



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 07:12 AM UTC

PDB ID : 8RW1 / pdb_00008rw1
EMDB ID : EMD-19541
Title : Structure of a yeast 48S-AUC preinitiation complex in closed conformation
Authors : Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on : 2024-02-02
Resolution : 3.35 Å (reported)
Based on initial model : 6FYX

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

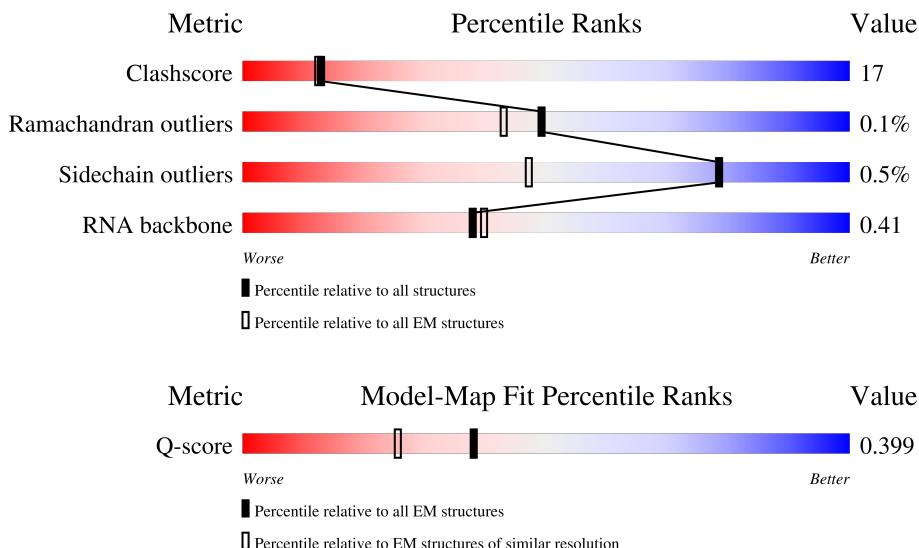
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 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.



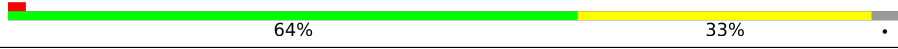
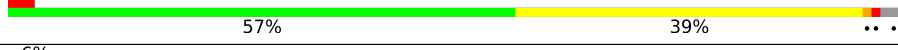
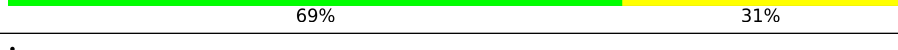
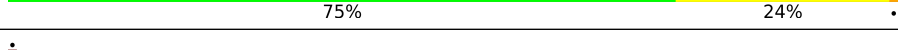
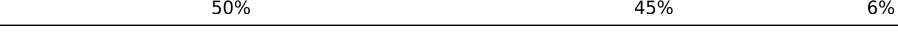
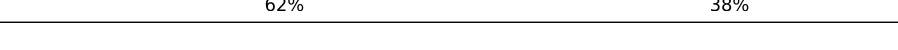
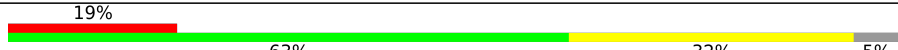
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14390 (2.85 - 3.85)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1798	
2	A	254	
3	B	255	

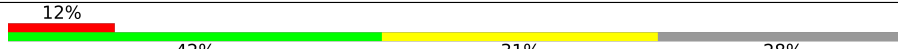
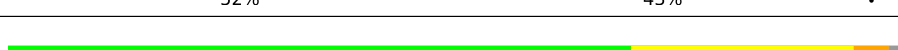
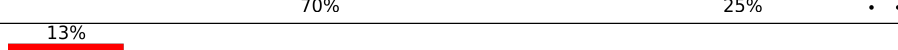
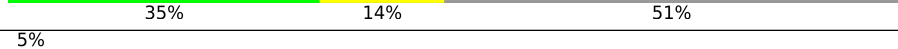
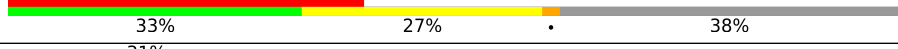
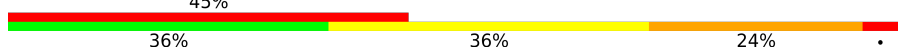
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Mol	Chain	Length	Quality of chain
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q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

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

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 86000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called KLLA0E23673p.

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

- Molecule 10 is a protein called KLLA0A10483p.

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

- Molecule 11 is a protein called KLLA0F18040p.

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

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

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

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

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

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

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

- Molecule 15 is a protein called KLLA0B11231p.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called KLLA0D10659p.

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

- Molecule 23 is a protein called KLLA0B08173p.

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

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

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

- Molecule 25 is a protein called KLLA0F07843p.

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

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

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

- Molecule 27 is a protein called KLLA0B01474p.

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

- Molecule 28 is a protein called KLLA0B01562p.

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

- Molecule 29 is a protein called KLLA0A07194p.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called KLLA0E12277p.

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

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

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

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

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

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

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

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

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

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

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

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

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

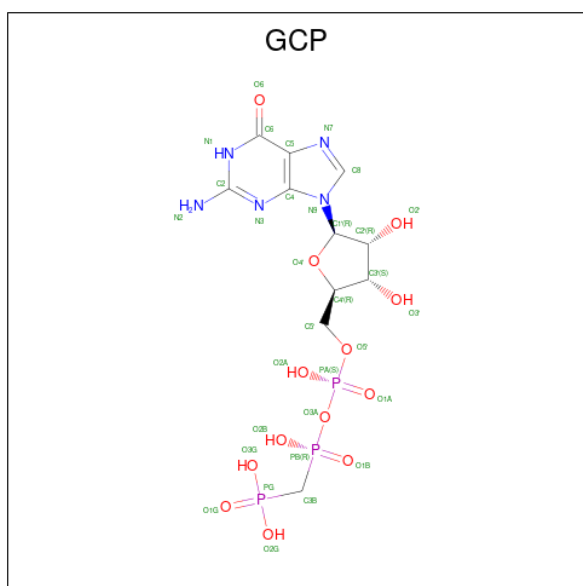
- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
42	2	112	Total	Mg	0
			112	112	
42	T	1	Total	Mg	0
			1	1	
42	i	1	Total	Mg	0
			1	1	
42	3	1	Total	Mg	0
			1	1	

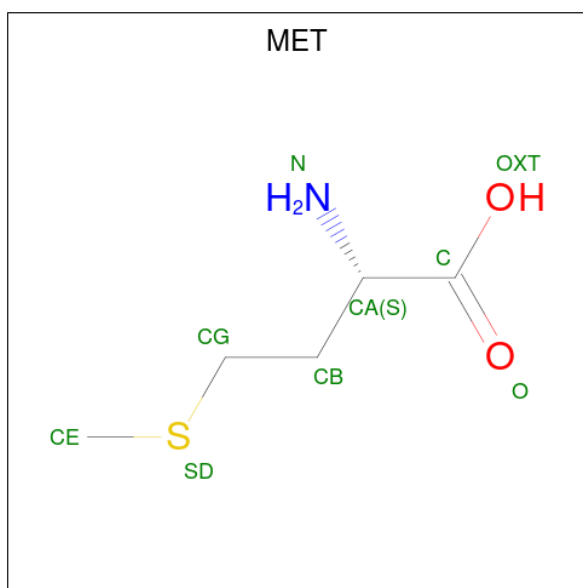
- Molecule 43 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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).



- Molecule 45 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



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

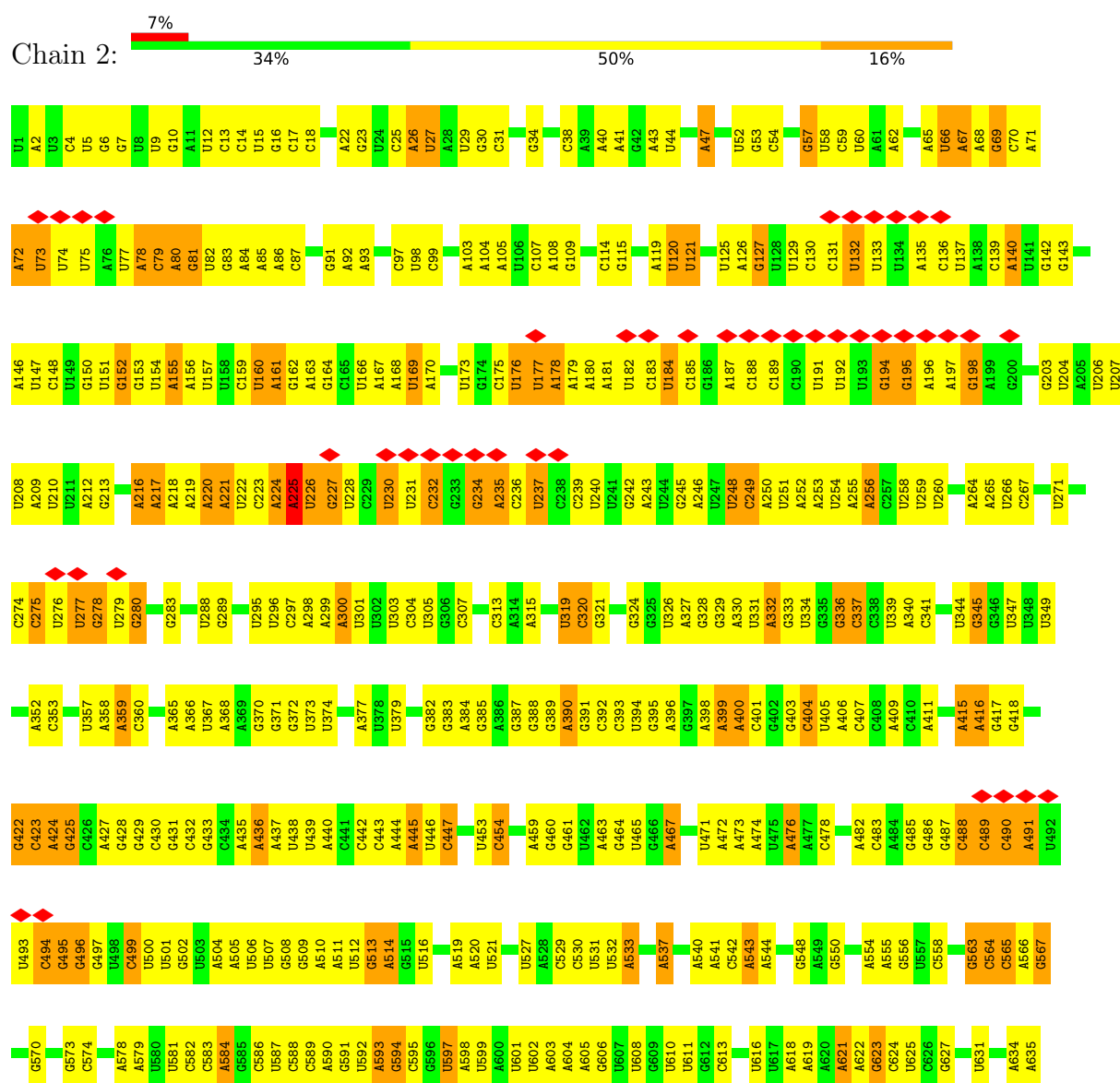
- Molecule 46 is water.

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

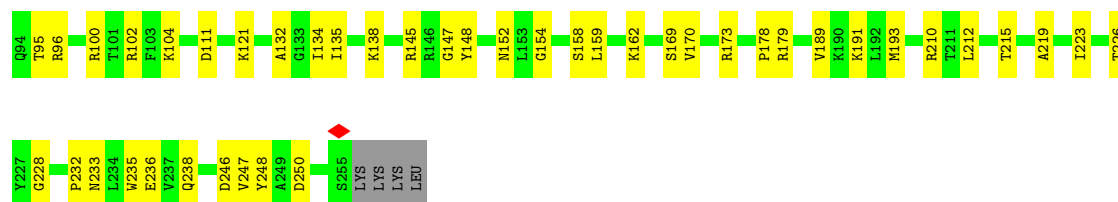
3 Residue-property plots

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.

