



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 04:28 PM UTC

PDB ID : 8S8H / pdb_00008s8h
EMDB ID : EMD-19805
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation (model py48S-AUC-2.2)
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-03-06
Resolution : 4.00 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:

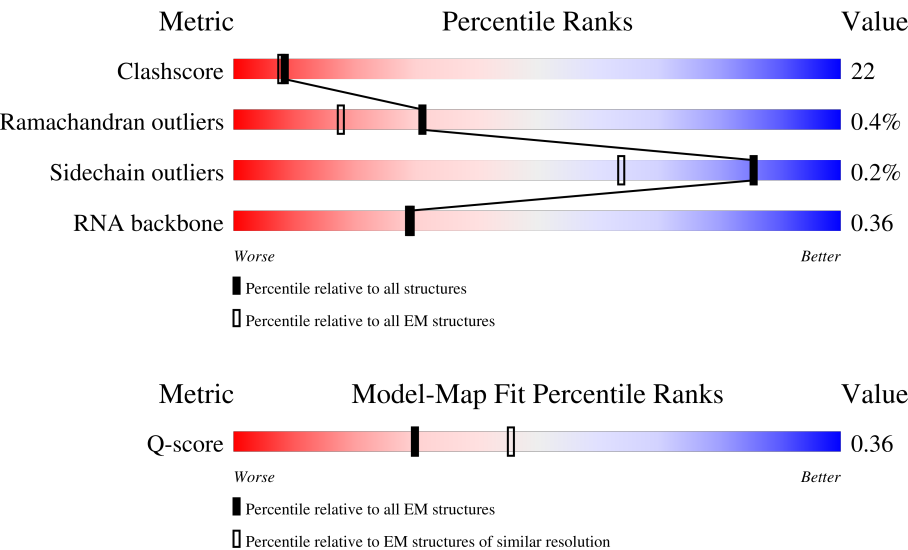
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.00 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.



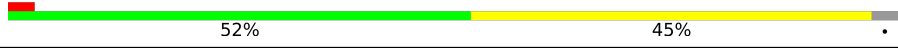
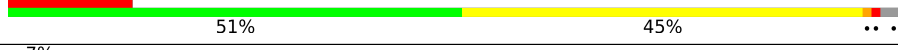
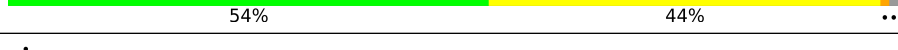
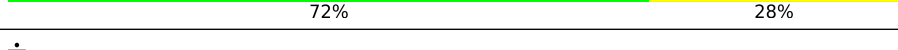
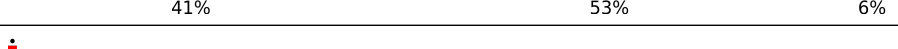
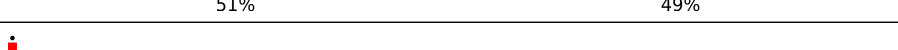
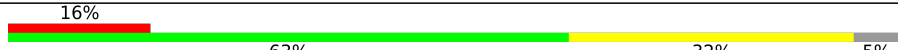
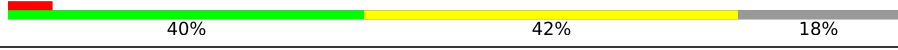
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	7% 21% 57% 21%
2	A	254	5% 47% 39% 14%
3	B	255	6% 45% 41% 12%

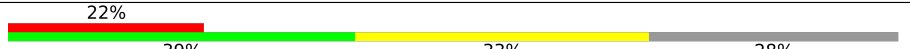
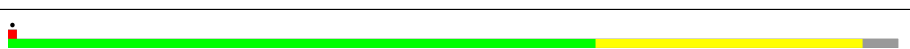
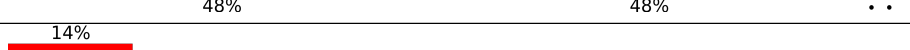
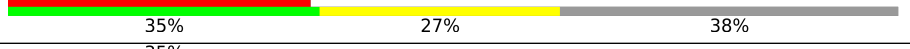
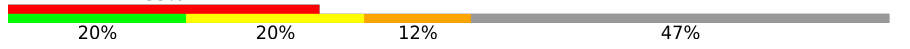
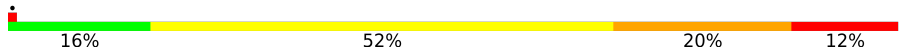
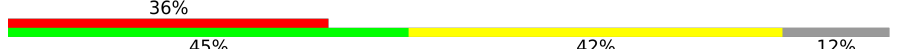
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Mol	Chain	Length	Quality of chain
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q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

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 86900 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
			2145	1369	358	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	134	Total	C	N	O	S	0	0
			1083	689	194	193	7		

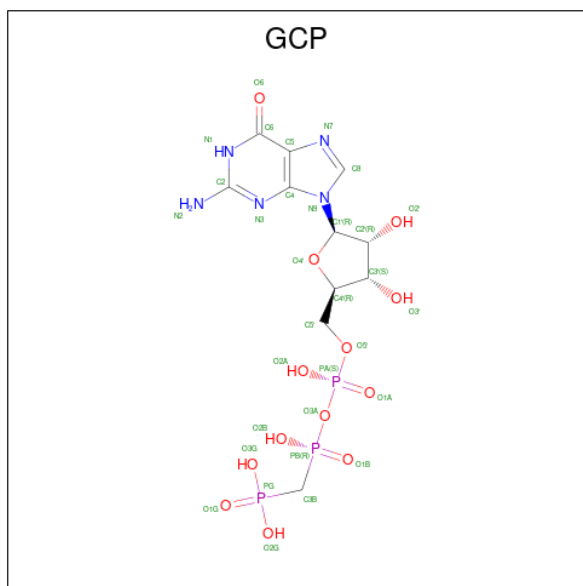
- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
42	2	111	Total 111	Mg 111	0
42	N	1	Total 1	Mg 1	0
42	Q	1	Total 1	Mg 1	0
42	i	1	Total 1	Mg 1	0
42	3	1	Total 1	Mg 1	0
42	k	1	Total 1	Mg 1	0

- Molecule 43 is ZINC ION (CCD ID: ZN) (formula: Zn).

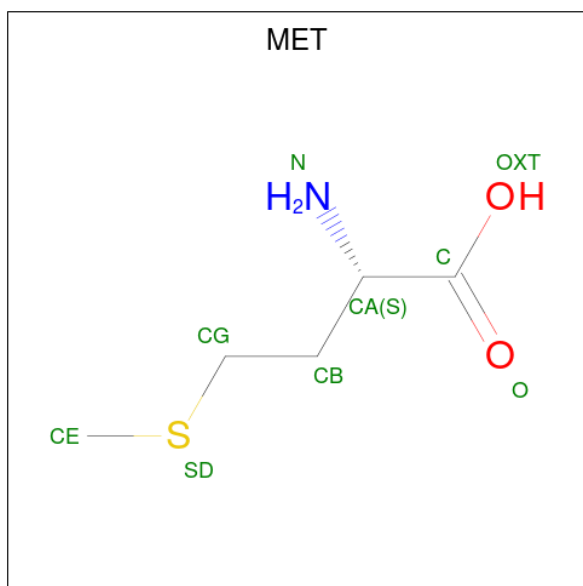
Mol	Chain	Residues	Atoms		AltConf
43	a	1	Total 1	Zn 1	0
43	b	1	Total 1	Zn 1	0
43	f	1	Total 1	Zn 1	0

- Molecule 44 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



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

- Molecule 45 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$) (labeled as "Ligand of Interest" by depositor).



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

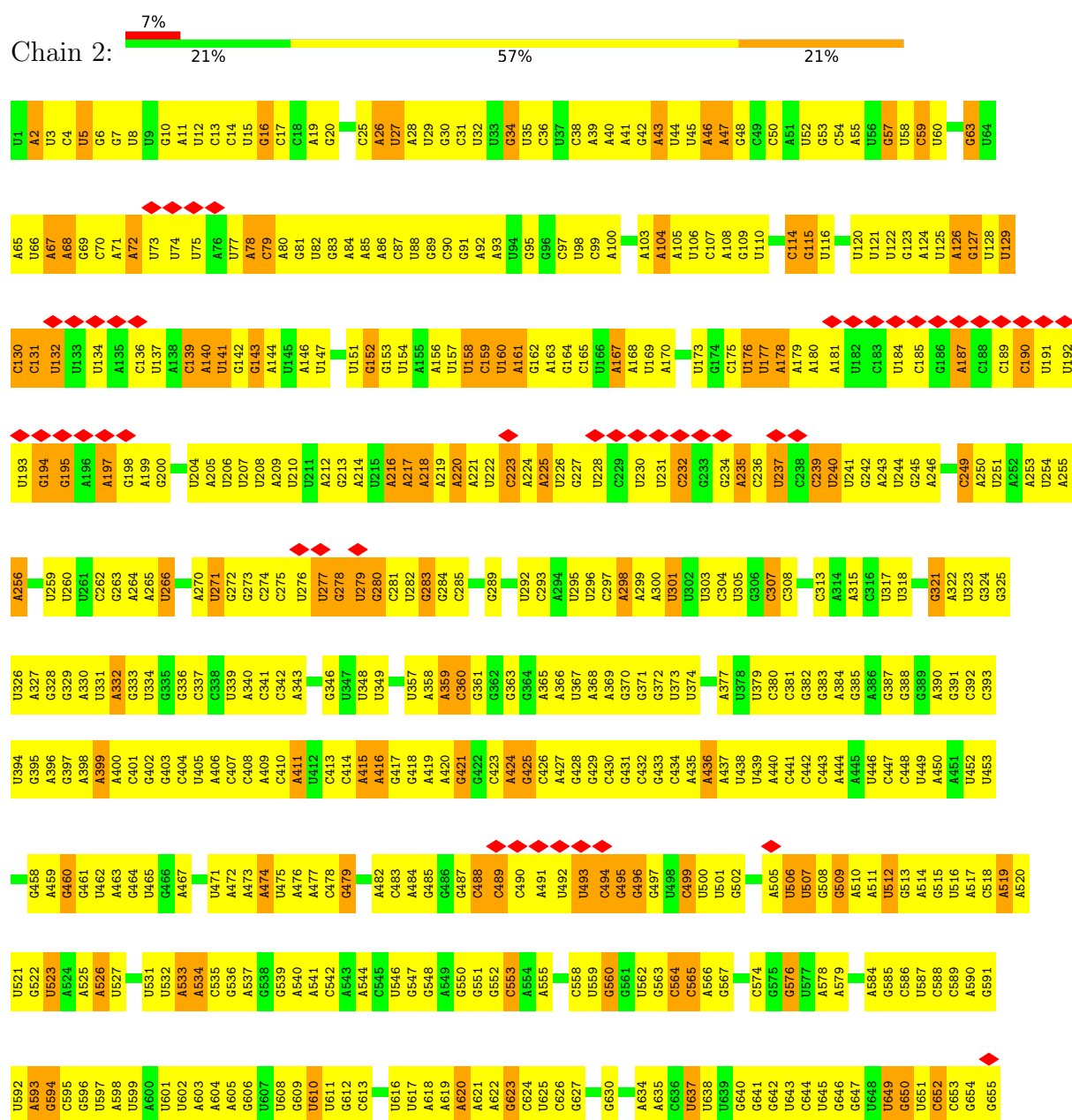
- Molecule 46 is water.

Mol	Chain	Residues	Atoms		AltConf
46	2	3	Total	O	0
			3	3	

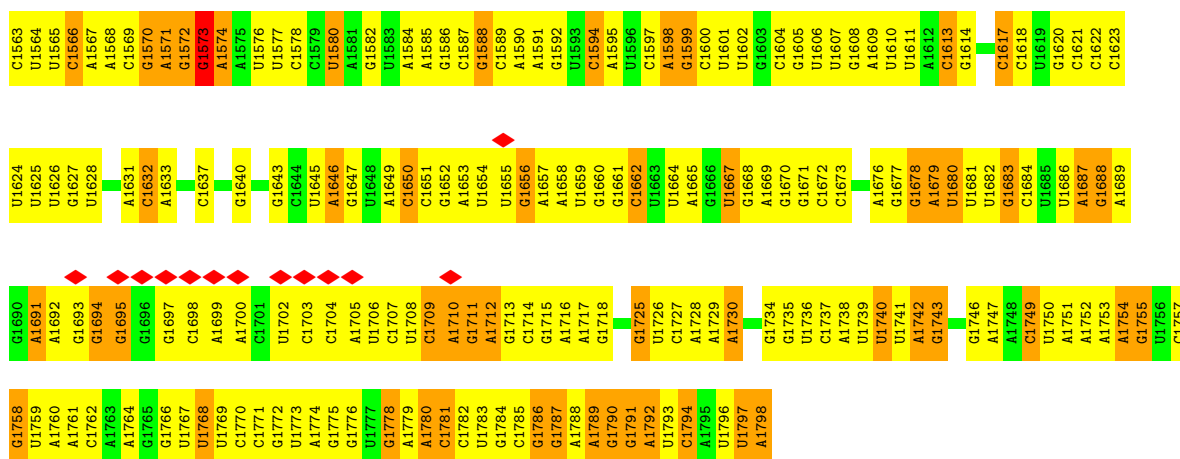
3 Residue-property plots

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.

