



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:10 AM UTC

PDB ID : 8S8G / pdb_00008s8g
EMDB ID : EMD-19804
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation (model py48S-AUC-2.1)
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:

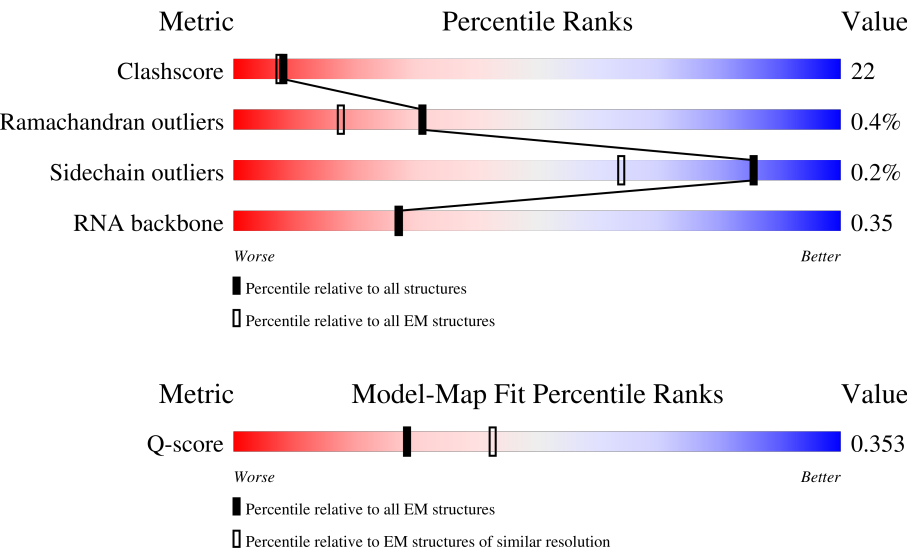
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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



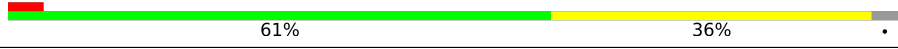
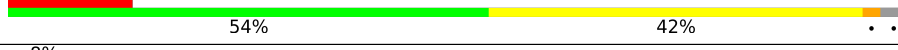
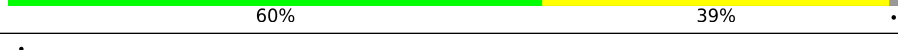
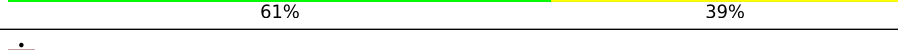
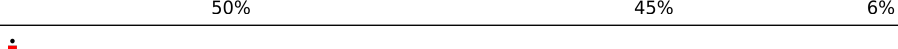
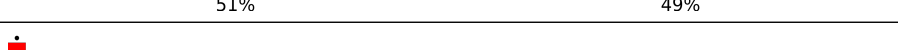
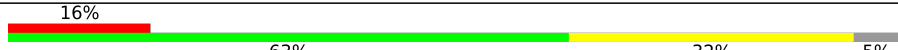
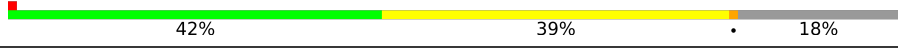
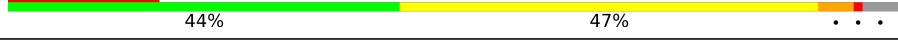
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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% 23% 56% 21%
2	A	254	5% 44% 42% 14%
3	B	255	5% 53% 35% 12%

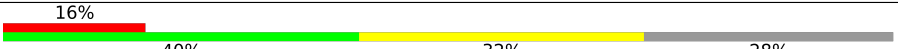
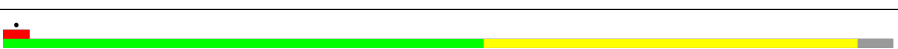
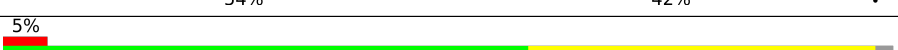
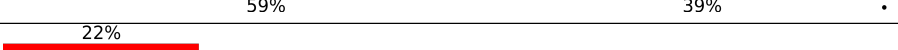
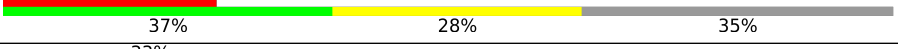
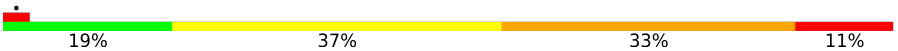
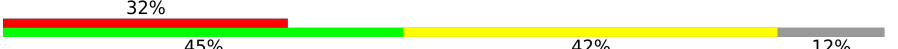
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Mol	Chain	Length	Quality of chain
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	M2G	1	26	-	-	X	-
38	5MC	1	48	-	-	X	-

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 86935 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		
			1483	950	270	263	0	0

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

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

- Molecule 9 is a protein called KLLA0E23673p.

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

- Molecule 10 is a protein called KLLA0A10483p.

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

- Molecule 11 is a protein called KLLA0F18040p.

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

- 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		
			955	585	191	176	3	0	0

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

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

- 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	99	Total	C	N	O	S	0	0
			799	494	153	147	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		

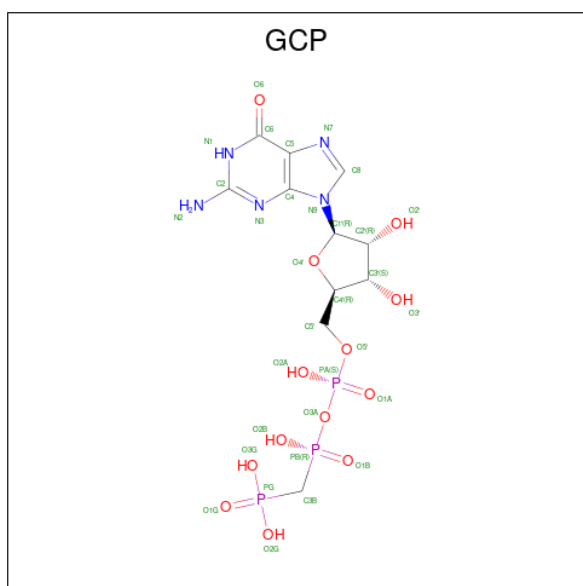
- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
42	2	113	Total	Mg	0
			113	113	
42	T	1	Total	Mg	0
			1	1	
42	i	1	Total	Mg	0
			1	1	
42	k	1	Total	Mg	0
			1	1	

- Molecule 43 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

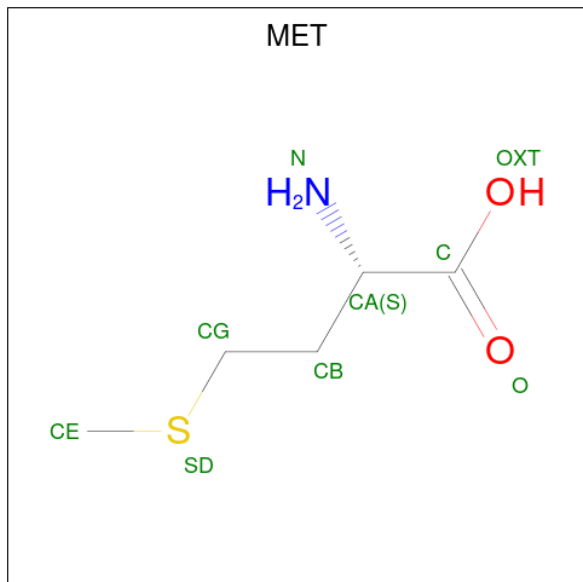
Mol	Chain	Residues	Atoms		AltConf
43	a	1	Total	Zn	0
			1	1	
43	b	1	Total	Zn	0
			1	1	
43	f	1	Total	Zn	0
			1	1	

- Molecule 44 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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
			Total	C	N	O	S	
45	k	1	8	5	1	1	1	0

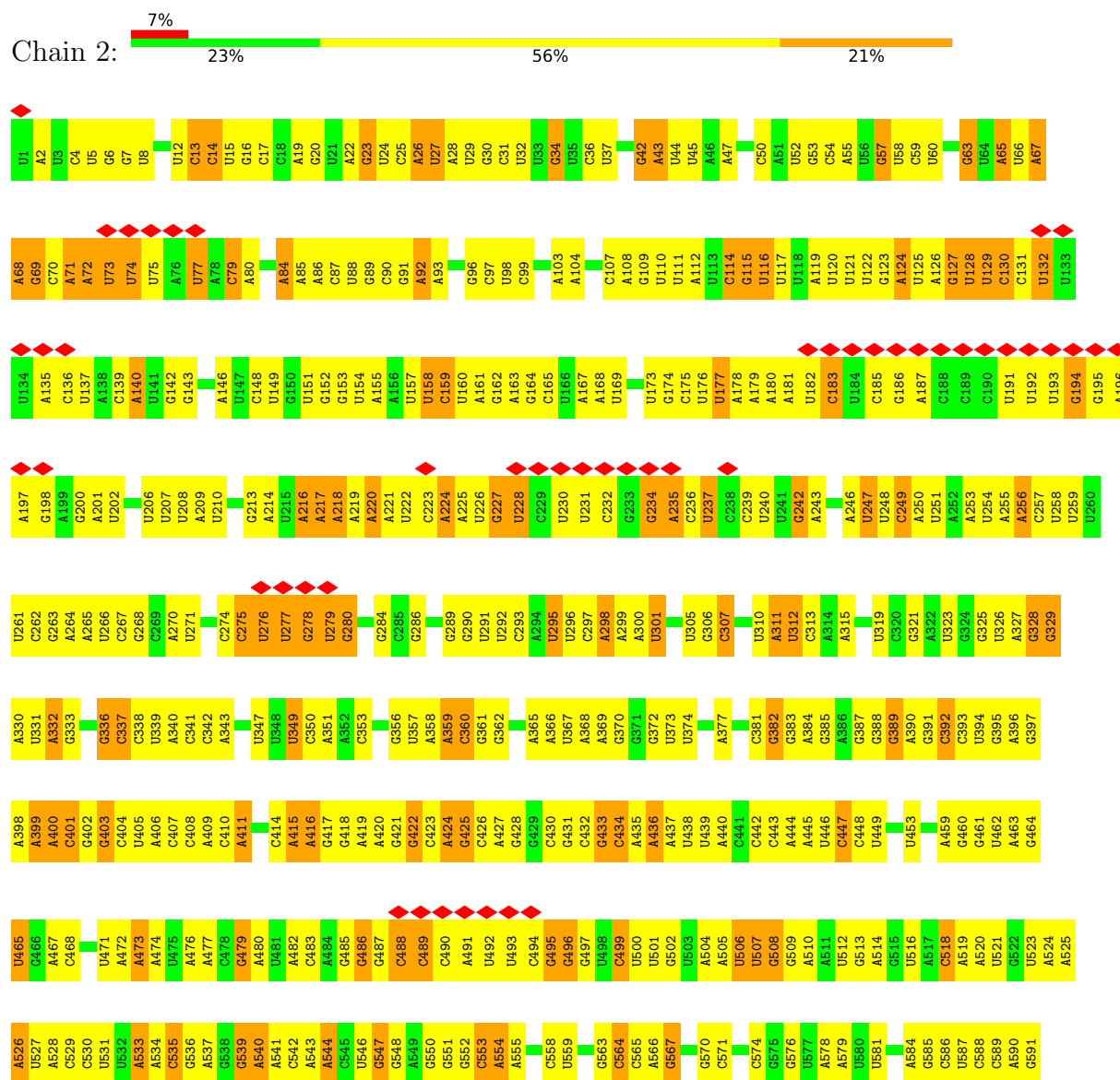
- Molecule 46 is water.

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

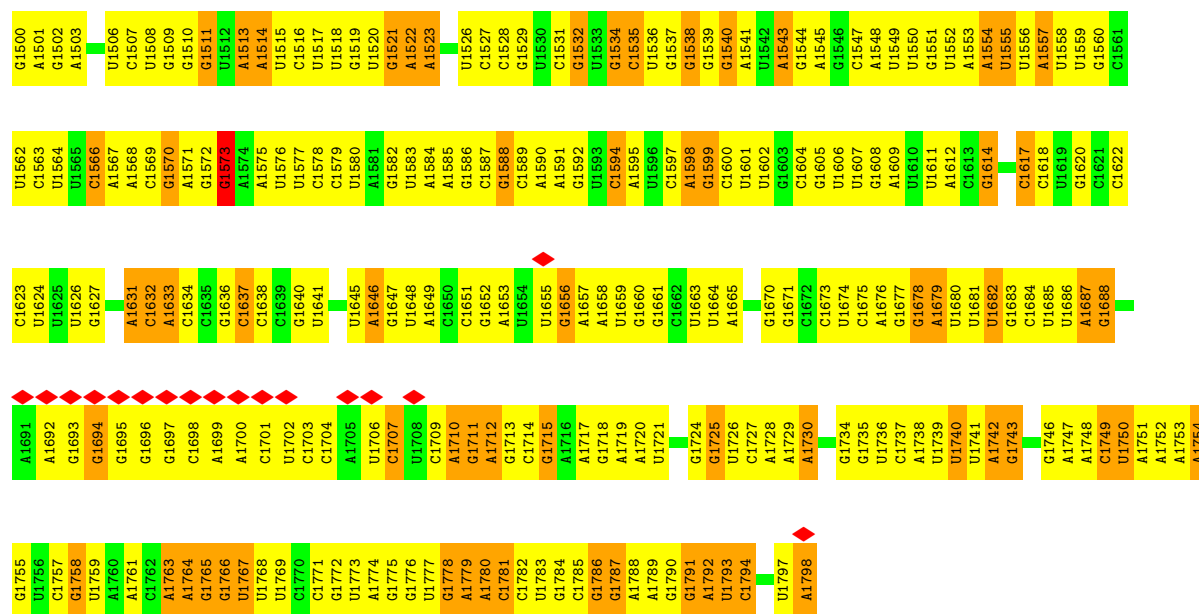
3 Residue-property plots

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.