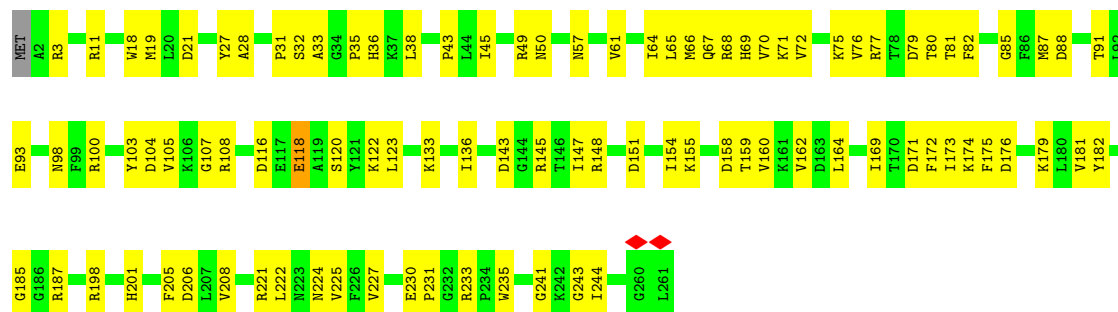
• Molecule 1: 18S ribosomal RNA



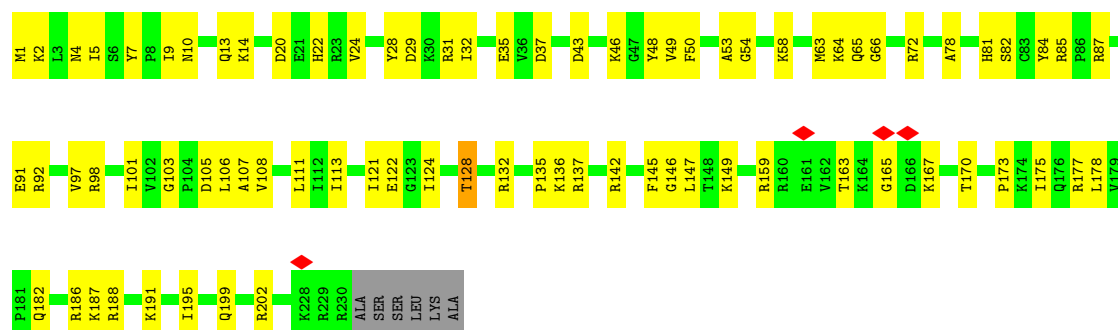
G1538	G1539	G1540	A1541	G1544	U1549	U1550	G1551	U1552	A1553	A1554	U1555	U1556	A1557	U1558	G1559	G1560	G1561	U1562	C1563	U1564	U1565	C1566	A1567	A1568	C1569	G1570	A1571	G1572	G1573	U1577	C1578	C1579	G1580	A1581	G1582	U1583	A1584	A1585	G1586	C1587	G1588	C1589	A1590	A1591	G1592	U1593	C1594	A1595	U1596	C1597	A1598	G1599	C1600	U1601	U1602	G1603
C1470	U1471	G1472	A1473	G1476	A1477	G1478	C1479	C1480	U1481	G1482	C1483	G1484	A1485	U1486	U1487	A1488	C1489	A1490	A1491	C1492	C1493	U1494	C1498	A1499	C1499	G1500	A1501	G1502	A1503	U1506	C1507	U1508	G1509	G1510	U1511	U1512	A1513	A1514	U1515	C1516	U1517	U1518	G1519	U1520	G1521	A1522	U1523	C1527	U1528	C1531	G1532	U1533	U1534	U1535	U1536	G1537
U1396	C1397	G1400	C1401	C1402	G1403	A1404	U1405	A1406	G1407	A1408	A1409	G1410	U1411	U1412	U1413	A1414	A1415	G1416	C1424	A1425	G1426	G1427	U1428	C1429	U1430	G1431	A1434	C1437	C1438	A1442	G1443	A1444	C1445	G1446	U1447	U1448	C1449	U1450	G1451	C1455	C1456	C1457	A1458	C1459	G1460	C1463	G1464	A1465	U1466	A1467	U1468	A1469				
A1324	G1329	A1330	C1331	C1332	U1333	U1334	A1335	A1336	C1337	C1338	U1339	A1340	A1343	A1344	A1345	U1346	A1347	G1348	G1349	G1350	U1351	U1352	G1353	C1354	U1355	G1356	G1357	C1358	A1359	C1360	U1361	G1362	G1363	G1366	G1367	U1368	U1369	U1370	U1373	C1374	U1375	U1379	A1380	G1381	A1382	A1386	C1387	U1388	A1389	U1390	U1391	A1392	C1393			
U1254	A1255	U1256	U1257	U1258	U1259	G1260	U1261	G1262	G1263	G1266	G1267	U1268	G1269	G1272	C1273	A1274	U1275	G1276	C1279	G1280	C1283	U1284	G1287	U1288	U1289	U1290	G1291	U1292	G1293	G1294	A1295	G1296	U1297	G1298	U1299	U1300	U1301	U1302	U1306	U1309	U1313	U1314	G1315	C1316	G1317	U1318	U1319	A1320	A1321	C1322	G1323					
A1188	C1189	B8N1190	C1191	U1114	A1192	C1193	C1194	A1195	C1196	G1197	G1198	G1199	G1200	A1201	A1202	C1204	U1205	C1206	A1207	C1208	C1209	A1210	G1211	G1212	U1213	A1216	G1217	A1218	C1219	A1220	U1224	A1225	G1227	G1228	A1229	U1230	C1234	A1235	G1236	A1237	U1238	U1239	G1240	A1241	G1242	A1243	G1244	U1245	C1247	U1248	U1249	U1250	C1251			
A1112	G1113	U1114	A1115	U1116	G1121	A1124	G1125	G1126	G1129	A1130	A1131	A1132	A1136	A1137	A1141	A1142	U1143	U1144	G1145	A1146	C1147	G1148	G1149	A1150	A1151	G1152	C1155	A1156	C1157	C1158	A1159	C1160	A1161	A1162	G1163	G1164	A1165	G1166	U1167	G1168	G1169	A1170	G1171	C1172	C1173	A1182	A1183	U1184	U1185	U1186	G1187					
A1038	G1039	G1040	G1041	A1042	U1043	C1044	G1047	U1048	G1049	G1050	U1051	G1052	U1055	U1056	U1057	C1058	U1059	U1060	A1061	U1062	C1066	C1069	U1070	G1071	G1072	G1073	C1074	A1075	G1076	C1077	U1078	U1079	A1080	C1081	G1082	A1085	A1086	A1087	U1088	A1091	A1092	C1095	U1096	G1099	G1100	G1101	U1102	G1106	G1107	G1108						
A965	A969	A970	G971	A972	G975	A976	A977	A978	A982	G983	G984	G985	G986	A987	U988	C989	G990	A991	U995	G996	A997	U998	U1003	C1006	G1007	U1008	C1009	G1010	U1011	A1012	G1013	U1014	C1015	U1016	U1017	A1018	C1021	A1022	A1025	A1026	C1027	U1028	A1029	U1030	G1031	C1032	C1033	G1034	A1035	C1036	U1037					
C896	A897	G898	A899	G900	G901	U902	G903	A904	G912	G913	A914	U915	U916	U917	A918	G919	U920	G921	A922	U923	G924	A925	C926	U927	A928	A929	U930	U931	A932	C933	G934	G935	A938	U939	A940	G941	U944	U945	U946	G947	C948	C949	A950	A951	G952	U953	A954	C955	U956	U957	U958	A959	U960	A961		
U830	U831	U832	G833	U834	U835	G836	G837	U838	U839	U840	A841	U842	A843	A846	C847	G852	U853	A854	U855	U856	C857	U860	A861	U862	U863	A864	G865	G866	A867	U868	U869	U870	U871	U872	C873	G874	G875	G876	G877	G878	C882	A883	G884	U885	A886	U887	U888	C889	G892	U893	A894	U895				
U698	U699	U700	U701	G702	G703	C704	U705	A706	A707	C708	C709	U710	U711	G712	U713	C714	U715	C716	C717	U718	U719	A721	G722	G723	G724	U725	G726	C727	A728	G729	U730	C731	G732	A733	A734	C735	C736	A737	G738	U739	A740	C741	U742	U743	U748	U749	U750	G751	A753	A754	A755	U758	U759	A760	G761	
U637	U638	U639	G640	G641	G642	U643	U644	U645	U646	G647	U648	U649	G650	U651	C652	G653	G654	U655	U656	C657	C658	G659	A660	C661	U662	U663	U664	A665	U666	G667	U668	C669	G670	C671	G672	A674	C675	U676	G677	G678	U679	U680	U681	U682	C683	A684	U685	C686	C687	G688	C692	U693	U694	U695	C696	C697



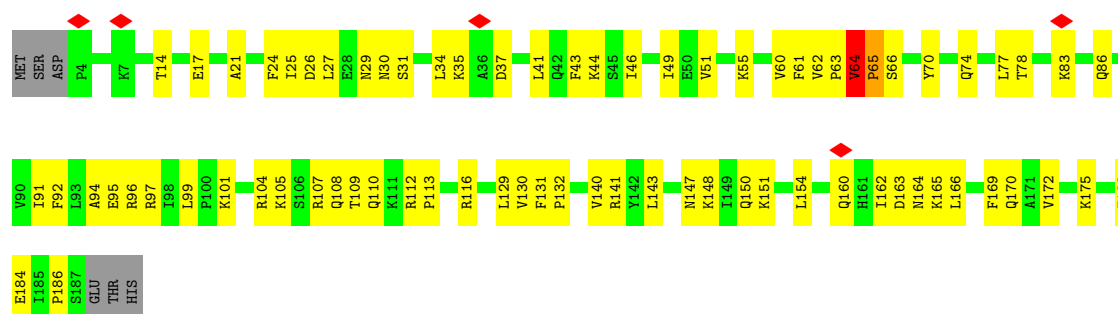
• Molecule 5: 40S ribosomal protein S4



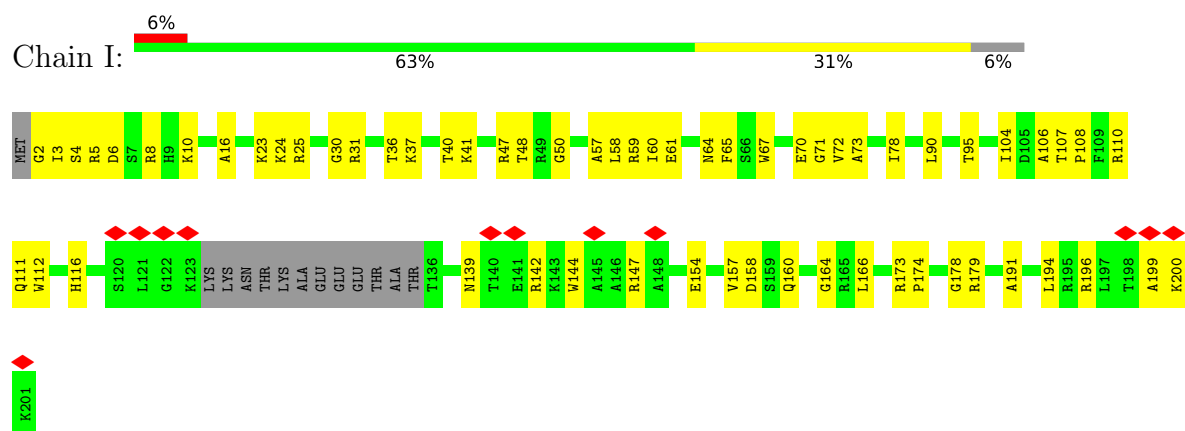
• Molecule 6: Small ribosomal subunit protein eS6



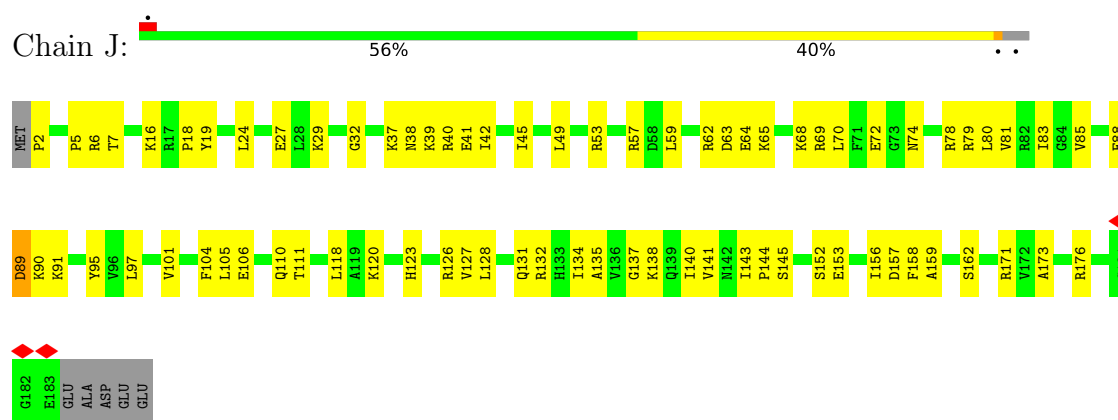
• Molecule 7: 40S ribosomal protein S7



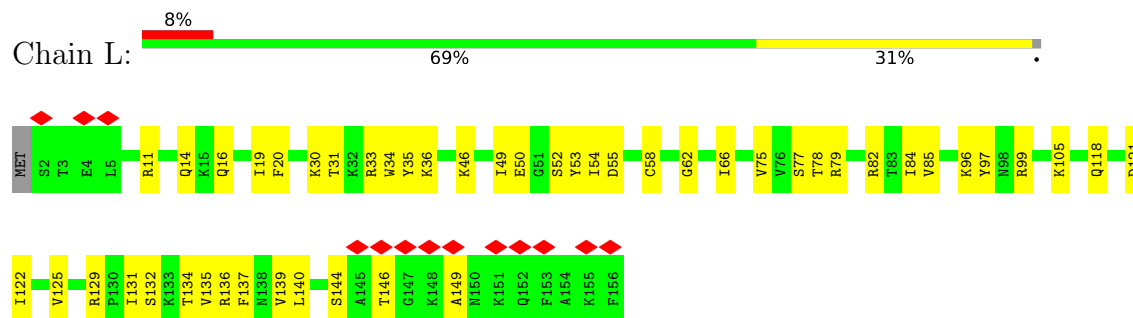
• Molecule 8: 40S ribosomal protein S8



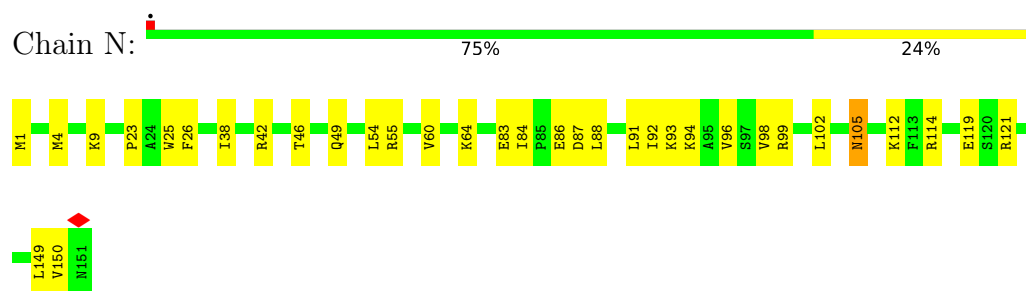
• Molecule 9: KLLA0E23673p



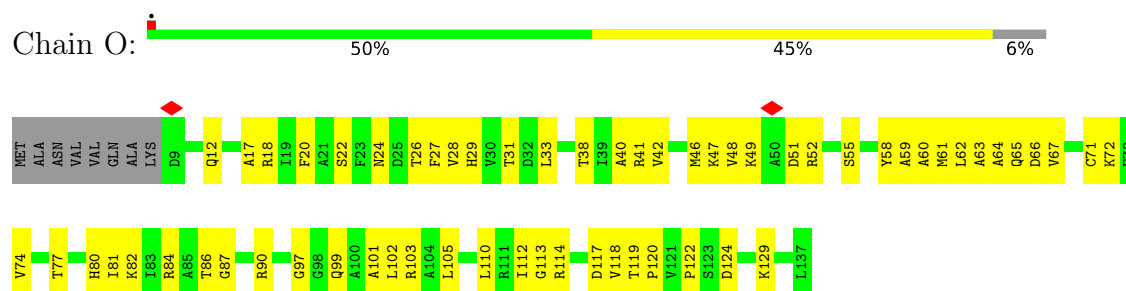
• Molecule 10: KLLA0A10483p



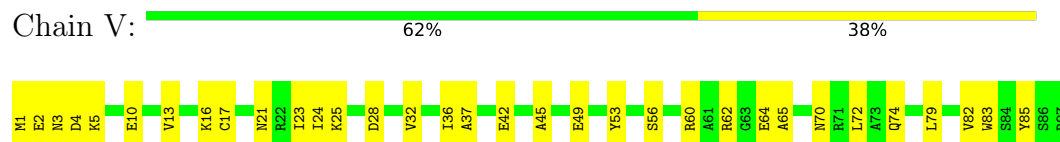
• Molecule 11: KLLA0F18040p



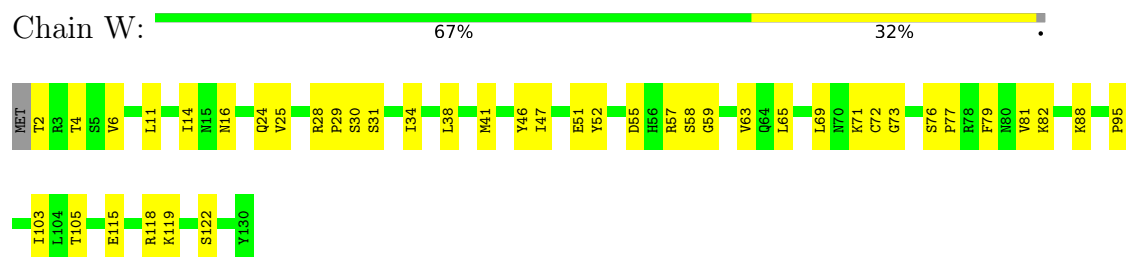
• Molecule 12: Small ribosomal subunit protein uS11



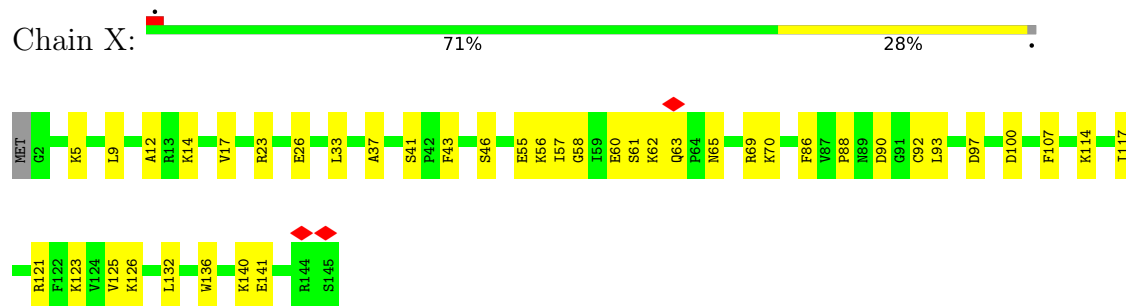
- Molecule 13: 40S ribosomal protein S21



