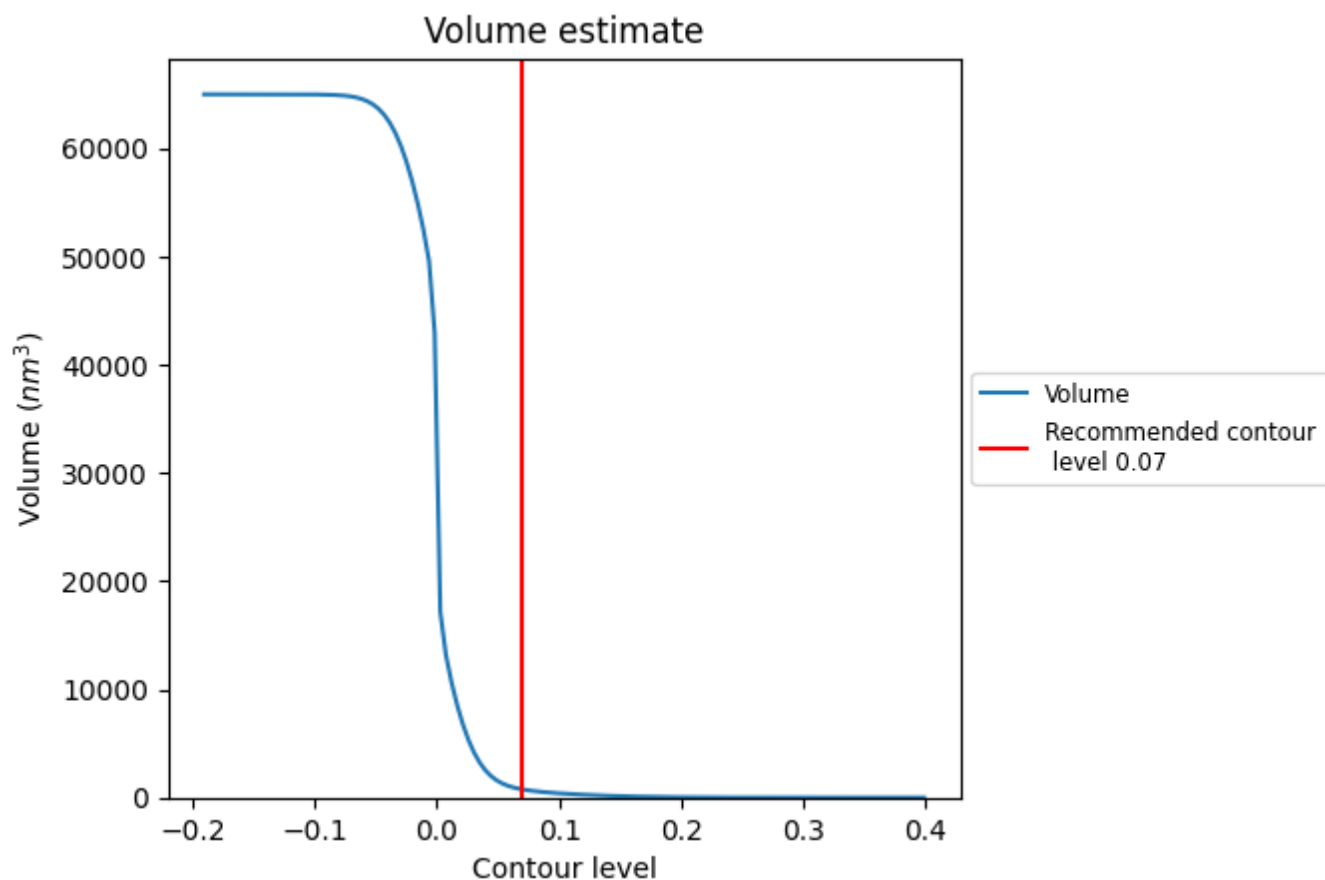
This section contains the results of statistical analysis of the map.

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.

