



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 11:37 AM UTC

PDB ID : 5UZ4 / pdb_00005uz4
EMDB ID : EMD-8621
Title : The cryo-EM structure of YjeQ bound to the 30S subunit suggests a fidelity checkpoint function for this protein in ribosome assembly
Authors : Razi, A.; Guarne, A.; Ortega, J.
Deposited on : 2017-02-24
Resolution : 5.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

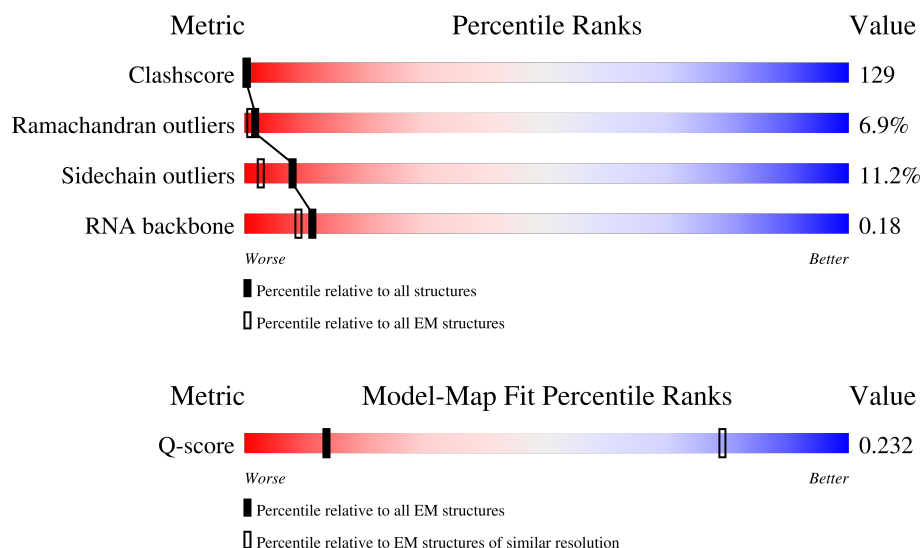
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.80 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	511 (5.30 - 6.30)

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	A	1527	
2	C	233	
3	D	206	

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Mol	Chain	Length	Quality of chain
4	E	167	
5	F	131	
6	G	179	
7	H	130	
8	I	130	
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	S	92	
19	T	87	
20	B	241	
21	Z	334	

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
23	GGM	Z	402	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 53225 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 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1527	Total	C	N	O	P	0	0
			32767	14614	6014	10613	1526		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	A	G	conflict	GB 1095872043

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	205	Total	C	N	O	S	0	0
			1639	1023	314	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	149	Total	C	N	O	S	0	0
			1160	721	222	213	4		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	129	Total	C	N	O	S	0	0
			975	613	172	184	6		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			951	587	195	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	109	Total	C	N	O	S	0	0
			845	522	169	151	3		

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	98	Total	C	N	O	S	0	0
			759	472	157	127	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	86	Total	C	N	O	S	0	0
			700	431	144	124	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	51	Total	C	N	O	0	0
			414	264	77	73		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	79	Total	C	N	O	S	0	0
			619	393	117	107	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	233	Total	C	N	O	S	2	0
			1830	1154	328	340	8		

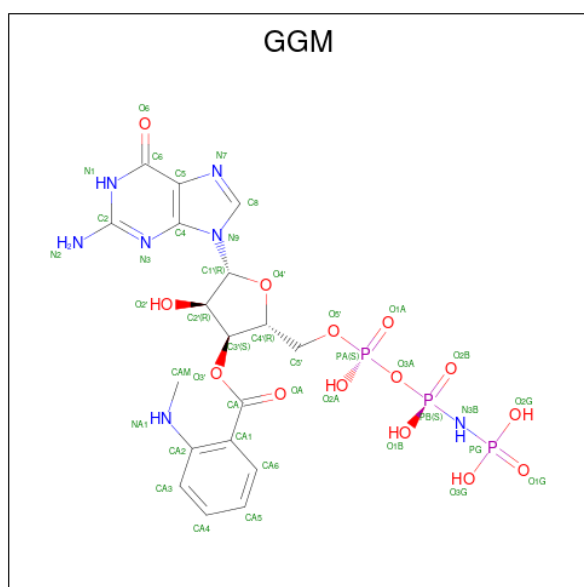
- Molecule 21 is a protein called Small ribosomal subunit biogenesis GTPase RsgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	323	Total	C	N	O	S	0	0
			2348	1463	397	479	9		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
22	Z	1	Total	Zn	0
			1	1	