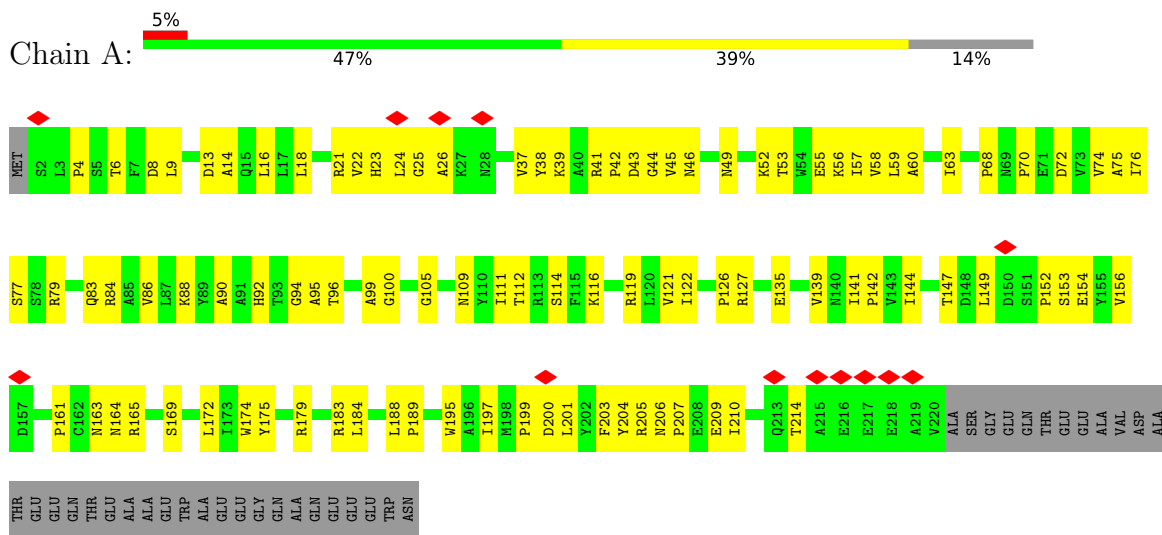
• Molecule 1: 18S ribosomal RNA



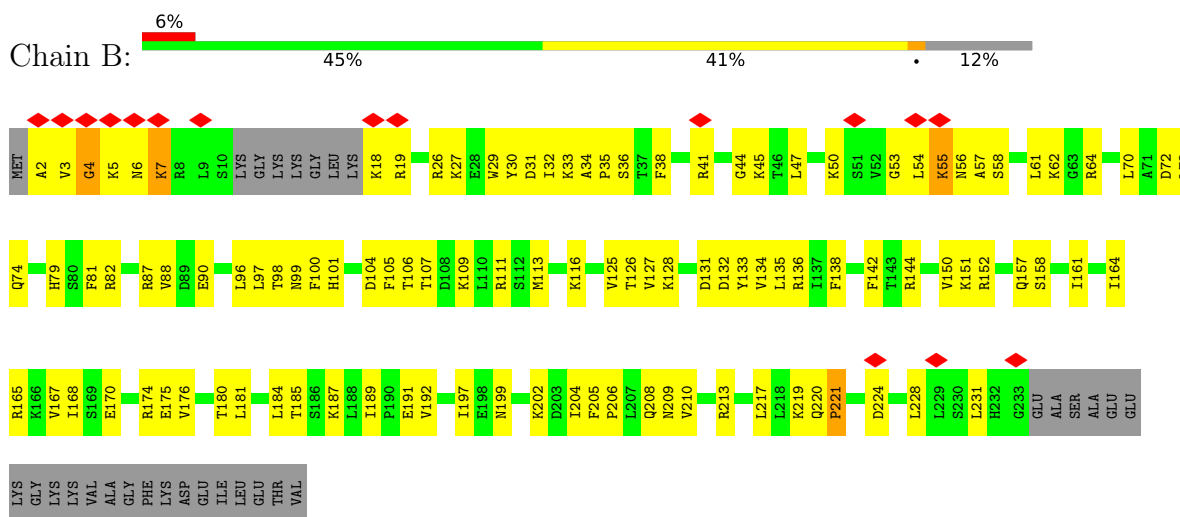
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A1501	U1432	G1363	G1298	A1237	G1168	U1103	G1040	A976	C909	G845	A780	U719	C657
A1503	G1433	C1364	A1299	U1238	G1169	C1104	G1041	A977	U910	A846	A781	G720	C658
		C1365	G1300	G1240	G1170	U1105	A1042	A978	G912		G782	U721	G659
U1506	G1437	G1366	U1301	G1241	G1171	G1106	C1043	A979	G913	G852	C783	G722	A660
C1507	C1438	U1368	U1302	G1242	G1172	G1108	C1044	G979	A914	A854	C784	G723	C661
		U1369		A1243		G1109	G1045		U915	A855	G786	G724	U862
G1510	U1441	C1370	C1305	G1244	G1177	G1110	G1046	A982	U916	G856	A787	G725	U863
U1511	A1442			C1245	C1178	G1111	U1048	G984	U917	G857	A788	U726	U864
G1512	G1443	C1371	U1309	U1246	C1179	G1112	G1049	G985	A918	U858	A789	G727	U865
A1513	U1372	U1372	U1310	C1247	G1180	G1113	G1050	G986	U919	U859	A790	G728	U866
A1514	A1444	U1373		U1248	U1181	G1114	U1051	A987	U920	U860	A791	C729	A665
U1515		U1376	U1313	U1249	A1182	A1115	G1052	U988	G921	A861	A792	A728	U866
C1516	U1447	C1377	G1314	U1250	A1183		U1053	G989	A922	A862	U793	G729	G667
U1517	A1448	U1378	G1315	C1251	U1184	U1119	U1054	G990	A923	U863	U794	G730	U868
U1518	U1450	U1379	G1316	U1252		C1120	U1055	A991	G924	A864	A795	C731	C669
G1519	A1380	A1380	G1317	U1253	G1187	G1121	U1056	A992	A925	G865	C796	G732	G670
U1520		G1381		G1254	A1188	C1122	U1057		U927	G866	C797	A733	C671
G1521	C1454		A1320	U1255	C1189	A1123	U1058	U995	A928	G867	A798	C734	G672
A1522	G1455		A1321	U1256	B8N1190	A1124	C1059	G996	A929	A868	U799	C735	
A1523	C1457		G1322	U1257		G1125	U1060	A997	C930	C869	U799		
	A1458		G1323	U1258	A1193	G1126	U1061	U998	A931	G870	G801		
U1526	C1459	U1390	A1324	U1259	C1194		U1062	U999	A932	G871	A802	C736	C675
C1527		G1391	A1325	G1260	A1195	A1131	U1063	A1000	C933	U872	A803	C737	U876
C1528	G1464	G1392	C1326	U1261	C1196	A1132		C873	C934	C873	U804	C738	G677
G1529	C1465		G1327	G1262	G1197	C1133	G1066	U1003	G935	G874	A811	G739	G678
U1530	U1466	U1393	A1328	G1263	G1198	U1134	C1067	A1004	G936	G875	U812	A740	U879
G1531	A1467	C1394	G1329	U1264	G1199	U1135	A1068	C1005	A938	G876	U813	C741	U880
C1532	C1468	C1395	A1330	G1265	G1200	U1136	C1069	G1007	A939	G877	G814	U742	U881
U1533	A1469	A1398	G1331	G1266	A1201	A1137	C1069	U1008	A940	G878	G815	U743	U882
G1534	C1470	A1399	C1332	G1267	A1202	A1138	C1070	C1009	G941	C879	A816	U744	C683
C1535	U1471	G1400	U1333	U1268	A1203	G1139	C1071	U1010	U944	U881	G817	U745	A884
U1536	A1472	C1401	U1334	G1269	C1204	G1140	G1072	A1011	U945	A882	U818	C747	A885
G1537	A1473	G1403	A1335	G1270	U1205	A1141	A1075	A1012	U946	A883	U819	U748	A886
C1538	C1474	G1404	U1336	U1271	C1206	U1142	C1076	G1013	U947	G884	U820	U749	C687
G1539	G1475	U1405	C1337	G1272	A1207	U1143	C1077	U888	A950	A886	G822	U750	G888
U1540	A1476	U1406	C1338	G1273	C1208	U1144	U1078	C1015		U887	G823	G751	A890
A1541	A1477	G1407	U1339	A1274	C1209	G1145	U1079	U1016	A951	U888	U824	A752	U891
U1542	G1478	A1408	A1340	U1275	A1210	U1146	A1080	C1020	G952	A890	U825	A753	C692
A1543	C1479	U1409	C1341	G1276	G1211	A1147	C1081	A1021	G953	A891	C826	A754	C693
G1544	A1480	G1410	U1342	G1277	G1212	G1148	A1082	A1022	A954	U892	A755	U755	U894
A1545	A1481	U1411	A1343	C1278		G1149	G1083	C1023	C955	U893	A756	A757	U895
C1546	G1482		A1344	C1279	C1215	A1150	A1084	U1024		G894	U827	U758	C696
C1547	C1483	U1412	A1345	G1280	A1216	A1151	G1084	U1025	U958	A890	U832	U759	C697
U1548	G1484	U1413	U1346	U1281	G1217	G1152	A1085	A1026	U959	C896	U833	A760	U898
A1549	A1485	G1414	A1347	U1282	A1218	G1153	A1086	U1027	U960	A897	U834	G761	U899
U1550	G1486	A1415		C1283	A1219	G1154	A1087	C1028	C961	G898	U835	A762	C700
G1551	U1487	G1416	G1350	U1284	A1220	C1155	A1087	U1029	A962	G900	G836	G763	U701
U1552	A1488	G1417	U1351	U1285		U1156		A1030	U964	G901	G837	U764	G702
A1553	C1489	C1418	U1352	A1286	U1224	C1157	A1090	G1033	A966	U902	U938	G765	G703
U1554	A1490		G1353	G1287		C1158	A1091	G1034	U967	U903	U939	U766	C704
U1555	A1491	A1423	C1354	U1288	G1227	A1159	A1092	A1031	A968	G904	U940	C767	
U1556	C1424	U1289	U1355	U1289	G1228	C1160		C1032	U969	G905	C941	C768	A707
A1557	G1356	G1290	G1357	G1291	A1229	C1161	U1096	G1033	A966	U902	U942	C773	C708
U1558	G1357	U1230	C1358	U1292	U1230	A1162	U1097	G1034	A967	U903	A905	C774	C709
U1559	G1427	C1359	C1358	U1293	A1233	G1163	U1098	A1035	C968	A904	C942	C775	G711
G1560	U1428	C1360	A1359	G1294	A1234	G1164	U1098	C1036	U969	A906	U943	C776	G712
C1561	C1498		U1361	A1295	A1235	G1166	G1100	U1037		A907	U944	C777	C713
U1562								A1038	A972	U907	A843	C778	C714
													C715
													C716
													C717



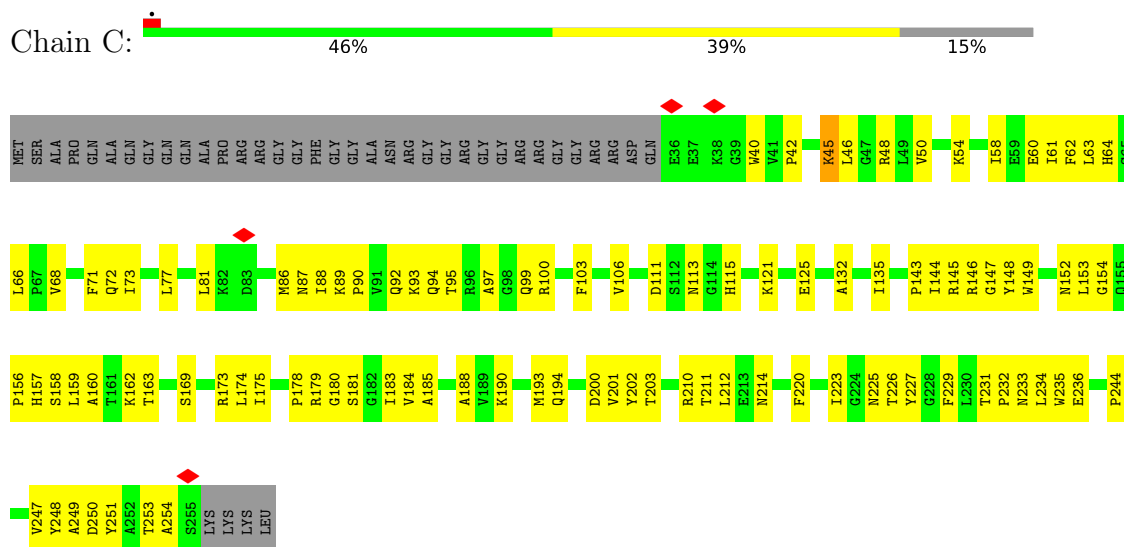
• Molecule 2: Small ribosomal subunit protein uS2



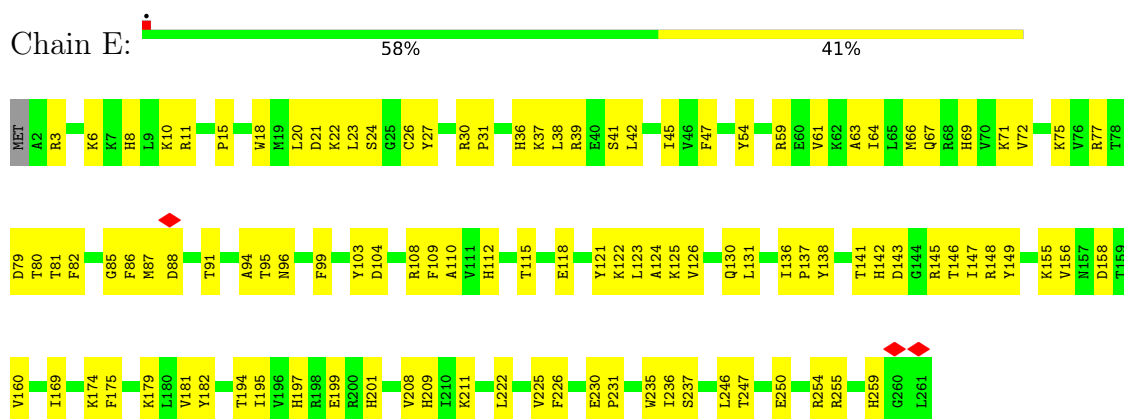
• Molecule 3: Small ribosomal subunit protein eS1



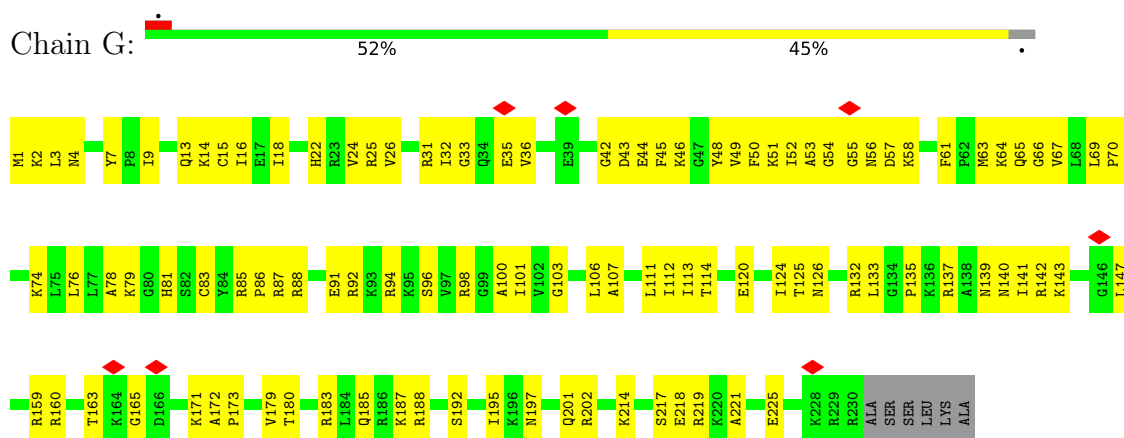
• Molecule 4: Small ribosomal subunit protein uS5