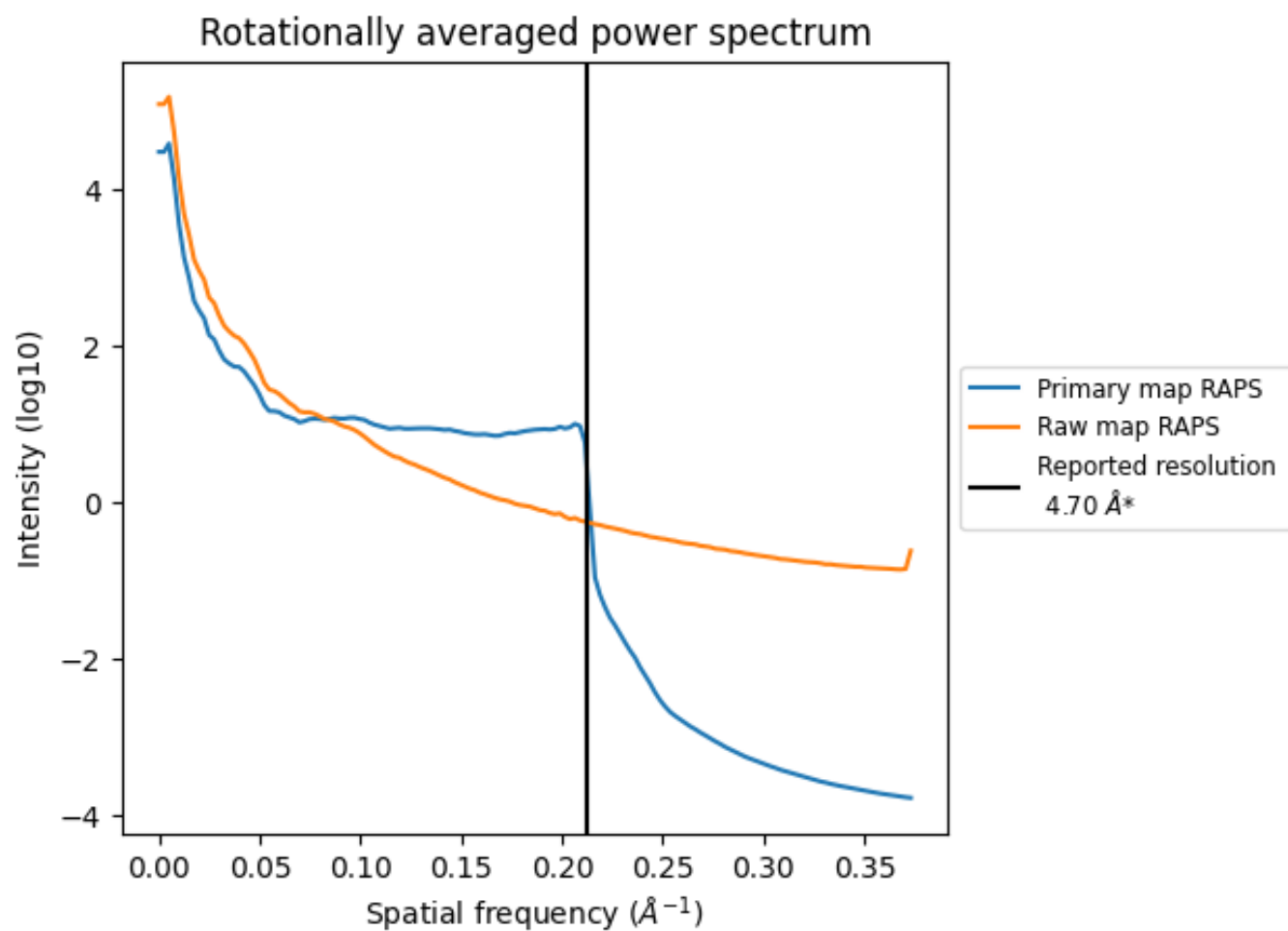
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 756 nm³; this corresponds to an approximate mass of 683 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 ⓘ