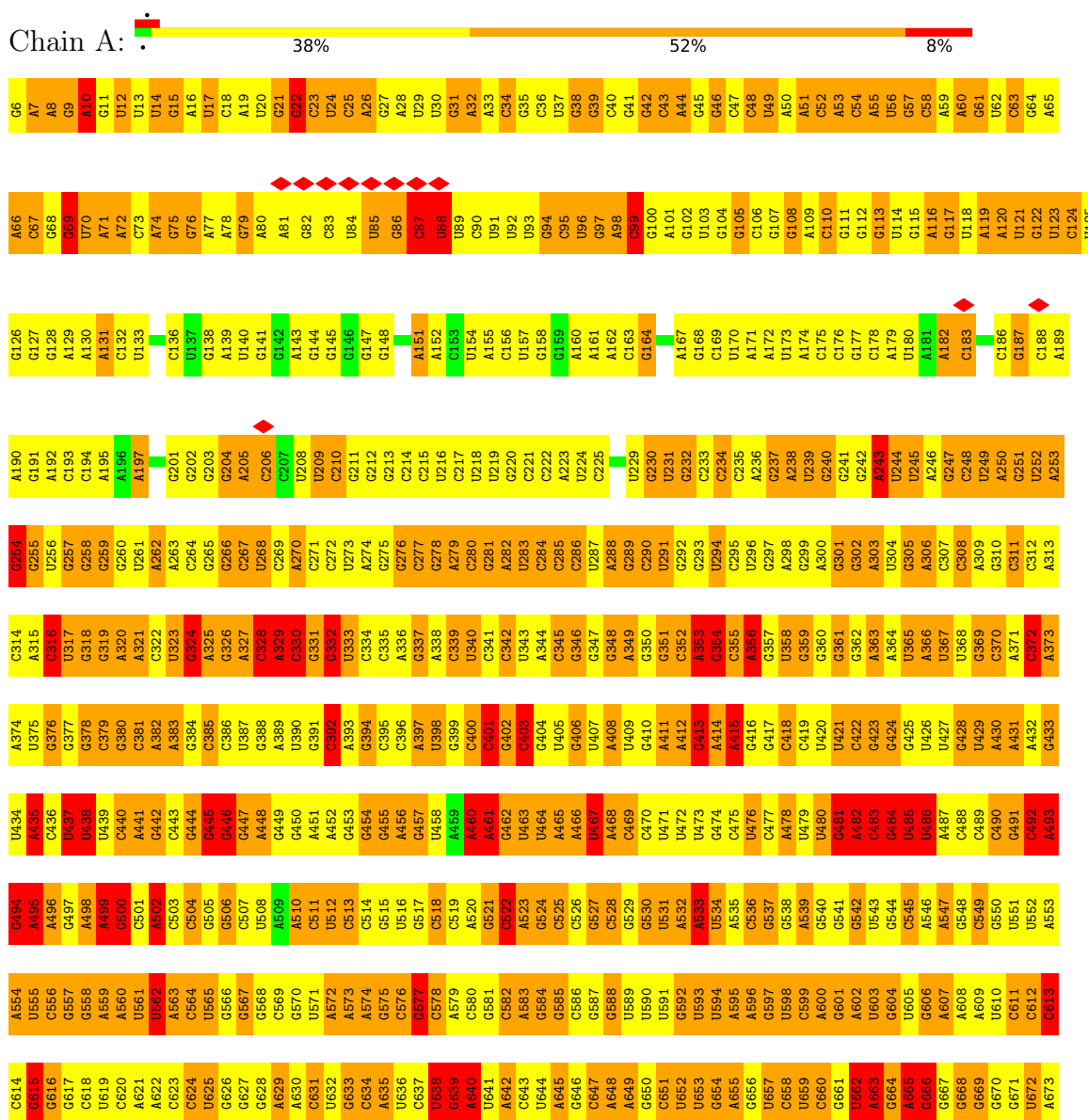
- Molecule 23 is 3'-O-(N-methylantraniloyl)-beta:gamma-imidoguanosine-5'-triphosphate (CCD ID: GGM) (formula: C₁₈H₂₄N₇O₁₄P₃).



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.

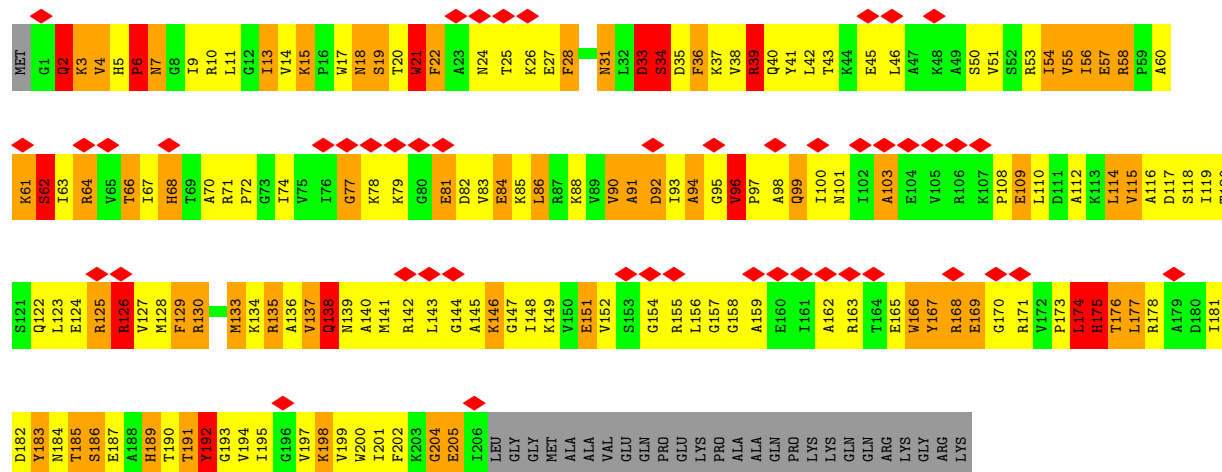
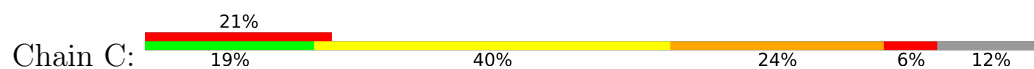
• Molecule 1: 16S RIBOSOMAL RNA