• Molecule 5: 40S ribosomal protein S4

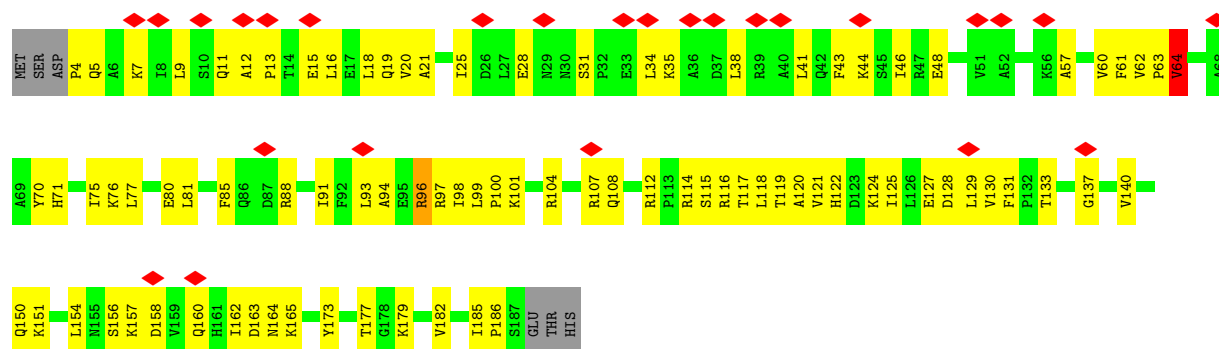


• Molecule 6: Small ribosomal subunit protein eS6

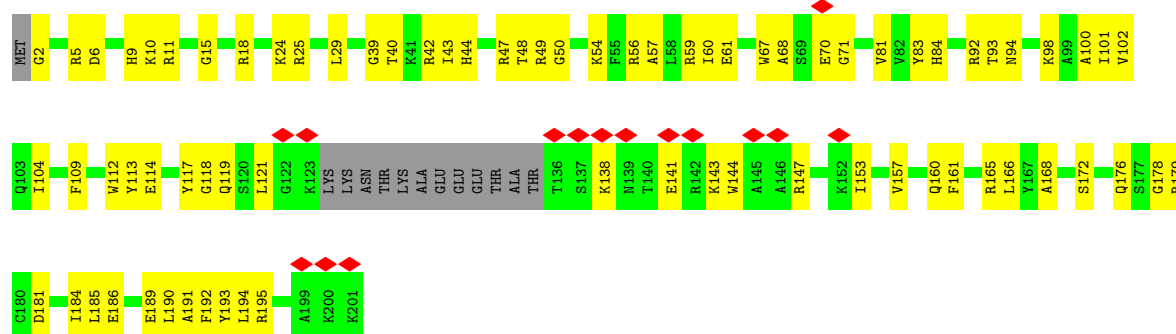


• Molecule 7: 40S ribosomal protein S7

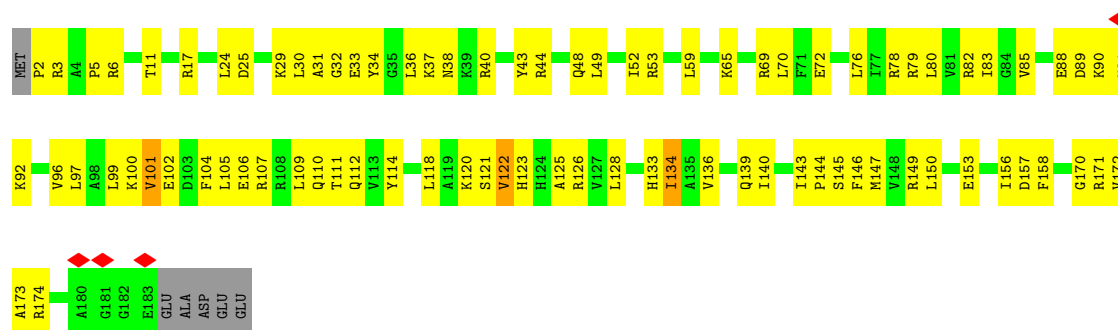




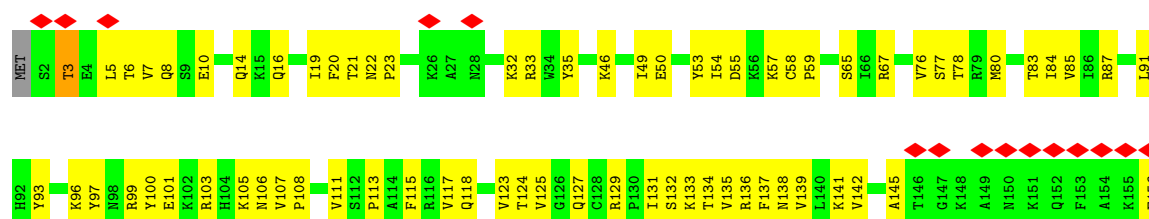
• Molecule 8: 40S ribosomal protein S8



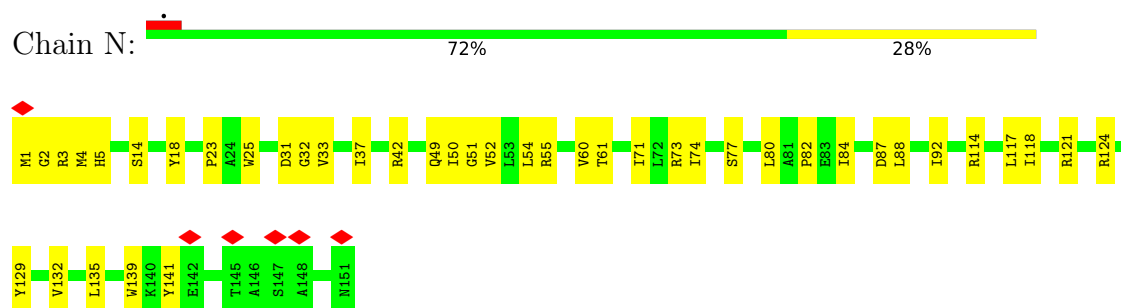
• Molecule 9: KLLA0E23673p



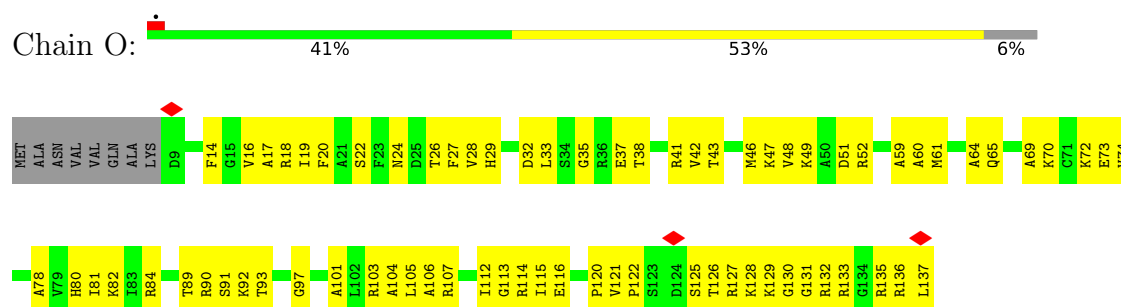
• Molecule 10: KLLA0A10483p



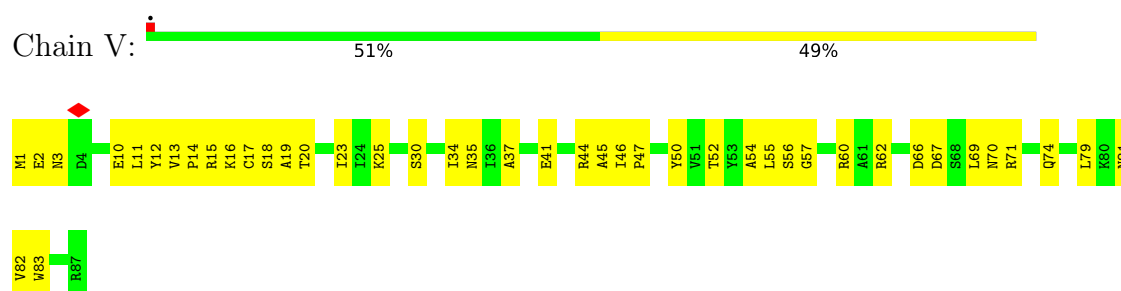
- Molecule 11: KLLA0F18040p



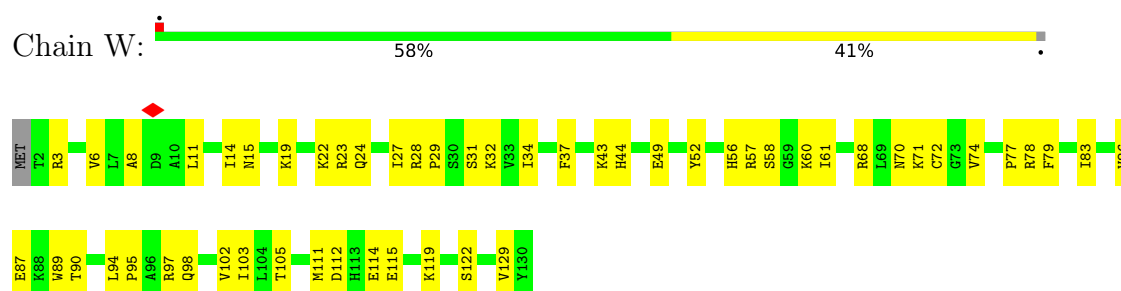
- Molecule 12: Small ribosomal subunit protein uS11



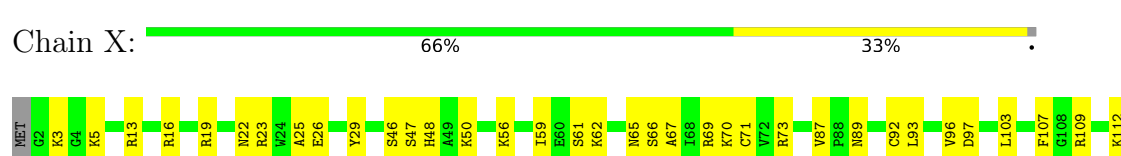
- Molecule 13: 40S ribosomal protein S21



- Molecule 14: Small ribosomal subunit protein uS8



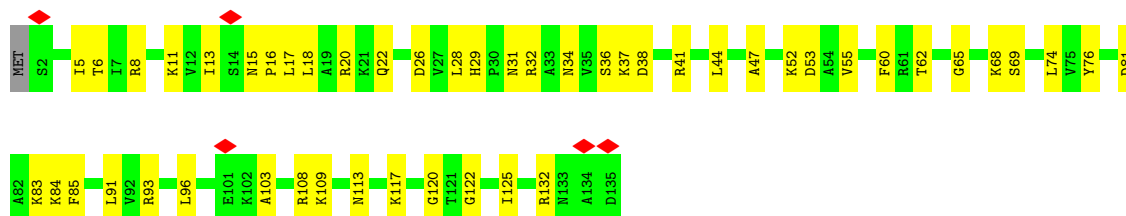
- Molecule 15: KLLA0B11231p





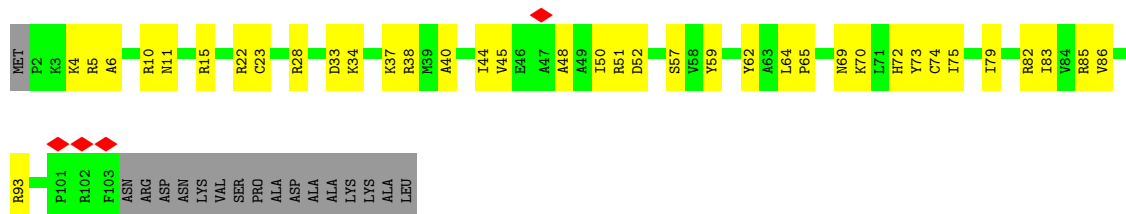
- Molecule 16: 40S ribosomal protein S24

Chain Y: 63% 36%



- Molecule 17: 40S ribosomal protein S26

Chain a: 55% 31% 14%



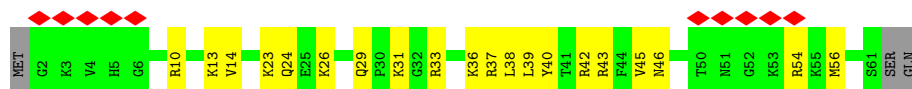
- Molecule 18: 40S ribosomal protein S27

Chain b: 57% 41%



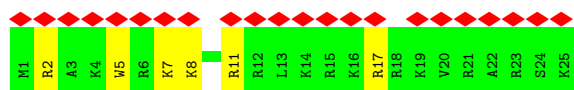
- Molecule 19: 40S ribosomal protein S30

Chain e: 16% 63% 32% 5%



- Molecule 20: 40S ribosomal protein L41-A

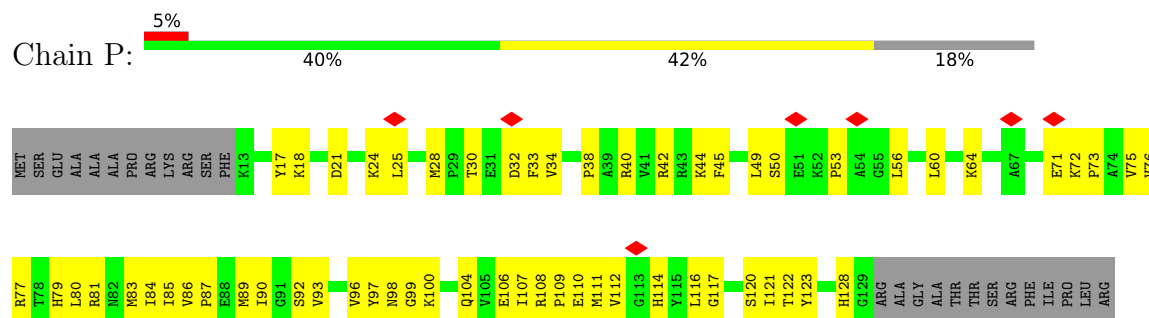
Chain h: 88% 76% 24%



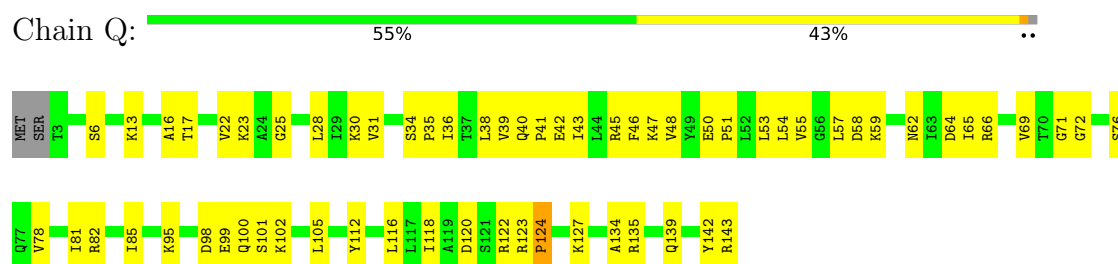
- Molecule 21: 40S ribosomal protein S3



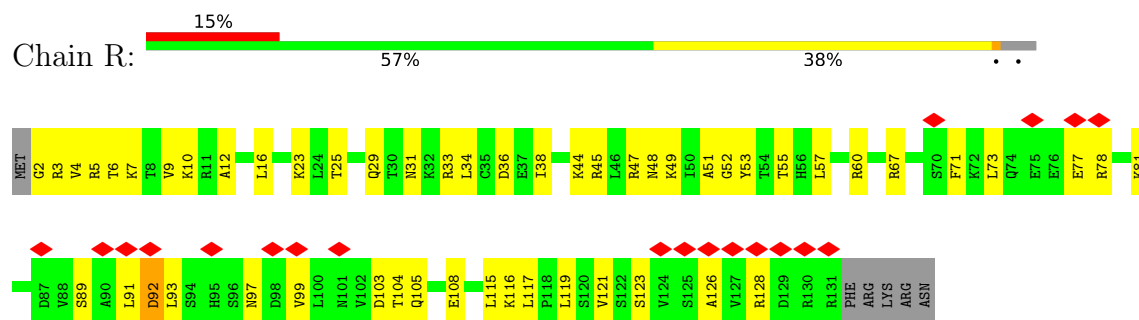
- Molecule 25: KLLA0F07843p



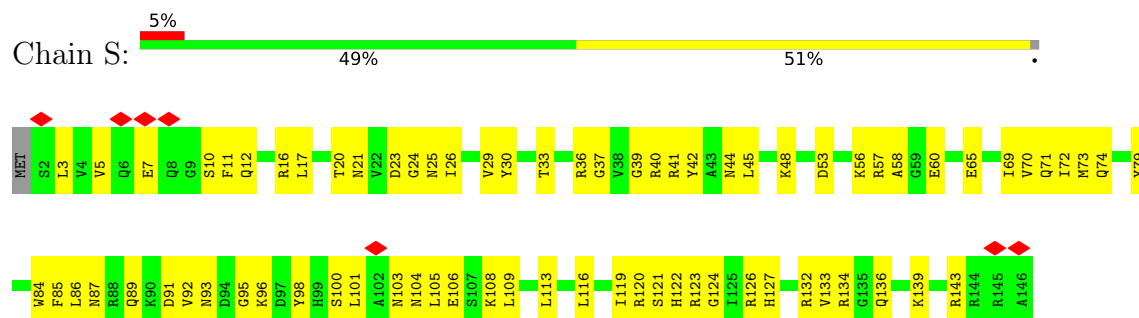
- Molecule 26: Small ribosomal subunit protein uS9