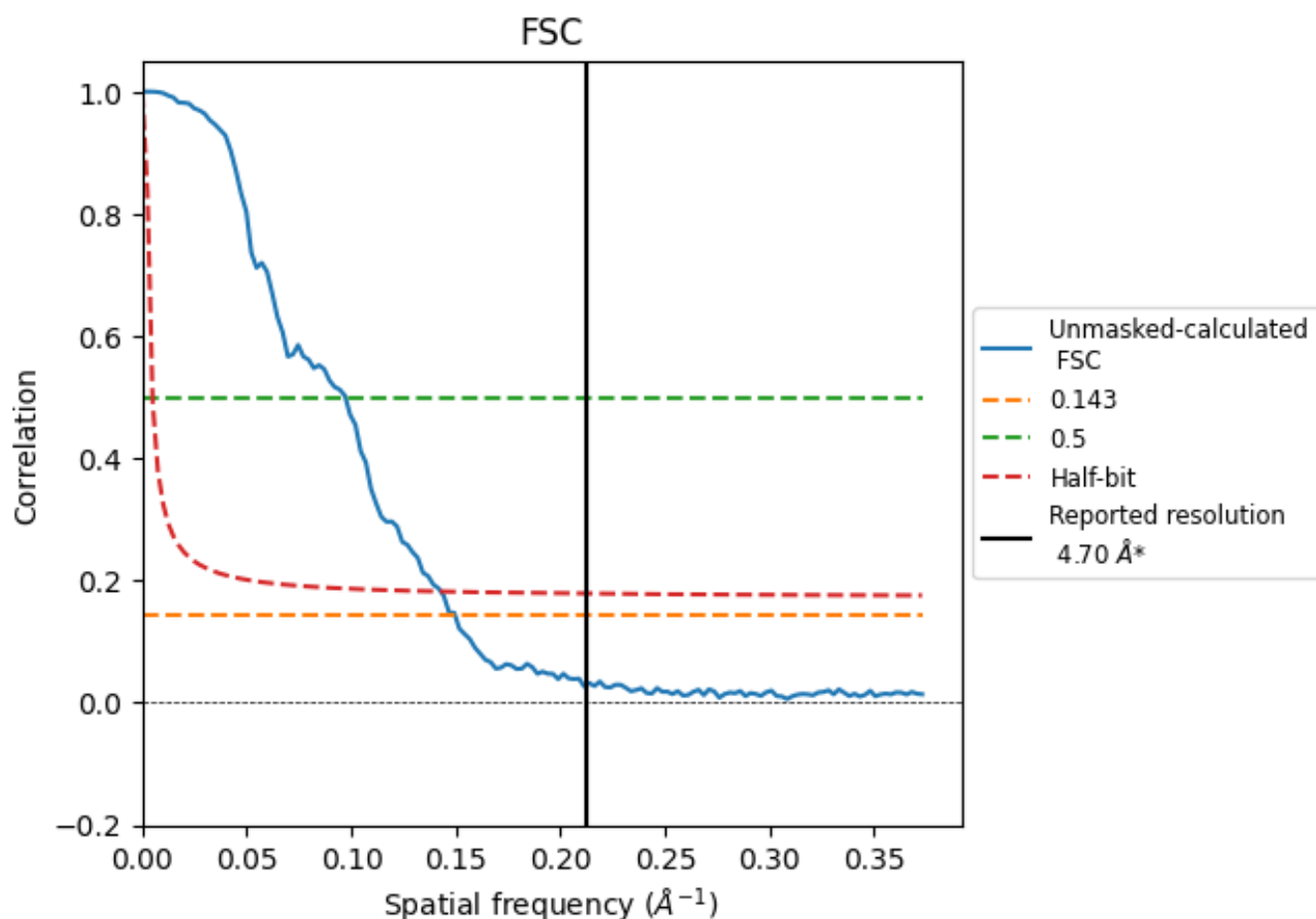


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

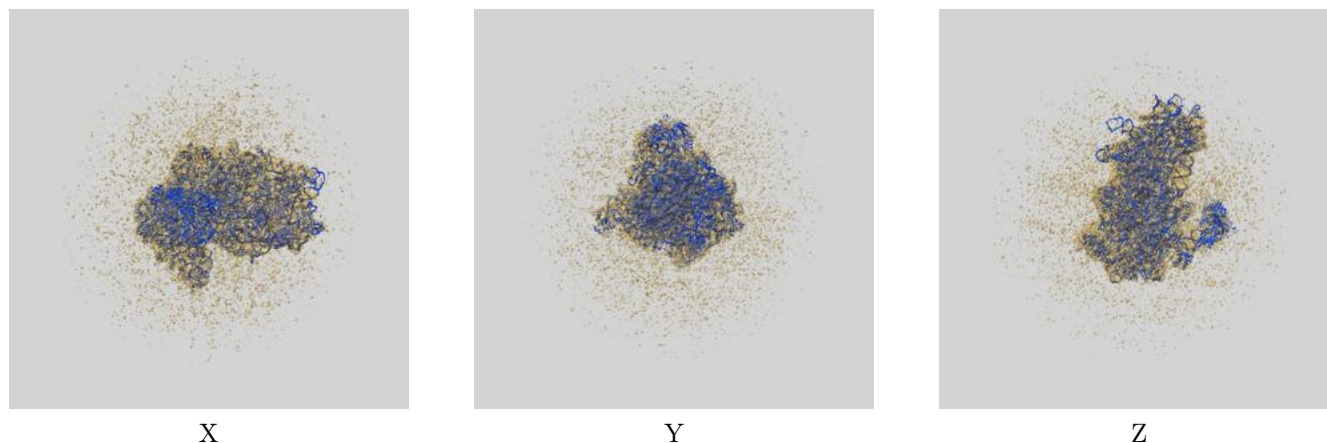
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.68	10.29	7.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.68 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