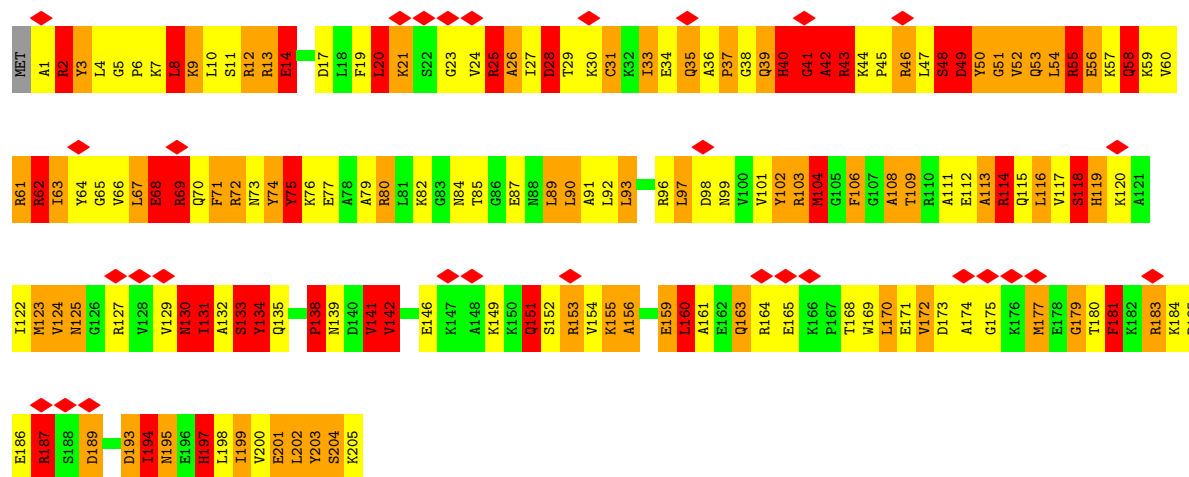
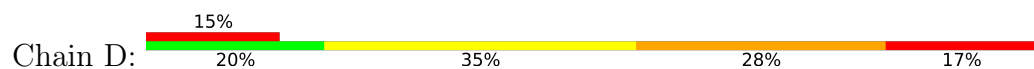
G1454	A1394	G1334	A1274	G1154	G1094	G1034	A974	A914	U854	A794	G734	G674
G1455	C1395	U1335	A1275	A1155	U1095	A1035	A975	A915	U855	C795	C735	A675
A1456	A1396	G1336	G1276	G1156	C1096	A1036	G976	U916	C856	C796	C736	A676
G1457	C1397	G1337	C1277	A1157	C1097	C1037	A977	G917	C857	C797	C737	U677
G1458	A1398	G1338	G1278	C1158	G1098	C1038	A978	A918	G858	U798	C738	U678
G1459	C1399	G1339	G1279	U1159	C1099	G1039	C979	A919	G859	G799	C739	C679
C1460	A1400	A1340	A1280	G1160	C1100	U1040	C980	U920	A860	G800	U740	C680
G1461	C1401	U1341	C1281	C1161	A1101	G1041	U981	U921	G861	A801	G741	A681
C1462	G1402	G1342	C1282	C1162	A1102	A1042	U982	G922	C862	G802	G742	G682
U1463	C1403	G1343	U1283	A1163	C1103	G1043	A983	A923	U863	G803	A743	G683
U1464	C1404	C1344	U1284	G1164	G1104	A1044	C984	C924	U864	U804	C744	U684
A1465	U1345	U1345	A1285	U1165	A1105	A1045	C985	G925	A865	C805	G745	G685
A1466	C1406	A1346	C1286	G1166	G1106	C1046	U986	G926	C866	C806	G746	G686
C1467	U1406	G1347	A1287	A1167	C1107	G1047	G987	G927	G867	A807	A747	A687
A1468	U1348	C1348	U1288	U1168	G1108	G1048	U988	G928	C868	C808	G748	G688
A1469	A1349	A1289	A1229	A1169	C1109	U1049	U989	G929	U869	G809	A749	C689
C1470	G1409	A1350	C1230	A1170	A1110	G1050	C990	C930	U870	C810	G750	G690
U1471	A1410	U1351	G1231	A1171	C1111	C1051	U991	C931	U871	C811	U751	G691
C1472	C1411	G1352	U1232	C1172	C1112	U1052	U992	C932	U872	G812	G752	U692
G1473	C1412	G1353	G1233	U1173	C1113	G1053	G993	C933	U873	U813	A753	G693
U1474	A1413	C1354	C1234	G1174	C1114	C1054	A994	C934	G874	A814	C754	A694
G1475	G1414	G1355	U1235	A1175	U1115	A1055	C995	A935	U875	A815	G755	A695
A1476	U1415	G1356	A1236	A1176	U1116	U1056	A996	C936	C876	A816	C756	A696
G1477	G1416	A1357	C1237	G1177	U1117	G1057	U997	A937	U877	C817	U757	U697
U1478	U1417	U1358	A1238	G1178	U1118	G1058	C998	A938	A878	G818	C758	G698
C1479	A1418	C1359	A1239	A1179	C1119	C1059	C999	G939	C879	A819	A759	G699
A1480	G1419	A1360	U1240	U1180	U1120	U1060	C1000	C940	C880	U820	G760	G700
U1481	U1420	G1361	G1241	A1181	C1121	G1061	C1001	G941	G881	G821	G761	U701
G1482	A1421	A1362	G1242	G1182	U1122	U1062	C1002	G942	C882	U822	U762	G702
A1483	C1422	A1363	C1243	U1183	U1123	C1063	G1003	U943	C883	C823	G763	A703
C1484	G1423	G1364	G1244	G1184	G1124	U1064	A1004	G944	U884	G824	C764	G704
G1485	U1424	G1365	C1245	G1185	U1125	U1065	A1005	G945	G885	A825	G765	A705
U1486	A1425	C1366	A1246	G1186	U1126	C1066	G1006	A946	G886	C826	A766	G706
G1487	G1426	G1367	U1247	G1187	U1127	A1067	U1007	G947	G887	U827	A767	A707
G1488	C1427	A1368	A1248	A1188	C1128	G1068	U1008	C948	C888	G828	U768	C708
U1489	U1428	C1369	C1249	U1189	C1129	C1069	U1009	A949	A889	G829	G769	C709
C1490	A1429	G1370	A1250	G1190	A1130	U1070	U1010	U950	G890	G830	C770	U709
G1491	A1430	G1371	A1251	A1191	C1131	C1071	C1011	G951	U891	A831	G771	G710
A1492	C1431	U1372	A1252	C1192	C1132	G1072	A1012	U952	A892	G832	U772	G711
A1493	G1432	G1373	G1253	G1193	C1133	U1073	G1013	G953	C893	G833	G773	A712
G1494	A1433	A1374	A1254	U1194	U1134	G1074	A1014	G954	G894	U834	G774	G713
C1495	C1434	A1375	G1255	C1195	U1135	U1075	G1015	U955	G895	U835	G775	G714
U1496	U1435	U1376	A1256	A1196	C1136	U1076	A1016	U956	C896	G836	G776	A715
G1497	G1436	A1377	A1257	A1197	C1137	G1077	U1017	U957	C897	U837	A777	A716
U1498	A1437	C1378	G1258	G1198	C1138	U1078	G1018	U958	G898	G838	G778	U717
A1499	G1438	G1379	C1259	U1199	G1139	G1079	A1019	A959	C899	C839	C779	A718
U1500	C1439	U1380	G1260	C1200	C1140	A1080	A1019	U960	A900	C840	A780	C719
C1501	U1381	A1261	A1261	A1201	C1141	U1081	G1020	U961	A901	C841	A781	C720
U1502	U1440	C1382	C1262	U1202	G1142	A1082	A1021	C962	G902	U842	A782	G721
A1503	A1441	C1383	C1263	C1203	G1143	U1083	A1022	C963	G903	U843	C783	G722
G1504	G1442	C1384	U1264	A1204	C1144	G1084	U1023	A964	U904	U844	A784	U723
G1505	C1443	G1385	A1265	U1205	A1145	U1085	U1025	U965	G895	G845	G785	G724
U1506	U1444	G1386	C1266	G1206	A1146	U1086	G1026	G966	A906	A846	G786	G725
A1507	A1445	G1387	G1267	G1207	C1147	G1087	C1027	C967	A907	G847	A787	C726
C1508	U1446	C1388	C1268	C1208	U1148	G1088	C1028	A968	A908	U848	U788	G727
U1509	A1447	A1389	A1269	C1209	C1149	G1089	U1029	A969	C909	C849	U789	A728
C1510	C1448	U1390	G1270	C1210	U1150	U1090	U1030	C970	C910	A850	A790	A729
U1511	U1449	G1391	A1271	U1211	A1151	A1091	C1031	C971	U911	G851	G791	G730
G1512	U1450	C1392	G1272	U1212	A1152	A1092	C1032	C972	U912	G852	A792	G731
A1513	A1451	U1393	C1273	A1213	C1153	A1093	G1033	G973	A913	C853	U793	G732
												G733