- Molecule 27: KLLA0B01474p

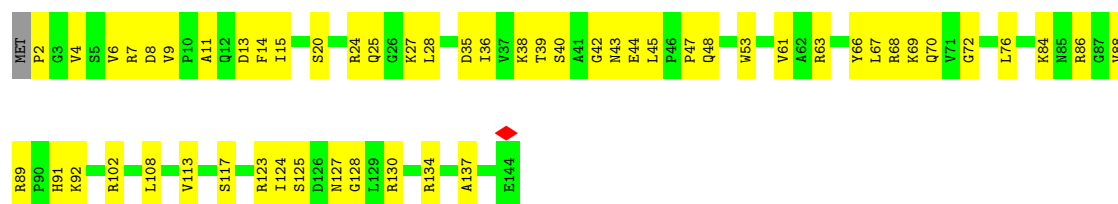


- Molecule 28: KLLA0B01562p



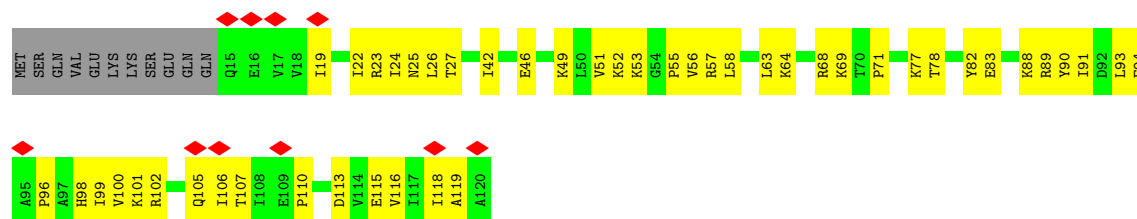
- Molecule 29: KLLA0A07194p

Chain T: 



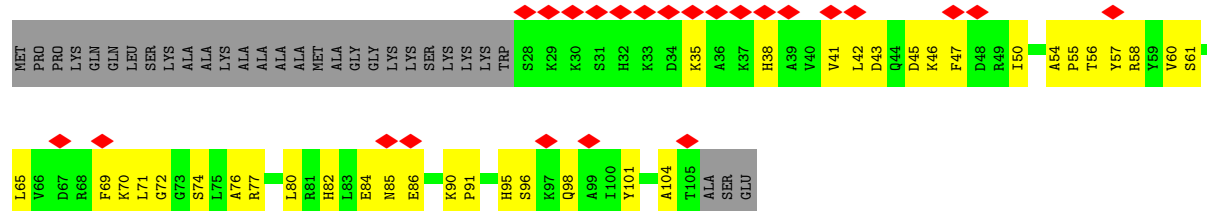
- Molecule 30: Small ribosomal subunit protein uS10

Chain U: 



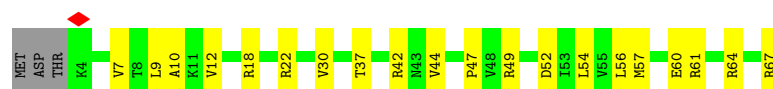
- Molecule 31: 40S ribosomal protein S25

Chain Z: 



- Molecule 32: Small ribosomal subunit protein eS28

Chain c: 



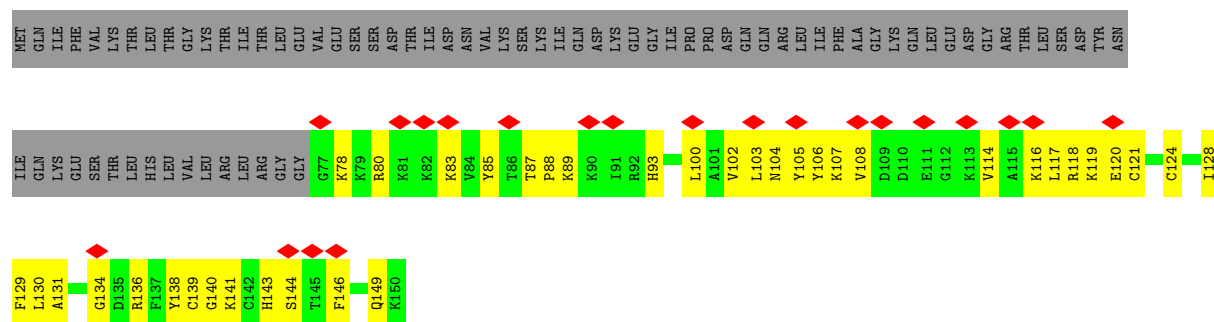
- Molecule 33: Small ribosomal subunit protein uS14

Chain d: 

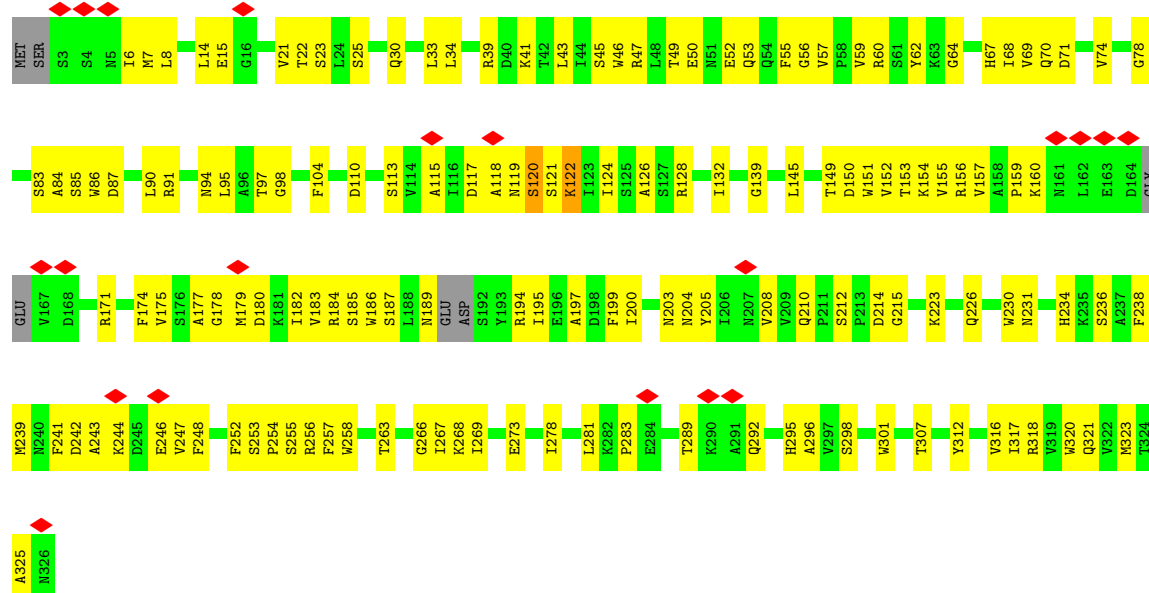


- Molecule 34: Small ribosomal subunit protein eS31

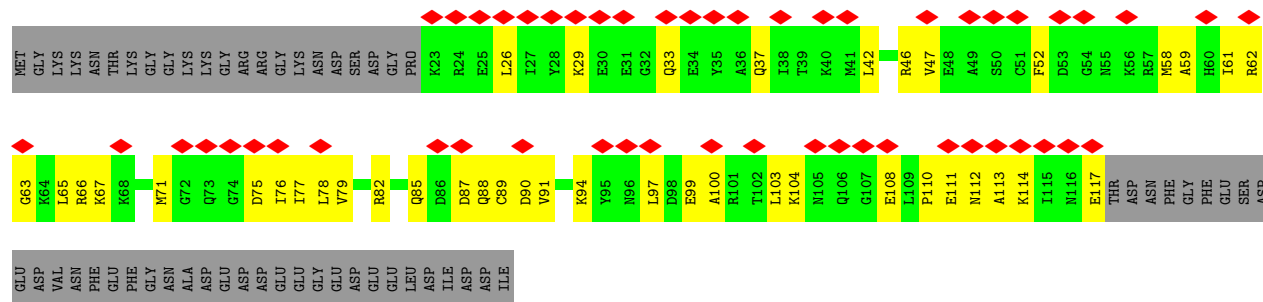
Chain f: 



• Molecule 35: KLLA0E12277p

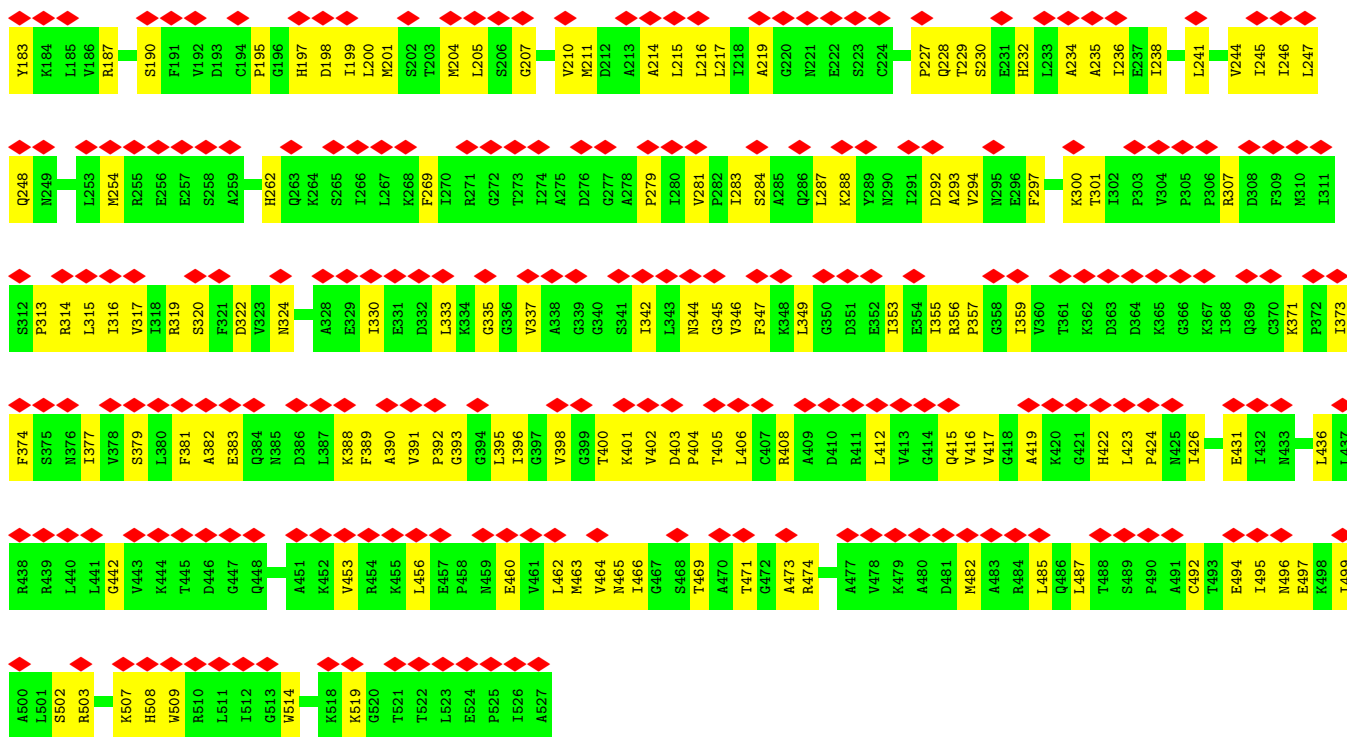


• Molecule 36: Eukaryotic translation initiation factor 1A

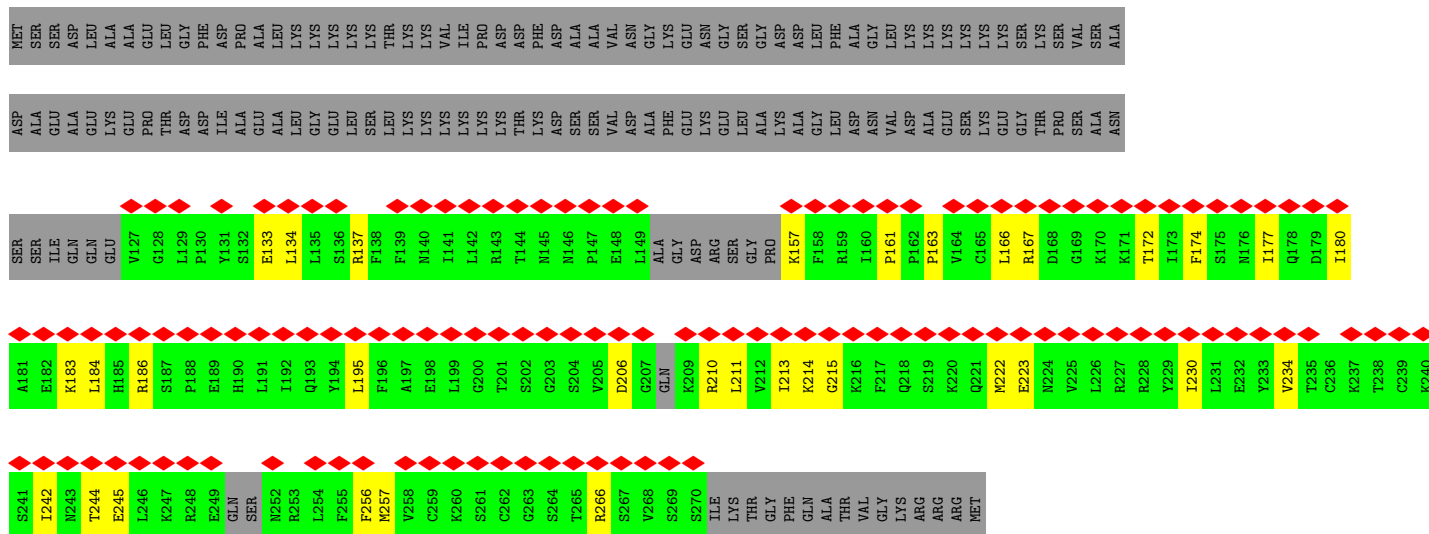
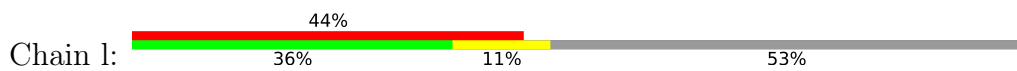


• Molecule 37: mRNA (5'-R(P*AP*AP*U)-3')





- Molecule 41: Eukaryotic translation initiation factor 2 subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24107	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	0.481	Depositor
Minimum map value	-0.273	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: 5MC, T6A, B8N, ZN, MA6, M2G, 2MG, 1MA, H2U, RIA, 1MG, MG, GCP, 7MG, PSU

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	0.22	0/42410	0.35	0/66079
2	A	0.21	0/1742	0.47	2/2383 (0.1%)
3	B	0.24	0/1820	0.52	0/2448
4	C	0.27	0/1678	0.50	0/2277
5	E	0.24	0/2122	0.48	0/2861
6	G	0.16	0/1855	0.39	0/2479
7	H	0.25	0/1507	0.52	0/2028
8	I	0.22	0/1515	0.41	0/2029
9	J	0.26	0/1495	0.48	0/2001
10	L	0.28	0/1276	0.51	0/1718
11	N	0.21	0/1218	0.40	0/1638
12	O	0.24	0/966	0.53	0/1297
13	V	0.23	0/696	0.50	1/938 (0.1%)
14	W	0.27	0/1039	0.46	0/1399
15	X	0.25	0/1137	0.49	0/1516
16	Y	0.21	0/1075	0.41	0/1433
17	a	0.23	0/810	0.47	0/1087
18	b	0.23	0/619	0.48	0/837
19	e	0.22	0/480	0.47	0/640
20	h	0.20	0/234	0.47	0/300
21	D	0.22	0/1800	0.44	0/2421
22	F	0.24	0/1628	0.45	0/2198
23	K	0.21	0/831	0.48	0/1123
24	M	0.33	0/891	0.62	0/1201
25	P	0.23	0/942	0.55	0/1269
26	Q	0.26	0/1125	0.80	2/1510 (0.1%)
27	R	0.28	0/1044	0.53	0/1402
28	S	0.19	0/1208	0.50	0/1624
29	T	0.22	0/1129	0.40	0/1520
30	U	0.21	0/857	0.42	0/1158
31	Z	0.31	0/603	0.46	0/814
32	c	0.21	0/501	0.42	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.23	0/473	0.46	1/629 (0.2%)
34	f	0.18	0/597	0.59	0/795
35	g	0.22	0/2523	0.47	0/3434
36	i	0.18	0/773	0.48	0/1031
37	3	0.15	0/595	0.28	0/920
38	1	0.25	1/1529 (0.1%)	0.51	4/2376 (0.2%)
39	j	0.21	0/2177	0.52	0/2931
40	k	0.17	0/3657	0.45	0/4946
41	l	0.14	0/1099	0.38	0/1469
All	All	0.22	1/91676 (0.0%)	0.42	10/132832 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	37	T6A	O3'-P	5.11	1.61	1.56