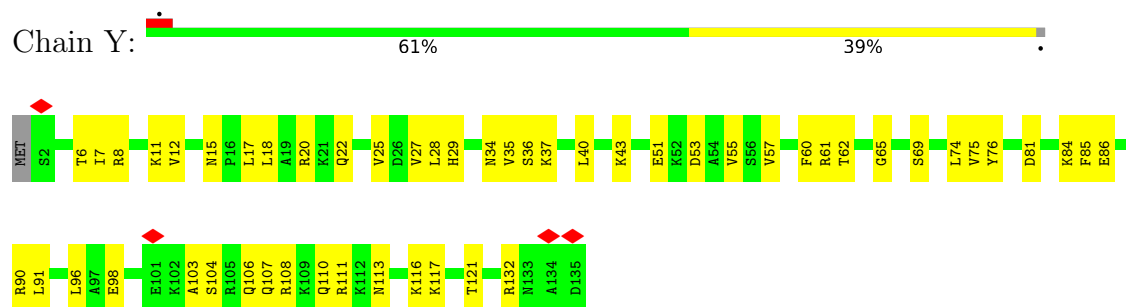
- Molecule 14: Small ribosomal subunit protein uS8



- Molecule 15: KLLA0B11231p

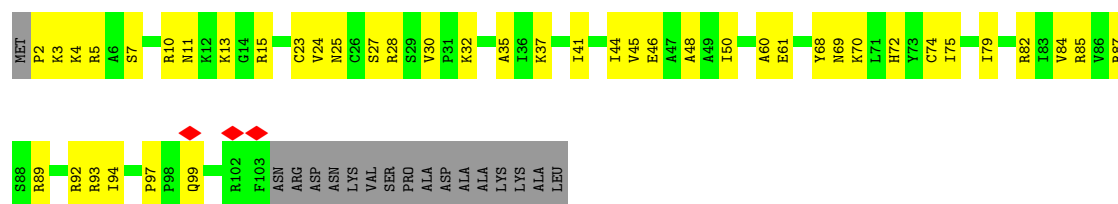


- Molecule 16: 40S ribosomal protein S24



- Molecule 17: 40S ribosomal protein S26

Chain a: 



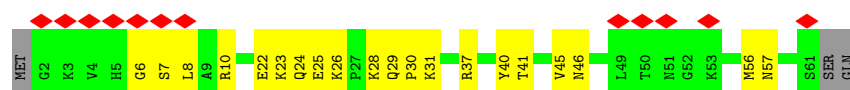
- Molecule 18: 40S ribosomal protein S27

Chain b: 



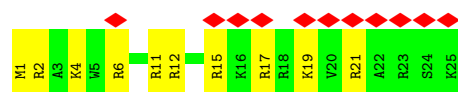
- Molecule 19: 40S ribosomal protein S30

Chain e: 



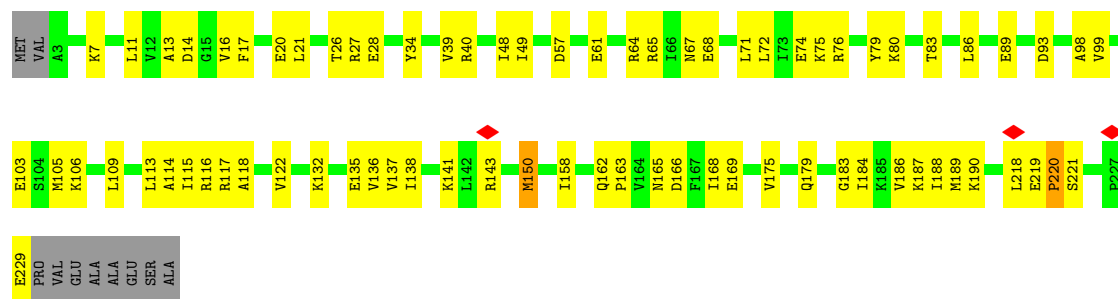
- Molecule 20: 40S ribosomal protein L41-A

Chain h: 



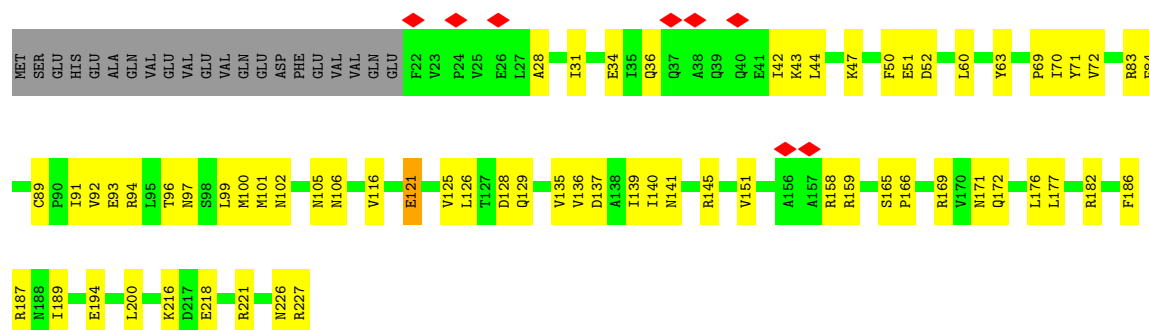
- Molecule 21: 40S ribosomal protein S3

Chain D: 

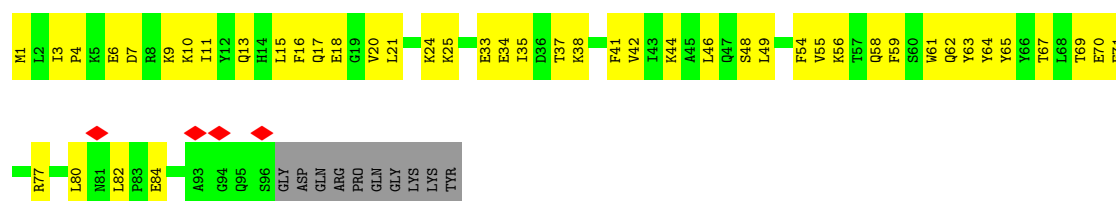


- Molecule 22: KLLA0D10659p

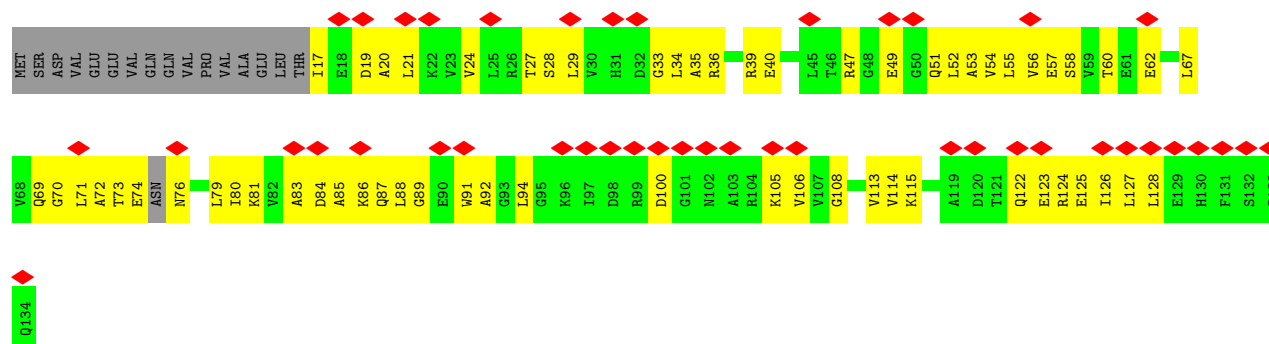
Chain F: 



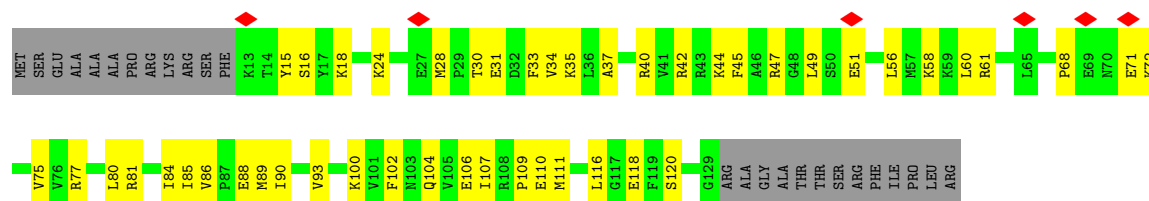
• Molecule 23: KLLA0B08173p



• Molecule 24: 40S ribosomal protein S12

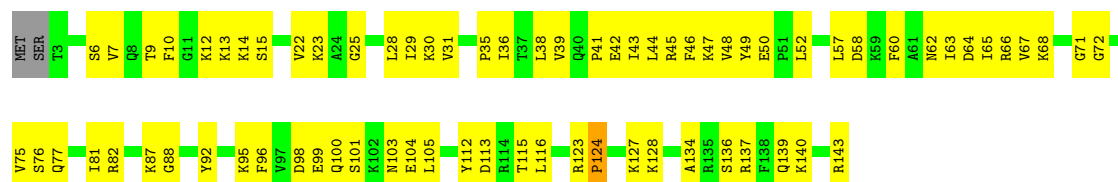


• Molecule 25: KLLA0F07843p

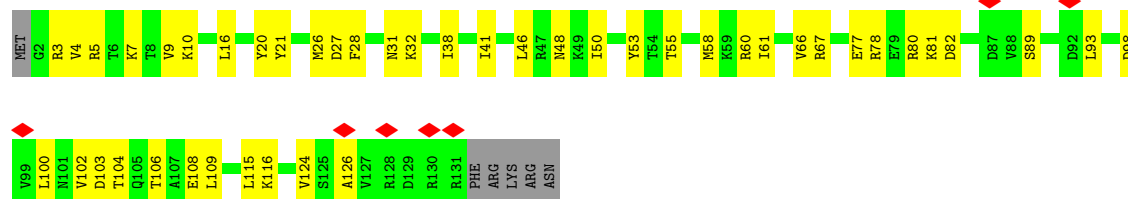


• Molecule 26: Small ribosomal subunit protein uS9

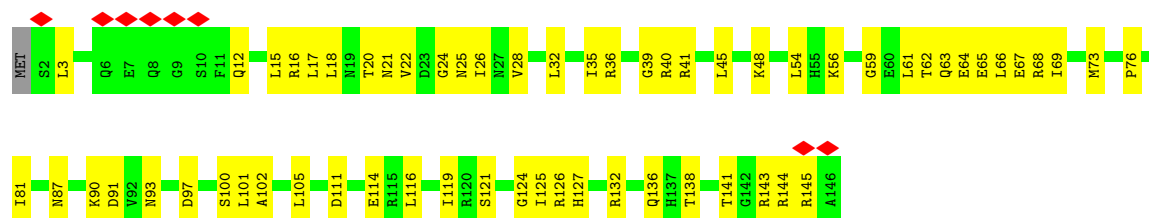




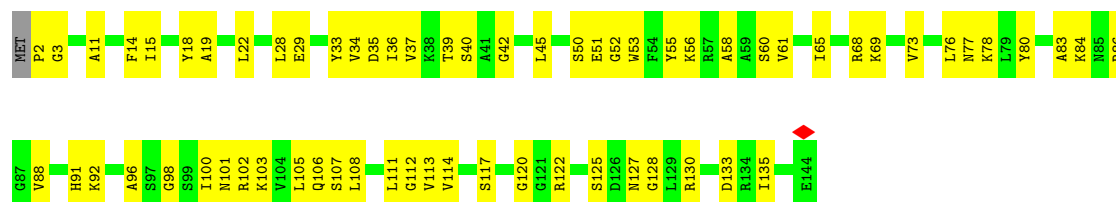
• Molecule 27: KLLA0B01474p



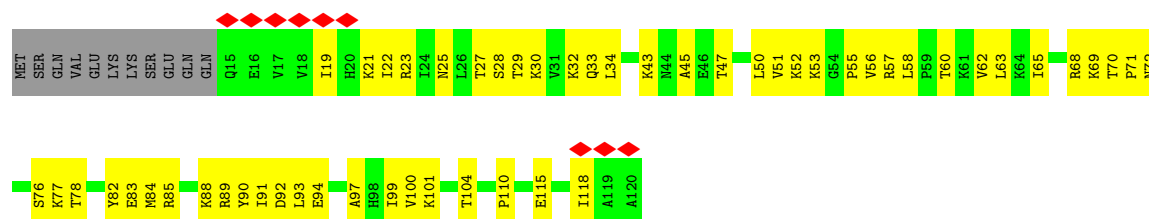
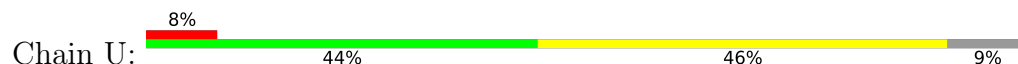
• Molecule 28: KLLA0B01562p



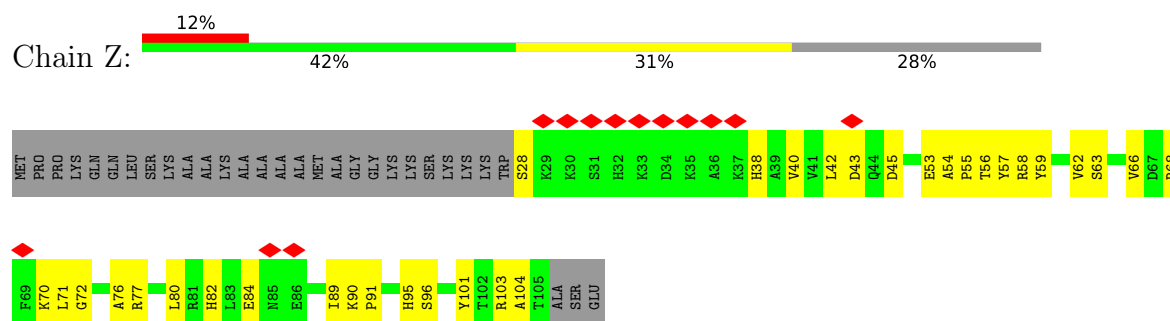
• Molecule 29: KLLA0A07194p



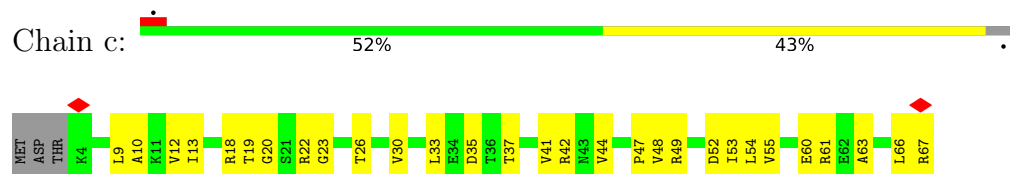
• Molecule 30: Small ribosomal subunit protein uS10



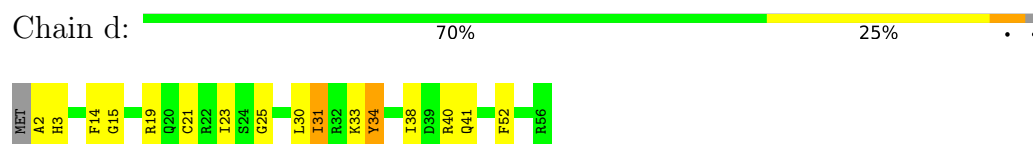
- Molecule 31: 40S ribosomal protein S25