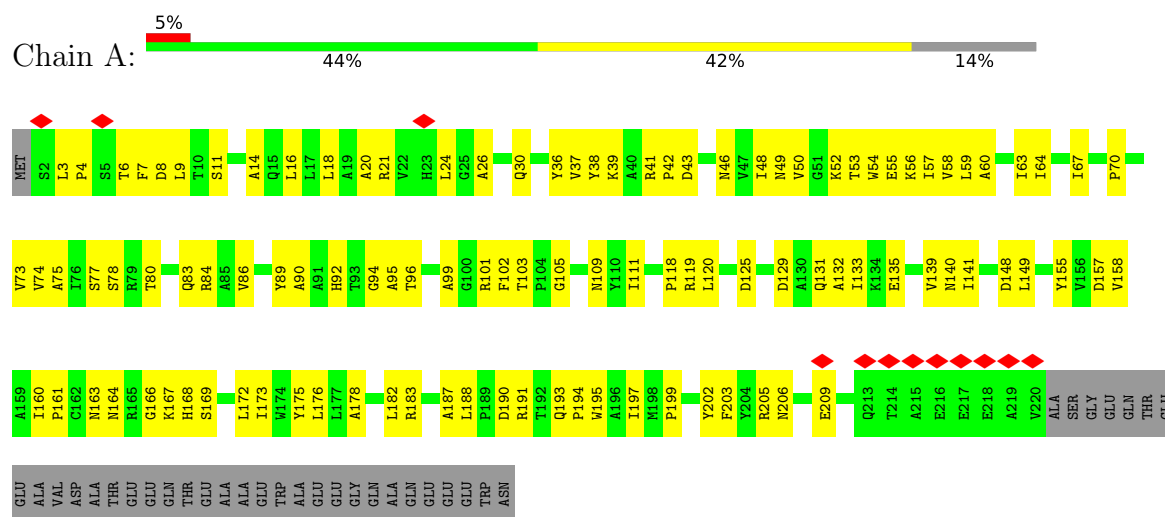
• Molecule 1: 18S ribosomal RNA



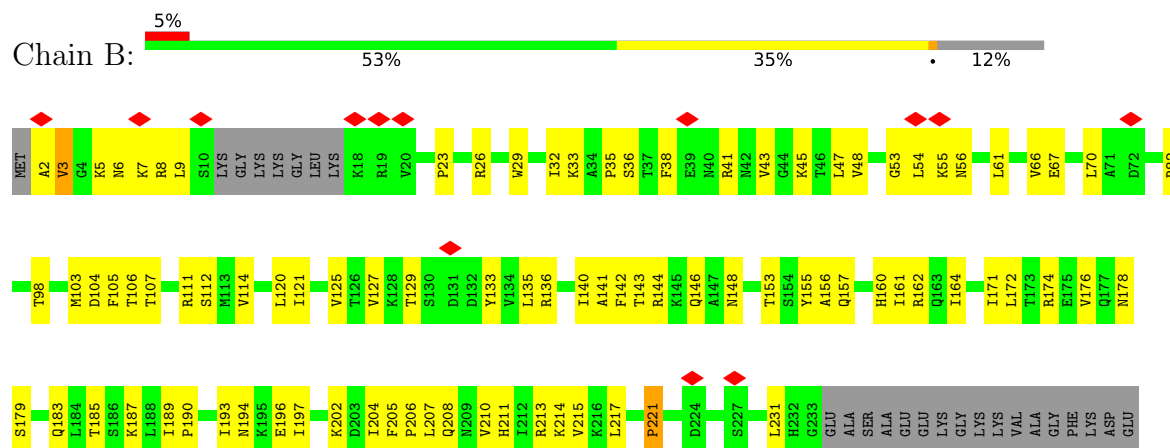
C1439	C1440	U1441	A1442	G1443	A1444		U1447	U1448	C1449	U1450	G1451	G1452	G1453	C1454	C1455	G1456	C1457	A1458	C1459	G1460	C1461	G1462	G1463	G1464	C1465	U1466	C1467	C1468	A1469	C1470	U1471	G1472	A1473	C1474	G1475	G1476	A1477	G1478	C1479	C1480	A1481	G1482	C1483	A1484	A1485	G1486	U1487	A1488	C1489	A1490	A1491	C1492	C1493	G1494	U1495	G1496	G1497	C1498	C1499				
G1370	A1371		U1376			U1379	A1380	G1381	A1382	G1383	G1384	G1385	G1386	C1387	U1388	A1389	U1390	C1391	G1392		U1396	C1397	A1398	A1399	G1400	C1401	C1402	G1403	A1404	U1405	G1406	C1407	A1408	U1409	G1410	U1411	U1412	U1413	G1414	A1415	G1416	G1417	C1418		A1423	C1424	A1425	G1426	G1427	U1428	C1429	U1430	G1431	U1432	G1433	A1434	U1435	G1436	U1437	C1438			
G1307	C1308	U1309	U1310	A1311	A1312	U1313	U1314	C1315	C1316	G1317	A1318	U1319	A1320	C1321	C1322	G1323	A1324	A1325	C1326	G1327	A1328	G1329	A1330	C1331	C1332	U1333	U1334	A1335	A1336	C1337	C1338	U1339	A1340	A1343	A1344	A1345	U1346	A1347	G1348	G1349		G1353	C1354	U1355	G1356	G1357	C1358	A1359	C1360	U1361	U1362	G1363	C1364	U1365	G1366	U1367	U1368	U1369					
A1243	G1244	C1245	U1246	C1247	U1248	U1249	U1250	C1251	U1252	U1253	G1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	G1262	G1263	G1264	U1265	G1266	C1267	U1268	G1269		C1272	C1273	U1274	U1275	G1276	G1277	C1278	C1279	G1280	U1281	U1282	C1283	U1284	U1285	A1286	G1287	U1288	U1289	G1290	G1291	U1292	G1293		G1296	U1297	G1298	A1299	U1300	U1301	U1302		U1306				
U1180	U1181	A1182	A1183	U1184	U1185		A1188	C1189	B8N1190	C1191	A1192	A1193	C1194	A1195	C1196	G1197	A1198	G1199	G1200	A1201	A1202	A1203		C1206	A1207	C1208	C1209	C1210	A1211	G1212	U1213	C1214	C1215	A1216	G1217	A1218	C1219	A1220	C1221	A1222	A1223	U1224	A1225	A1226	G1227	A1228	A1229	U1230		A1233	C1234	A1235	G1236	A1237	U1238	U1239	G1240	A1241	G1242				
A1115	U1116	G1117		G1121	C1122	A1123	A1124	G1125	C1126	C1127		A1131	A1132	C1133	U1134	U1135	A1136	A1137		G1140	A1141	A1142	U1143	U1144	G1145	A1146	C1147	U1148	G1149	A1150	A1151	U1152	G1153	C1154	C1155	A1156	C1157	C1158	A1159	C1160	C1161	A1162	G1163	G1164	A1165	G1166	U1167	G1168	G1169	A1170	C1171	C1172	C1173	U1174	G1175	C1176	G1177	C1178	C1179				
U1048	G1049	U1050	U1051	G1052	U1053	U1054	U1055	U1056	U1057	C1058	U1059		U1062	G1063	A1064	U1065	C1066	A1067	A1068		C1071	G1072	G1073	C1074	A1075	C1076	C1077	U1078	U1079	A1080	C1081	G1082	A1083	G1084	A1085	A1086	A1087		A1090	A1091	A1092		C1095	U1096	U1097	U1098	G1099	G1100	G1101	U1102	U1103		G1106	G1107	G1108		A1112	U1114					
G979		A982	G983	G984	G985	G986	A987	U988	C989	G990	A991	A992	G993	A994	U995	A996	A997	U998		A1002	U1003		C1006	G1007	G941	C942	A943	U944	U945	U946	G947	C948	C949	A950	A951	G952	G953	A954	C955	G956	U957	U958	U959	U960	C961	A962	U963	G1033	G1034	U964	A965	A966	U967	C968	A969		A973	G974	G975	A976	A977	G1045	
U915	U916	U917	A918	U919	U920	G921	A922	G923	A924	G925	U926	A927	A928		U931	A932	C933	U934		A938	A939		A940	G941	C942	A943	U944	U945	U946	G947	C948	C949	A950	A951	G952	G953	A954	C955	G956	U957	U958	U959	U960	C961	A962	U963	G1033	G1034	U964	A965	A966	U967	C968	A969		A973	G974	G975	A976	A977	G1045		
U853	A854	A855	U856	U857	A858	U859	U860	A861	A862	U863	A864	U865	G866	G867	A868	C869	G870	G871	U872		G875	G876	G877	G878	C879	A880	U881	U882	U883	G884	U885	A886	U887	G888	C889	U890	U891	U892	U893	G894	U895	U896	A897	G898	U899	G833	U834	G900	G901	U902	G903	A904	A905	A906		C909	U910	U911	G912	G913			
C785	G786	A787	A788	U789	U790	U791	U792	U793	U794		A798	U799	G800	G801	A802	A803		A806	U807	G808	G809	A810	U811	A812	A813	G814	G815	A816	C817	G818	U819	U820	A821	G822	G823	U824	U825	C826	U827	A828	U829	U830	U831	U832	G833	U834	G900	G901	U902	G903	A904	A905	A906		C909	U910	U911	G912	G913				
U658	G659	A660	C661	U662	U663	U664	A665	U666		U667	U668	C669	G670	C671	G672	A673	C674	G675		U679	U680	U681	U682	U683	A684	U685	C686	U687	G688		U691	C692	U693	U694	U695	U696	U697	U698	U699	C700	U701	G702	U703	C704	U705	U706	A707	U708	U709	U710	G711	U712	U713	C714	U715	C716	C717	U718	U719	G720			
U592	A593	G594	C595	G596	U597	A598	U599	A600	U601	U602		A605	G606	U607	U608	G609	U610	U611	G612	C613		A618	A619	A620	A621	A622	G623	C624	U625	C626	G627	U628	A629		U632		A635	C636	U637	U638	U639	G640	G641	G642	U643	C644	U645	G646	G647	U648	U649	G650	U651	C652	C653	G654	G655	U656	C657				



• Molecule 2: Small ribosomal subunit protein uS2

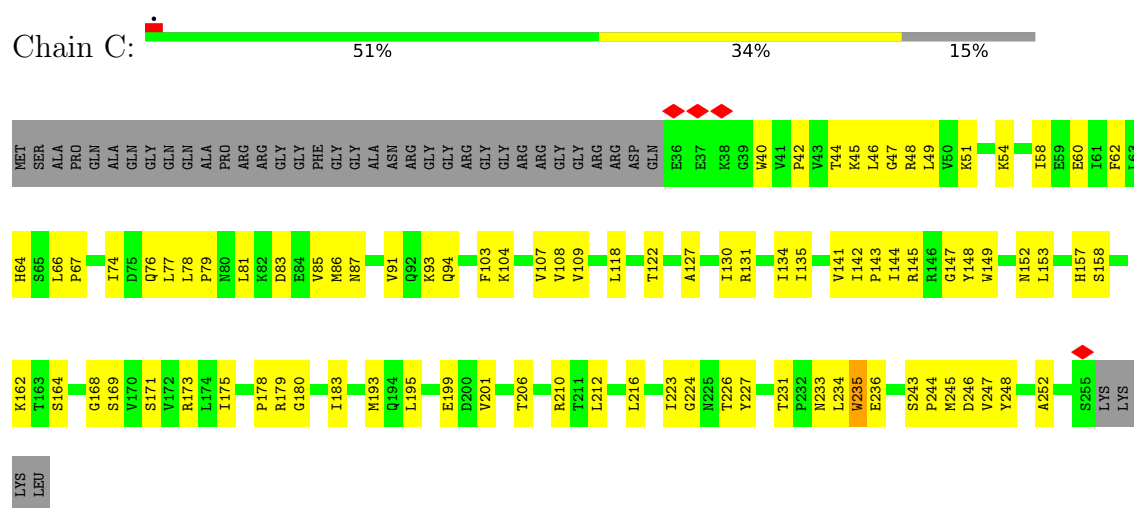


• Molecule 3: Small ribosomal subunit protein eS1

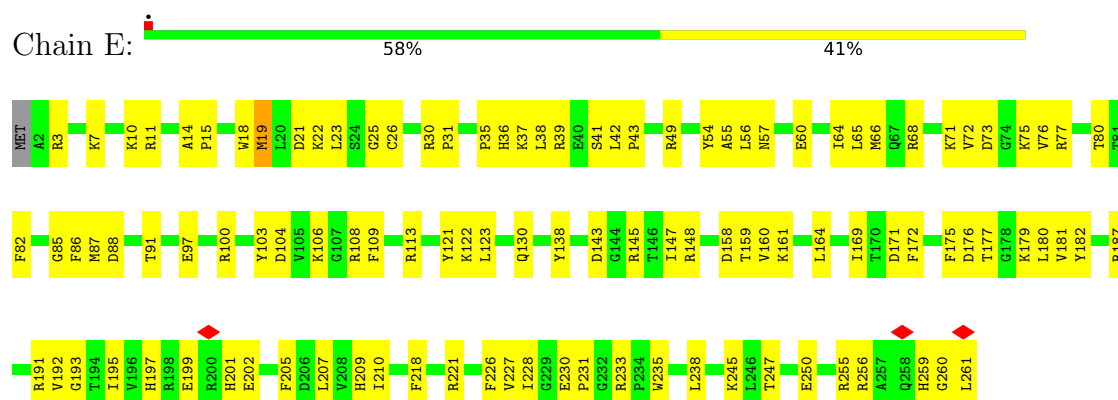


ILE
LEU
GLU
THR
VAL

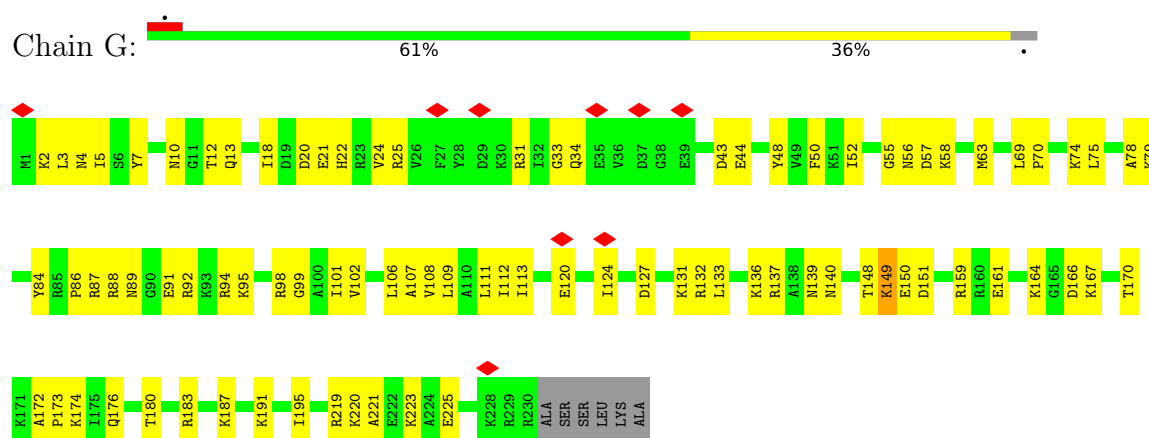
• Molecule 4: Small ribosomal subunit protein uS5