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Q	124	PRO	CA-C-N	15.92	143.49	121.20
26	Q	124	PRO	C-N-CA	15.92	143.49	121.20
38	1	45	U	C4'-C3'-O3'	8.08	125.12	113.00
38	1	45	U	N1-C1'-C2'	-7.12	101.32	112.00
2	A	197	ILE	CA-C-N	6.27	130.21	120.68

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	19213	1408	0
2	A	1702	0	1695	78	0
3	B	1796	0	1874	130	0
4	C	1648	0	1727	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2078	0	2157	108	0
6	G	1832	0	1919	89	0
7	H	1483	0	1579	94	0
8	I	1489	0	1504	84	0
9	J	1471	0	1554	82	0
10	L	1248	0	1311	62	0
11	N	1195	0	1263	41	0
12	O	955	0	987	77	0
13	V	687	0	682	38	0
14	W	1021	0	1056	51	0
15	X	1119	0	1198	45	0
16	Y	1061	0	1111	46	0
17	a	797	0	835	42	0
18	b	609	0	630	27	0
19	e	472	0	508	28	0
20	h	233	0	284	11	0
21	D	1774	0	1855	57	0
22	F	1609	0	1679	92	0
23	K	809	0	810	48	0
24	M	885	0	917	62	0
25	P	923	0	960	56	0
26	Q	1105	0	1170	70	0
27	R	1033	0	1082	50	0
28	S	1189	0	1211	79	0
29	T	1110	0	1124	52	0
30	U	845	0	913	44	0
31	Z	594	0	590	35	0
32	c	499	0	536	18	0
33	d	461	0	448	34	0
34	f	584	0	600	37	0
35	g	2469	0	2403	118	0
36	i	764	0	763	38	0
37	3	536	0	277	11	0
38	1	1639	0	852	61	0
39	j	2145	0	2216	109	0
40	k	3596	0	3713	146	0
41	l	1083	0	1123	22	0
42	2	111	0	0	0	0
42	3	1	0	0	0	0
42	N	1	0	0	0	0
42	Q	1	0	0	0	0
42	i	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	k	1	0	0	0	0
43	a	1	0	0	0	0
43	b	1	0	0	0	0
43	f	1	0	0	0	0
44	k	32	0	13	4	0
45	k	8	0	8	4	0
46	2	3	0	0	0	0
All	All	86900	0	68350	3295	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 22.

The worst 5 of 3295 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)
3:B:5:LYS:NZ	3:B:7:LYS:HA	1.36	1.40
7:H:94:ALA:O	7:H:96:ARG:HD2	1.27	1.29
3:B:5:LYS:NZ	3:B:7:LYS:CA	2.13	1.11
7:H:94:ALA:O	7:H:96:ARG:CD	2.00	1.09
24:M:95:GLY:HA3	24:M:104:ARG:HH11	1.19	1.08

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%)	192 (87%)	25 (11%)	4 (2%)	6	34
4	C	218/259 (84%)	195 (89%)	22 (10%)	1 (0%)	24	60
5	E	258/261 (99%)	234 (91%)	24 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	228/236 (97%)	215 (94%)	13 (6%)	0	100	100
7	H	182/190 (96%)	159 (87%)	22 (12%)	1 (0%)	24	60
8	I	184/201 (92%)	166 (90%)	18 (10%)	0	100	100
9	J	180/188 (96%)	155 (86%)	22 (12%)	3 (2%)	7	36
10	L	153/156 (98%)	132 (86%)	21 (14%)	0	100	100
11	N	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
12	O	127/137 (93%)	106 (84%)	21 (16%)	0	100	100
13	V	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
14	W	127/130 (98%)	114 (90%)	13 (10%)	0	100	100
15	X	142/145 (98%)	120 (84%)	22 (16%)	0	100	100
16	Y	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
17	a	100/119 (84%)	82 (82%)	18 (18%)	0	100	100
18	b	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
19	e	58/63 (92%)	51 (88%)	7 (12%)	0	100	100
20	h	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
21	D	225/237 (95%)	209 (93%)	15 (7%)	1 (0%)	30	65
22	F	204/227 (90%)	173 (85%)	28 (14%)	3 (2%)	8	38
23	K	94/106 (89%)	80 (85%)	14 (15%)	0	100	100
24	M	113/134 (84%)	92 (81%)	19 (17%)	2 (2%)	6	34
25	P	115/142 (81%)	92 (80%)	23 (20%)	0	100	100
26	Q	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
27	R	128/136 (94%)	109 (85%)	16 (12%)	3 (2%)	5	31
28	S	143/146 (98%)	125 (87%)	18 (13%)	0	100	100
29	T	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
30	U	104/117 (89%)	91 (88%)	13 (12%)	0	100	100
31	Z	76/108 (70%)	69 (91%)	6 (8%)	1 (1%)	9	41
32	c	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
33	d	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
34	f	72/150 (48%)	53 (74%)	19 (26%)	0	100	100
35	g	314/326 (96%)	287 (91%)	25 (8%)	2 (1%)	21	57
36	i	93/153 (61%)	80 (86%)	13 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	j	263/304 (86%)	245 (93%)	17 (6%)	1 (0%)	30	65
40	k	468/527 (89%)	433 (92%)	32 (7%)	3 (1%)	21	57
41	l	126/285 (44%)	122 (97%)	4 (3%)	0	100	100
All	All	5796/6582 (88%)	5167 (89%)	604 (10%)	25 (0%)	31	65

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	7	LYS
7	H	64	VAL
22	F	103	GLY
27	R	92	ASP
35	g	120	SER

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%)	202 (100%)	0	100	100
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%)	192 (100%)	0	100	100
7	H	164/170 (96%)	162 (99%)	2 (1%)	63	73
8	I	147/159 (92%)	146 (99%)	1 (1%)	76	79
9	J	153/158 (97%)	153 (100%)	0	100	100
10	L	136/137 (99%)	135 (99%)	1 (1%)	76	79
11	N	128/128 (100%)	128 (100%)	0	100	100
12	O	97/104 (93%)	97 (100%)	0	100	100
13	V	73/73 (100%)	73 (100%)	0	100	100
14	W	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	X	119/120 (99%)	119 (100%)	0	100	100
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%)	172 (99%)	2 (1%)	65	74
23	K	88/96 (92%)	88 (100%)	0	100	100
24	M	93/109 (85%)	92 (99%)	1 (1%)	65	74
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%)	115 (99%)	1 (1%)	70	76
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%)	263 (100%)	1 (0%)	84	84
36	i	80/130 (62%)	80 (100%)	0	100	100
39	j	240/274 (88%)	240 (100%)	0	100	100
40	k	393/449 (88%)	393 (100%)	0	100	100
41	l	125/246 (51%)	125 (100%)	0	100	100
All	All	4975/5595 (89%)	4966 (100%)	9 (0%)	85	87

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	R	92	ASP
35	g	122	LYS
10	L	3	THR

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Mol	Chain	Res	Type
22	F	40	GLN
22	F	104	ARG

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

Mol	Chain	Res	Type
22	F	171	ASN
40	k	415	GLN
28	S	74	GLN
40	k	384	GLN
41	l	218	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	581 (32%)	24 (1%)
37	3	25/49 (51%)	14 (56%)	0
38	1	72/75 (96%)	31 (43%)	6 (8%)
All	All	1894/1922 (98%)	626 (33%)	30 (1%)

5 of 626 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	5	U
1	2	16	G
1	2	17	C

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1240	G
38	1	44	A
1	2	1470	C
38	1	74	C
38	1	8	U

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	4.66	14 (40%)	50,57,60	2.10	13 (26%)
1	5MC	2	1637	1	19,22,23	3.75	8 (42%)	26,32,35	1.00	1 (3%)
1	PSU	2	998	1	18,21,22	4.36	7 (38%)	21,30,33	1.94	5 (23%)
1	B8N	2	1190	1	25,29,30	3.31	8 (32%)	28,42,45	2.12	8 (28%)
38	M2G	1	26	38	24,27,28	2.63	7 (29%)	33,40,43	1.70	8 (24%)
1	5MC	2	1006	1	19,22,23	3.70	8 (42%)	26,32,35	1.03	2 (7%)
38	1MG	1	9	38	23,26,27	3.27	7 (30%)	33,39,42	2.26	8 (24%)
38	H2U	1	47	38	18,21,22	3.15	4 (22%)	19,30,33	1.43	4 (21%)
38	7MG	1	46	38	23,26,27	3.52	10 (43%)	27,39,42	2.26	9 (33%)
1	2MG	2	1570	1	23,26,27	2.94	9 (39%)	33,38,41	2.20	12 (36%)
1	PSU	2	465	1	18,21,22	4.33	7 (38%)	21,30,33	1.91	5 (23%)
1	PSU	2	120	1	18,21,22	4.32	7 (38%)	21,30,33	2.07	5 (23%)
38	2MG	1	10	38	23,26,27	2.86	9 (39%)	33,38,41	2.16	10 (30%)
38	T6A	1	37	38	31,34,35	1.81	8 (25%)	43,49,52	2.19	12 (27%)
1	PSU	2	766	1	18,21,22	4.38	7 (38%)	21,30,33	2.05	6 (28%)
38	H2U	1	16	38	18,21,22	3.08	4 (22%)	19,30,33	1.46	4 (21%)
38	1MA	1	58	38	21,25,26	3.10	6 (28%)	30,37,40	2.40	8 (26%)
1	PSU	2	1289	1	18,21,22	4.33	7 (38%)	21,30,33	1.89	5 (23%)
38	5MC	1	48	38	19,22,23	3.79	8 (42%)	26,32,35	1.15	1 (3%)
38	5MC	1	49	38	19,22,23	3.91	8 (42%)	26,32,35	1.05	1 (3%)
1	7MG	2	1573	1	23,26,27	3.46	10 (43%)	27,39,42	2.31	9 (33%)
1	2MG	2	1426	42,1	23,26,27	2.85	9 (39%)	33,38,41	2.39	11 (33%)
1	MA6	2	1780	1	23,26,27	1.40	4 (17%)	33,38,41	3.48	13 (39%)

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	-	5/17/51/52	0/4/4/4
1	5MC	2	1637	1	-	1/7/25/26	0/2/2/2
1	PSU	2	998	1	-	0/7/25/26	0/2/2/2
1	B8N	2	1190	1	-	5/16/34/35	0/2/2/2
38	M2G	1	26	38	-	4/11/29/30	0/3/3/3
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
38	1MG	1	9	38	-	2/7/25/26	0/3/3/3
38	H2U	1	47	38	-	4/7/38/39	0/2/2/2
38	7MG	1	46	38	-	2/7/37/38	0/3/3/3
1	2MG	2	1570	1	-	1/9/27/28	0/3/3/3
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
1	PSU	2	120	1	-	0/7/25/26	0/2/2/2
38	2MG	1	10	38	-	2/9/27/28	0/3/3/3
38	T6A	1	37	38	-	5/23/41/42	0/3/3/3
1	PSU	2	766	1	-	2/7/25/26	0/2/2/2
38	H2U	1	16	38	-	6/7/38/39	0/2/2/2
38	1MA	1	58	38	-	2/7/25/26	0/3/3/3
1	PSU	2	1289	1	-	1/7/25/26	0/2/2/2
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2
38	5MC	1	49	38	-	3/7/25/26	0/2/2/2
1	7MG	2	1573	1	-	4/7/37/38	0/3/3/3
1	2MG	2	1426	42,1	-	0/9/27/28	0/3/3/3
1	MA6	2	1780	1	-	6/11/29/30	0/3/3/3

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	64	RIA	C1'-C2'	-16.39	1.32	1.52
1	2	766	PSU	C6-C5	11.53	1.48	1.35
1	2	1289	PSU	C6-C5	11.43	1.47	1.35
1	2	465	PSU	C6-C5	11.41	1.47	1.35
1	2	998	PSU	C6-C5	11.41	1.47	1.35

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	N1-C6-N6	-13.37	100.56	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	C5-C6-N6	8.82	139.29	125.33
1	2	1426	2MG	C2-N3-C4	6.97	120.72	112.00
38	1	58	1MA	C1'-N9-C8	-6.90	107.13	126.73
1	2	1570	2MG	C2-N3-C4	6.45	120.07	112.00

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1573	7MG	O4'-C4'-C5'-O5'
1	2	1780	MA6	O4'-C4'-C5'-O5'
1	2	1780	MA6	C5-C6-N6-C10
1	2	1780	MA6	N1-C6-N6-C10
38	1	9	1MG	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	1	64	RIA	5	0
1	2	998	PSU	1	0
38	1	26	M2G	1	0
1	2	1006	5MC	1	0
38	1	9	1MG	1	0
38	1	47	H2U	1	0
38	1	46	7MG	1	0
1	2	1570	2MG	1	0
38	1	10	2MG	1	0
38	1	37	T6A	2	0
38	1	16	H2U	1	0
38	1	58	1MA	2	0
1	2	1289	PSU	1	0
38	1	48	5MC	1	0
1	2	1573	7MG	4	0
1	2	1426	2MG	2	0
1	2	1780	MA6	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
45	MET	k	603	-	6,7,8	0.48	0	2,7,9	0.25	0
44	GCP	k	601	-	32,34,34	3.18	12 (37%)	49,54,54	1.65	9 (18%)

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
45	MET	k	603	-	-	0/5/6/8	-
44	GCP	k	601	-	-	7/19/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	k	601	GCP	O4'-C1'	8.85	1.62	1.42
44	k	601	GCP	C2'-C1'	-7.35	1.30	1.53
44	k	601	GCP	O4'-C4'	-6.15	1.31	1.45
44	k	601	GCP	PB-O3A	5.92	1.65	1.58
44	k	601	GCP	PA-O3A	5.14	1.65	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	601	GCP	C5-C4-N3	-5.29	119.97	128.39
44	k	601	GCP	C2-N3-C4	4.47	119.99	112.30
44	k	601	GCP	N9-C4-N3	3.07	132.09	125.95
44	k	601	GCP	PB-O3A-PA	-3.04	122.46	132.37
44	k	601	GCP	N9-C8-N7	-2.97	107.89	113.40