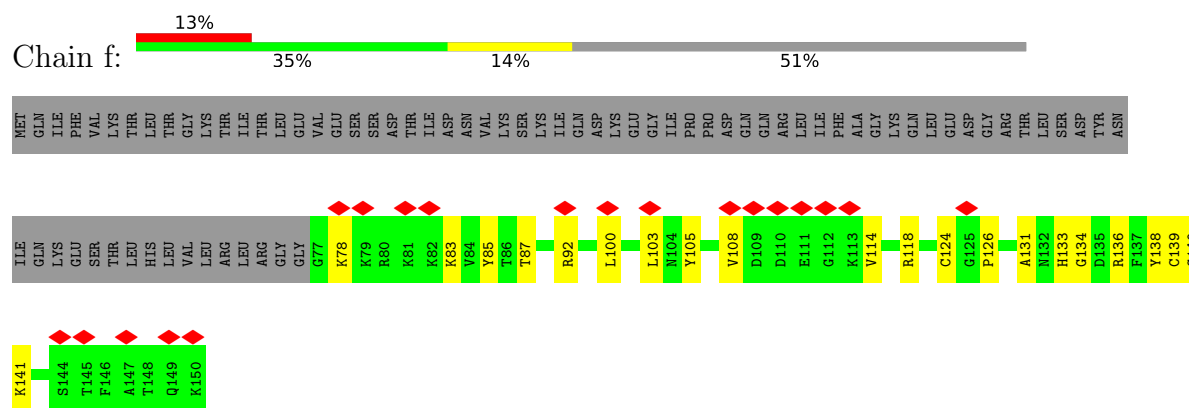
- Molecule 32: Small ribosomal subunit protein eS28



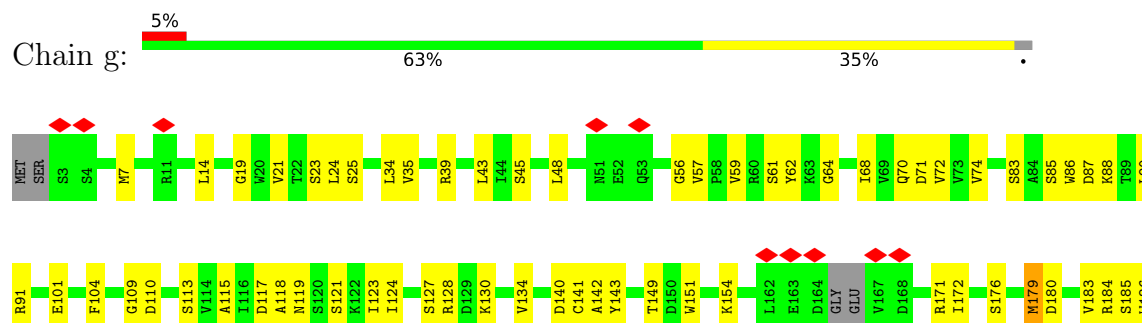
- Molecule 33: Small ribosomal subunit protein uS14

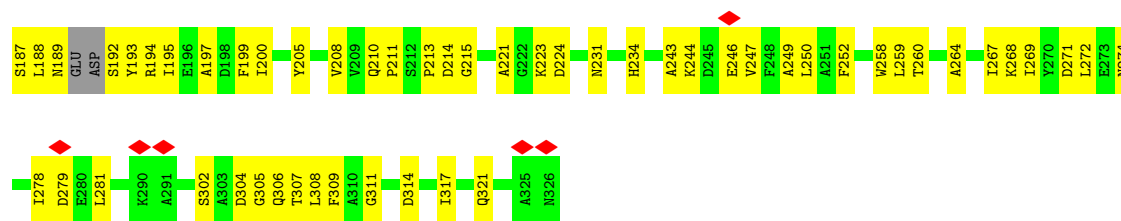


- Molecule 34: Small ribosomal subunit protein eS31

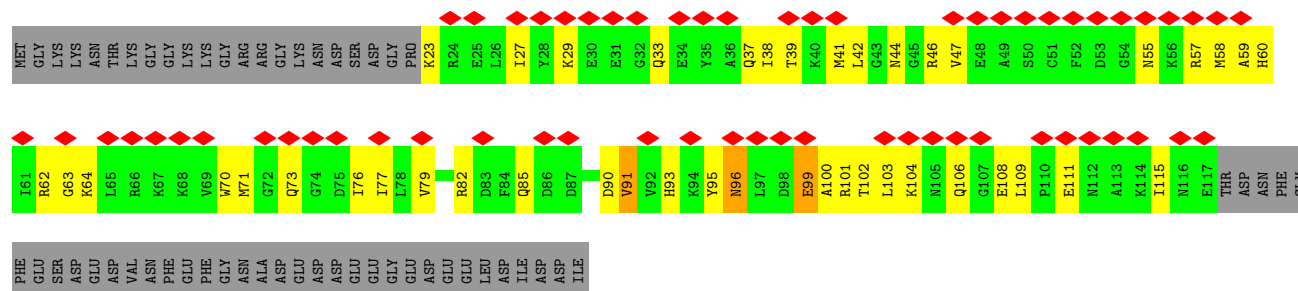
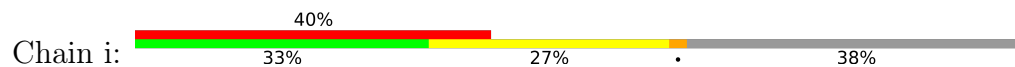


- Molecule 35: KLLA0E12277p

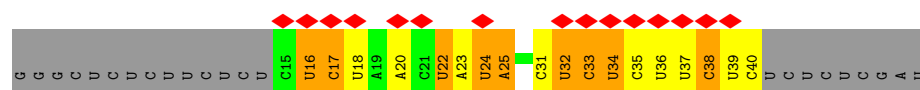
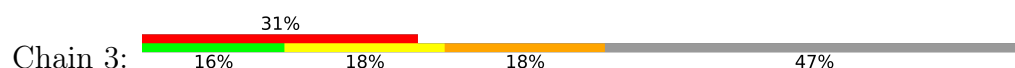




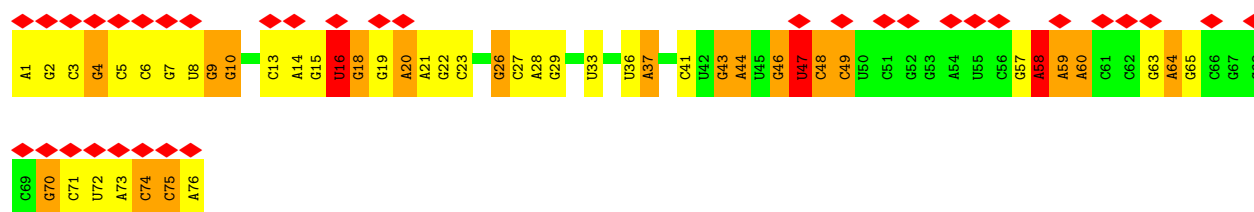
• Molecule 36: Eukaryotic translation initiation factor 1A



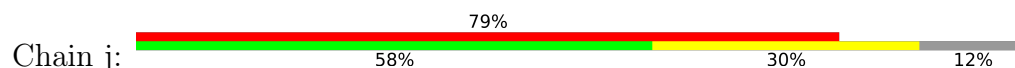
• Molecule 37: mRNA (5'-R(P*AP*AP*U)-3')

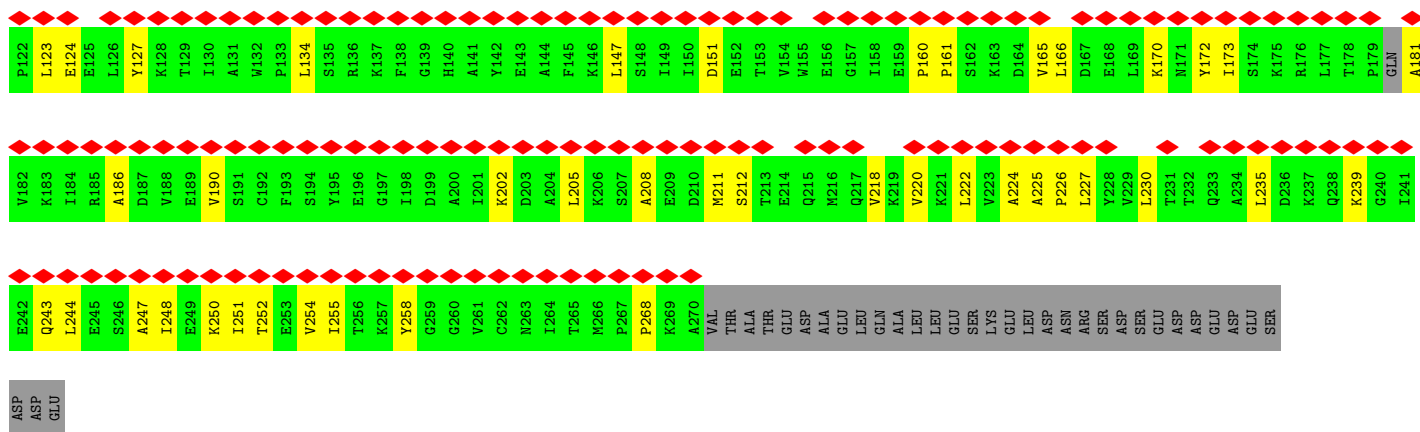


• Molecule 38: Met-tRNA_i

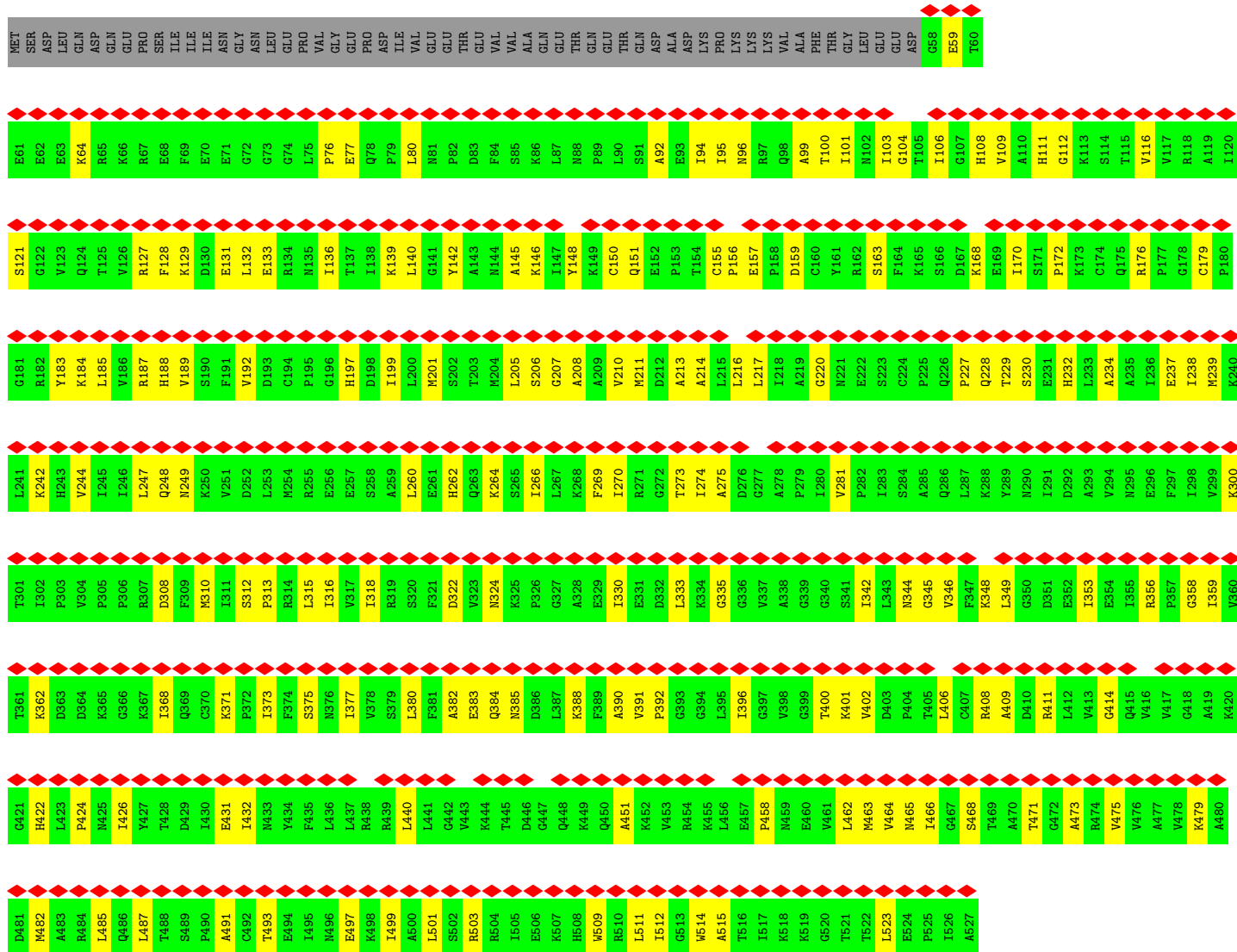
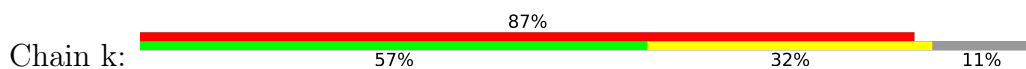


• Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha

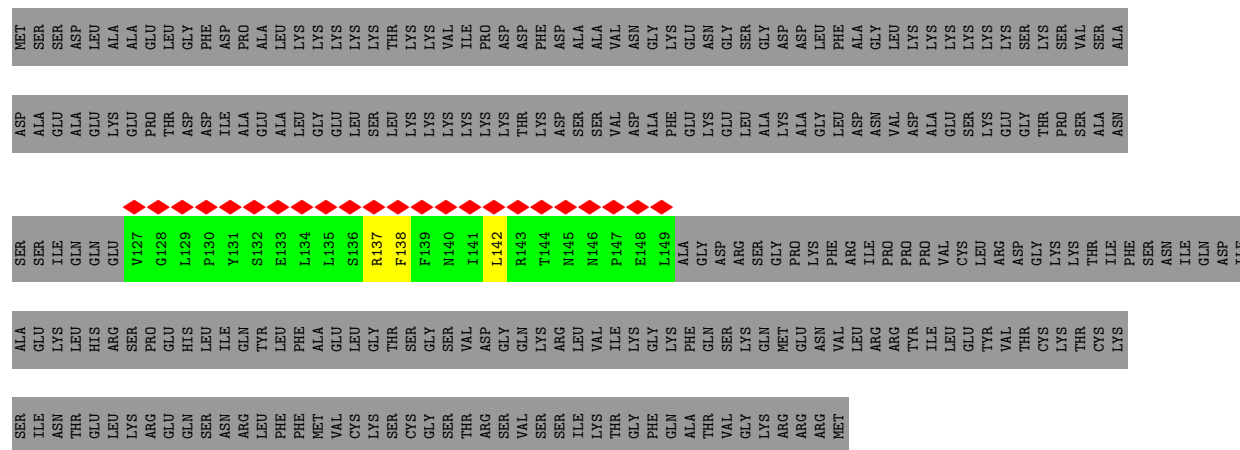




• Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma



Chain 1: 8% 7% 92%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66519	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	0.868	Depositor
Minimum map value	-0.475	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	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: H2U, 5MC, B8N, RIA, GCP, M2G, 1MA, 2MG, PSU, MG, MA6, 1MG, ZN, 7MG, T6A