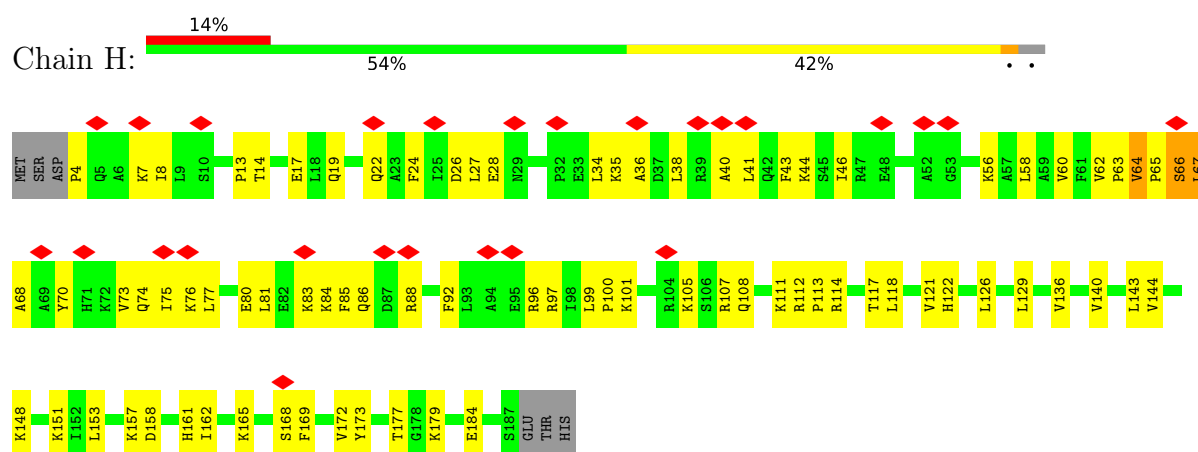
• Molecule 5: 40S ribosomal protein S4



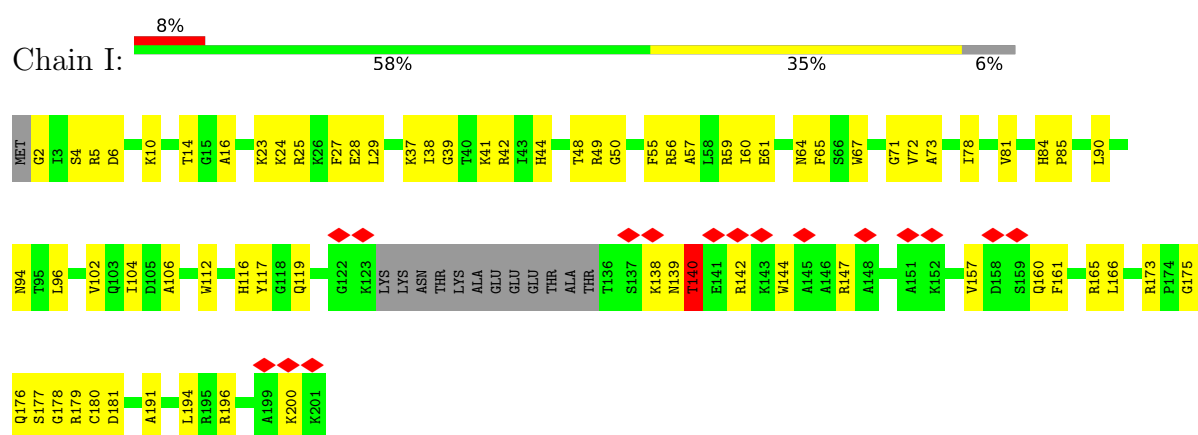
• Molecule 6: Small ribosomal subunit protein eS6



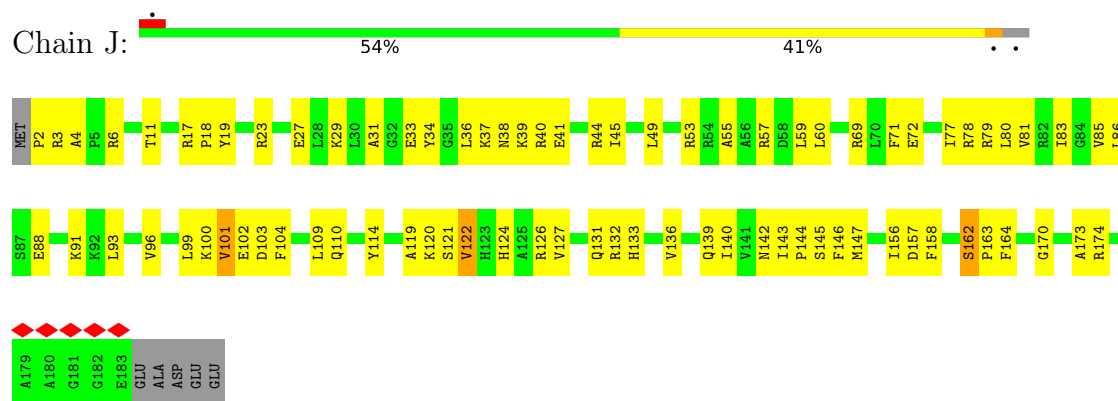
• Molecule 7: 40S ribosomal protein S7



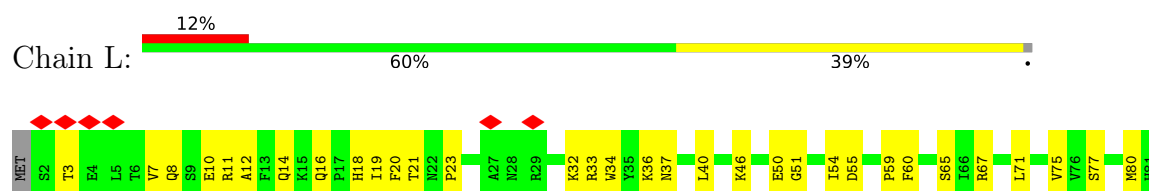
• Molecule 8: 40S ribosomal protein S8

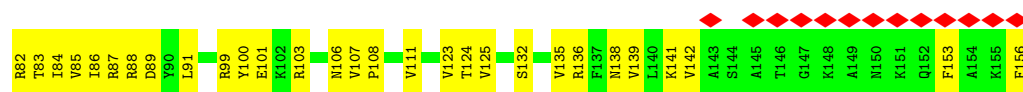


• Molecule 9: KLLA0E23673p



• Molecule 10: KLLA0A10483p

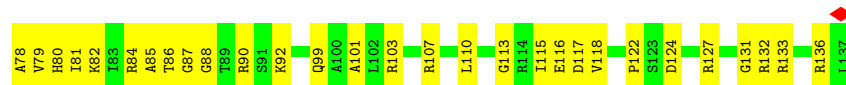
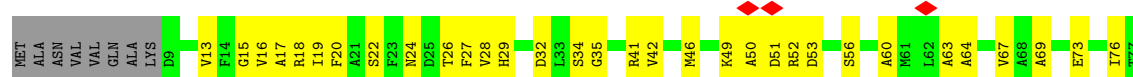




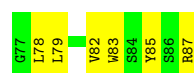
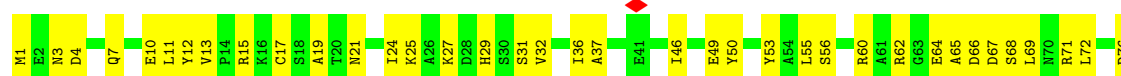
• Molecule 11: KLLA0F18040p



• Molecule 12: Small ribosomal subunit protein uS11



• Molecule 13: 40S ribosomal protein S21



• Molecule 14: Small ribosomal subunit protein uS8



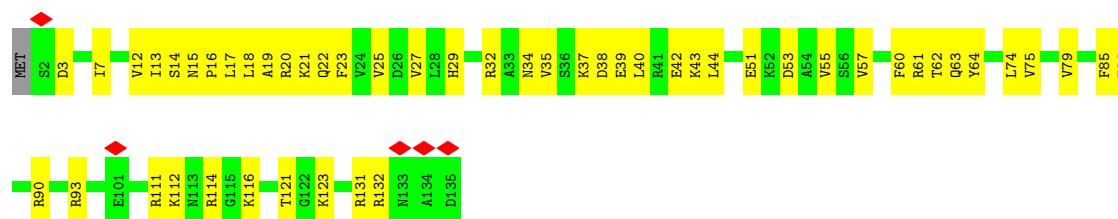
• Molecule 15: KLLA0B11231p

Chain X: 



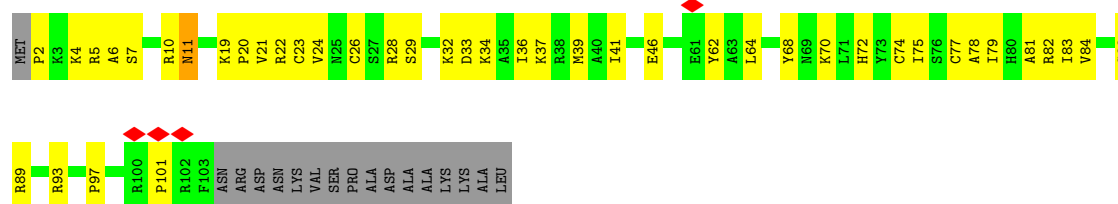
- Molecule 16: 40S ribosomal protein S24

Chain Y: 



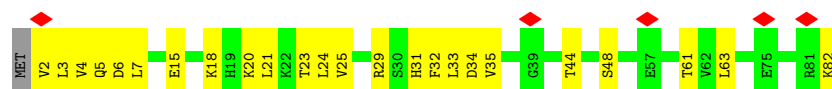
- Molecule 17: 40S ribosomal protein S26

Chain a: 



- Molecule 18: 40S ribosomal protein S27

Chain b: 



- Molecule 19: 40S ribosomal protein S30

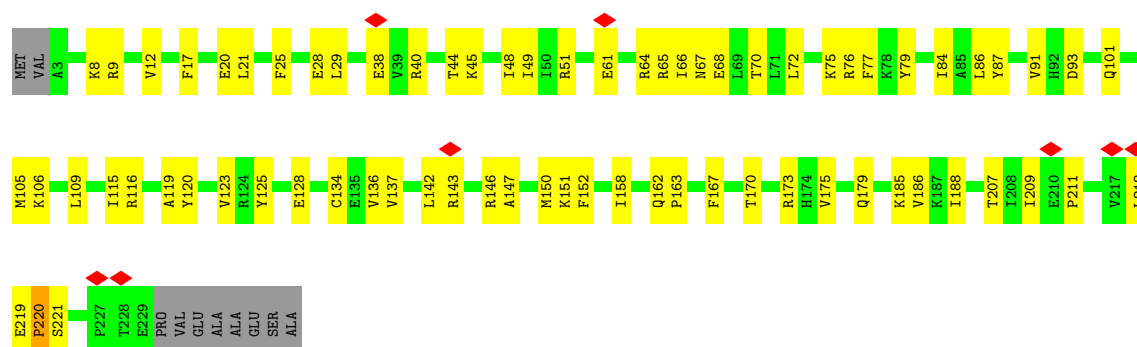
Chain e: 



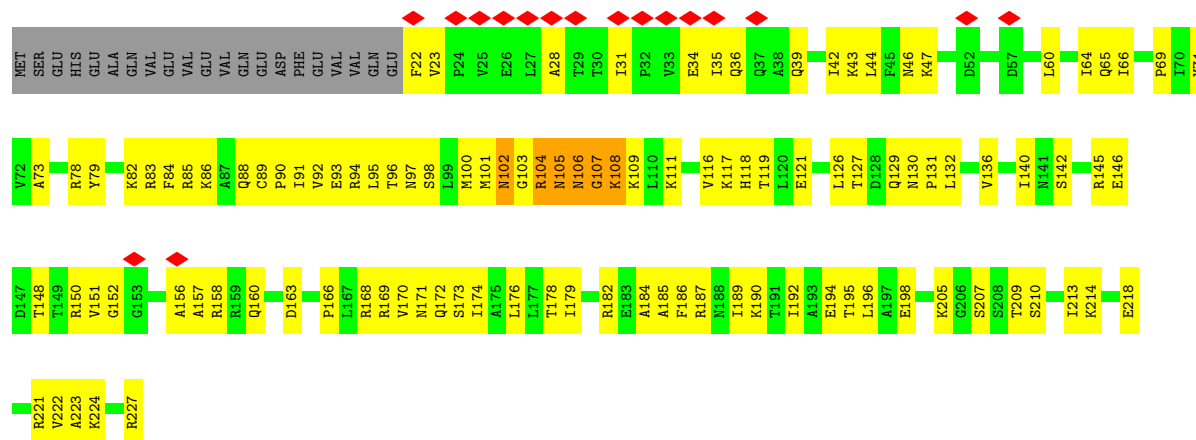
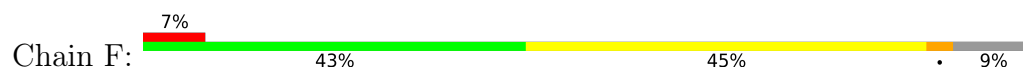
- Molecule 20: 40S ribosomal protein L41-A

Chain h: 

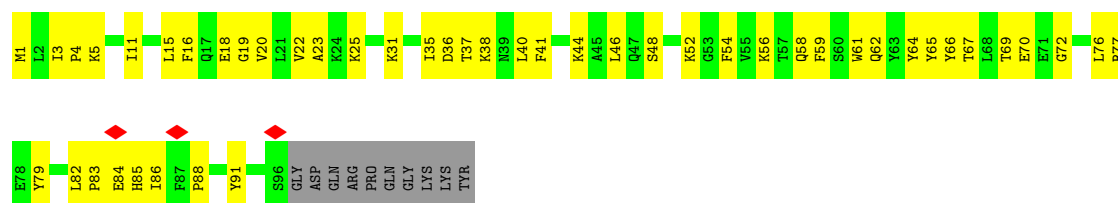
- Molecule 21: 40S ribosomal protein S3



- Molecule 22: KLLA0D10659p

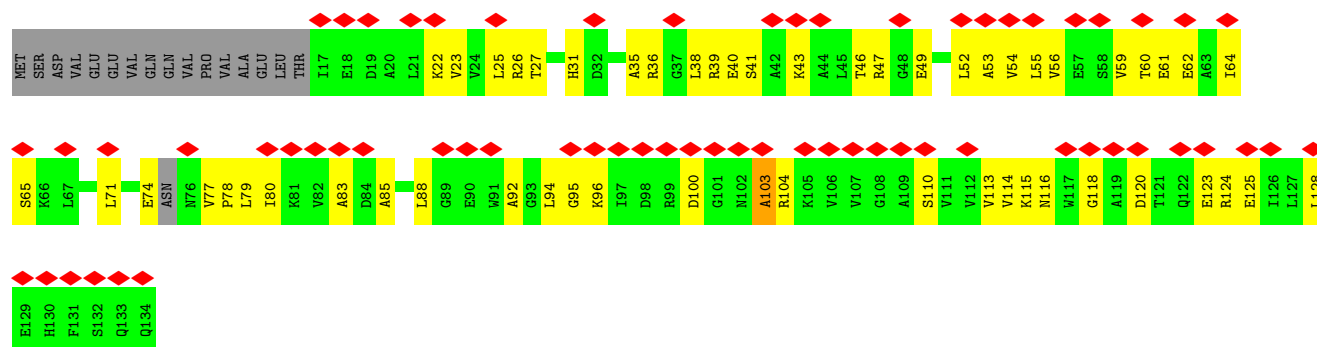


- Molecule 23: KLLA0B08173p

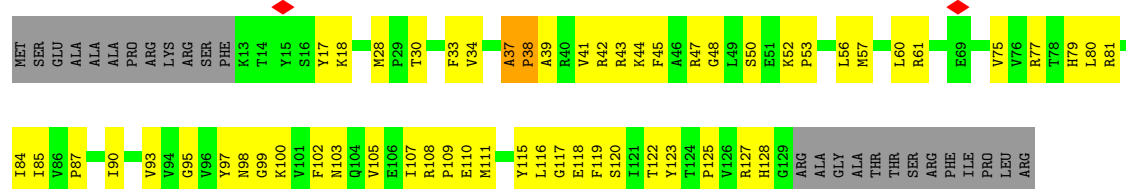


- Molecule 24: 40S ribosomal protein S12

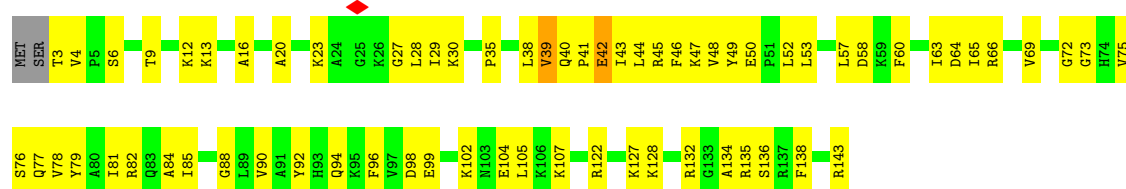




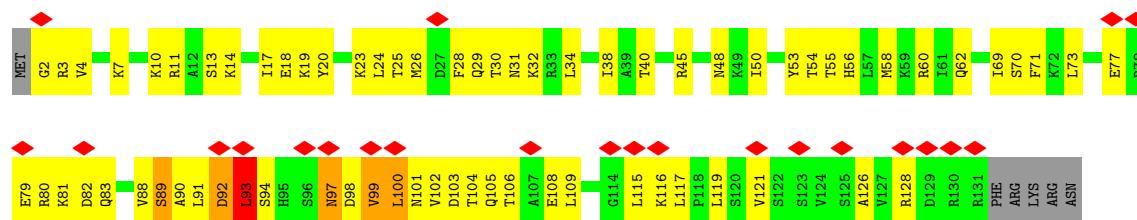
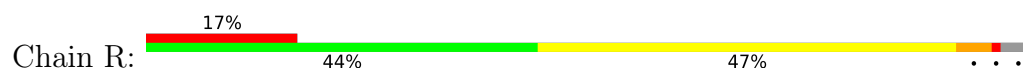
• Molecule 25: KLLA0F07843p