• Molecule 2: 30S ribosomal protein S3

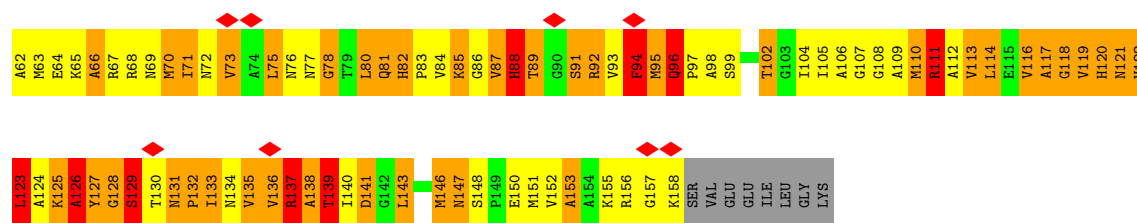


• Molecule 3: 30S ribosomal protein S4

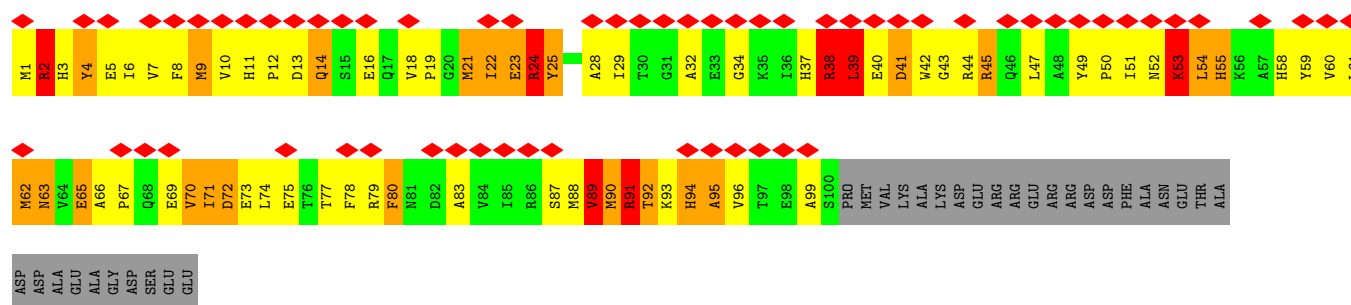
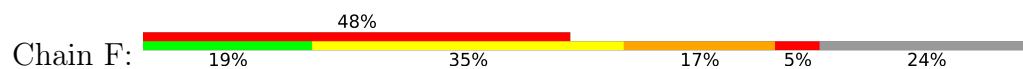


• Molecule 4: 30S ribosomal protein S5

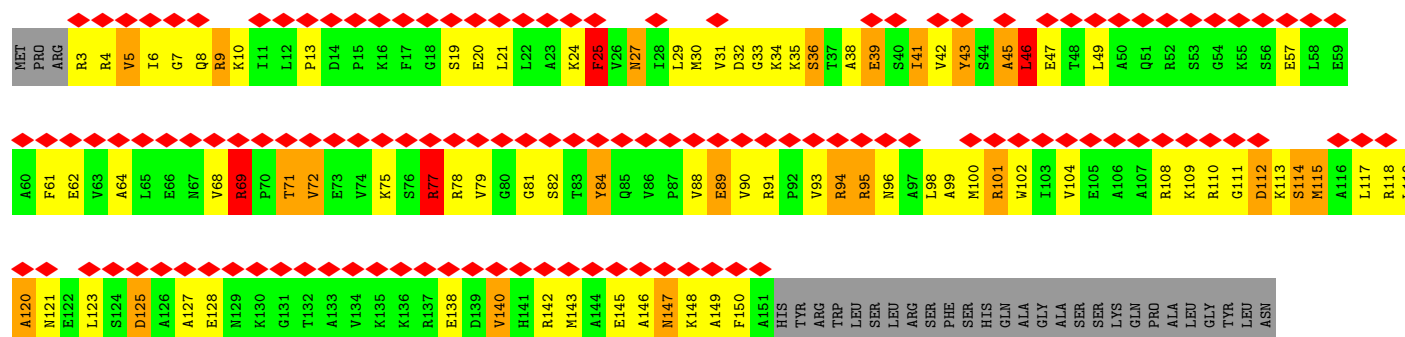




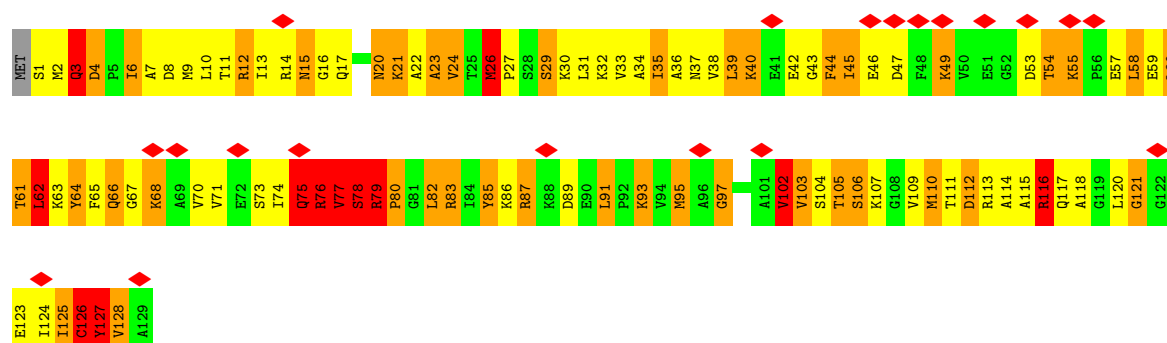
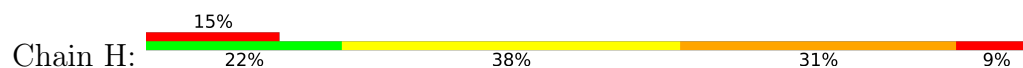
• Molecule 5: 30S ribosomal protein S6