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	0.16	0/42410	0.31	4/66079 (0.0%)
2	A	0.19	0/1742	0.44	2/2383 (0.1%)
3	B	0.20	0/1820	0.46	1/2448 (0.0%)
4	C	0.20	0/1678	0.37	0/2277
5	E	0.19	0/2122	0.45	0/2861
6	G	0.14	0/1855	0.36	0/2479
7	H	0.20	0/1507	0.58	2/2028 (0.1%)
8	I	0.18	0/1515	0.44	0/2029
9	J	0.20	0/1495	0.45	1/2001 (0.0%)
10	L	0.19	0/1276	0.44	0/1718
11	N	0.17	0/1218	0.39	0/1638
12	O	0.21	0/966	0.51	0/1297
13	V	0.19	0/696	0.43	0/938
14	W	0.22	0/1039	0.42	0/1399
15	X	0.16	0/1137	0.37	0/1516
16	Y	0.19	0/1075	0.43	0/1433
17	a	0.22	0/810	0.52	0/1087
18	b	0.17	0/619	0.42	0/837
19	e	0.20	0/480	0.49	0/640
20	h	0.20	0/234	0.41	0/300
21	D	0.18	0/1800	0.42	0/2421
22	F	0.18	0/1628	0.45	0/2198
23	K	0.21	0/831	0.60	0/1123
24	M	0.17	0/891	0.50	0/1201
25	P	0.17	0/942	0.48	0/1269
26	Q	0.22	0/1125	0.57	2/1510 (0.1%)
27	R	0.17	0/1044	0.42	0/1402
28	S	0.17	0/1208	0.48	0/1624
29	T	0.22	0/1129	0.51	0/1520
30	U	0.18	0/857	0.48	0/1158
31	Z	0.18	0/603	0.49	0/814
32	c	0.17	0/501	0.41	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.18	0/473	0.40	0/629
34	f	0.13	0/597	0.43	0/795
35	g	0.15	0/2523	0.40	0/3434
36	i	0.20	0/773	0.53	0/1031
37	3	0.09	0/595	0.20	0/920
38	1	0.17	0/1529	0.27	0/2376
39	j	0.16	0/2171	0.47	0/2924
40	k	0.14	0/3657	0.41	0/4946
41	l	0.21	0/194	0.44	0/263
All	All	0.17	0/90765	0.38	12/131619 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	65	PRO	N-CA-C	-8.35	102.94	114.80
1	2	225	A	C4'-C3'-O3'	6.78	123.17	113.00
2	A	35	PRO	CA-N-CD	-6.75	102.55	112.00
1	2	225	A	N9-C1'-C2'	-6.63	102.05	112.00
9	J	2	PRO	CA-N-CD	-6.36	103.10	112.00

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	961	0
2	A	1702	0	1695	72	0
3	B	1796	0	1874	68	0
4	C	1648	0	1727	51	0
5	E	2078	0	2157	79	0
6	G	1832	0	1919	72	0
7	H	1483	0	1579	72	0
8	I	1489	0	1504	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	1471	0	1554	65	0
10	L	1248	0	1311	46	0
11	N	1195	0	1263	31	0
12	O	955	0	987	66	0
13	V	687	0	682	34	0
14	W	1021	0	1056	42	0
15	X	1119	0	1198	38	0
16	Y	1061	0	1111	47	0
17	a	797	0	835	41	0
18	b	609	0	630	20	0
19	e	472	0	508	21	0
20	h	233	0	284	9	0
21	D	1774	0	1855	67	0
22	F	1609	0	1679	59	0
23	K	809	0	810	46	0
24	M	885	0	917	53	0
25	P	923	0	960	47	0
26	Q	1105	0	1170	73	0
27	R	1033	0	1082	43	0
28	S	1189	0	1211	53	0
29	T	1110	0	1124	55	0
30	U	845	0	913	44	0
31	Z	594	0	590	35	0
32	c	499	0	536	23	0
33	d	461	0	448	22	0
34	f	584	0	600	20	0
35	g	2469	0	2403	92	0
36	i	764	0	763	48	0
37	3	536	0	277	10	0
38	1	1639	0	853	36	0
39	j	2139	0	2205	78	0
40	k	3596	0	3713	127	0
41	l	190	0	191	3	0
42	2	112	0	0	0	0
42	3	1	0	0	0	0
42	T	1	0	0	0	0
42	i	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	1	0
45	k	8	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2	3	0	0	0	0
All	All	86000	0	67408	2504	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 17.

The worst 5 of 2504 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:2:ALA:N	12:O:49:LYS:HE3	1.60	1.16
24:M:67:LEU:O	24:M:71:LEU:HD13	1.50	1.10
1:2:824:U:H3	1:2:847:C:N4	1.54	1.04
12:O:51:ASP:HB2	39:j:89:ARG:HH12	1.21	1.00
1:2:1586:G:H1	1:2:1606:U:H3	1.05	0.95

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%)	194 (89%)	23 (11%)	0	100	100
3	B	221/255 (87%)	204 (92%)	17 (8%)	0	100	100
4	C	218/259 (84%)	207 (95%)	11 (5%)	0	100	100
5	E	258/261 (99%)	237 (92%)	21 (8%)	0	100	100
6	G	228/236 (97%)	218 (96%)	10 (4%)	0	100	100
7	H	182/190 (96%)	171 (94%)	10 (6%)	1 (0%)	24	52
8	I	184/201 (92%)	169 (92%)	15 (8%)	0	100	100
9	J	180/188 (96%)	169 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
11	N	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
12	O	127/137 (93%)	115 (91%)	12 (9%)	0	100	100
13	V	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
14	W	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
15	X	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
16	Y	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
17	a	100/119 (84%)	85 (85%)	15 (15%)	0	100	100
18	b	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
19	e	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	214 (95%)	10 (4%)	1 (0%)	30	58
22	F	204/227 (90%)	188 (92%)	16 (8%)	0	100	100
23	K	94/106 (89%)	84 (89%)	10 (11%)	0	100	100
24	M	113/134 (84%)	101 (89%)	12 (11%)	0	100	100
25	P	115/142 (81%)	108 (94%)	7 (6%)	0	100	100
26	Q	139/143 (97%)	129 (93%)	10 (7%)	0	100	100
27	R	128/136 (94%)	120 (94%)	8 (6%)	0	100	100
28	S	143/146 (98%)	126 (88%)	17 (12%)	0	100	100
29	T	141/144 (98%)	130 (92%)	11 (8%)	0	100	100
30	U	104/117 (89%)	94 (90%)	10 (10%)	0	100	100
31	Z	76/108 (70%)	70 (92%)	6 (8%)	0	100	100
32	c	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
33	d	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
34	f	72/150 (48%)	59 (82%)	13 (18%)	0	100	100
35	g	314/326 (96%)	291 (93%)	23 (7%)	0	100	100
36	i	93/153 (61%)	83 (89%)	10 (11%)	0	100	100
39	j	263/304 (86%)	247 (94%)	15 (6%)	1 (0%)	30	58
40	k	468/527 (89%)	429 (92%)	39 (8%)	0	100	100
41	l	21/285 (7%)	20 (95%)	1 (5%)	0	100	100
All	All	5691/6582 (86%)	5269 (93%)	419 (7%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	64	VAL
39	j	17	ASP
21	D	220	PRO

5.3.2 Protein sidechains [i](#)

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	80
4	C	177/203 (87%)	177 (100%)	0	100	100
5	E	223/224 (100%)	222 (100%)	1 (0%)	84	82
6	G	192/200 (96%)	190 (99%)	2 (1%)	68	74
7	H	164/170 (96%)	162 (99%)	2 (1%)	63	72
8	I	147/159 (92%)	146 (99%)	1 (1%)	76	77
9	J	153/158 (97%)	152 (99%)	1 (1%)	76	77
10	L	136/137 (99%)	136 (100%)	0	100	100
11	N	128/128 (100%)	126 (98%)	2 (2%)	55	67
12	O	97/104 (93%)	96 (99%)	1 (1%)	68	74
13	V	73/73 (100%)	72 (99%)	1 (1%)	59	69
14	W	110/111 (99%)	110 (100%)	0	100	100
15	X	119/120 (99%)	119 (100%)	0	100	100
16	Y	108/109 (99%)	107 (99%)	1 (1%)	70	75
17	a	83/100 (83%)	82 (99%)	1 (1%)	63	72
18	b	71/72 (99%)	70 (99%)	1 (1%)	59	69
19	e	51/55 (93%)	51 (100%)	0	100	100
20	h	23/23 (100%)	22 (96%)	1 (4%)	26	52
21	D	188/196 (96%)	187 (100%)	1 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	F	174/194 (90%)	173 (99%)	1 (1%)	78	79
23	K	88/96 (92%)	88 (100%)	0	100	100
24	M	93/109 (85%)	92 (99%)	1 (1%)	65	73
25	P	99/119 (83%)	98 (99%)	1 (1%)	68	74
26	Q	117/119 (98%)	117 (100%)	0	100	100
27	R	116/124 (94%)	116 (100%)	0	100	100
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%)	45 (96%)	2 (4%)	26	52
34	f	60/133 (45%)	60 (100%)	0	100	100
35	g	264/272 (97%)	263 (100%)	1 (0%)	84	82
36	i	80/130 (62%)	77 (96%)	3 (4%)	29	55
39	j	239/274 (87%)	239 (100%)	0	100	100
40	k	393/449 (88%)	393 (100%)	0	100	100
41	l	22/246 (9%)	22 (100%)	0	100	100
All	All	4871/5595 (87%)	4845 (100%)	26 (0%)	78	80

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	b	3	LEU
22	F	121	GLU
36	i	96	ASN
21	D	150	MET
24	M	74	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
24	M	51	GLN
29	T	77	ASN
40	k	425	ASN

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Mol	Chain	Res	Type
25	P	104	GLN
27	R	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1797/1798 (99%)	525 (29%)	32 (1%)
37	3	25/49 (51%)	16 (64%)	0
38	1	72/75 (96%)	26 (36%)	3 (4%)
All	All	1894/1922 (98%)	567 (29%)	35 (1%)

5 of 567 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1552	U
1	2	1571	A
38	1	43	G
1	2	513	G
1	2	423	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	5MC	1	48	38	19,22,23	3.94	8 (42%)	26,32,35	1.02	2 (7%)
38	7MG	1	46	38	23,26,27	3.62	11 (47%)	27,39,42	2.20	9 (33%)
1	MA6	2	1780	1	23,26,27	1.39	4 (17%)	33,38,41	3.36	12 (36%)
38	H2U	1	47	38	18,21,22	3.24	4 (22%)	19,30,33	1.46	3 (15%)
38	RIA	1	64	38	35,38,39	1.30	4 (11%)	50,57,60	1.82	11 (22%)
1	B8N	2	1190	1	25,29,30	3.36	7 (28%)	28,42,45	1.97	8 (28%)
38	1MG	1	9	38	23,26,27	3.32	7 (30%)	33,39,42	2.32	8 (24%)
38	T6A	1	37	38	31,34,35	1.82	7 (22%)	43,49,52	2.19	14 (32%)
1	5MC	2	1006	1	19,22,23	3.69	8 (42%)	26,32,35	1.20	3 (11%)
1	PSU	2	120	1	18,21,22	4.40	7 (38%)	21,30,33	2.03	5 (23%)
1	2MG	2	1426	1,42	23,26,27	2.87	8 (34%)	33,38,41	2.20	10 (30%)
38	M2G	1	26	38	24,27,28	2.69	8 (33%)	33,40,43	1.74	8 (24%)
1	2MG	2	1570	1	23,26,27	2.92	8 (34%)	33,38,41	2.15	10 (30%)
1	PSU	2	766	1	18,21,22	4.36	8 (44%)	21,30,33	2.02	6 (28%)
38	5MC	1	49	38	19,22,23	3.95	8 (42%)	26,32,35	1.04	2 (7%)
1	7MG	2	1573	1,38	23,26,27	3.56	10 (43%)	27,39,42	2.24	9 (33%)
1	5MC	2	1637	1	19,22,23	3.80	8 (42%)	26,32,35	0.98	2 (7%)
38	H2U	1	16	38	18,21,22	3.14	4 (22%)	19,30,33	1.45	4 (21%)
1	PSU	2	1289	1	18,21,22	4.42	7 (38%)	21,30,33	2.01	5 (23%)
1	PSU	2	465	1	18,21,22	4.36	7 (38%)	21,30,33	1.95	5 (23%)
1	PSU	2	998	1	18,21,22	4.39	7 (38%)	21,30,33	2.02	6 (28%)
38	2MG	1	10	38	23,26,27	2.91	8 (34%)	33,38,41	2.22	10 (30%)
38	1MA	1	58	38	21,25,26	3.14	6 (28%)	30,37,40	2.38	8 (26%)

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	5MC	1	48	38	-	3/7/25/26	0/2/2/2
38	7MG	1	46	38	-	1/7/37/38	0/3/3/3
1	MA6	2	1780	1	-	3/11/29/30	0/3/3/3
38	H2U	1	47	38	-	5/7/38/39	0/2/2/2
38	RIA	1	64	38	-	12/17/51/52	0/4/4/4
1	B8N	2	1190	1	-	5/16/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	1MG	1	9	38	-	2/7/25/26	0/3/3/3
38	T6A	1	37	38	-	3/23/41/42	0/3/3/3
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
1	PSU	2	120	1	-	0/7/25/26	0/2/2/2
1	2MG	2	1426	1,42	-	0/9/27/28	0/3/3/3
38	M2G	1	26	38	-	4/11/29/30	0/3/3/3
1	2MG	2	1570	1	-	0/9/27/28	0/3/3/3
1	PSU	2	766	1	-	0/7/25/26	0/2/2/2
38	5MC	1	49	38	-	2/7/25/26	0/2/2/2
1	7MG	2	1573	1,38	-	2/7/37/38	0/3/3/3
1	5MC	2	1637	1	-	0/7/25/26	0/2/2/2
38	H2U	1	16	38	-	6/7/38/39	0/2/2/2
1	PSU	2	1289	1	-	0/7/25/26	0/2/2/2
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
1	PSU	2	998	1	-	4/7/25/26	0/2/2/2
38	2MG	1	10	38	-	2/9/27/28	0/3/3/3
38	1MA	1	58	38	-	2/7/25/26	0/3/3/3

The worst 5 of 164 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1289	PSU	C6-C5	11.70	1.48	1.35
1	2	120	PSU	C6-C5	11.55	1.48	1.35
1	2	766	PSU	C6-C5	11.53	1.48	1.35
1	2	465	PSU	C6-C5	11.49	1.48	1.35
1	2	998	PSU	C6-C5	11.46	1.48	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	-12.57	101.53	116.86
1	2	1780	MA6	C5-C6-N6	8.30	138.47	125.33
38	1	10	2MG	C2-N3-C4	6.81	120.52	112.00
38	1	58	1MA	C1'-N9-C8	-6.68	107.76	126.73
38	1	9	1MG	C1'-N9-C4	-6.56	107.12	126.49

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1190	B8N	C31-C32-C33-N34
1	2	1780	MA6	O4'-C4'-C5'-O5'
38	1	9	1MG	O4'-C4'-C5'-O5'
38	1	16	H2U	C4'-C5'-O5'-P
38	1	26	M2G	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	1	47	H2U	2	0
38	1	64	RIA	6	0
38	1	37	T6A	2	0
1	2	1006	5MC	2	0
1	2	120	PSU	1	0
1	2	1570	2MG	1	0
1	2	1573	7MG	2	0
1	2	1637	5MC	2	0
38	1	16	H2U	1	0
1	2	1289	PSU	1	0
1	2	998	PSU	1	0
38	1	58	1MA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 118 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	3.17	12 (37%)	49,54,54	1.64	9 (18%)
45	MET	k	602	-	6,7,8	0.47	0	2,7,9	0.23	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	-	-	2/19/38/38	0/3/3/3
45	MET	k	602	-	-	0/5/6/8	-