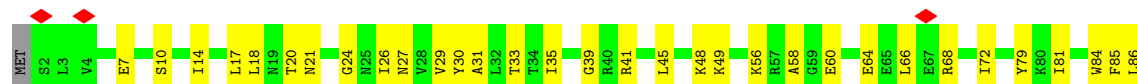
• Molecule 26: Small ribosomal subunit protein uS9

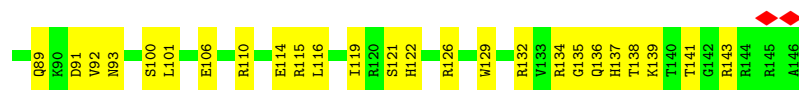


• Molecule 27: KLLA0B01474p

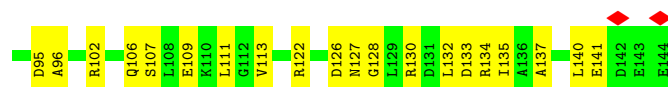


• Molecule 28: KLLA0B01562p

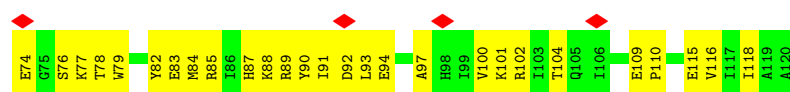
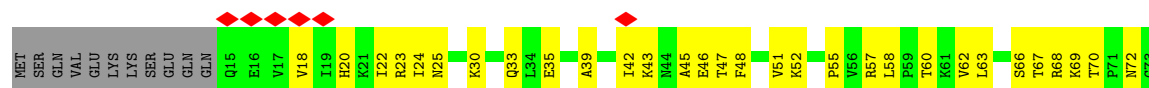




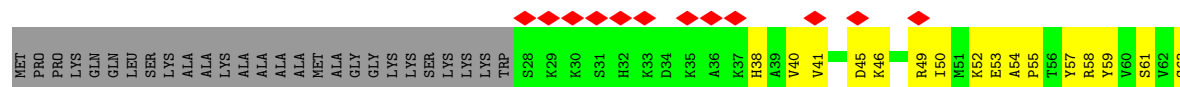
• Molecule 29: KLLA0A07194p



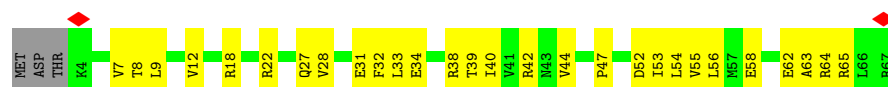
• Molecule 30: Small ribosomal subunit protein uS10



• Molecule 31: 40S ribosomal protein S25



• Molecule 32: Small ribosomal subunit protein eS28

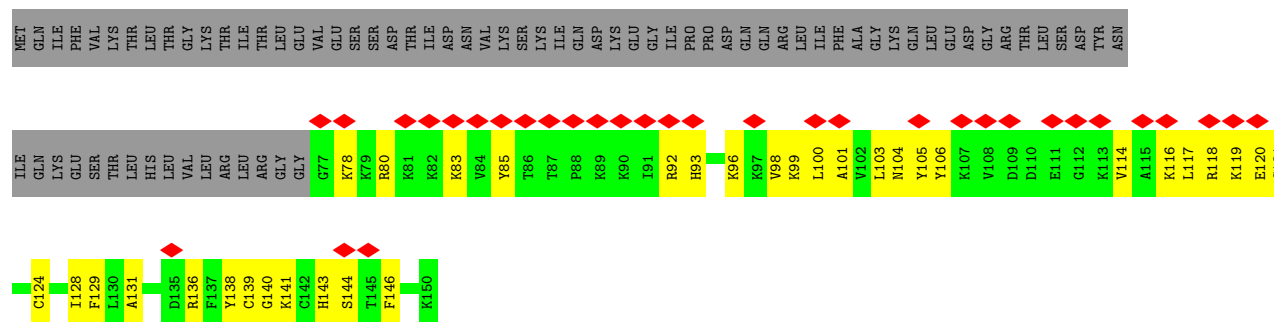
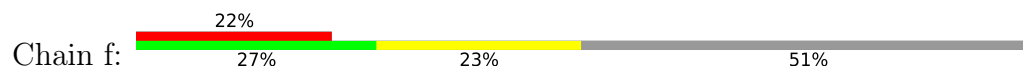


• Molecule 33: Small ribosomal subunit protein uS14

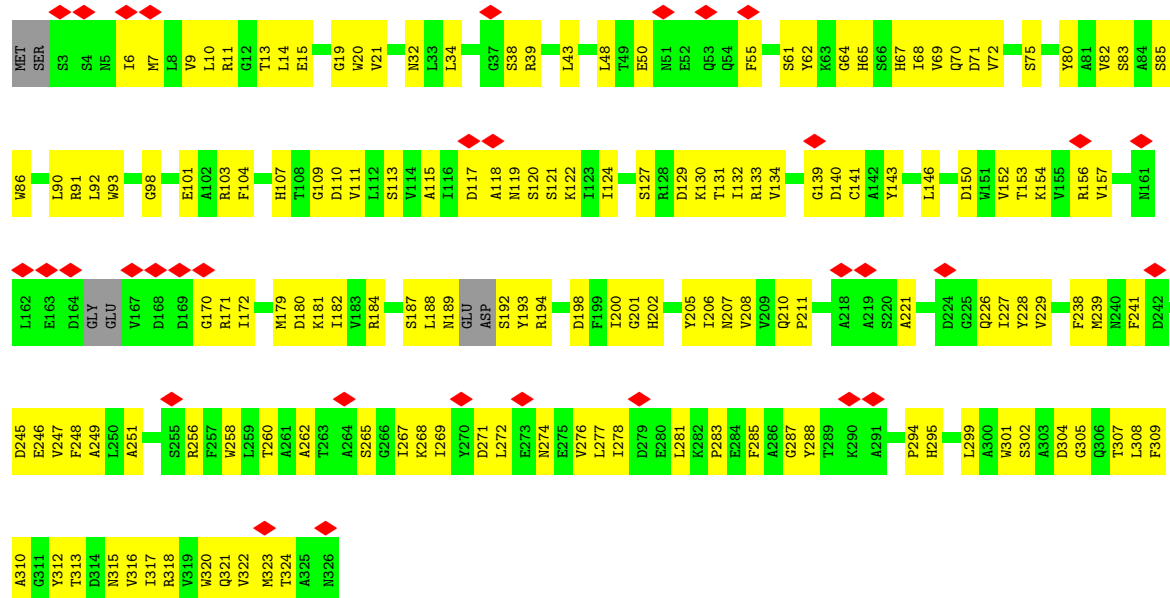




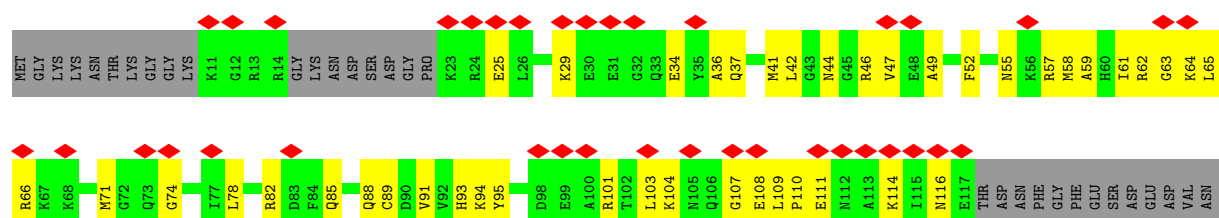
- Molecule 34: Small ribosomal subunit protein eS31

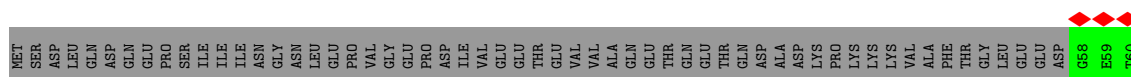


- Molecule 35: KLLA0E12277p



- Molecule 36: Eukaryotic translation initiation factor 1A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30016	Depositor
Resolution determination method	FSC 3 SIGMA 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	0.506	Depositor
Minimum map value	-0.346	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	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, B8N, H2U, ZN, 7MG, 2MG, MA6, T6A, 1MG, PSU, M2G, 1MA, GCP, MG, RIA

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	0.14	0/42410	0.35	0/66079
2	A	0.19	0/1742	0.46	0/2383
3	B	0.20	0/1820	0.48	0/2448
4	C	0.23	0/1678	0.53	1/2277 (0.0%)
5	E	0.19	0/2122	0.48	2/2861 (0.1%)
6	G	0.18	0/1855	0.43	0/2479
7	H	0.26	0/1507	0.56	0/2028
8	I	0.31	1/1515 (0.1%)	0.50	0/2029
9	J	0.24	0/1495	0.55	1/2001 (0.0%)
10	L	0.17	0/1276	0.46	0/1718
11	N	0.21	0/1218	0.49	0/1638
12	O	0.22	0/966	0.51	0/1297
13	V	0.23	0/696	0.46	0/938
14	W	0.27	0/1039	0.52	0/1399
15	X	0.18	0/1137	0.45	0/1516
16	Y	0.17	0/1075	0.41	0/1433
17	a	0.26	0/810	0.59	1/1087 (0.1%)
18	b	0.20	0/619	0.48	0/837
19	e	0.20	0/480	0.50	0/640
20	h	0.23	0/234	0.49	0/300
21	D	0.24	0/1800	0.49	0/2421
22	F	0.19	0/1628	0.62	5/2198 (0.2%)
23	K	0.16	0/831	0.45	0/1123
24	M	0.17	0/891	0.58	0/1201
25	P	0.29	0/942	0.71	5/1269 (0.4%)
26	Q	0.28	0/1125	0.55	0/1510
27	R	0.31	0/1044	0.60	0/1402
28	S	0.19	0/1208	0.49	0/1624
29	T	0.19	0/1129	0.40	0/1520
30	U	0.26	0/857	0.56	0/1158
31	Z	0.16	0/603	0.41	0/814
32	c	0.17	0/501	0.45	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.23	0/473	0.53	0/629
34	f	0.17	0/597	0.49	0/795
35	g	0.19	0/2523	0.50	0/3434
36	i	0.17	0/807	0.43	0/1072
37	3	0.10	0/595	0.28	0/920
38	1	0.25	0/1529	0.58	3/2376 (0.1%)
39	j	0.22	0/2177	0.55	0/2931
40	k	0.19	0/3657	0.48	0/4946
41	l	0.16	0/1099	0.47	1/1469 (0.1%)
All	All	0.19	1/91710 (0.0%)	0.43	19/132873 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	140	THR	N-CA	5.45	1.53	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	104	ARG	N-CA-C	-15.04	94.19	112.54
4	C	235	TRP	N-CA-C	10.00	122.17	111.28
22	F	107	GLY	N-CA-C	-8.56	100.92	111.45
25	P	37	ALA	CA-C-N	7.83	127.85	119.78
25	P	37	ALA	C-N-CA	7.83	127.85	119.78

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	19211	1349	0
2	A	1702	0	1695	98	0
3	B	1796	0	1874	83	0
4	C	1648	0	1727	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2078	0	2157	102	0
6	G	1832	0	1919	90	0
7	H	1483	0	1579	86	0
8	I	1489	0	1504	77	0
9	J	1471	0	1554	81	0
10	L	1248	0	1311	60	0
11	N	1195	0	1263	56	0
12	O	955	0	987	64	0
13	V	687	0	682	45	0
14	W	1021	0	1056	71	0
15	X	1119	0	1198	51	0
16	Y	1061	0	1111	52	0
17	a	797	0	835	52	0
18	b	609	0	629	17	0
19	e	472	0	508	21	0
20	h	233	0	284	14	0
21	D	1774	0	1855	60	0
22	F	1609	0	1679	120	0
23	K	809	0	810	43	0
24	M	885	0	917	43	0
25	P	923	0	960	70	0
26	Q	1105	0	1170	69	0
27	R	1033	0	1082	69	0
28	S	1189	0	1211	58	0
29	T	1110	0	1124	55	0
30	U	845	0	913	53	0
31	Z	594	0	590	37	0
32	c	499	0	536	27	0
33	d	461	0	448	31	0
34	f	584	0	601	47	0
35	g	2469	0	2403	134	0
36	i	799	0	804	41	0
37	3	536	0	277	10	0
38	1	1639	0	852	88	0
39	j	2145	0	2216	151	0
40	k	3596	0	3713	154	0
41	l	1083	0	1123	36	0
42	2	113	0	0	0	0
42	T	1	0	0	0	0
42	i	1	0	0	0	0
42	k	1	0	0	0	0
43	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	b	1	0	0	0	0
43	f	1	0	0	0	0
44	k	32	0	14	8	0
45	k	8	0	8	2	0
46	2	3	0	0	0	0
All	All	86935	0	68390	3374	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 3374 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)
8:I:140:THR:HG23	8:I:144:TRP:CZ3	1.47	1.48
38:1:26:M2G:HM22	38:1:44:A:N1	1.44	1.31
3:B:8:ARG:O	3:B:9:LEU:CD1	1.80	1.29
39:j:74:LEU:HB2	39:j:89:ARG:NH1	1.46	1.28
22:F:103:GLY:HA3	22:F:106:ASN:OD1	1.28	1.25