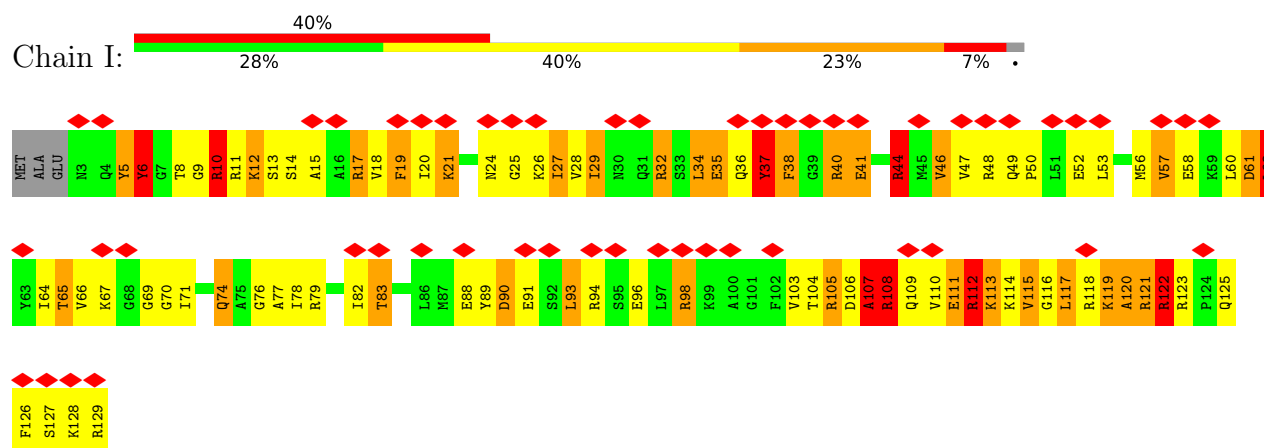
• Molecule 6: 30S ribosomal protein S7



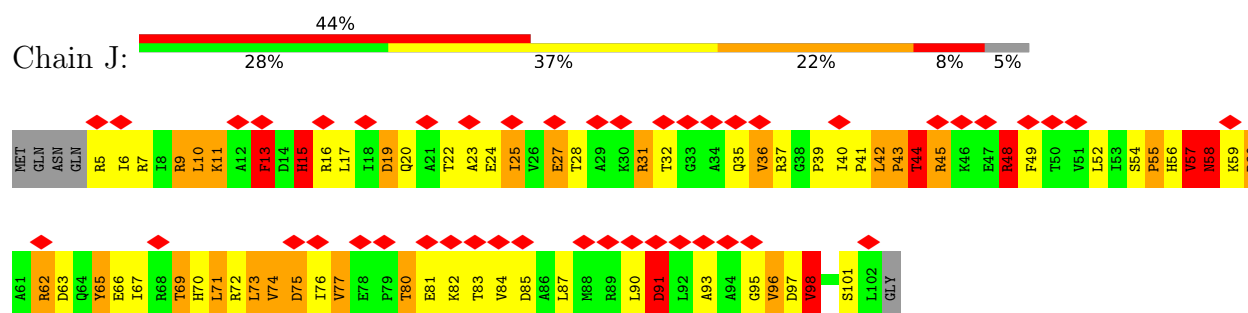
• Molecule 7: 30S ribosomal protein S8



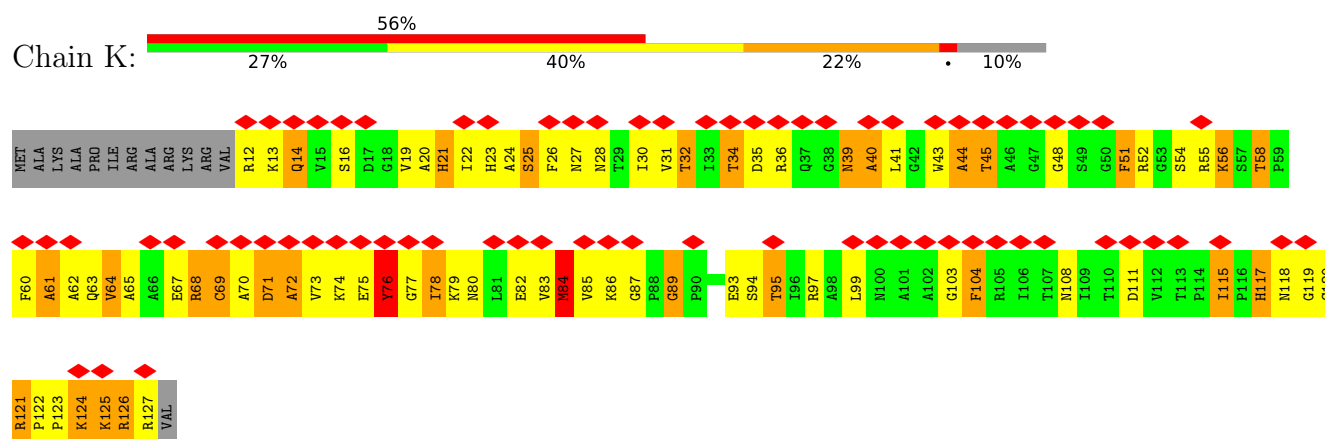
- Molecule 8: 30S ribosomal protein S9



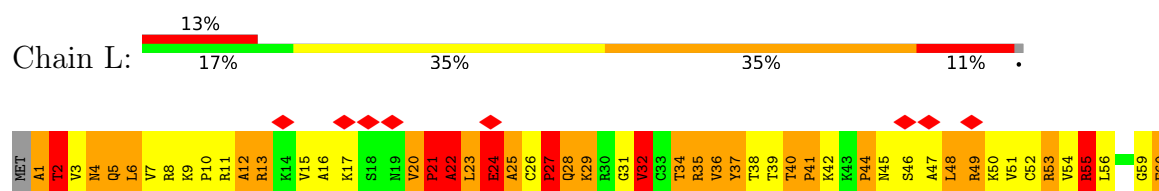
- Molecule 9: 30S ribosomal protein S10

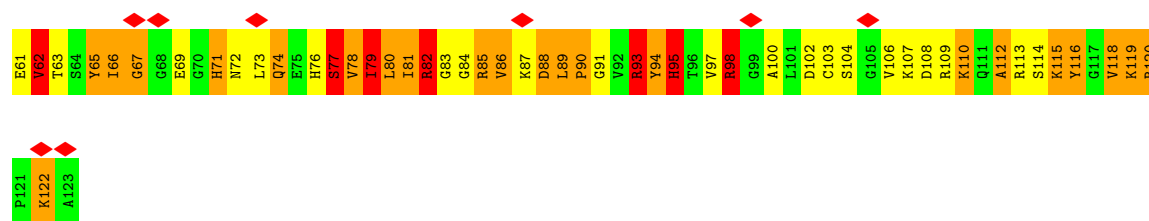


- Molecule 10: 30S ribosomal protein S11

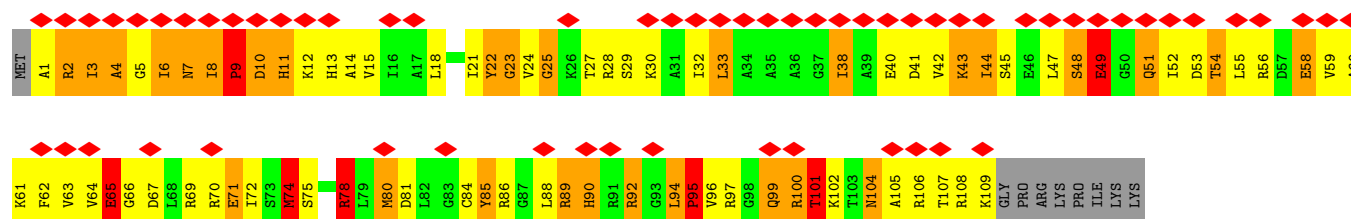
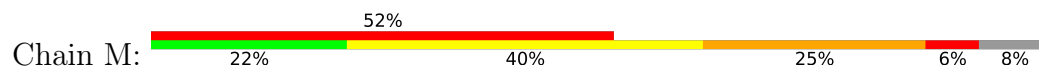