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'	8.68	1.62	1.42
44	k	601	GCP	C2'-C1'	-7.25	1.30	1.53
44	k	601	GCP	O4'-C4'	-6.19	1.31	1.45
44	k	601	GCP	PB-O3A	6.13	1.65	1.58
44	k	601	GCP	PA-O3A	5.30	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	-5.21	120.10	128.39
44	k	601	GCP	C2-N3-C4	4.50	120.05	112.30
44	k	601	GCP	N9-C8-N7	-2.97	107.90	113.40
44	k	601	GCP	N9-C4-N3	2.95	131.86	125.95
44	k	601	GCP	C2-N1-C6	-2.79	120.06	125.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	k	601	GCP	O4'-C4'-C5'-O5'
44	k	601	GCP	C3'-C4'-C5'-O5'

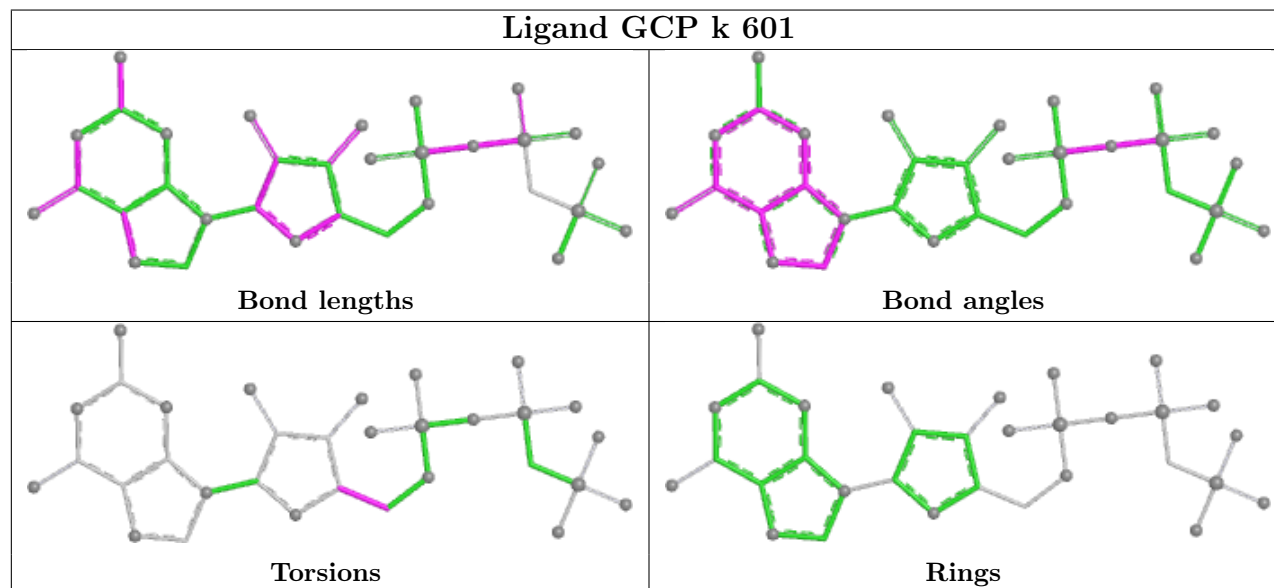
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	k	601	GCP	1	0
45	k	602	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	8.93
1	1	63:G	O3'	64:RIA	P	4.61
1	1	16:H2U	O3'	18:G	P	3.39

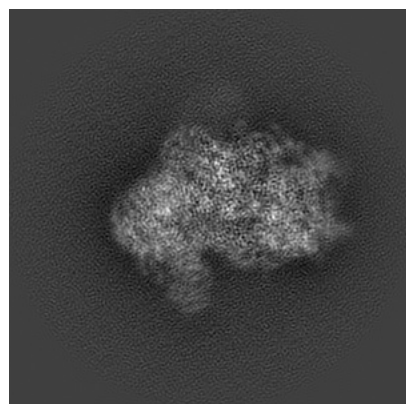
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19541. These allow visual inspection of the internal detail of the map and identification of artifacts.

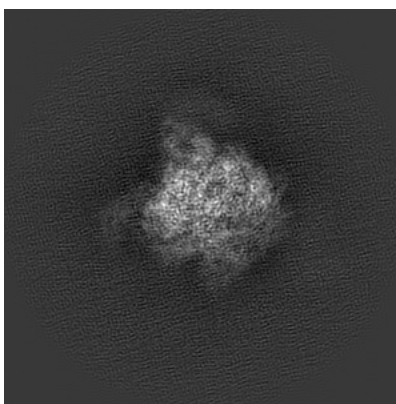
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

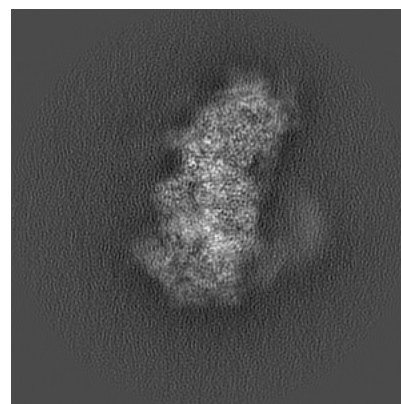
6.1.1 Primary map



X

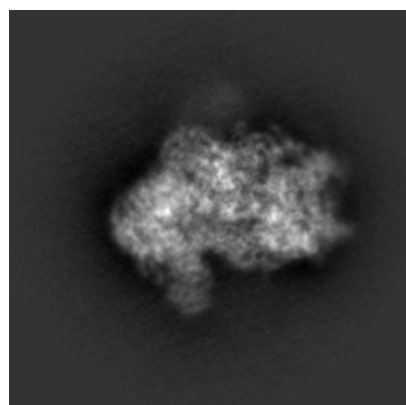


Y

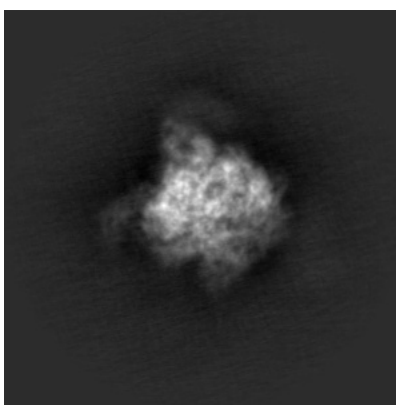


Z

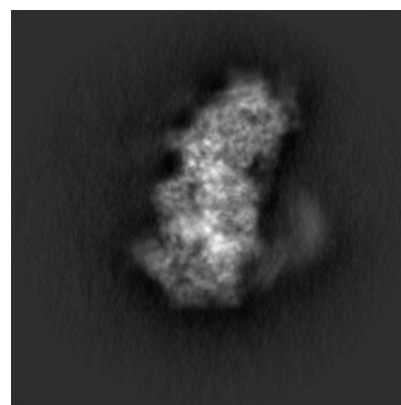
6.1.2 Raw map



X



Y

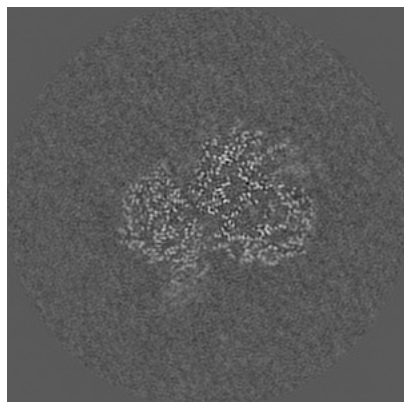


Z

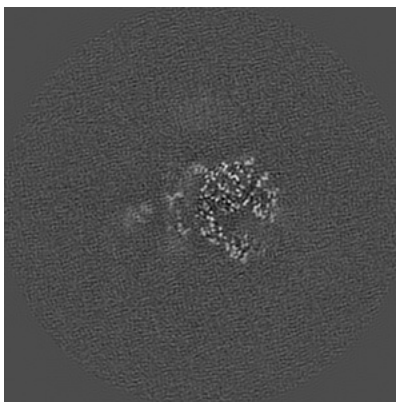
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

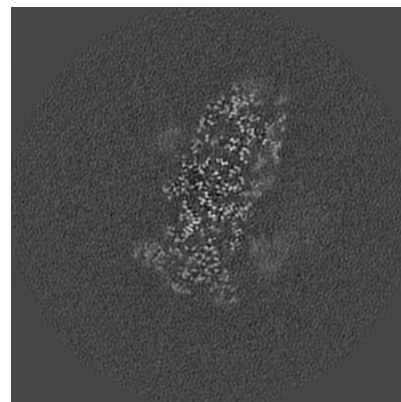
6.2.1 Primary map



X Index: 150

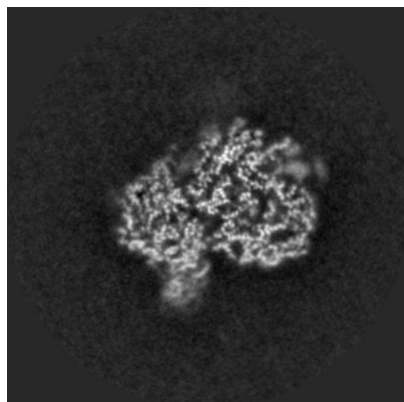


Y Index: 150

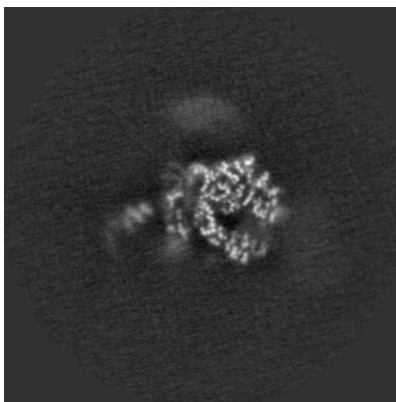


Z Index: 150

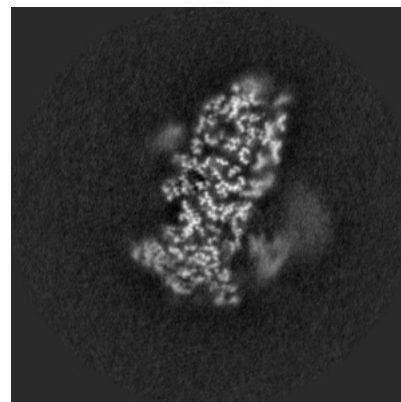
6.2.2 Raw map



X Index: 150



Y Index: 150

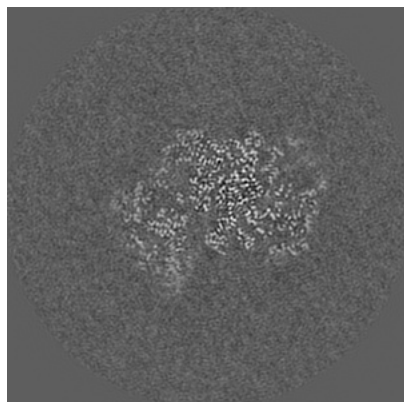


Z Index: 150

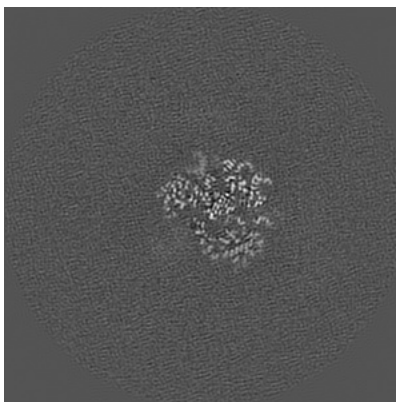
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

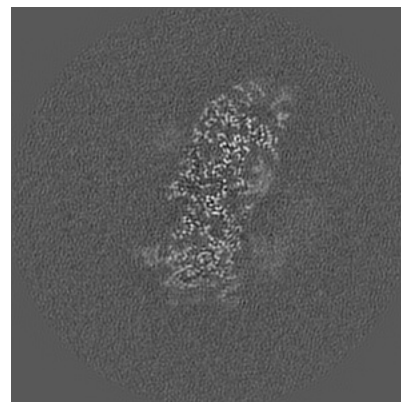
6.3.1 Primary map



X Index: 157

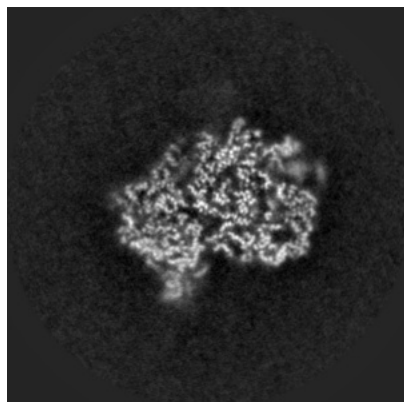


Y Index: 161

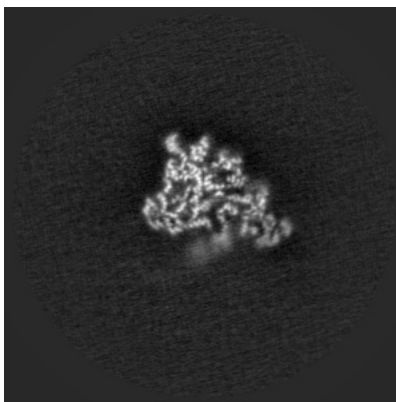


Z Index: 147

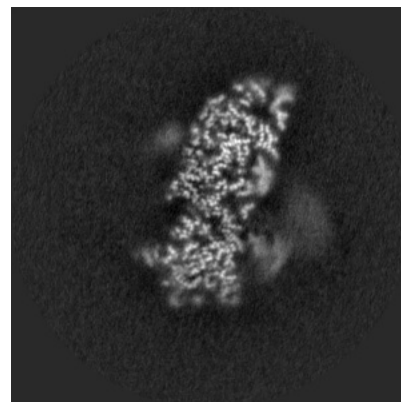
6.3.2 Raw map



X Index: 152



Y Index: 198

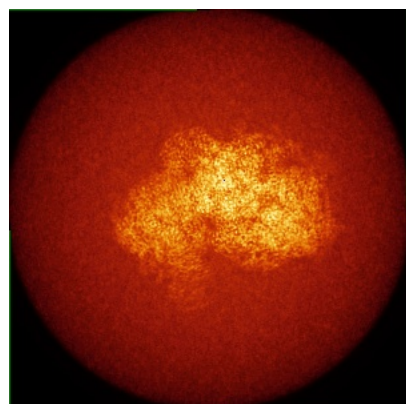


Z Index: 146

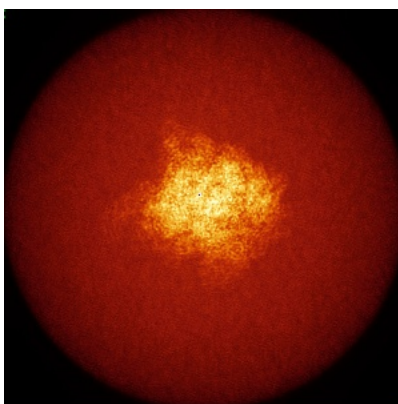
The images above show the largest variance slices of the map in three orthogonal directions.