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%)	191 (88%)	26 (12%)	0	100	100
3	B	221/255 (87%)	192 (87%)	27 (12%)	2 (1%)	14	48
4	C	218/259 (84%)	198 (91%)	19 (9%)	1 (0%)	24	60
5	E	258/261 (99%)	234 (91%)	24 (9%)	0	100	100
6	G	228/236 (97%)	214 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	182/190 (96%)	152 (84%)	28 (15%)	2 (1%)	11	44
8	I	184/201 (92%)	163 (89%)	20 (11%)	1 (0%)	24	60
9	J	180/188 (96%)	154 (86%)	22 (12%)	4 (2%)	5	31
10	L	153/156 (98%)	135 (88%)	18 (12%)	0	100	100
11	N	149/151 (99%)	138 (93%)	11 (7%)	0	100	100
12	O	127/137 (93%)	107 (84%)	20 (16%)	0	100	100
13	V	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
14	W	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
15	X	142/145 (98%)	122 (86%)	20 (14%)	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%)	68 (86%)	11 (14%)	0	100	100
19	e	58/63 (92%)	53 (91%)	5 (9%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	210 (93%)	14 (6%)	1 (0%)	30	65
22	F	204/227 (90%)	182 (89%)	21 (10%)	1 (0%)	24	60
23	K	94/106 (89%)	84 (89%)	10 (11%)	0	100	100
24	M	113/134 (84%)	91 (80%)	21 (19%)	1 (1%)	14	48
25	P	115/142 (81%)	97 (84%)	18 (16%)	0	100	100
26	Q	139/143 (97%)	119 (86%)	18 (13%)	2 (1%)	9	39
27	R	128/136 (94%)	104 (81%)	19 (15%)	5 (4%)	2	22
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%)	96 (92%)	8 (8%)	0	100	100
31	Z	76/108 (70%)	68 (90%)	8 (10%)	0	100	100
32	c	62/67 (92%)	55 (89%)	7 (11%)	0	100	100
33	d	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
34	f	72/150 (48%)	55 (76%)	17 (24%)	0	100	100
35	g	314/326 (96%)	277 (88%)	37 (12%)	0	100	100
36	i	95/153 (62%)	83 (87%)	12 (13%)	0	100	100
39	j	263/304 (86%)	238 (90%)	24 (9%)	1 (0%)	30	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	k	468/527 (89%)	433 (92%)	32 (7%)	3 (1%)	21	57
41	l	126/285 (44%)	120 (95%)	5 (4%)	1 (1%)	16	52
All	All	5798/6582 (88%)	5152 (89%)	621 (11%)	25 (0%)	31	65

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	6	ASN
8	I	140	THR
26	Q	42	GLU
27	R	93	LEU
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%)	201 (100%)	1 (0%)	81	82
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%)	191 (100%)	1 (0%)	81	82
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%)	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
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%)	82 (99%)	1 (1%)	63	73
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%)	173 (99%)	1 (1%)	78	81
23	K	88/96 (92%)	88 (100%)	0	100	100
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%)	116 (99%)	1 (1%)	70	76
27	R	116/124 (94%)	113 (97%)	3 (3%)	40	61
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	83/130 (64%)	83 (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	4978/5595 (89%)	4969 (100%)	9 (0%)	85	87

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

Mol	Chain	Res	Type
27	R	93	LEU
27	R	100	LEU
17	a	11	ASN
22	F	105	ASN
26	Q	40	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
26	Q	21	HIS
36	i	88	GLN
27	R	97	ASN
31	Z	38	HIS
40	k	144	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	593 (32%)	23 (1%)
37	3	25/49 (51%)	16 (64%)	0
38	1	71/75 (94%)	31 (43%)	8 (11%)
All	All	1893/1922 (98%)	640 (33%)	31 (1%)

5 of 640 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	13	C
1	2	14	C
1	2	17	C

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1198	G
38	1	27	C
1	2	1343	A
38	1	44	A
38	1	14	A

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	1MA	1	58	38	21,25,26	3.16	6 (28%)	30,37,40	2.51	8 (26%)
38	2MG	1	10	38	23,26,27	2.91	8 (34%)	33,38,41	2.18	11 (33%)
38	M2G	1	26	38	24,27,28	1.33	4 (16%)	33,40,43	2.08	8 (24%)
1	PSU	2	465	1	18,21,22	4.44	7 (38%)	21,30,33	1.90	5 (23%)
1	PSU	2	766	1	18,21,22	4.45	7 (38%)	21,30,33	2.11	6 (28%)
1	B8N	2	1190	1	25,29,30	3.35	7 (28%)	28,42,45	2.00	9 (32%)
38	5MC	1	49	38	19,22,23	3.94	8 (42%)	26,32,35	1.07	3 (11%)
1	5MC	2	1637	1	19,22,23	3.83	8 (42%)	26,32,35	0.93	1 (3%)
38	7MG	1	46	38	23,26,27	3.64	11 (47%)	27,39,42	2.21	9 (33%)
38	1MG	1	9	38	23,26,27	3.33	7 (30%)	33,39,42	2.30	8 (24%)
1	2MG	2	1426	1,42	23,26,27	2.90	8 (34%)	33,38,41	2.18	9 (27%)
1	7MG	2	1573	1,38	23,26,27	3.59	11 (47%)	27,39,42	2.22	9 (33%)
1	MA6	2	1780	1	23,26,27	1.40	4 (17%)	33,38,41	3.22	11 (33%)
38	5MC	1	48	38	19,22,23	3.84	8 (42%)	26,32,35	1.18	2 (7%)
38	T6A	1	37	38	31,34,35	1.81	7 (22%)	43,49,52	2.16	13 (30%)
38	H2U	1	16	38	18,21,22	3.13	4 (22%)	19,30,33	1.36	4 (21%)
1	5MC	2	1006	1	19,22,23	3.84	8 (42%)	26,32,35	1.11	3 (11%)
1	PSU	2	120	1	18,21,22	4.45	7 (38%)	21,30,33	1.98	6 (28%)
1	2MG	2	1570	1	23,26,27	2.92	8 (34%)	33,38,41	2.15	10 (30%)
1	PSU	2	998	1	18,21,22	4.42	7 (38%)	21,30,33	1.94	6 (28%)
1	PSU	2	1289	1	18,21,22	4.46	7 (38%)	21,30,33	1.86	5 (23%)
38	H2U	1	47	38	18,21,22	3.16	4 (22%)	19,30,33	1.43	4 (21%)
38	RIA	1	64	38	35,38,39	4.66	14 (40%)	50,57,60	1.97	12 (24%)

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	1MA	1	58	38	-	2/7/25/26	0/3/3/3
38	2MG	1	10	38	-	0/9/27/28	0/3/3/3

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

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	64	RIA	C1'-C2'	-16.24	1.32	1.52
1	2	1289	PSU	C6-C5	11.90	1.48	1.35
1	2	766	PSU	C6-C5	11.76	1.48	1.35
1	2	120	PSU	C6-C5	11.72	1.48	1.35
1	2	465	PSU	C6-C5	11.70	1.48	1.35

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1780	MA6	N1-C6-N6	-11.95	102.30	116.86
1	2	1780	MA6	C5-C6-N6	7.81	137.70	125.33
38	1	58	1MA	C1'-N9-C8	-7.34	105.89	126.73
38	1	26	M2G	C5-C4-N3	-6.79	117.58	128.39
1	2	1426	2MG	C2-N3-C4	6.63	120.30	112.00

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	766	PSU	O4'-C4'-C5'-O5'
1	2	1190	B8N	O4'-C4'-C5'-O5'
1	2	1289	PSU	O4'-C4'-C5'-O5'
1	2	1780	MA6	C5-C6-N6-C10
1	2	1780	MA6	N1-C6-N6-C10

There are no ring outliers.

21 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	1	58	1MA	2	0
38	1	10	2MG	6	0
38	1	26	M2G	9	0
1	2	465	PSU	1	0
1	2	766	PSU	1	0
1	2	1190	B8N	2	0
38	1	49	5MC	2	0
1	2	1637	5MC	2	0
38	1	46	7MG	3	0
38	1	9	1MG	4	0
1	2	1426	2MG	3	0
1	2	1573	7MG	2	0
1	2	1780	MA6	4	0
38	1	48	5MC	7	0
38	1	37	T6A	4	0
38	1	16	H2U	5	0
1	2	1006	5MC	1	0
1	2	1570	2MG	1	0
1	2	998	PSU	2	0
38	1	47	H2U	5	0
38	1	64	RIA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
44	GCP	k	601	-	32,34,34	1.47	7 (21%)	49,54,54	1.79	8 (16%)
45	MET	k	603	-	6,7,8	0.50	0	2,7,9	0.35	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
44	GCP	k	601	-	-	0/19/38/38	0/3/3/3
45	MET	k	603	-	-	1/5/6/8	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	k	601	GCP	C5-C4	3.19	1.47	1.38
44	k	601	GCP	PG-O3G	2.92	1.61	1.55
44	k	601	GCP	PG-O2G	2.90	1.61	1.55
44	k	601	GCP	PB-O3A	2.76	1.61	1.58
44	k	601	GCP	C6-N1	-2.41	1.34	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	601	GCP	C5-C4-N3	-6.19	118.54	128.39
44	k	601	GCP	C2-N3-C4	5.04	120.98	112.30
44	k	601	GCP	N9-C4-N3	4.57	135.09	125.95
44	k	601	GCP	PB-O3A-PA	-3.65	120.45	132.37
44	k	601	GCP	C6-C5-N7	3.21	136.13	130.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

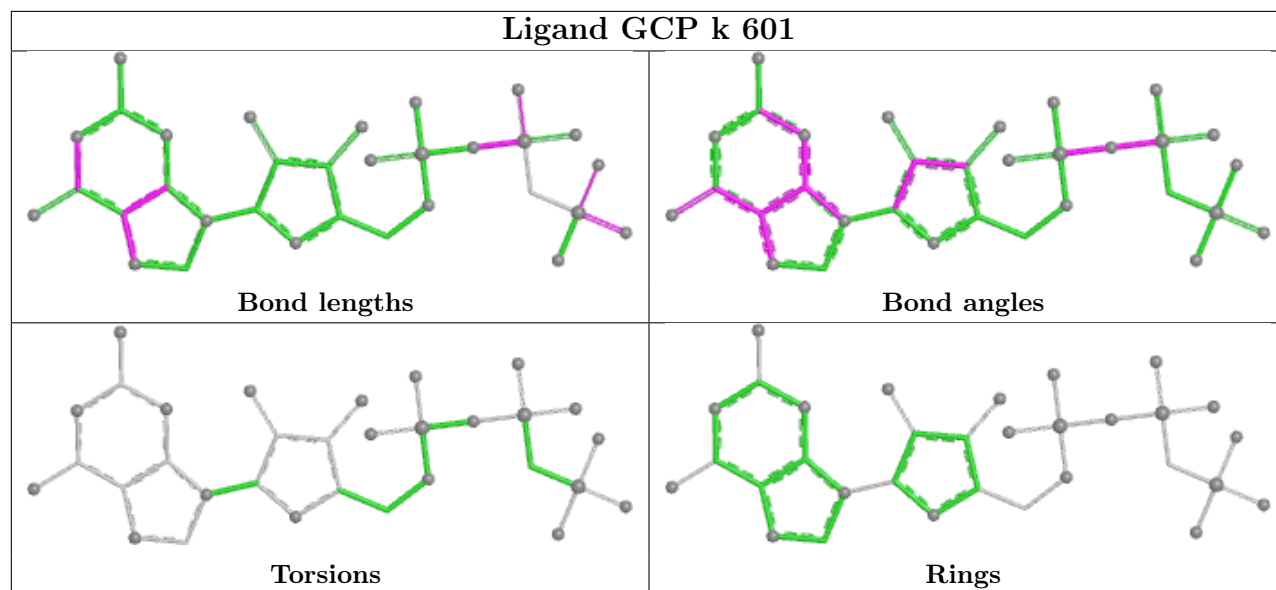
Mol	Chain	Res	Type	Atoms
45	k	603	MET	CB-CG-SD-CE

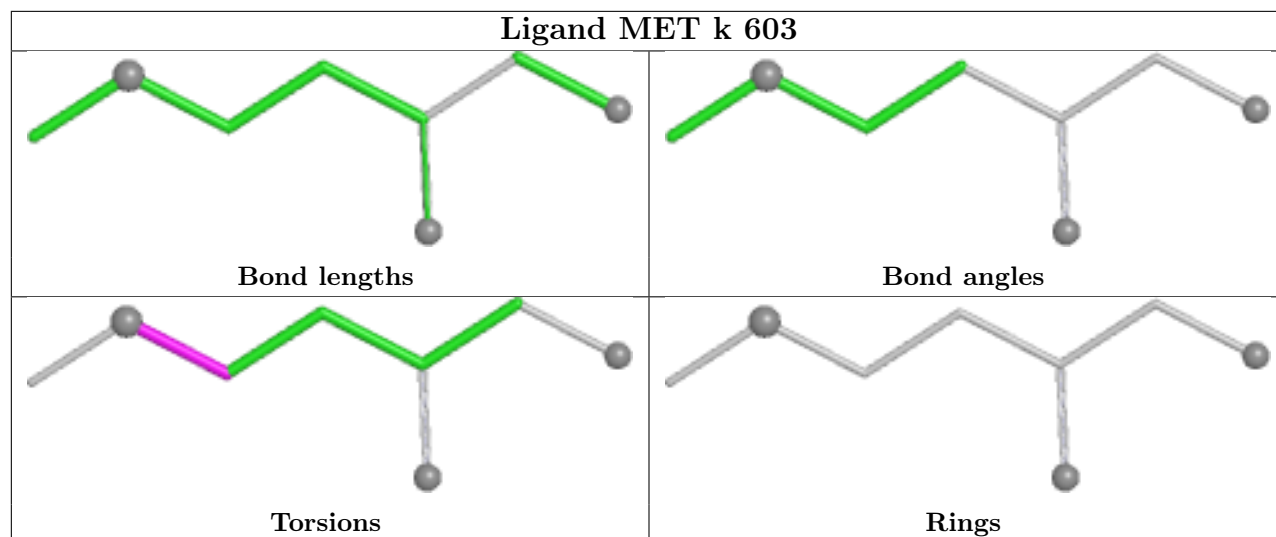
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	k	601	GCP	8	0
45	k	603	MET	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	8.39
1	1	16:H2U	O3'	18:G	P	4.94
1	1	63:G	O3'	64:RIA	P	3.65

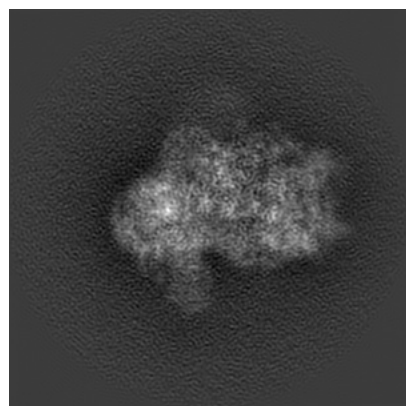
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19804. These allow visual inspection of the internal detail of the map and identification of artifacts.