- Molecule 11: 30S ribosomal protein S12

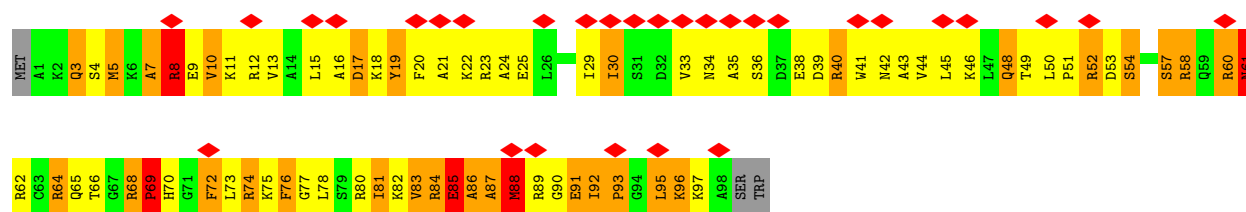
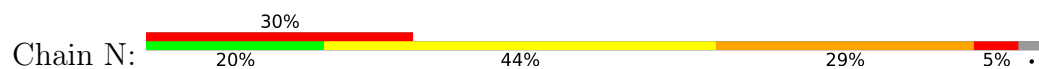




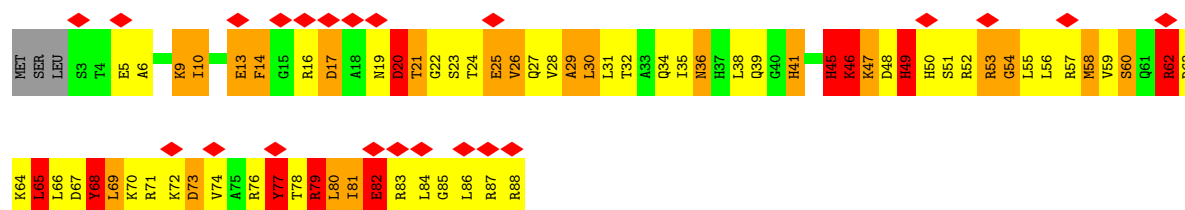
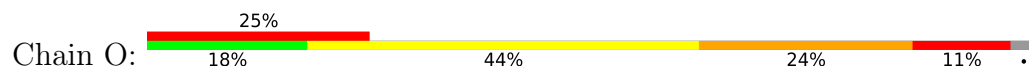
• Molecule 12: 30S ribosomal protein S13



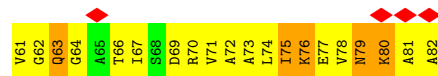
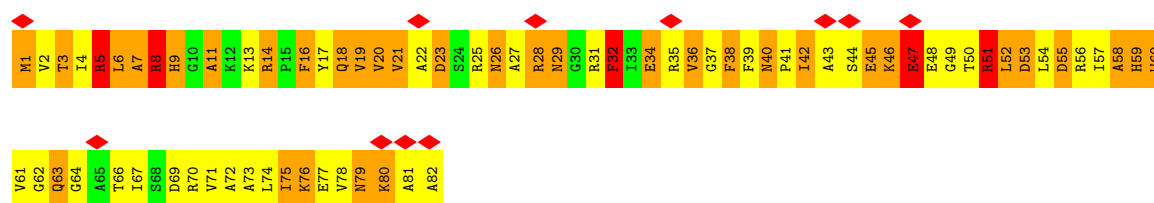
• Molecule 13: 30S ribosomal protein S14



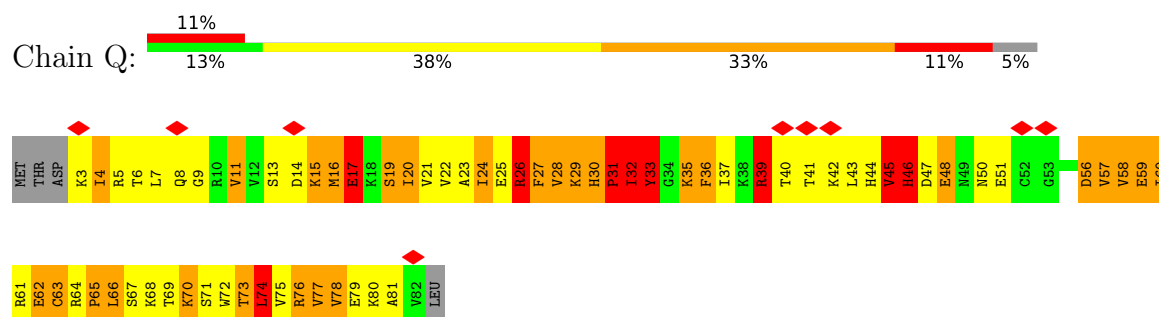
• Molecule 14: 30S ribosomal protein S15