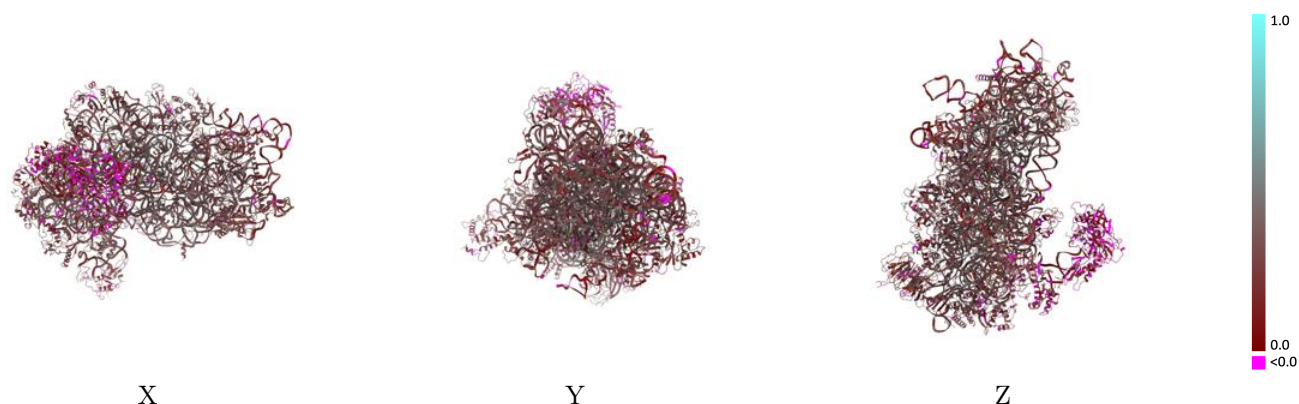
This section contains information regarding the fit between EMDB map EMD-19807 and PDB model 8S8J. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



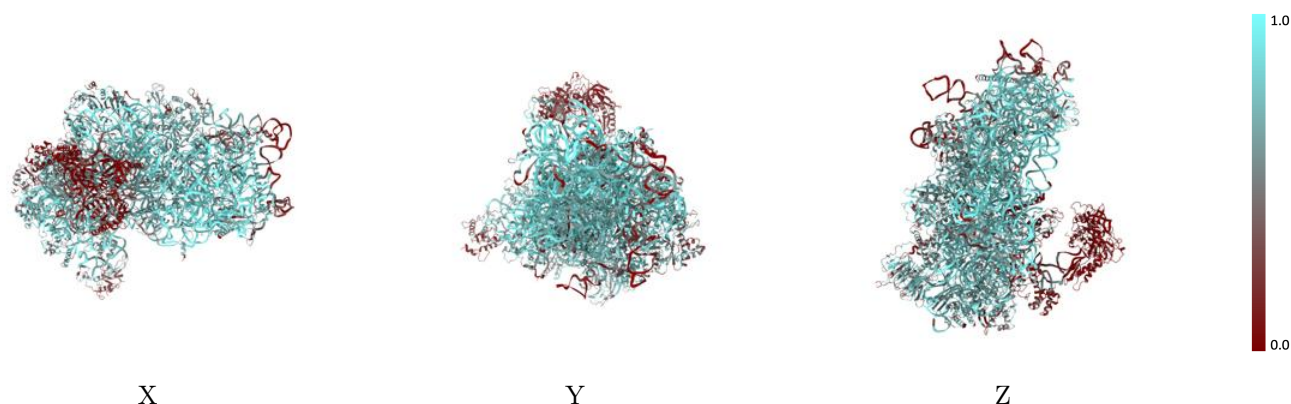
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