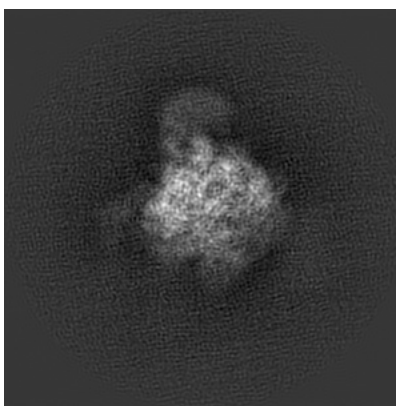
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

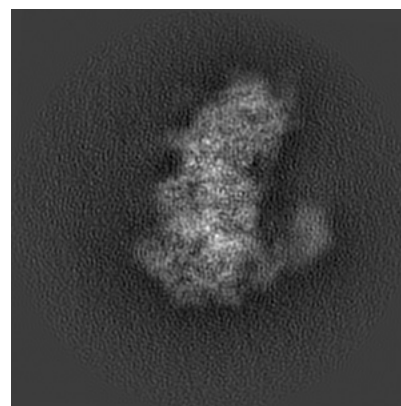
6.1.1 Primary map



X

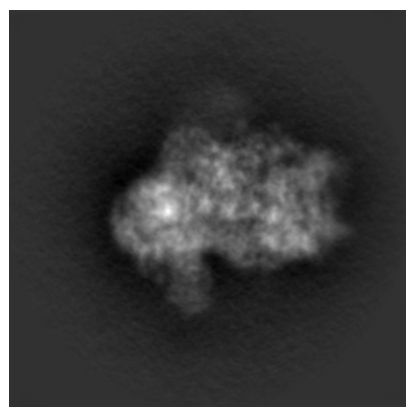


Y

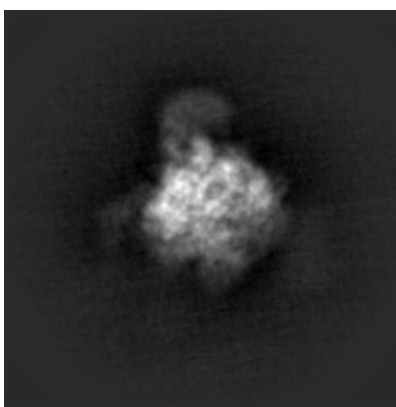


Z

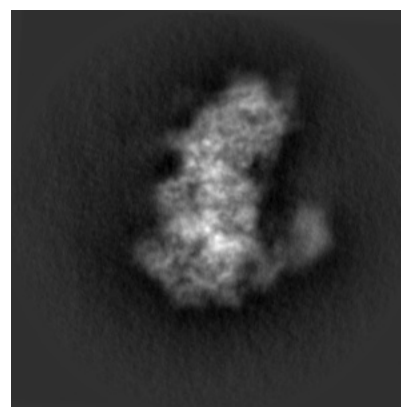
6.1.2 Raw map



X



Y

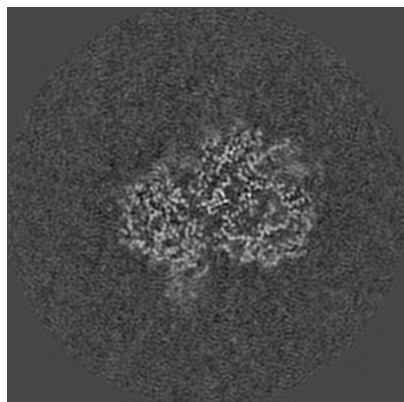


Z

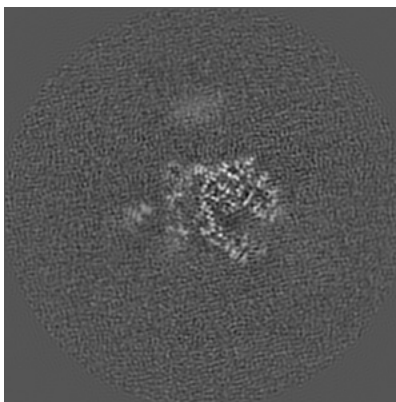
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

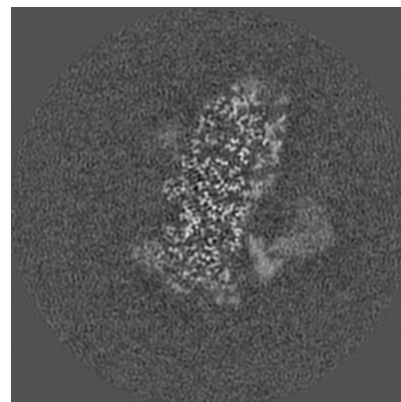
6.2.1 Primary map



X Index: 150

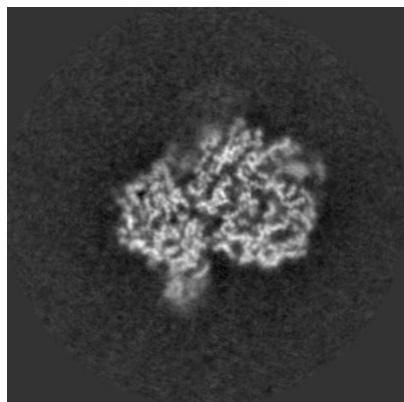


Y Index: 150

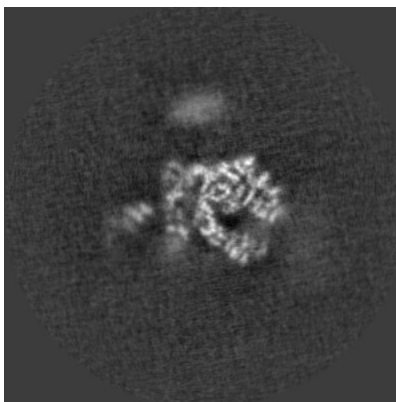


Z Index: 150

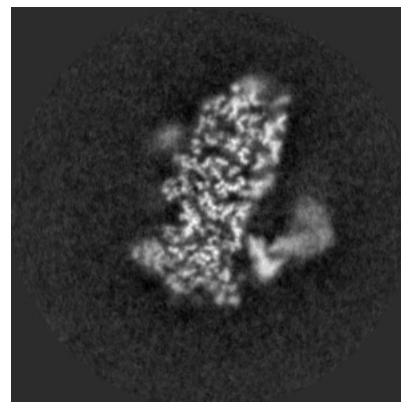
6.2.2 Raw map



X Index: 150



Y Index: 150

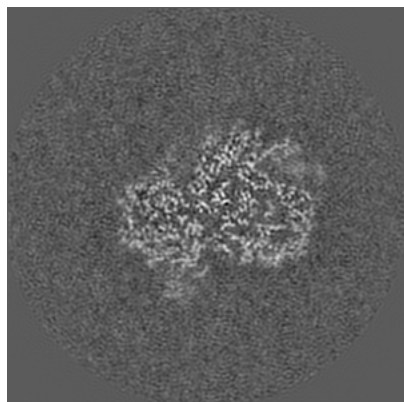


Z Index: 150

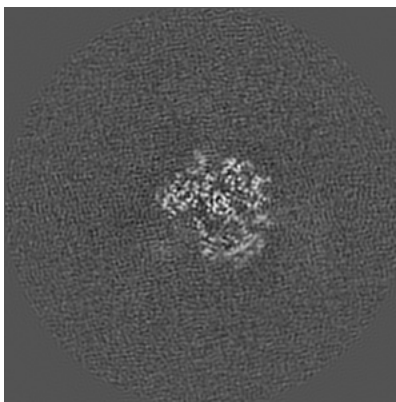
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

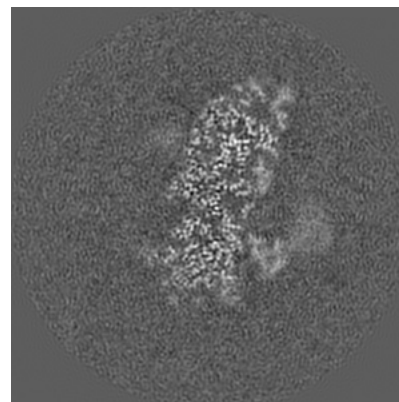
6.3.1 Primary map



X Index: 151

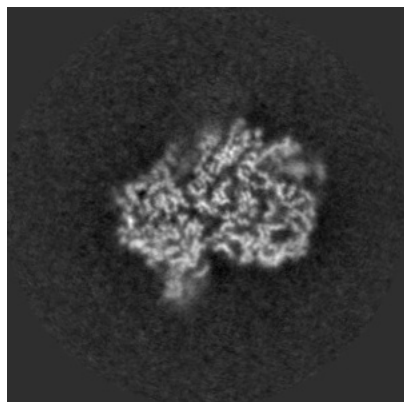


Y Index: 162

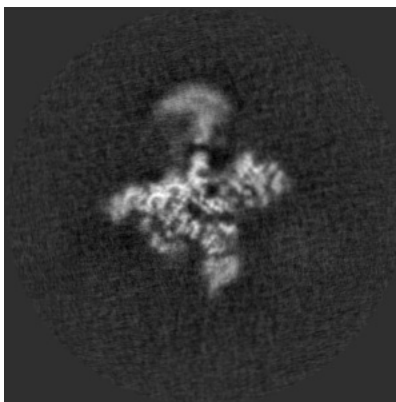


Z Index: 146

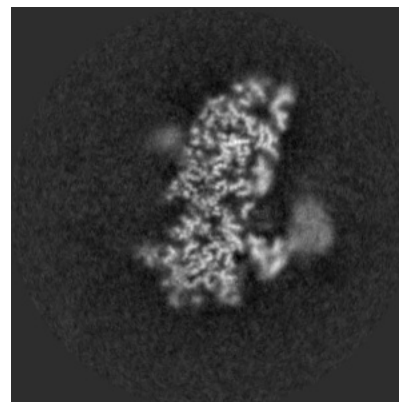
6.3.2 Raw map



X Index: 151



Y Index: 124

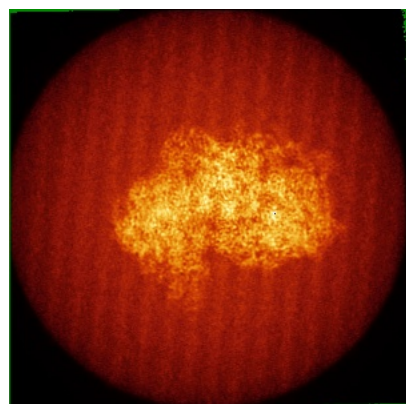


Z Index: 146

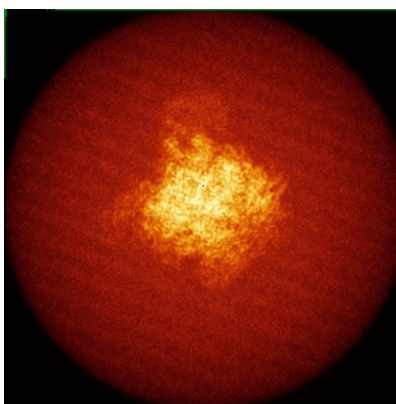
The images above show the largest variance slices of the map in three orthogonal directions.

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

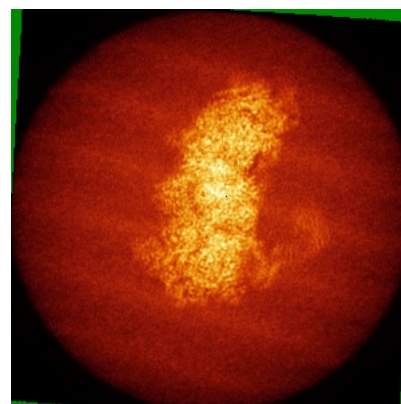
6.4.1 Primary map



X

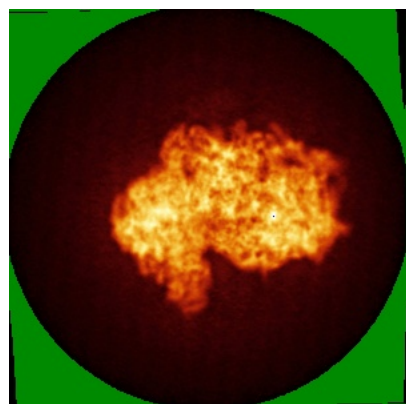


Y

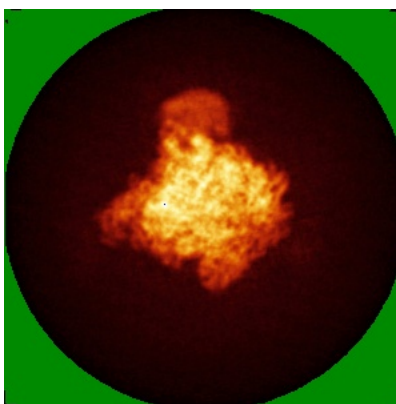


Z

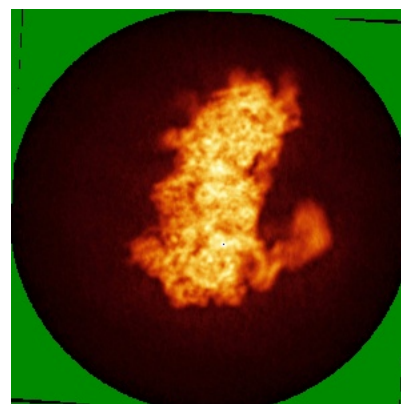
6.4.2 Raw map



X



Y

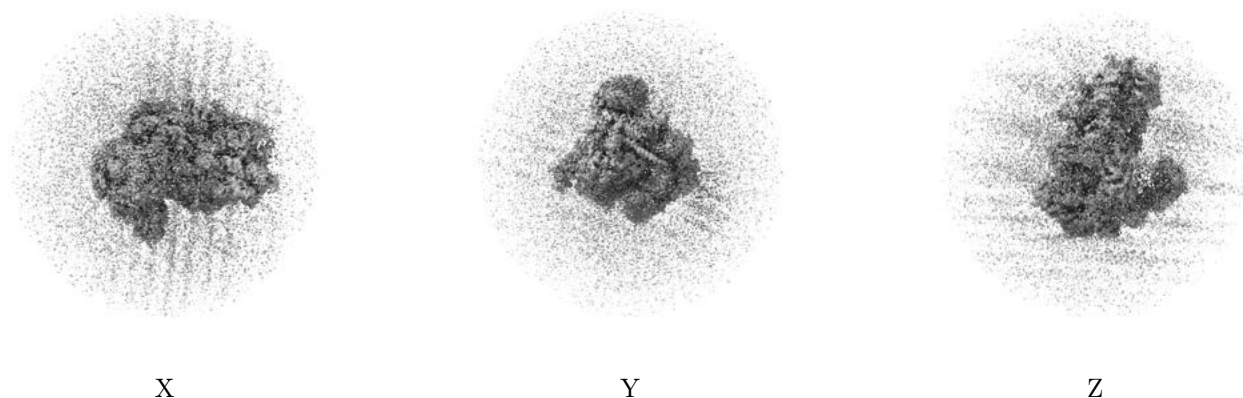


Z

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.