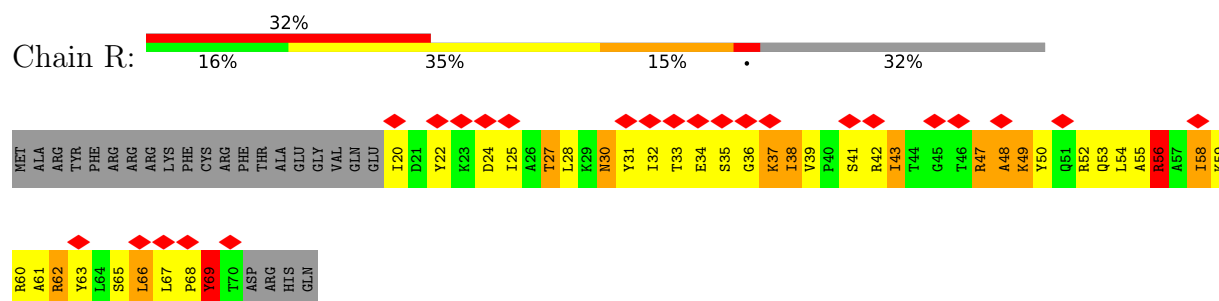
• Molecule 15: 30S ribosomal protein S16



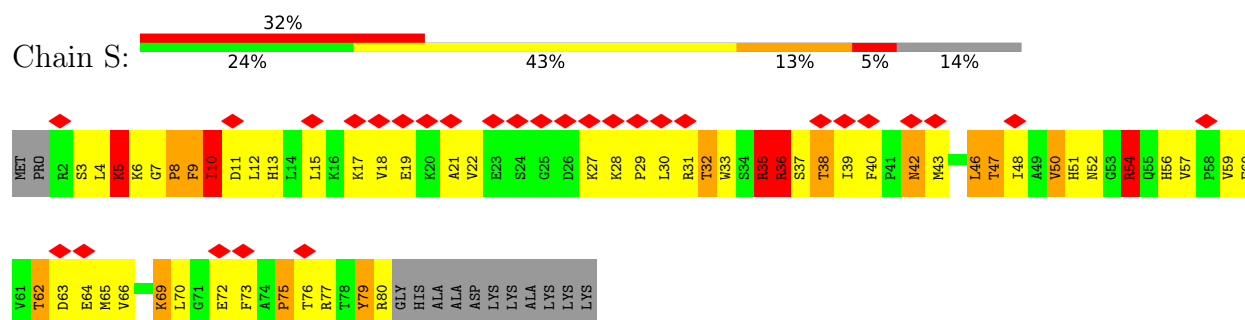
- Molecule 16: 30S ribosomal protein S17



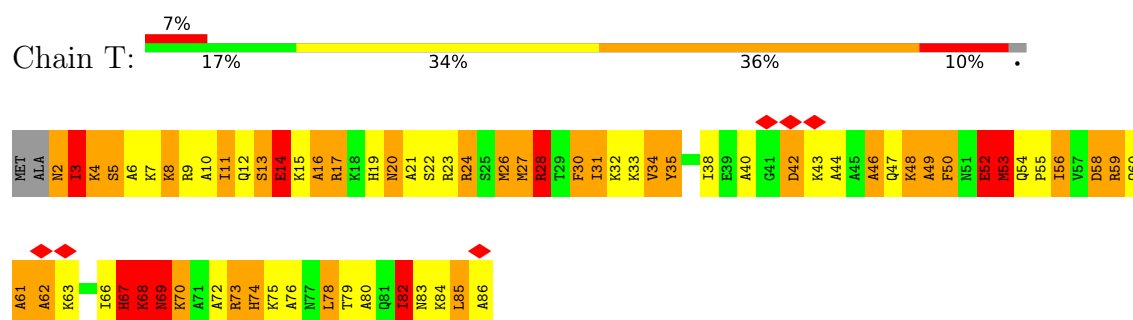
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19