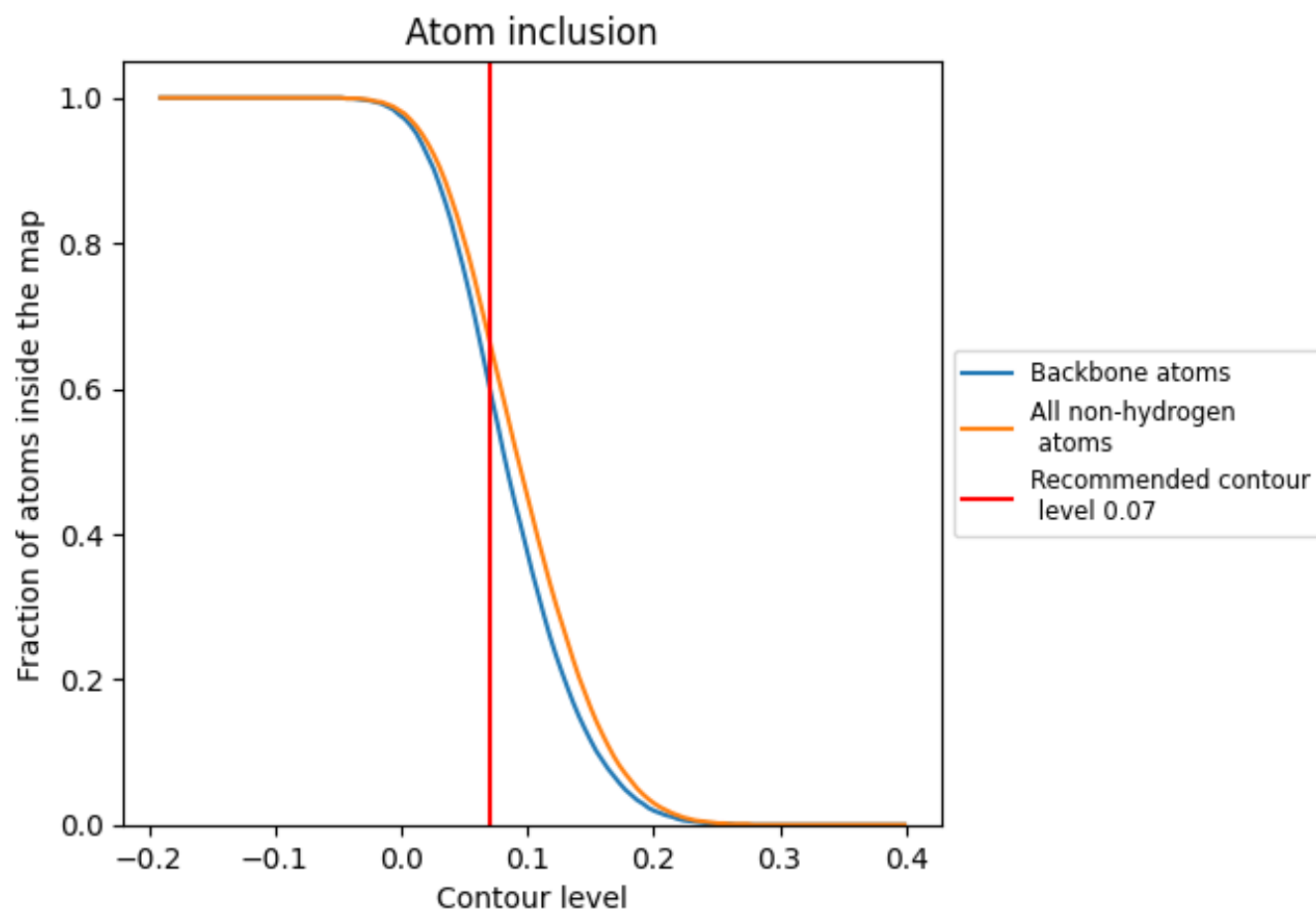
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 67% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.2860
1	 0.4260	 0.1860
2	 0.8270	 0.3100
3	 0.3390	 0.2960
A	 0.6820	 0.3010
B	 0.6330	 0.2720
C	 0.7150	 0.3430
D	 0.6510	 0.3170
E	 0.7210	 0.3290
F	 0.6500	 0.2940
G	 0.6970	 0.2800
H	 0.5190	 0.2870
I	 0.6620	 0.3110
J	 0.6820	 0.3110
K	 0.6530	 0.2680
L	 0.6300	 0.3290
M	 0.2510	 0.2140
N	 0.6900	 0.3140
O	 0.6670	 0.2990
P	 0.6890	 0.2790
Q	 0.7010	 0.2920
R	 0.5710	 0.2870
S	 0.6930	 0.2780
T	 0.7190	 0.2830
U	 0.5770	 0.2990
V	 0.7410	 0.3230
W	 0.6640	 0.3380
X	 0.7020	 0.3580
Y	 0.7160	 0.3100
Z	 0.3710	 0.2090
a	 0.6650	 0.3510
b	 0.6250	 0.3160
c	 0.5870	 0.3320
d	 0.7380	 0.3290
e	 0.5330	 0.3060



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Chain	Atom inclusion	Q-score
f	 0.3860	 0.2220
g	 0.6340	 0.2660
h	 0.1410	 0.2260
i	 0.2530	 0.2790
j	 0.1440	 0.1360
k	 0.0590	 0.0730
l	 0.0430	 0.0560
m	 0.2370	 0.1590