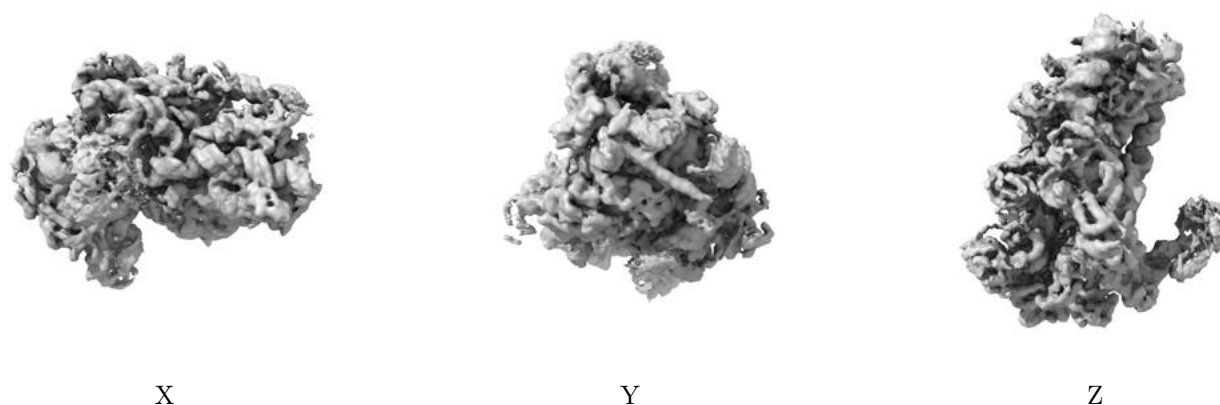
6.5 Orthogonal surface views [i](#)

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.

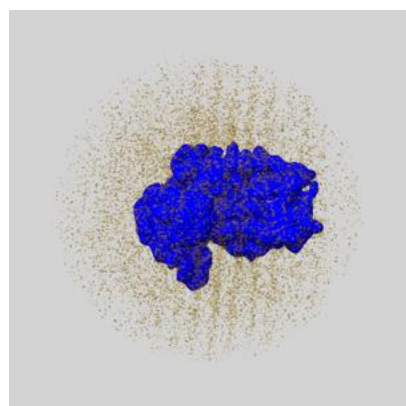
6.6 Mask visualisation [i](#)

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

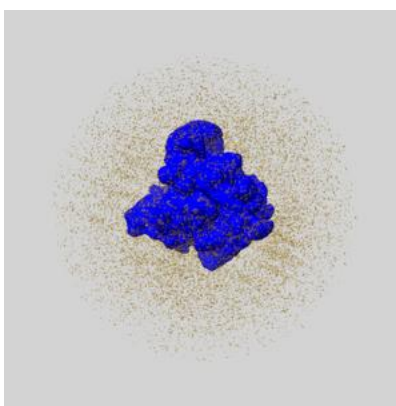
A mask typically either:

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

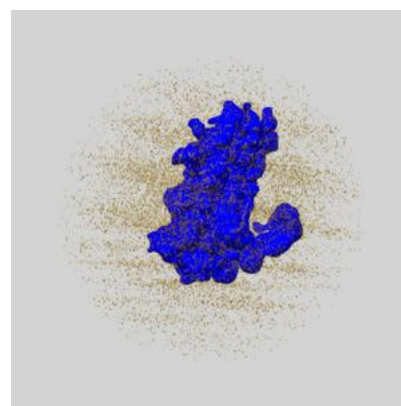
6.6.1 emd_19804_msk_1.map [i](#)



X



Y

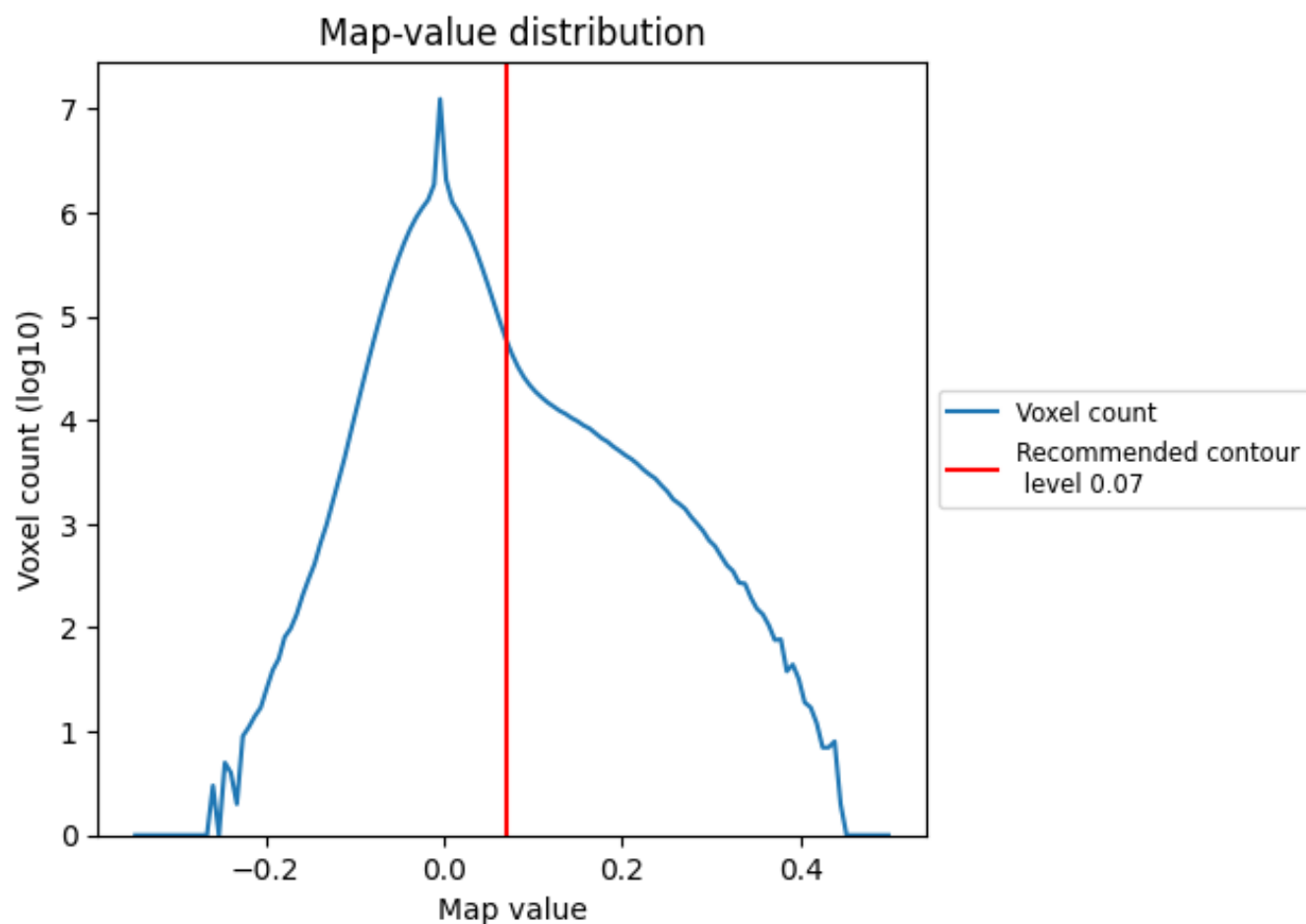


Z

7 Map analysis [i](#)

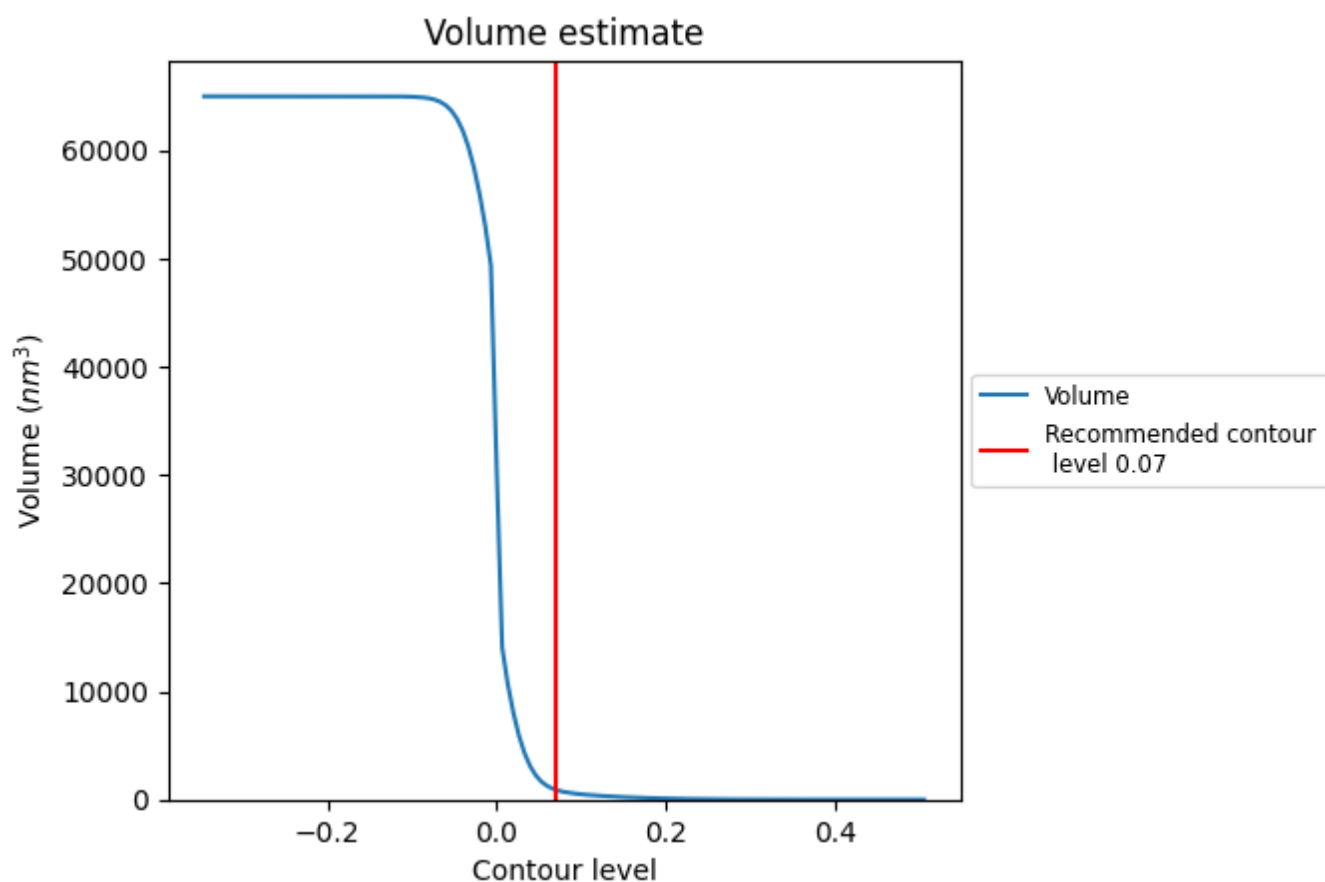
This section contains the results of statistical analysis of the map.

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.

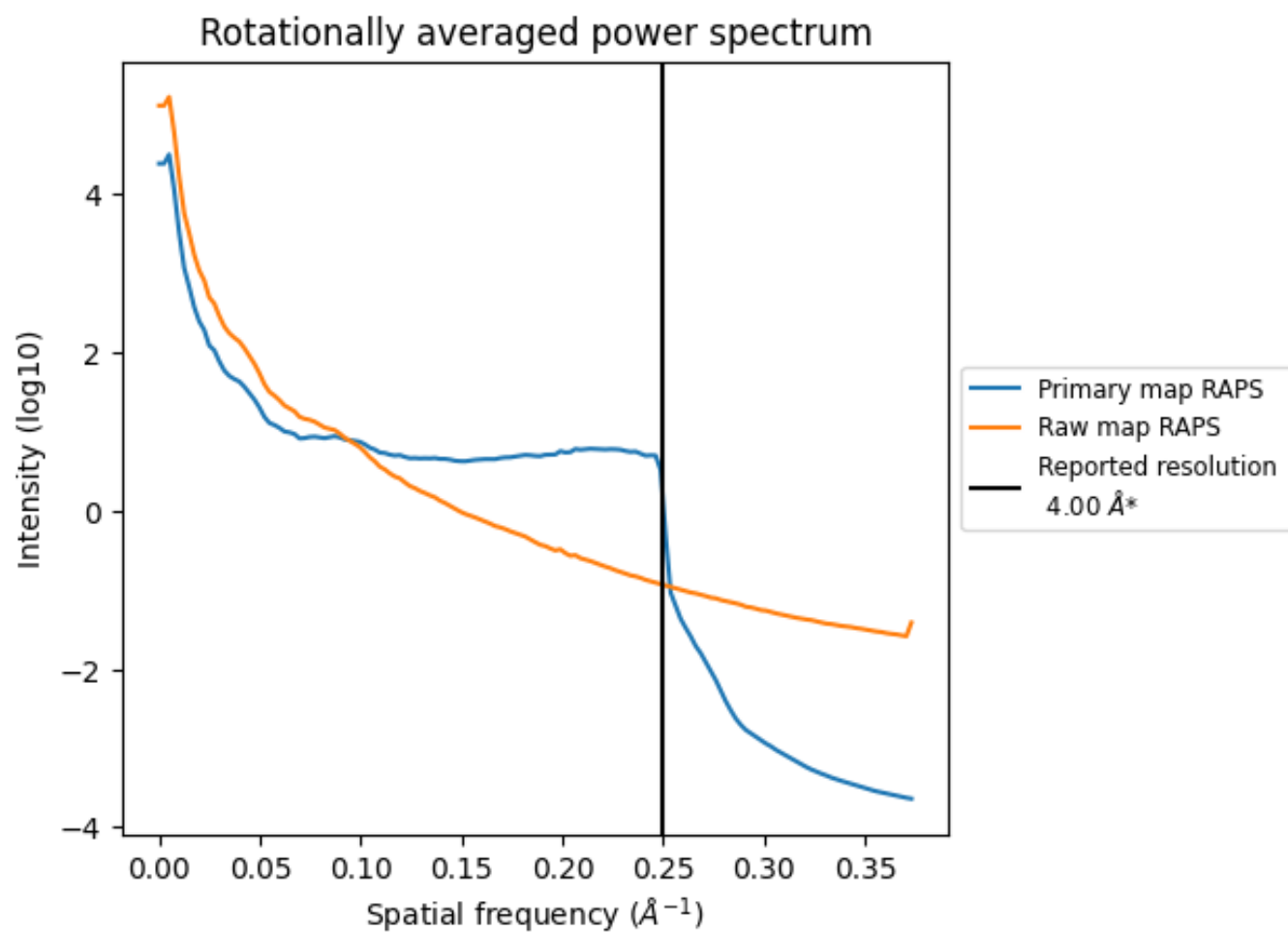
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 907 nm³; this corresponds to an approximate mass of 819 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 ⓘ