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

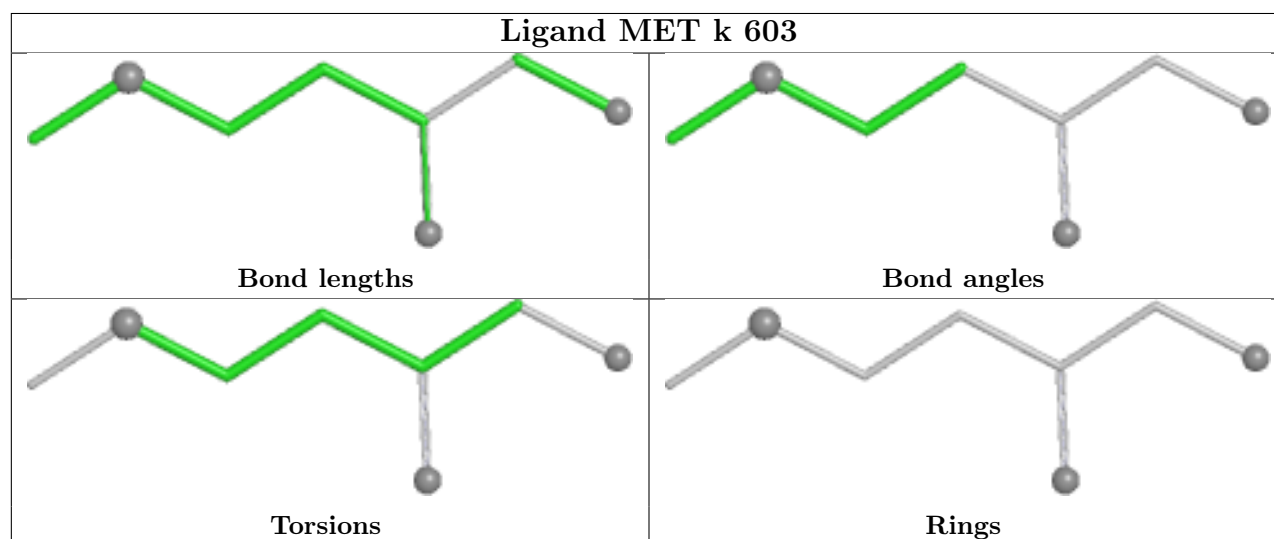
Mol	Chain	Res	Type	Atoms
44	k	601	GCP	PG-C3B-PB-O1B
44	k	601	GCP	PG-C3B-PB-O3A
44	k	601	GCP	C5'-O5'-PA-O3A
44	k	601	GCP	C5'-O5'-PA-O2A
44	k	601	GCP	O4'-C4'-C5'-O5'

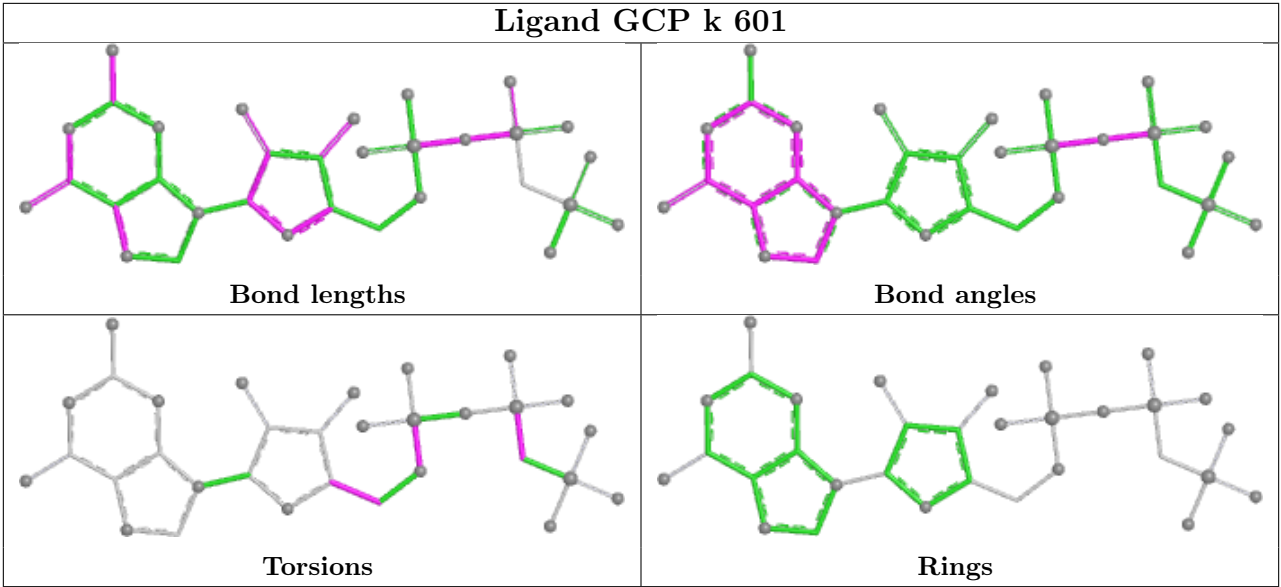
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	k	603	MET	4	0
44	k	601	GCP	4	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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	8.15
1	1	63:G	O3'	64:RIA	P	4.24
1	1	16:H2U	O3'	18:G	P	3.15

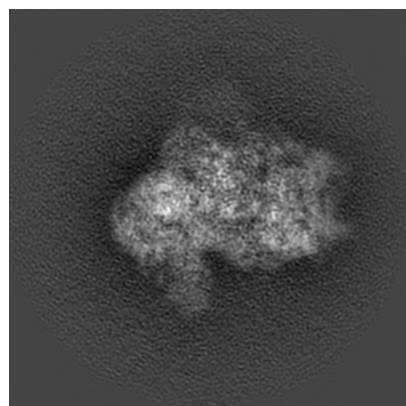
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19805. These allow visual inspection of the internal detail of the map and identification of artifacts.

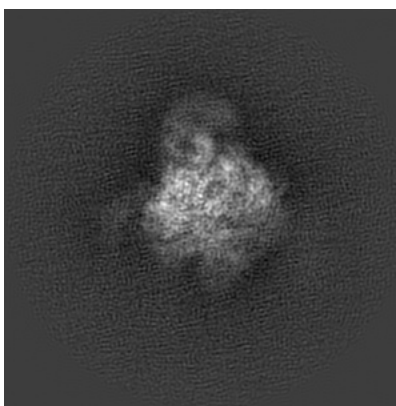
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

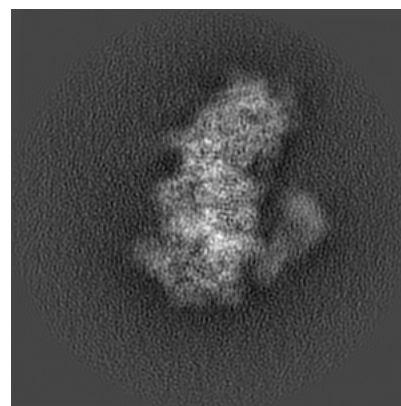
6.1.1 Primary map



X

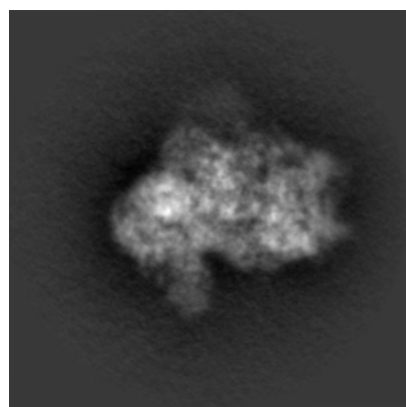


Y

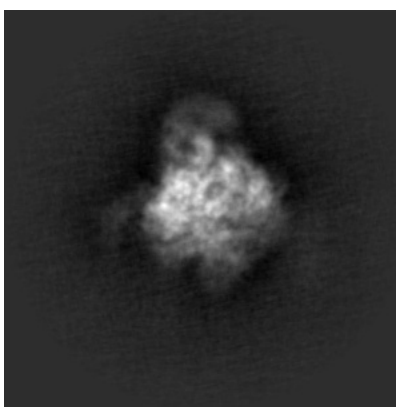


Z

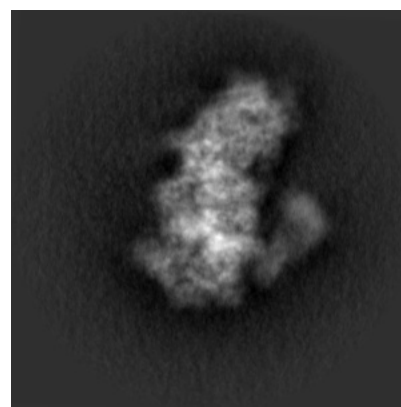
6.1.2 Raw map



X



Y

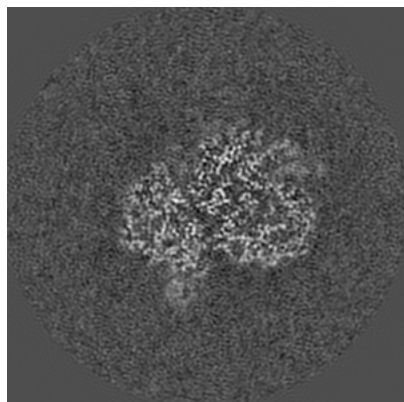


Z

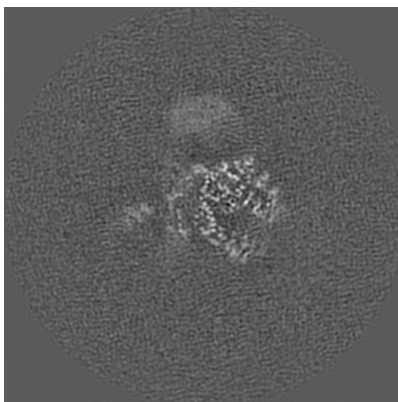
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

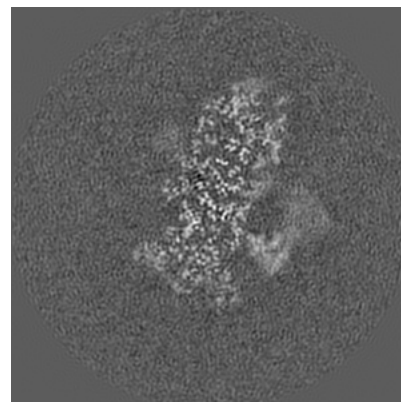
6.2.1 Primary map



X Index: 150

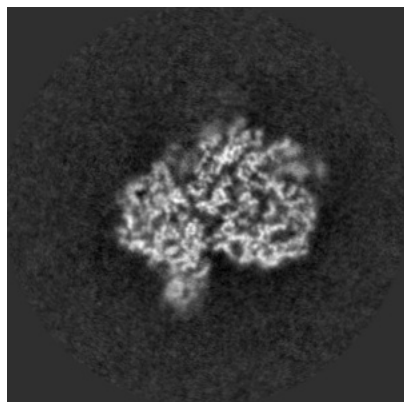


Y Index: 150

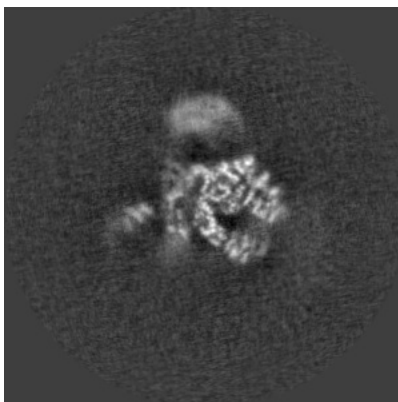


Z Index: 150

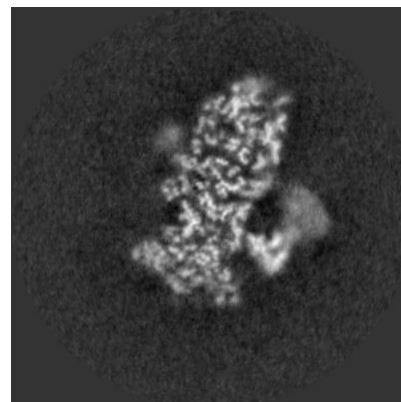
6.2.2 Raw map



X Index: 150



Y Index: 150

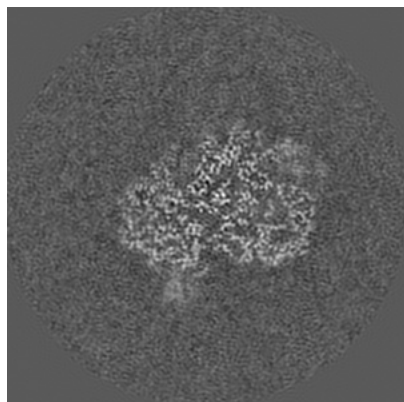


Z Index: 150

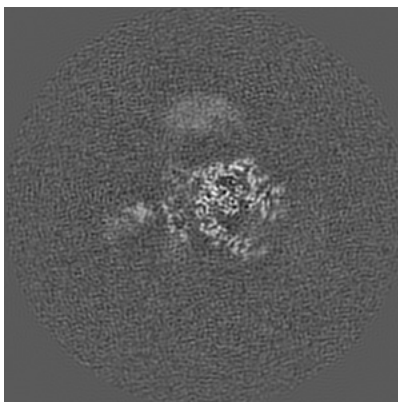
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

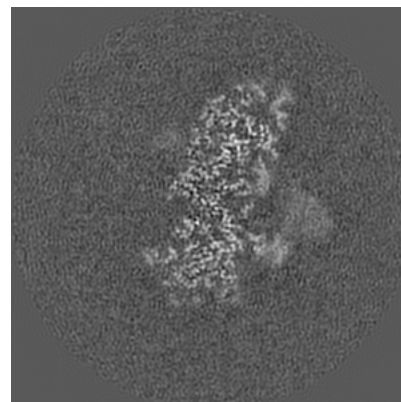
6.3.1 Primary map



X Index: 151

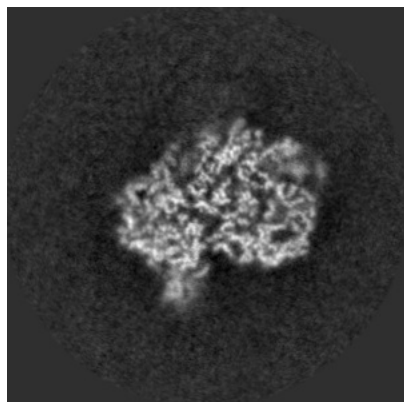


Y Index: 148

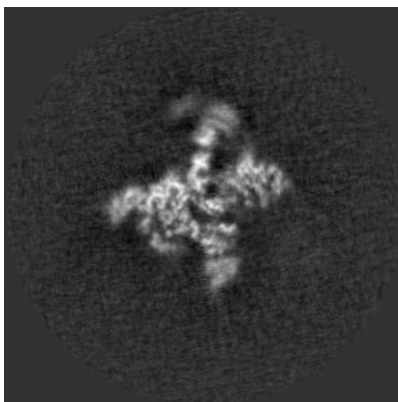


Z Index: 146

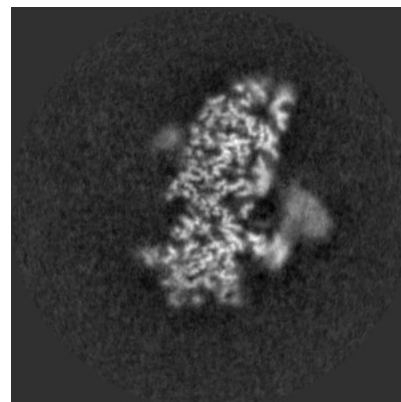
6.3.2 Raw map



X Index: 151



Y Index: 125

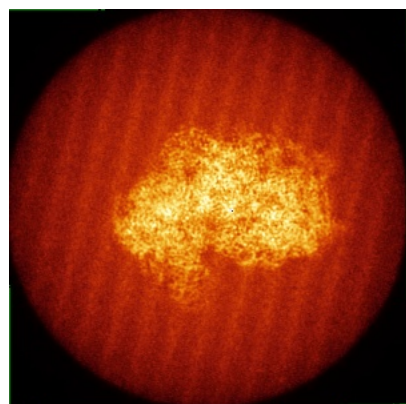


Z Index: 146

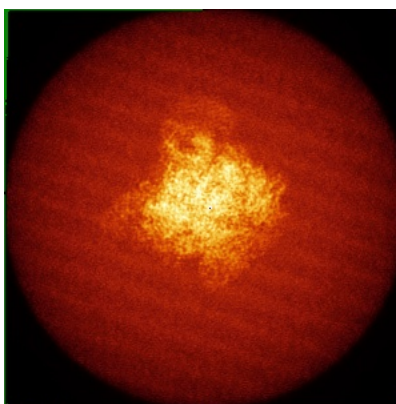
The images above show the largest variance slices of the map in three orthogonal directions.