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

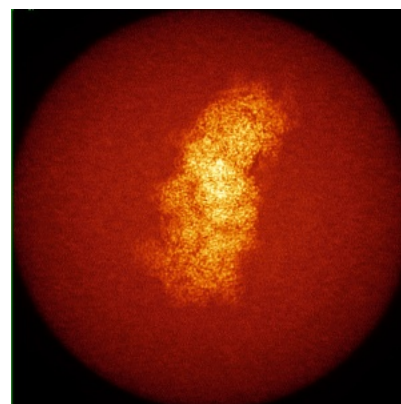
6.4.1 Primary map



X

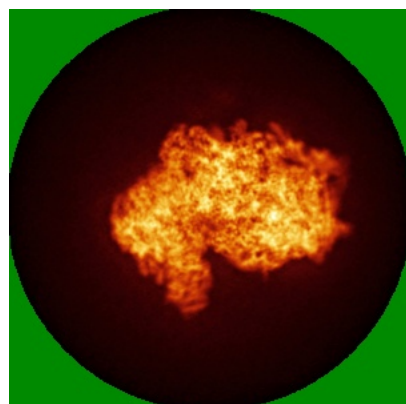


Y

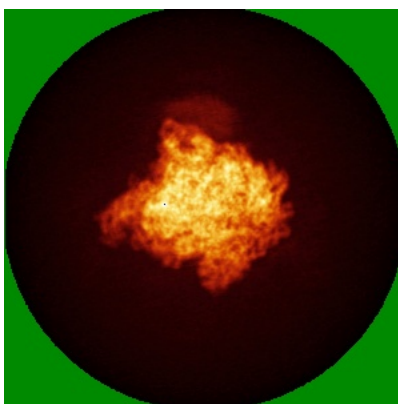


Z

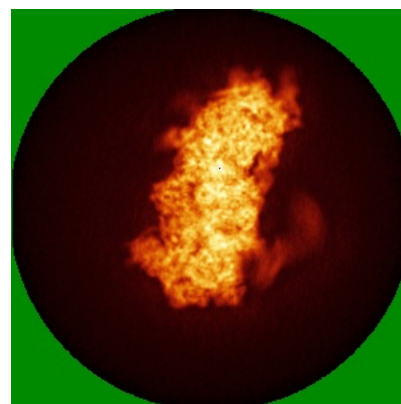
6.4.2 Raw map



X



Y

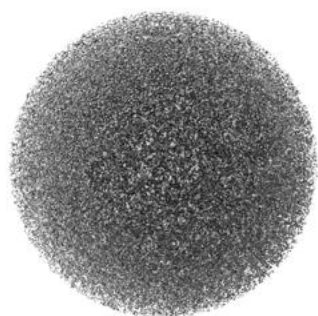


Z

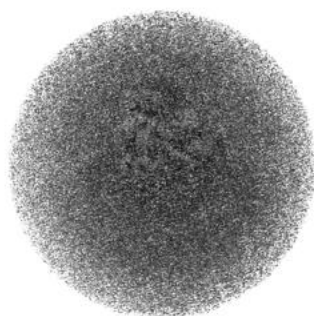
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

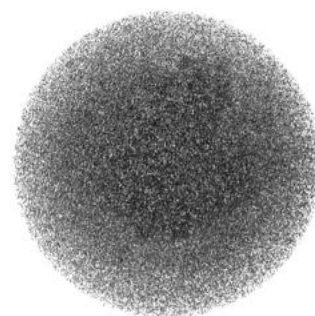
6.5.1 Primary map



X



Y



Z

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.

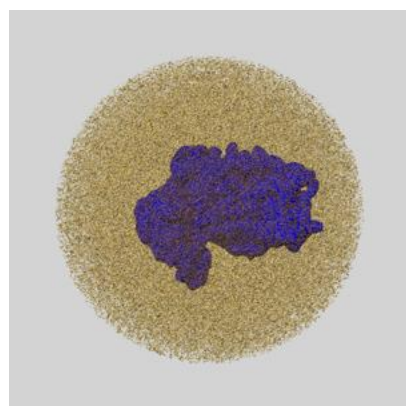
6.6 Mask visualisation [i](#)

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

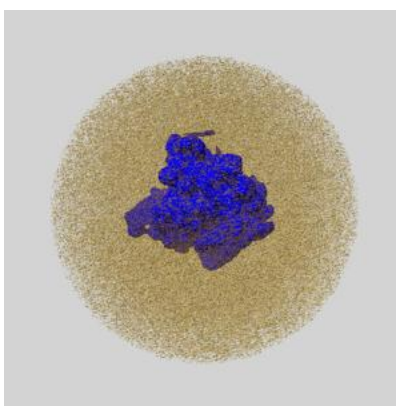
A mask typically either:

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

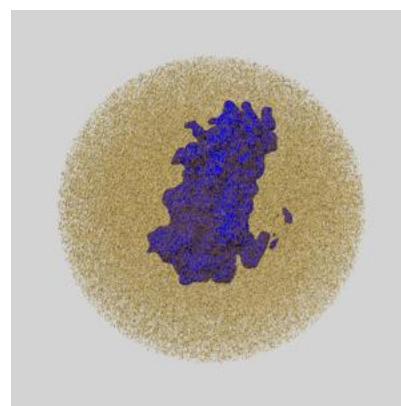
6.6.1 emd_19541_msk_1.map [i](#)



X



Y

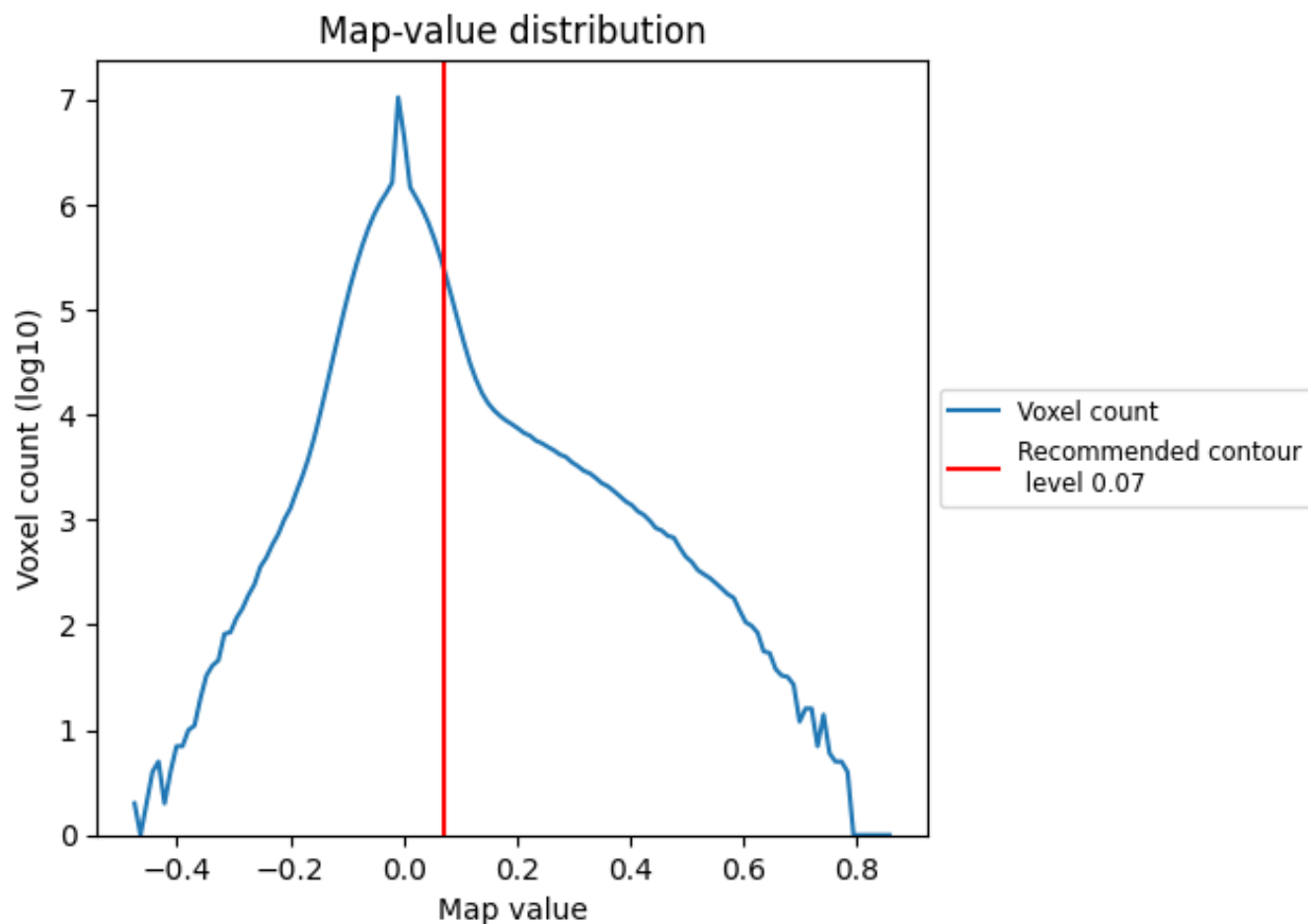


Z

7 Map analysis [i](#)

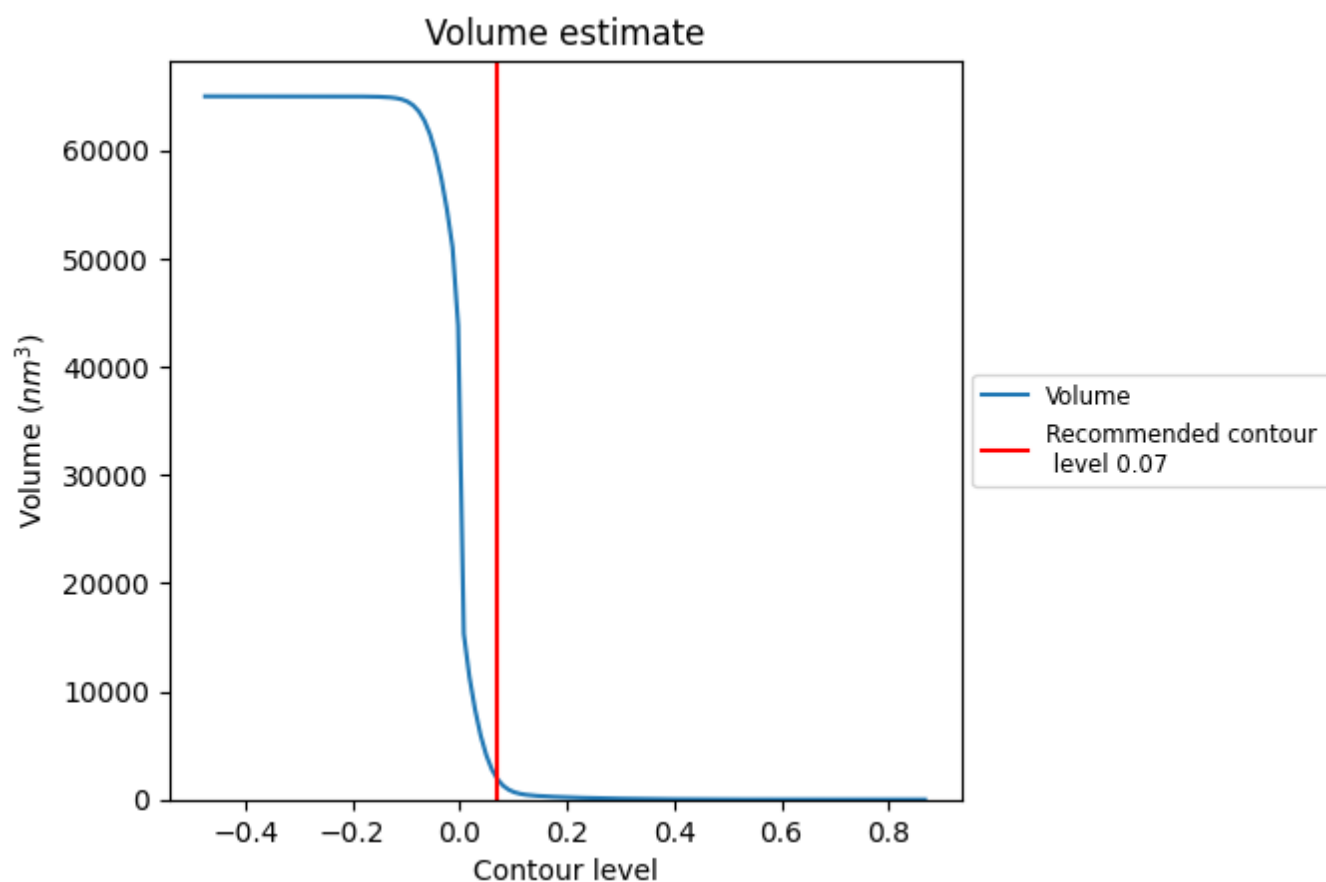
This section contains the results of statistical analysis of the map.

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.

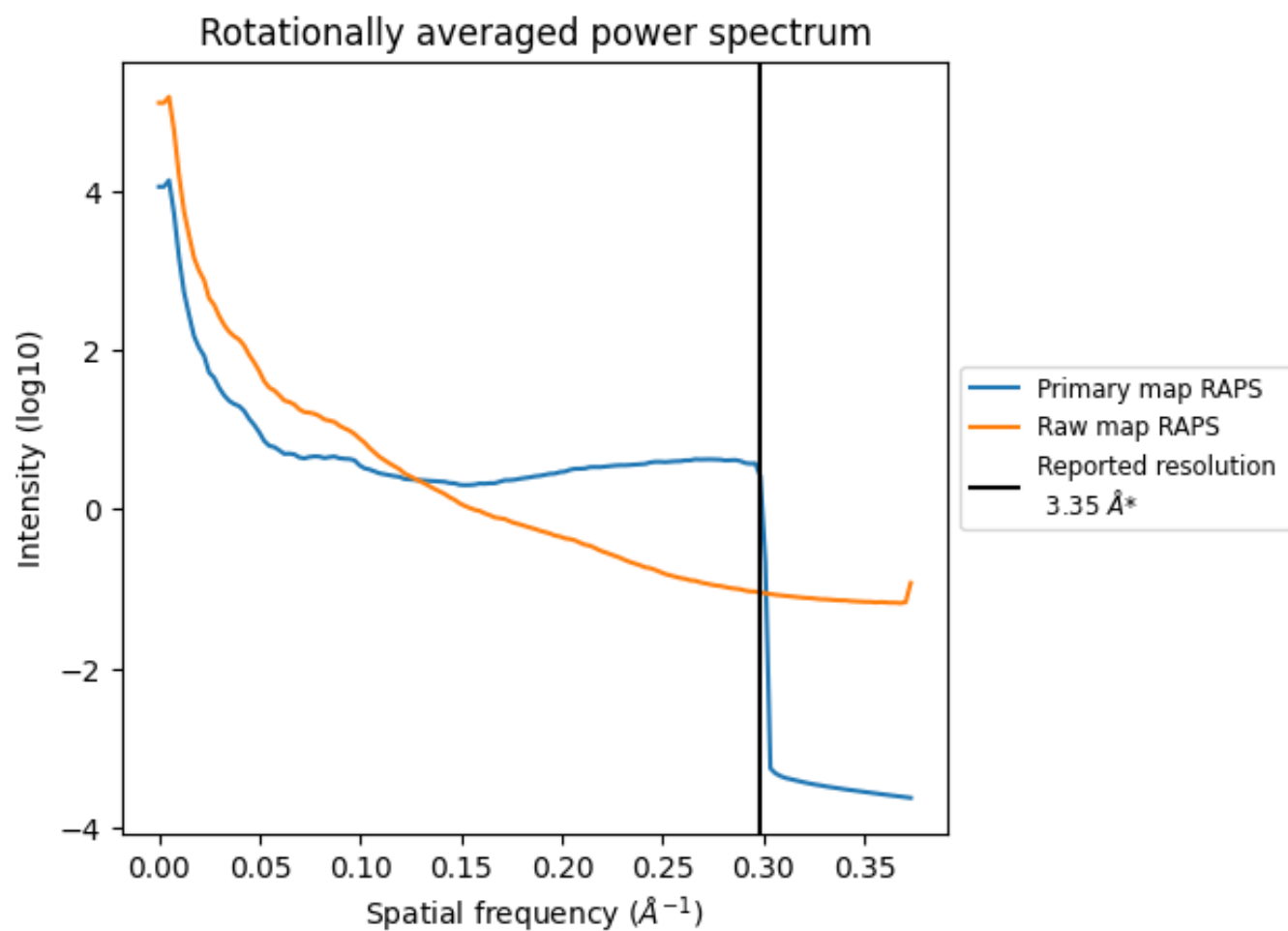
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1921 nm³; this corresponds to an approximate mass of 1736 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 ⓘ