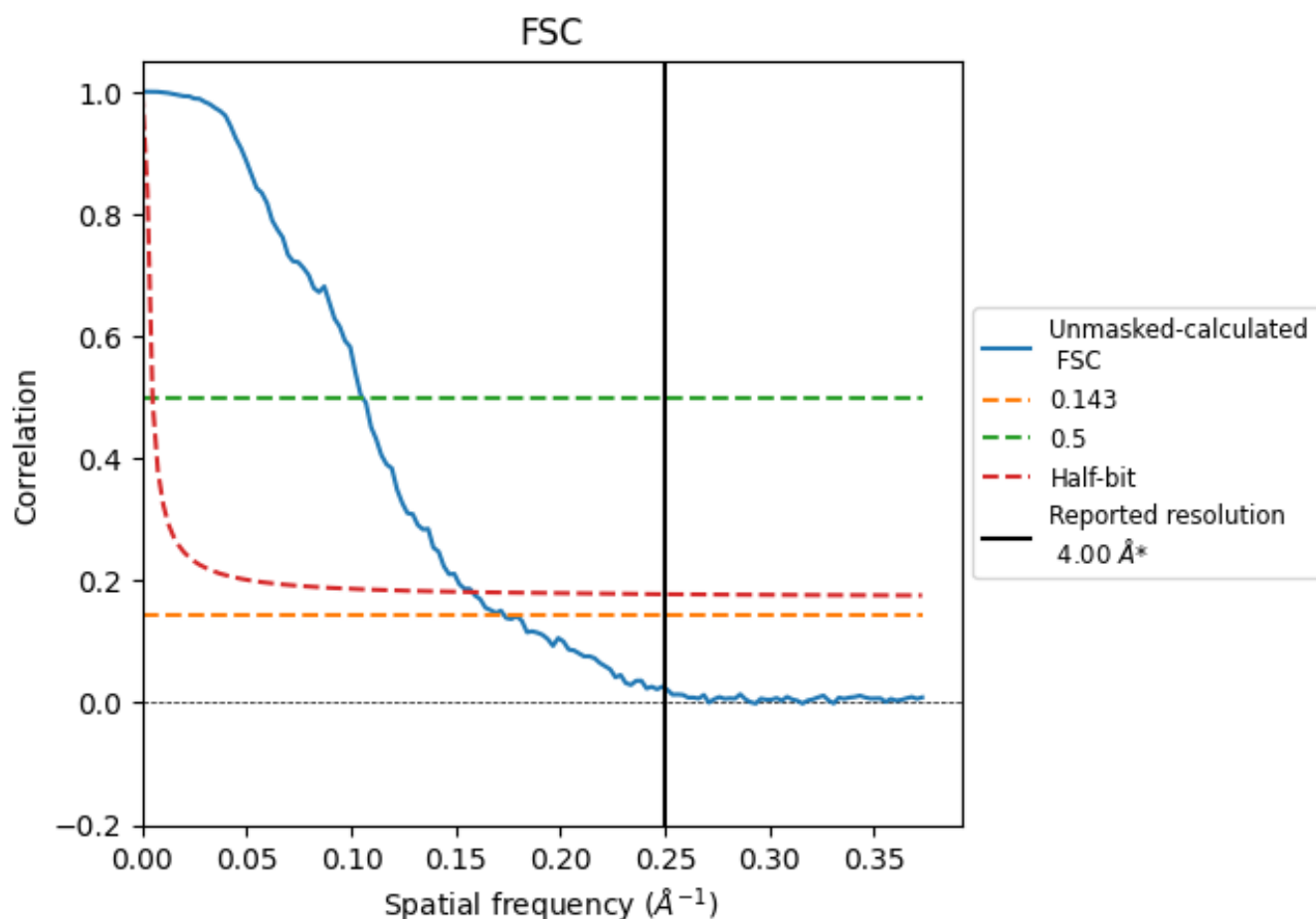


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

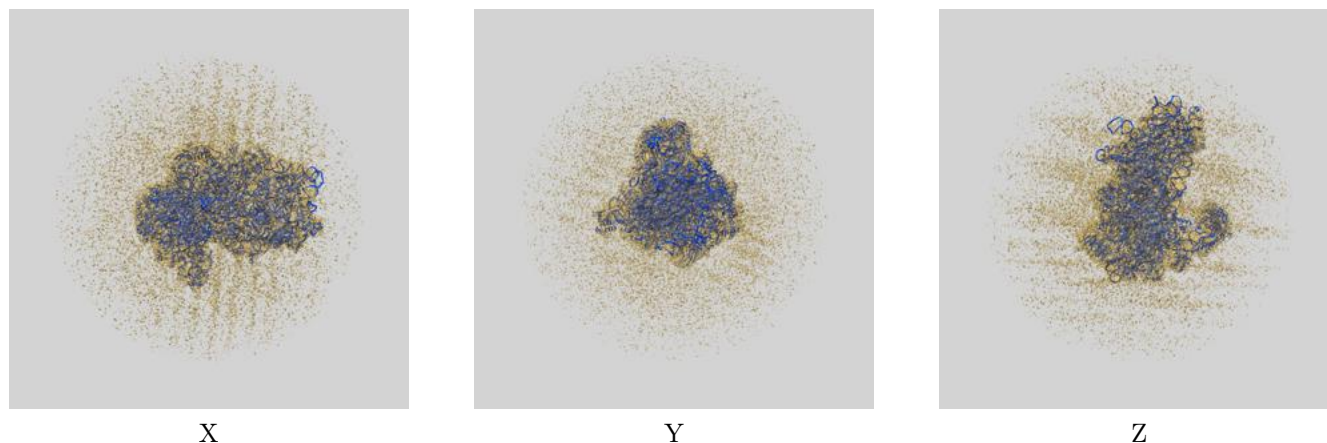
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Threesig
Reported by author	-	-	-	4.00
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	5.77	9.51	6.33	3.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

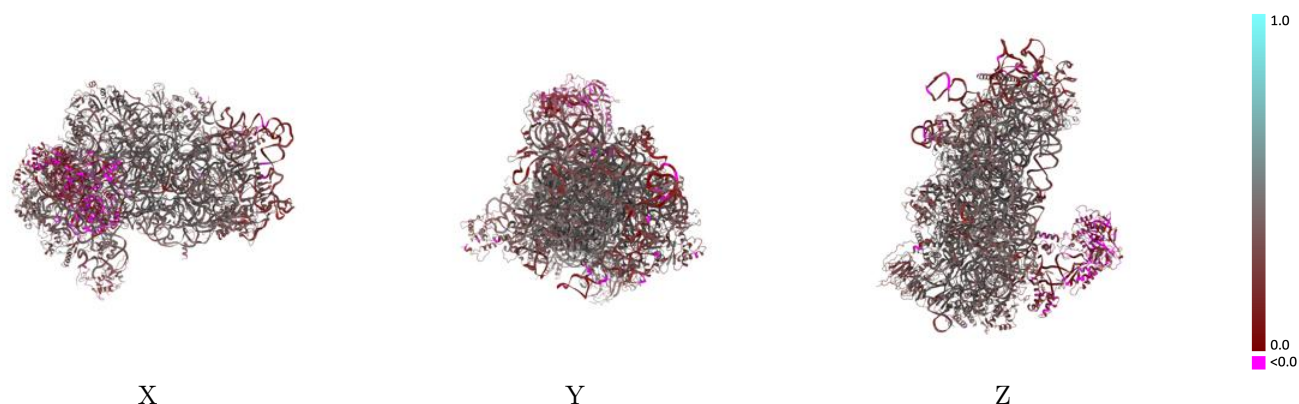
This section contains information regarding the fit between EMDB map EMD-19804 and PDB model 8S8G. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



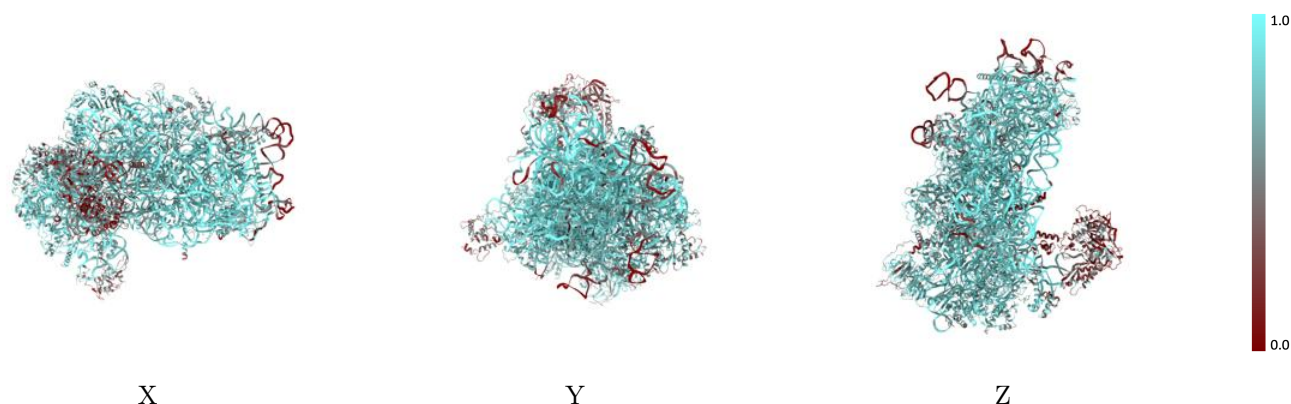
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



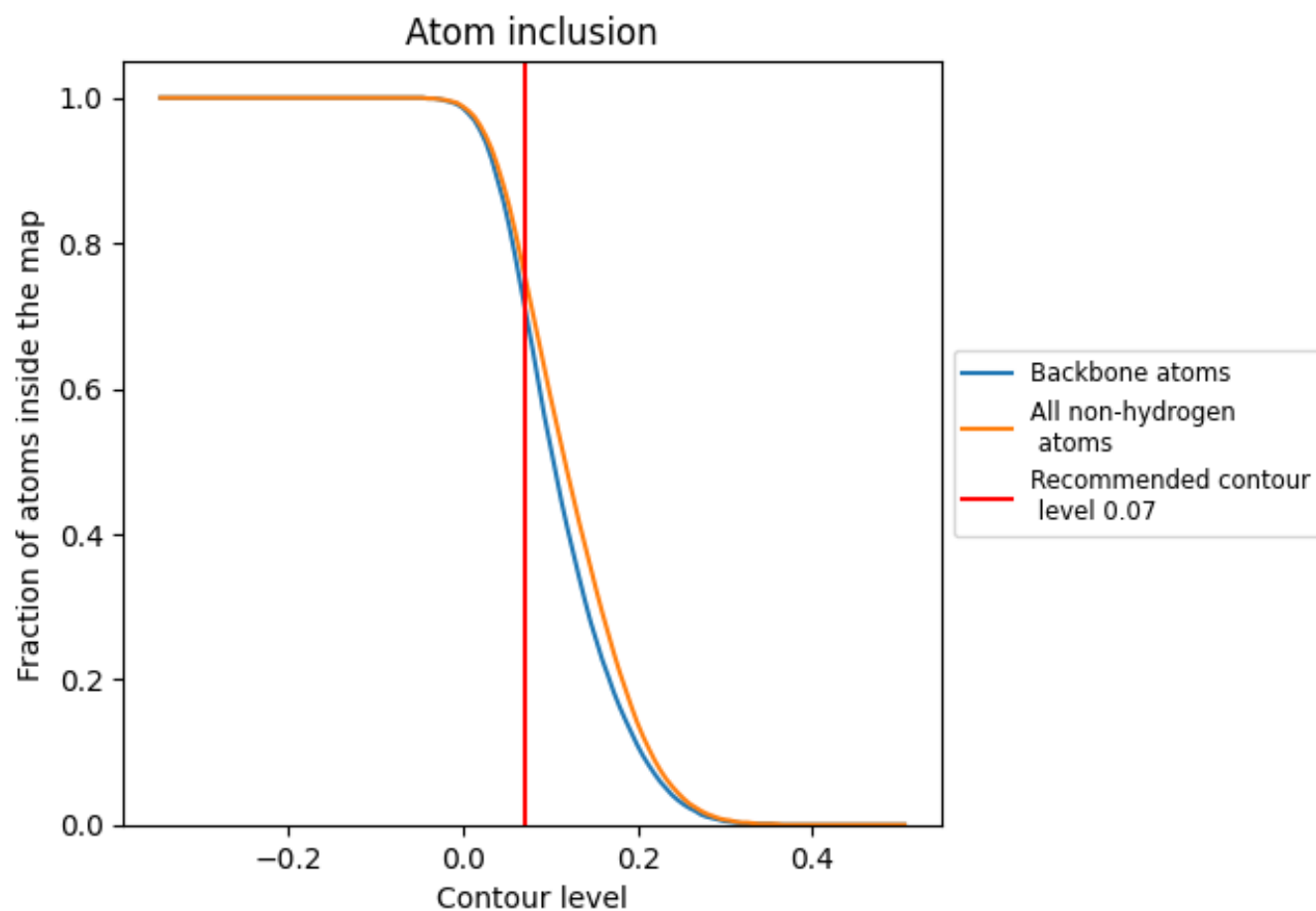
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 72% of all backbone atoms, 76% 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	 0.7610	 0.3530
1	 0.8150	 0.2240
2	 0.8710	 0.3690
3	 0.4010	 0.3040
A	 0.7570	 0.3840
B	 0.7550	 0.3810
C	 0.8110	 0.4300
D	 0.7430	 0.4010
E	 0.8260	 0.4230
F	 0.7410	 0.3910
G	 0.7640	 0.3430
H	 0.6620	 0.3580
I	 0.7480	 0.3760
J	 0.7940	 0.4120
K	 0.7560	 0.3470
L	 0.7420	 0.4110
M	 0.3470	 0.2380
N	 0.8100	 0.4050
O	 0.8030	 0.4130
P	 0.8140	 0.3610
Q	 0.7950	 0.3960
R	 0.6660	 0.3650
S	 0.8100	 0.3810
T	 0.8350	 0.3890
U	 0.7000	 0.3810
V	 0.8010	 0.4150
W	 0.7940	 0.4350
X	 0.7940	 0.4380
Y	 0.8110	 0.3940
Z	 0.6420	 0.3000
a	 0.7940	 0.4370
b	 0.7490	 0.4020
c	 0.7520	 0.4140
d	 0.8390	 0.4190
e	 0.7180	 0.3990



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Chain	Atom inclusion	Q-score
f	 0.4520	 0.2290
g	 0.7220	 0.3420
h	 0.1980	 0.2910
i	 0.5180	 0.3520
j	 0.5240	 0.1910
k	 0.2720	 0.0820
l	 0.0850	 0.1410