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

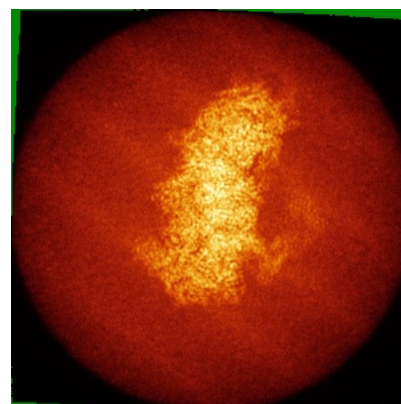
6.4.1 Primary map



X

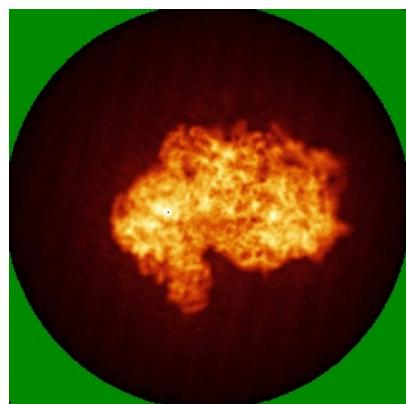


Y

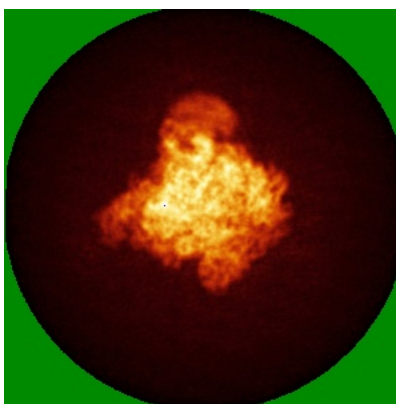


Z

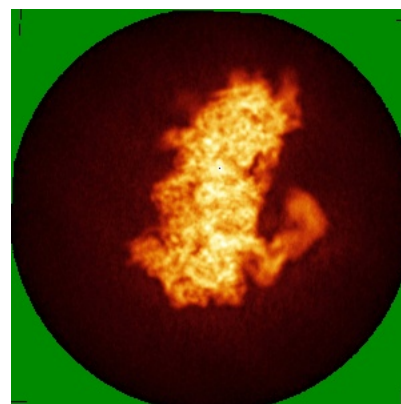
6.4.2 Raw map



X



Y

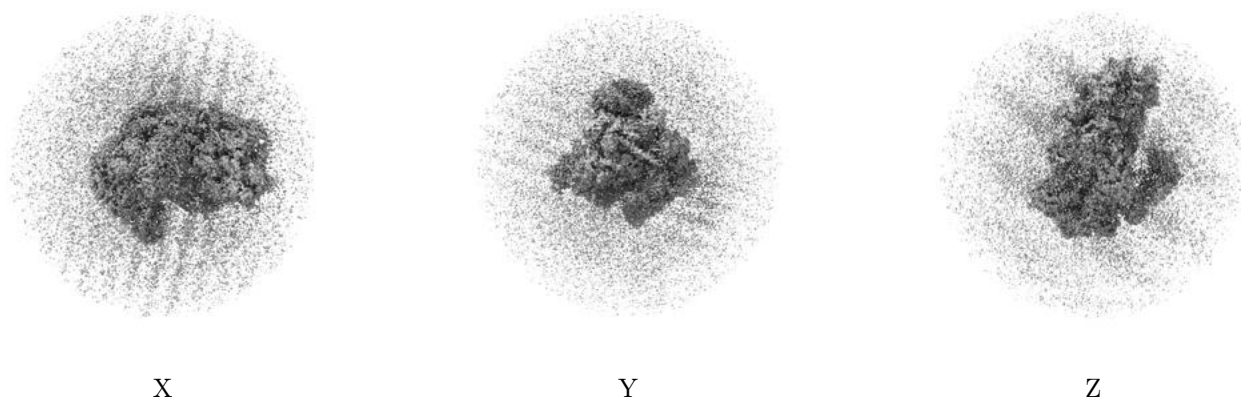


Z

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.

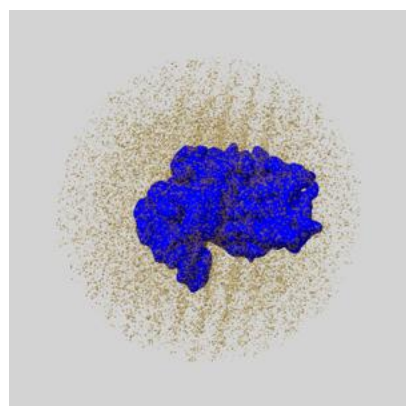
6.6 Mask visualisation [i](#)

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

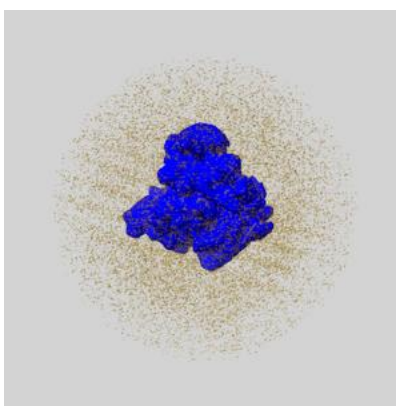
A mask typically either:

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

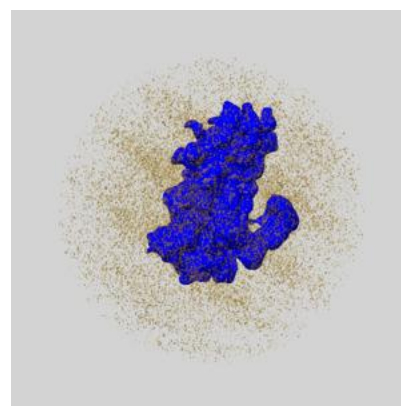
6.6.1 emd_19805_msk_1.map [i](#)



X



Y

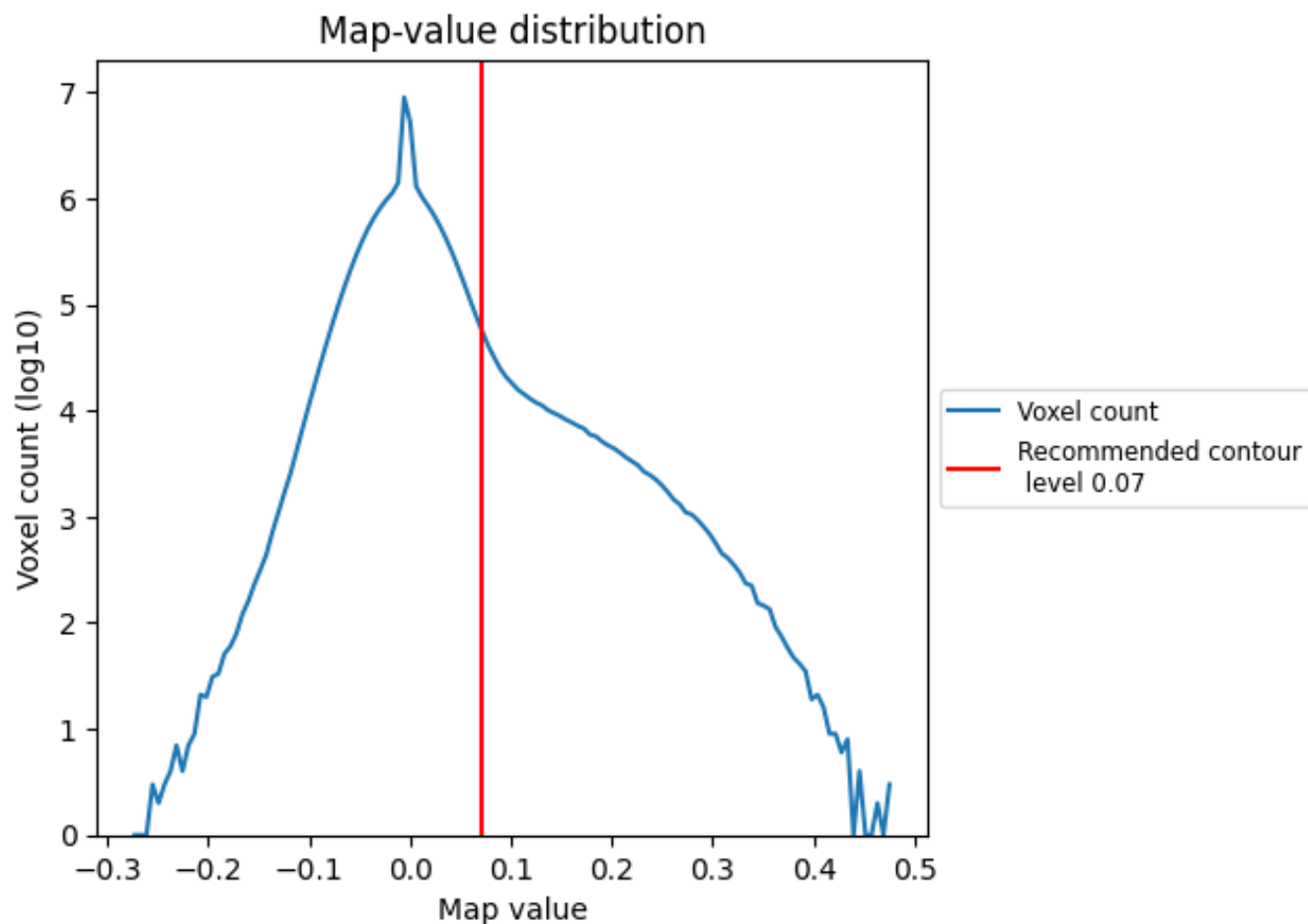


Z

7 Map analysis [i](#)

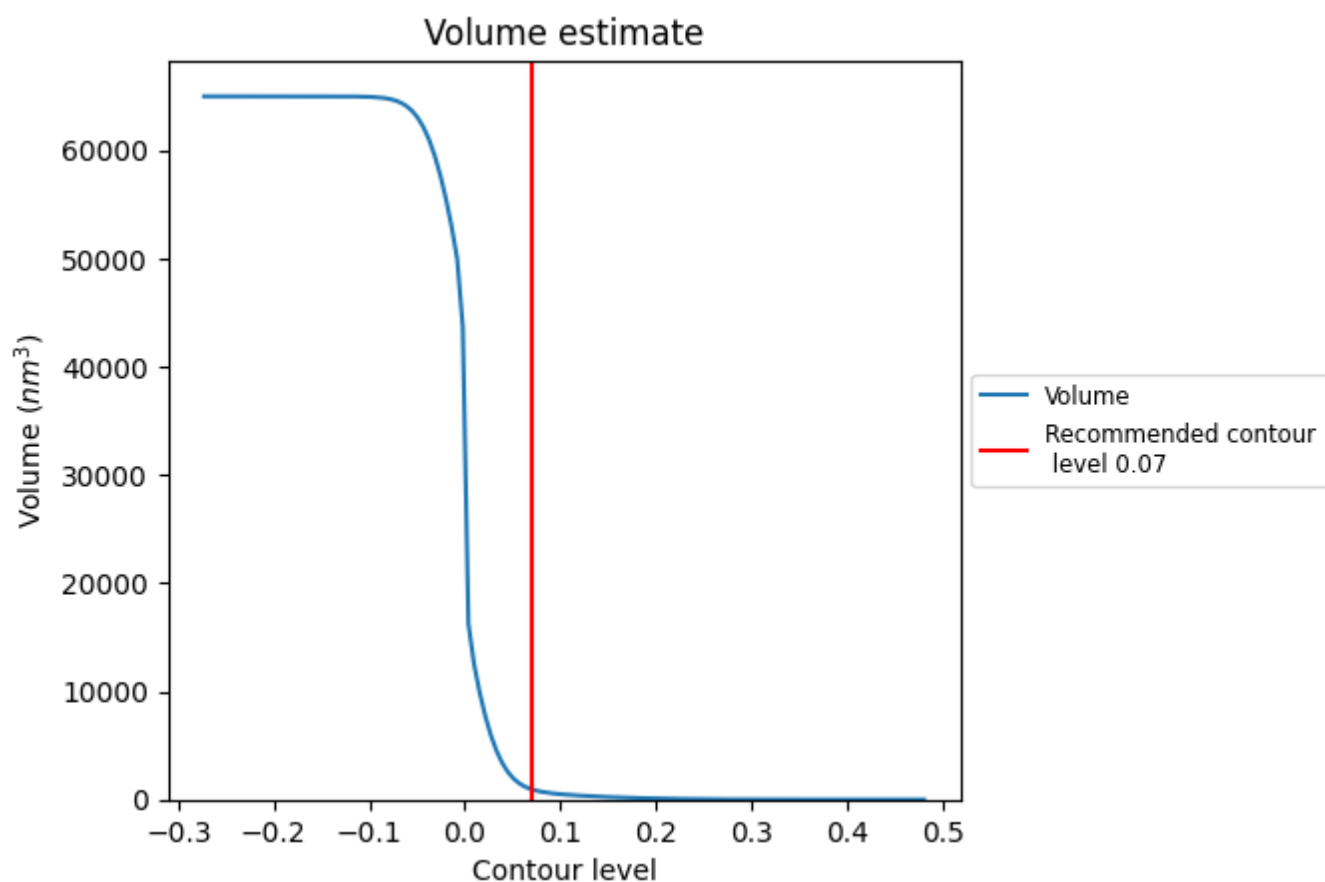
This section contains the results of statistical analysis of the map.

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.

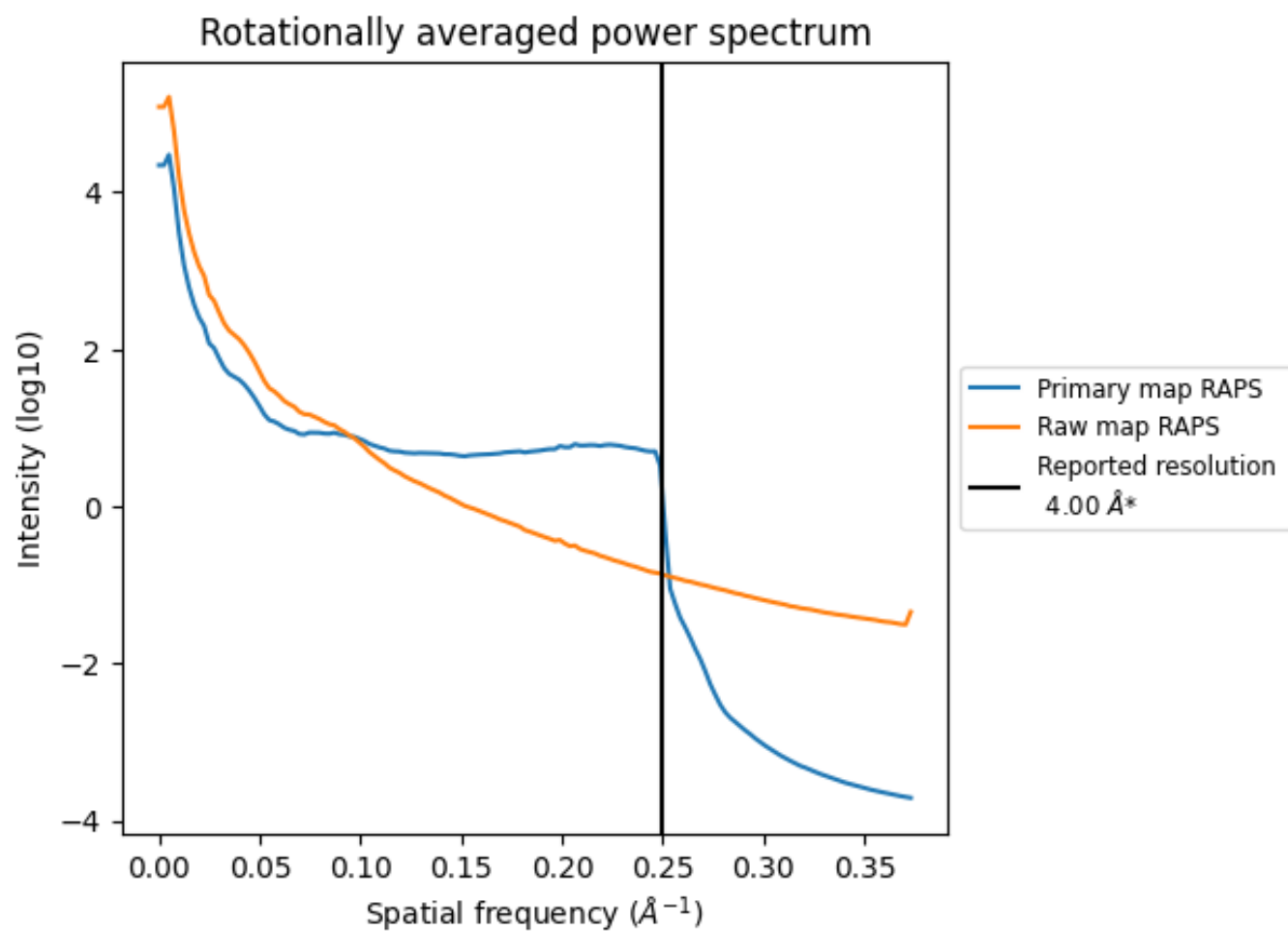
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 951 nm³; this corresponds to an approximate mass of 859 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 ⓘ