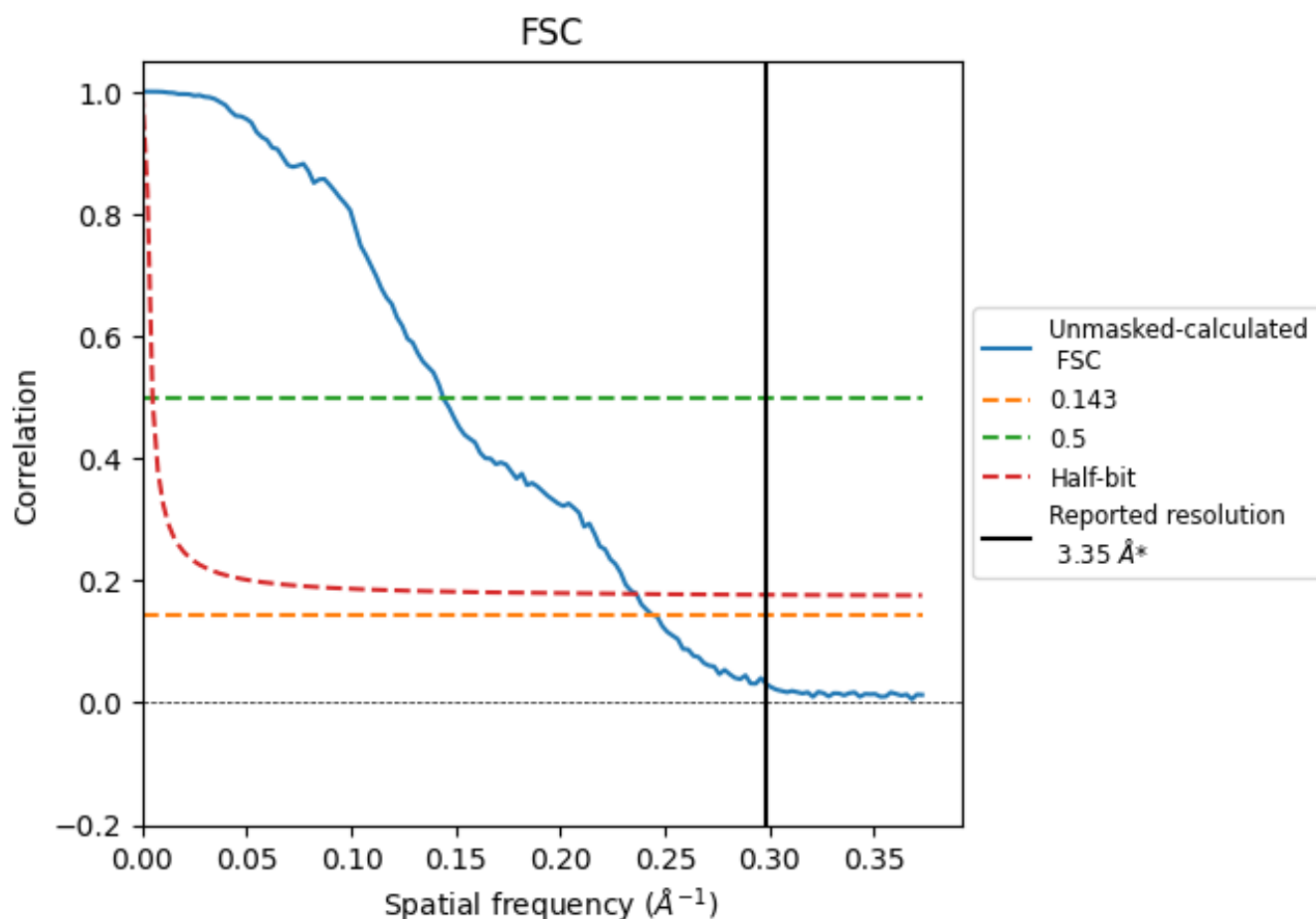


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

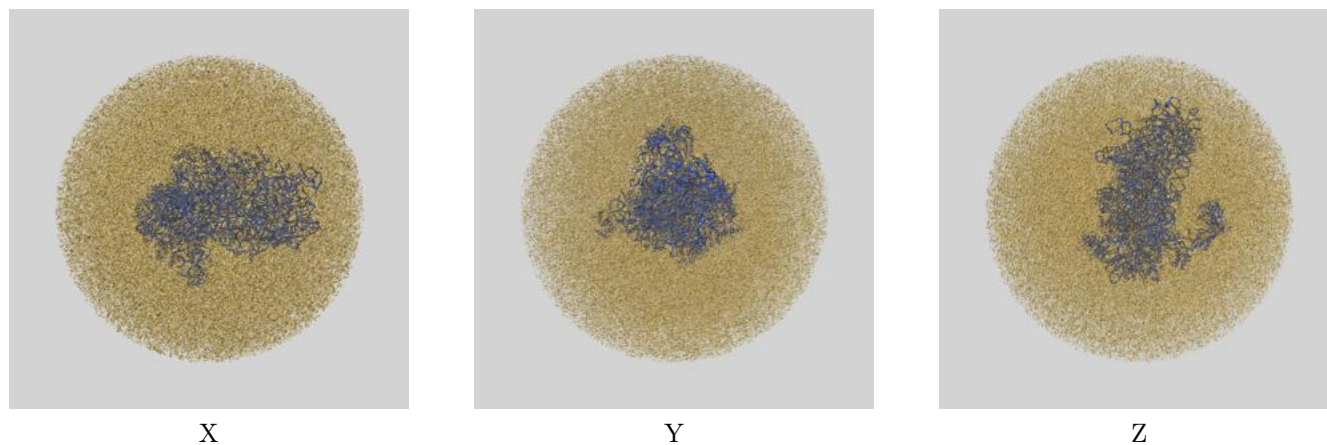
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	6.95	4.23

*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 4.09 differs from the reported value 3.35 by more than 10 %

9 Map-model fit [i](#)

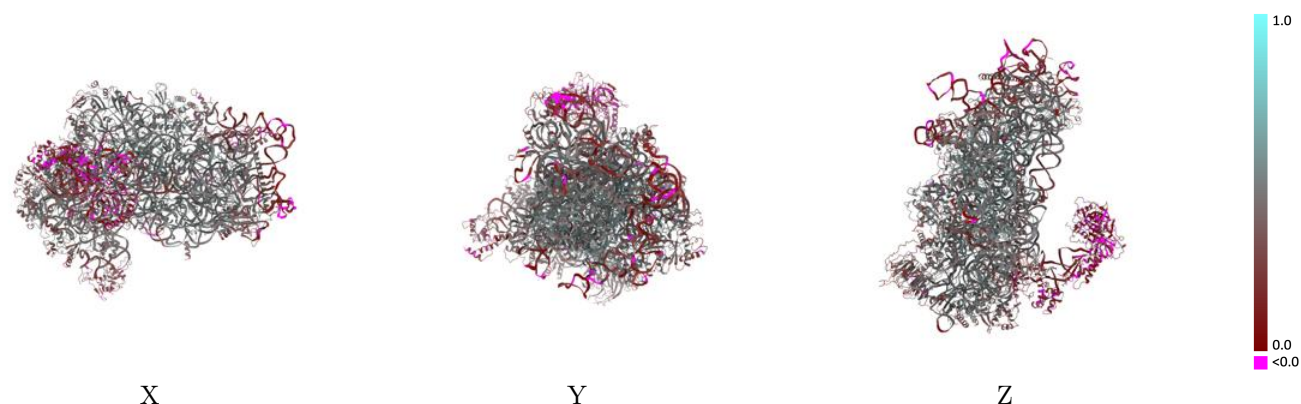
This section contains information regarding the fit between EMDB map EMD-19541 and PDB model 8RW1. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



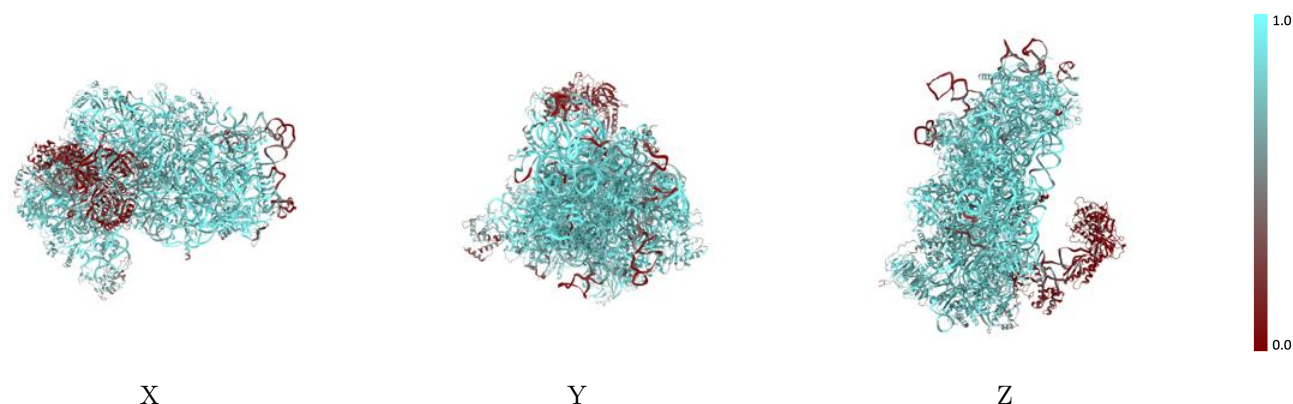
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



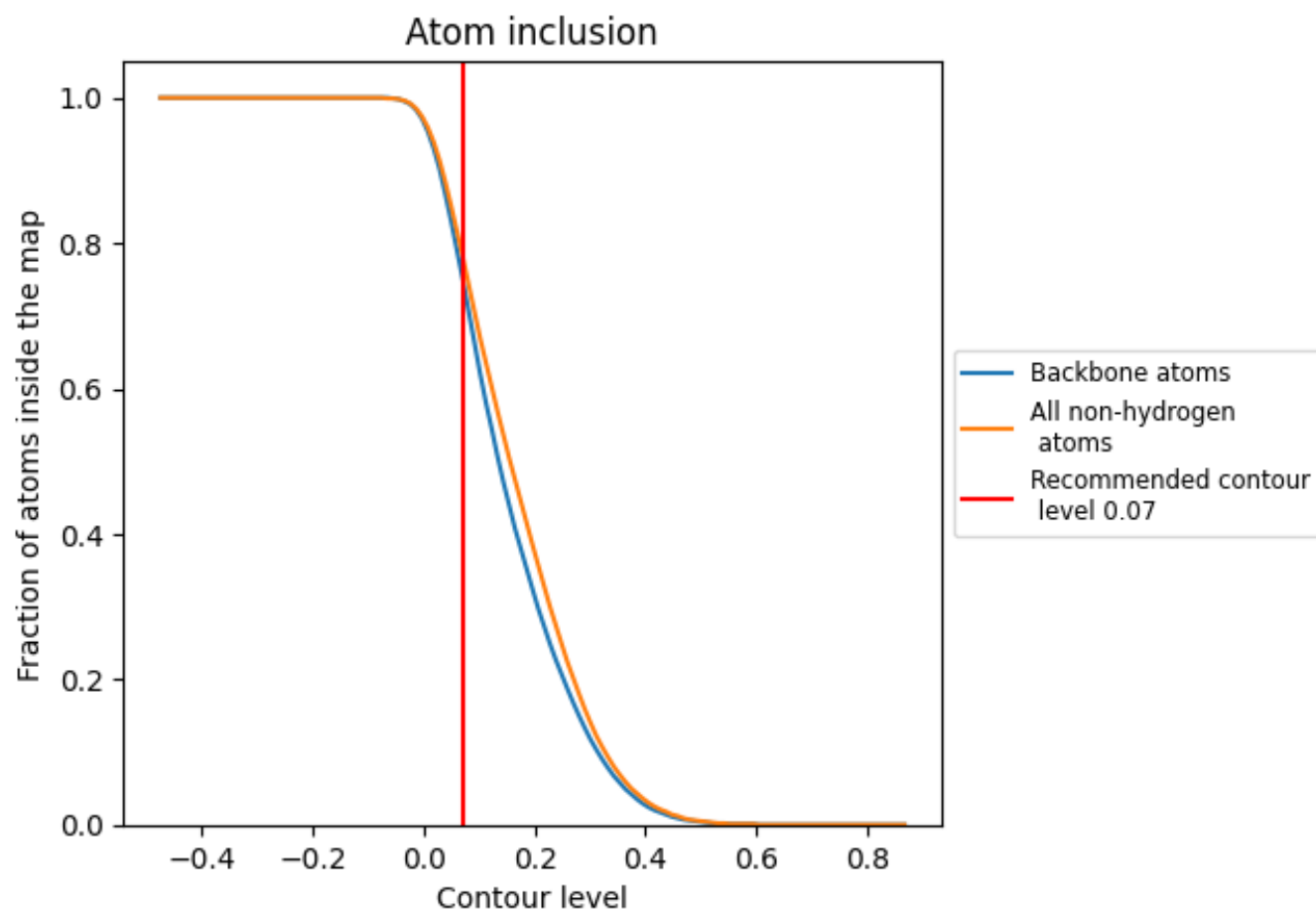
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 75% of all backbone atoms, 78% 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	 0.7830	 0.3990
1	 0.5110	 0.2620
2	 0.8800	 0.4190
3	 0.4730	 0.3100
A	 0.8730	 0.4670
B	 0.8280	 0.4290
C	 0.8950	 0.5070
D	 0.8060	 0.4210
E	 0.8840	 0.4810
F	 0.8060	 0.4480
G	 0.8040	 0.3770
H	 0.7650	 0.3900
I	 0.8460	 0.4440
J	 0.8740	 0.4790
K	 0.7980	 0.3890
L	 0.8270	 0.4520
M	 0.4560	 0.1800
N	 0.9050	 0.4800
O	 0.8750	 0.4640
P	 0.7980	 0.3770
Q	 0.8660	 0.4700
R	 0.7930	 0.4210
S	 0.7950	 0.3860
T	 0.8810	 0.4480
U	 0.7510	 0.3700
V	 0.8740	 0.4850
W	 0.9090	 0.5240
X	 0.8770	 0.4960
Y	 0.8620	 0.4480
Z	 0.6060	 0.2950
a	 0.8780	 0.4880
b	 0.8610	 0.4540
c	 0.8330	 0.4560
d	 0.9050	 0.5020
e	 0.7400	 0.4180



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Chain	Atom inclusion	Q-score
f	 0.6110	 0.2380
g	 0.7820	 0.3660
h	 0.4760	 0.3520
i	 0.3520	 0.3090
j	 0.1900	 0.1660
k	 0.0920	 0.1200
l	 0.0590	 0.1150