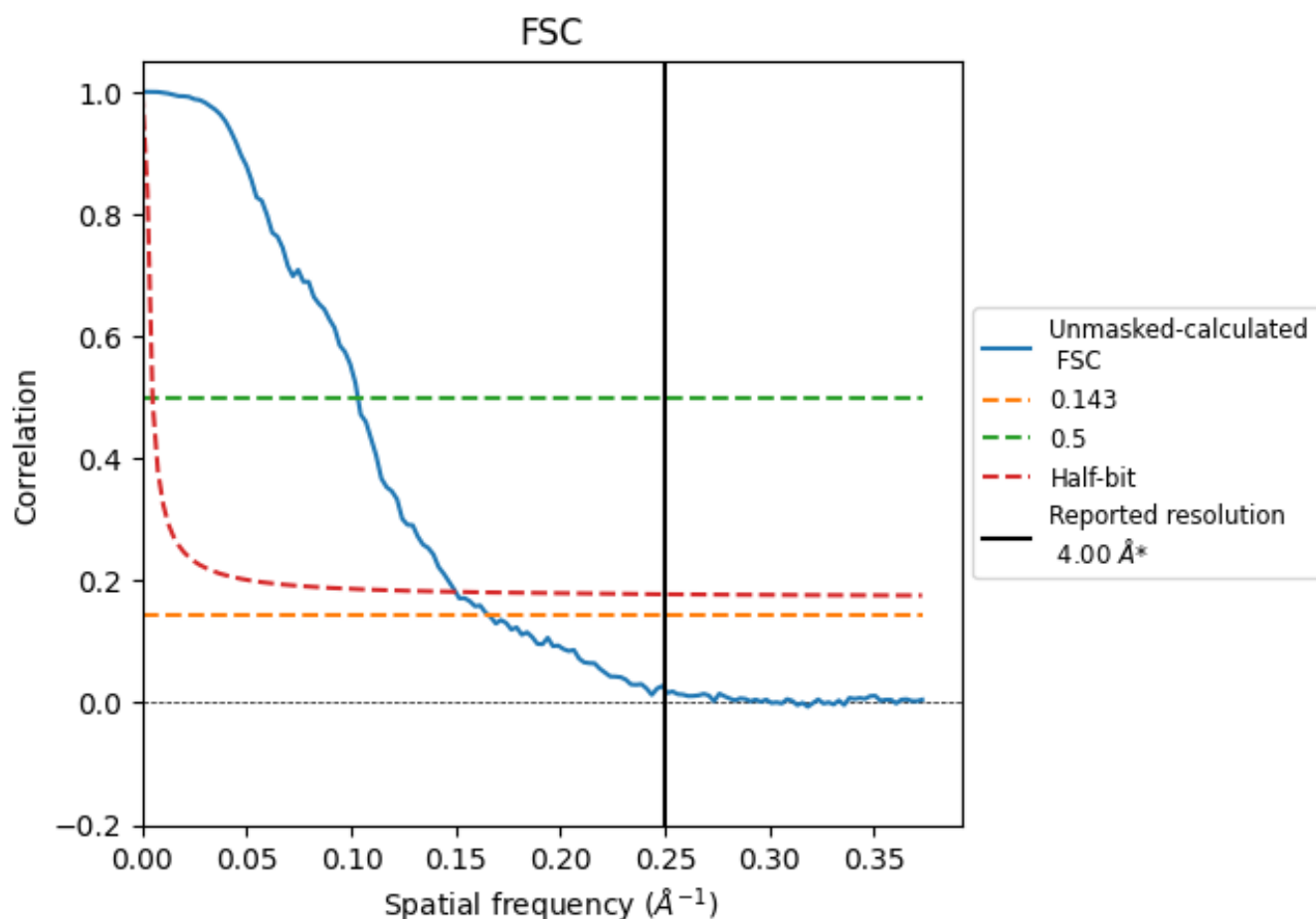


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

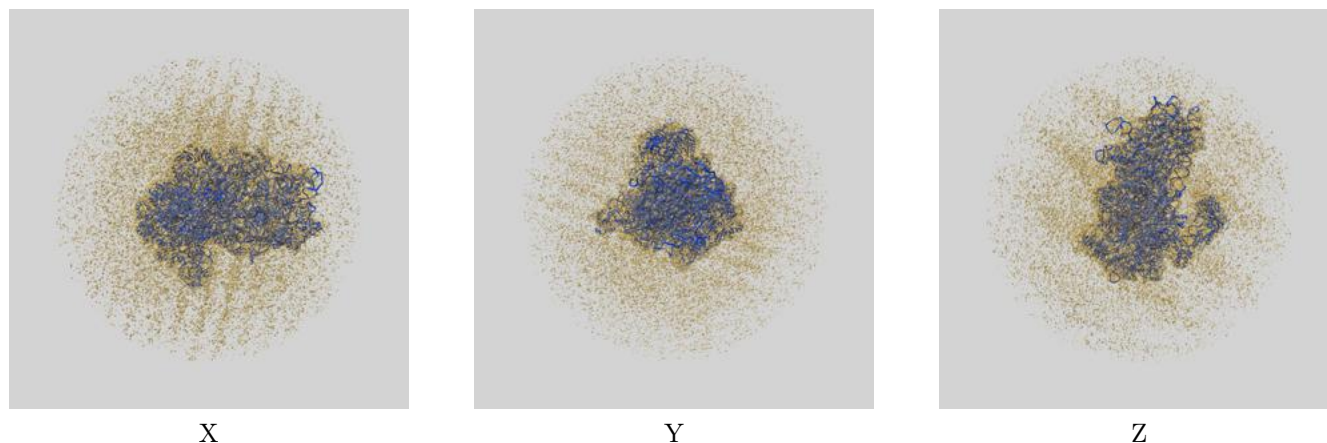
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.04	9.70	6.67

*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 6.04 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

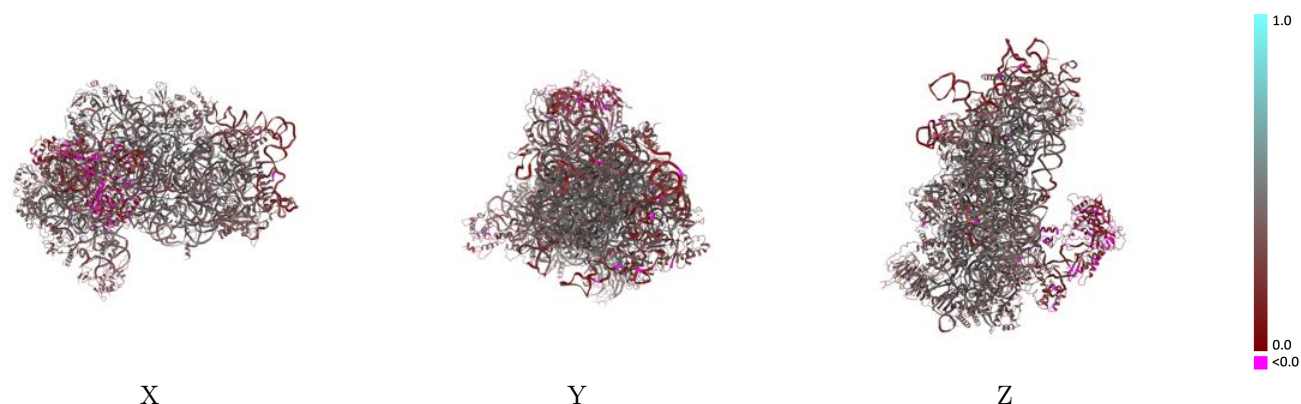
This section contains information regarding the fit between EMDB map EMD-19805 and PDB model 8S8H. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



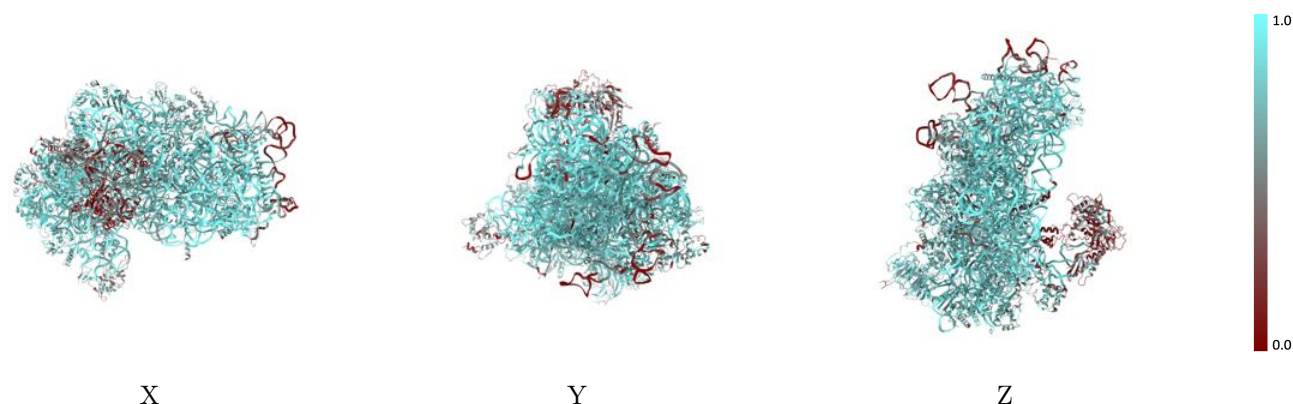
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



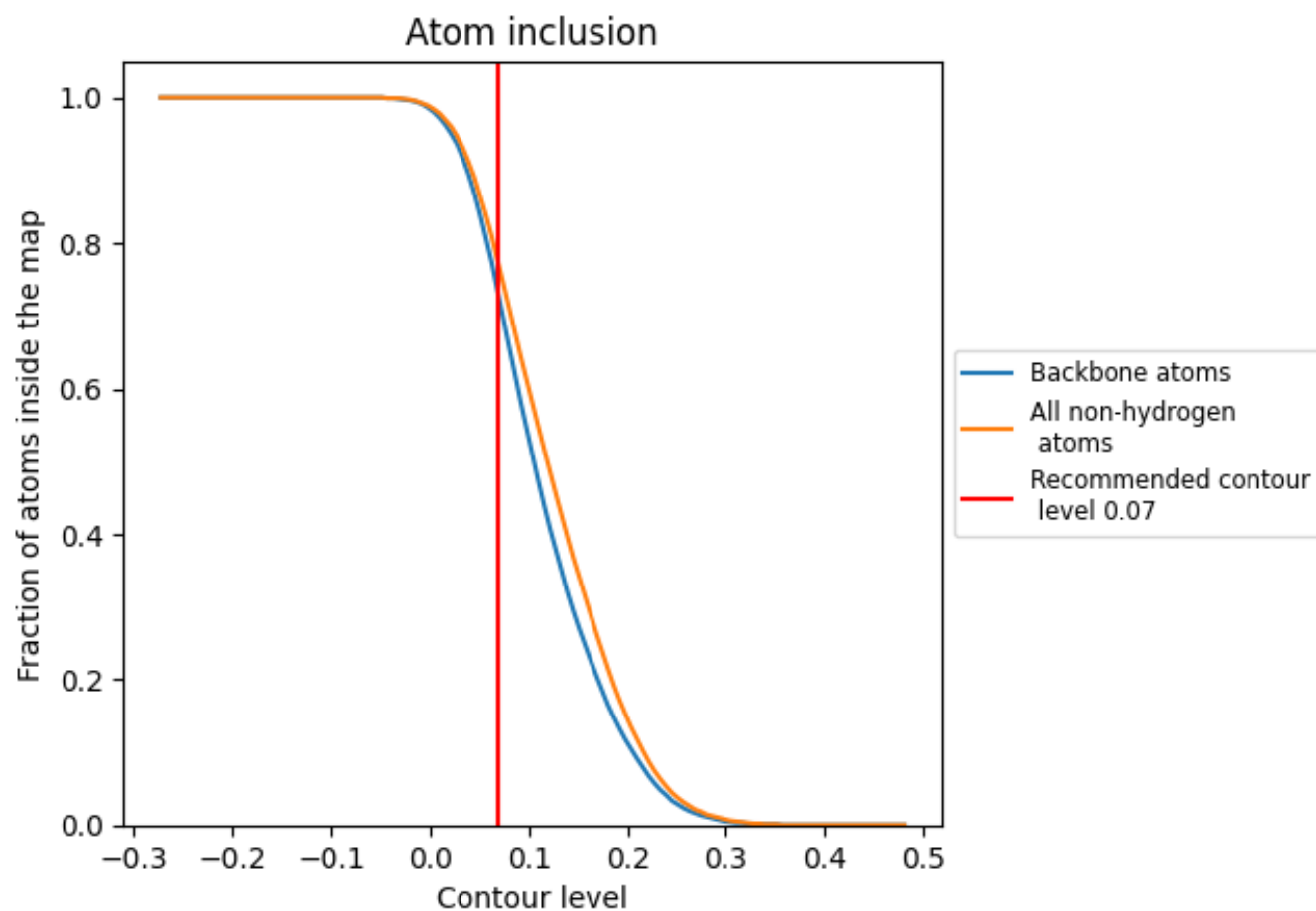
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 73% of all backbone atoms, 77% 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	 0.7690	 0.3600
1	 0.8750	 0.2670
2	 0.8740	 0.3730
3	 0.4320	 0.3120
A	 0.7700	 0.3900
B	 0.7600	 0.3840
C	 0.8050	 0.4320
D	 0.7640	 0.4040
E	 0.8160	 0.4340
F	 0.7730	 0.3950
G	 0.7800	 0.3580
H	 0.6280	 0.3480
I	 0.7840	 0.3970
J	 0.8170	 0.4180
K	 0.7570	 0.3530
L	 0.7580	 0.4190
M	 0.4450	 0.2470
N	 0.8070	 0.4080
O	 0.8250	 0.4080
P	 0.7800	 0.3670
Q	 0.8290	 0.4100
R	 0.6870	 0.3790
S	 0.7940	 0.3720
T	 0.8510	 0.3950
U	 0.6990	 0.3760
V	 0.8500	 0.4260
W	 0.8020	 0.4390
X	 0.8040	 0.4480
Y	 0.8290	 0.3960
Z	 0.5770	 0.3290
a	 0.8130	 0.4410
b	 0.7790	 0.3950
c	 0.8080	 0.4470
d	 0.8620	 0.4410
e	 0.7360	 0.4030



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Chain	Atom inclusion	Q-score
f	 0.5600	 0.2890
g	 0.7600	 0.3510
h	 0.1510	 0.2840
i	 0.4220	 0.3510
j	 0.4830	 0.1980
k	 0.2870	 0.1220
l	 0.1120	 0.1070