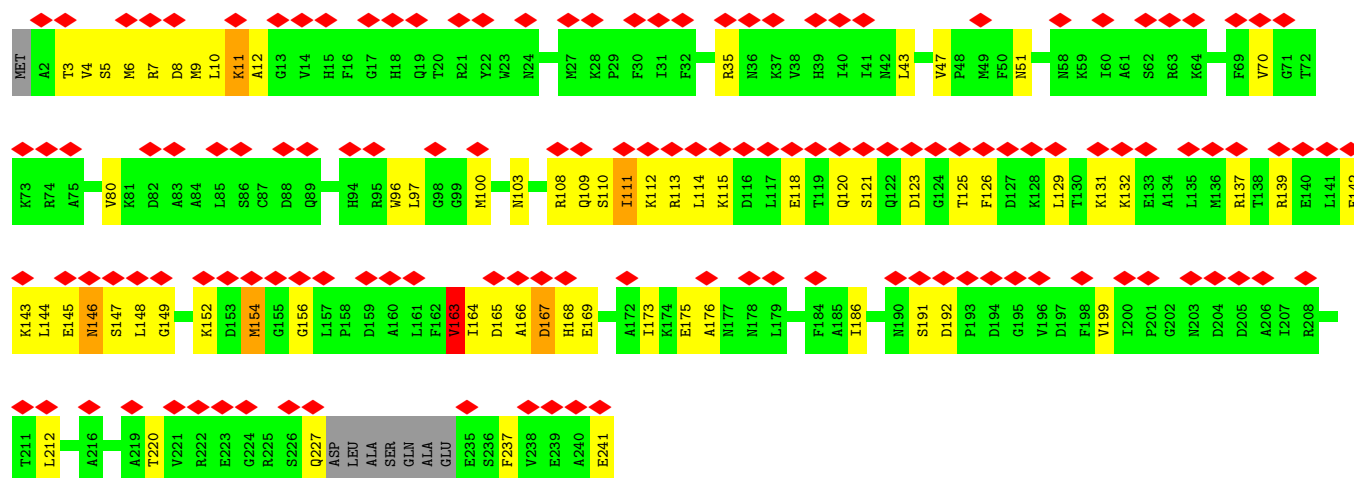


- Molecule 19: 30S ribosomal protein S20

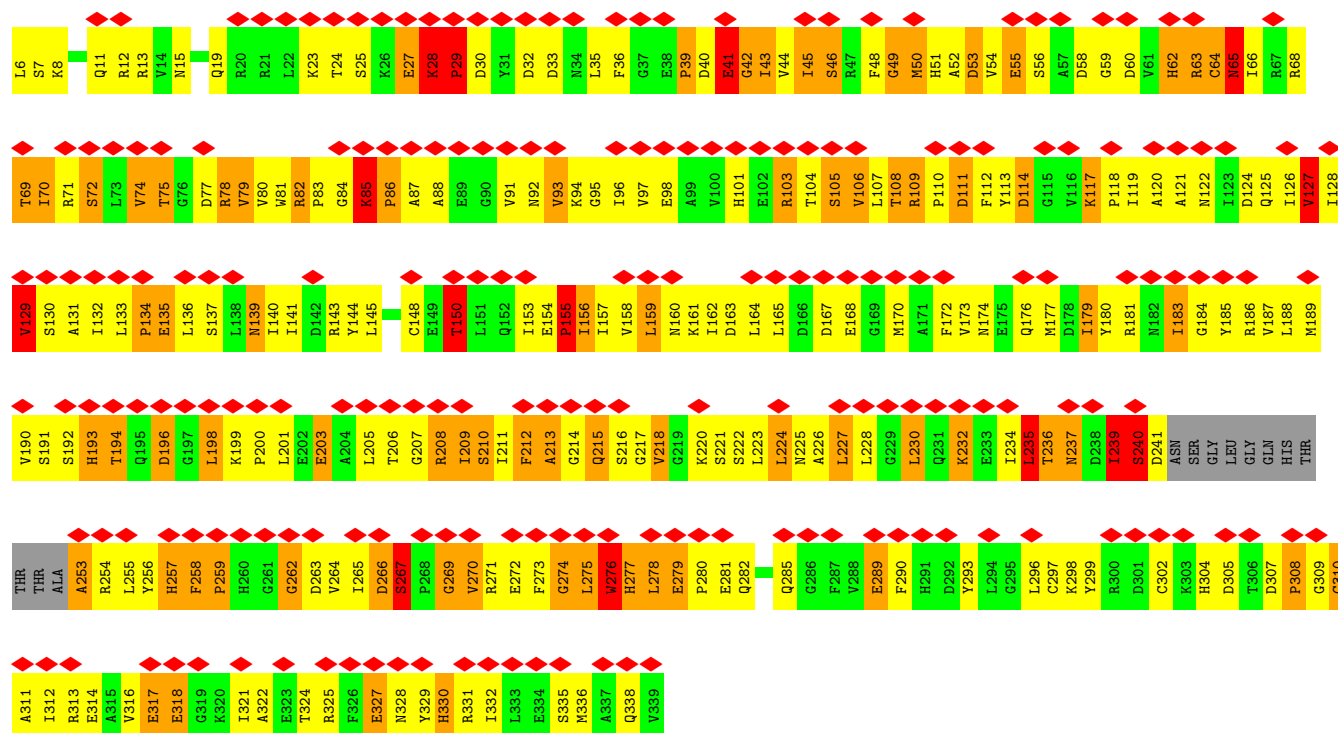
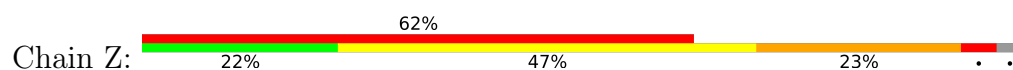


- Molecule 20: 30S ribosomal protein S2





• Molecule 21: Small ribosomal subunit biogenesis GTPase RsgA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130462	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	34482	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0309	Depositor
Map size (Å)	319.0, 319.0, 319.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.45, 1.45, 1.45	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	2.15	216/36645 (0.6%)	1.42	535/57061 (0.9%)
2	C	2.36	103/1651 (6.2%)	2.12	82/2225 (3.7%)
3	D	2.61	124/1661 (7.5%)	2.15	70/2223 (3.1%)
4	E	2.94	114/1118 (10.2%)	2.27	61/1504 (4.1%)
5	F	2.05	30/835 (3.6%)	2.11	35/1128 (3.1%)
6	G	1.89	26/1173 (2.2%)	2.11	49/1573 (3.1%)
7	H	2.72	89/985 (9.0%)	2.35	64/1322 (4.8%)
8	I	2.13	40/1034 (3.9%)	2.17	51/1375 (3.7%)
9	J	2.19	26/796 (3.3%)	2.23	43/1077 (4.0%)
10	K	2.01	29/885 (3.3%)	2.12	41/1195 (3.4%)
11	L	2.78	92/965 (9.5%)	2.30	57/1296 (4.4%)
12	M	1.96	22/851 (2.6%)	2.15	42/1136 (3.7%)
13	N	2.20	35/769 (4.6%)	1.97	19/1026 (1.9%)
14	O	2.39	46/708 (6.5%)	2.17	35/946 (3.7%)
15	P	2.65	58/659 (8.8%)	2.24	41/884 (4.6%)
16	Q	2.59	60/657 (9.1%)	2.30	35/881 (4.0%)
17	R	1.68	12/420 (2.9%)	1.53	6/565 (1.1%)
18	S	1.79	13/633 (2.1%)	1.88	27/853 (3.2%)
19	T	2.60	52/671 (7.7%)	2.28	33/888 (3.7%)
20	B	0.84	2/1864 (0.1%)	1.46	6/2511 (0.2%)
21	Z	1.22	27/2388 (1.1%)	1.68	91/3259 (2.8%)
All	All	2.15	1216/57368 (2.1%)	1.66	1423/84928 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	7
2	C	0	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	17
4	E	0	9
5	F	0	6
6	G	0	6
7	H	0	5
8	I	0	10
9	J	0	7
10	K	0	2
11	L	0	7
12	M	0	2
13	N	0	3
14	O	0	6
15	P	0	5
16	Q	0	2
17	R	0	2
18	S	0	4
19	T	0	4
21	Z	0	11
All	All	1	135

The worst 5 of 1216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	801	U	O3'-P	-72.71	0.52	1.61
1	A	1012	A	O3'-P	-72.63	0.52	1.61
1	A	901	A	O3'-P	-70.24	0.55	1.61
1	A	1310	G	O3'-P	-66.89	0.60	1.61
1	A	354	G	O3'-P	-66.26	0.61	1.61

The worst 5 of 1423 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	801	U	P-O3'-C3'	-62.09	27.07	120.20
1	A	316	C	O3'-P-O5'	38.84	162.26	104.00
1	A	1016	A	O3'-P-O5'	-38.19	46.72	104.00
20	B	111	ILE	O-C-N	36.46	160.96	121.94
1	A	882	C	O3'-P-O5'	34.83	156.25	104.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1243	C	C3'

5 of 135 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	437	U	Sidechain
1	A	438	U	Sidechain
1	A	496	A	Sidechain
1	A	521	G	Sidechain

5.2 Too-close contacts [i](#)

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	A	32767	0	16531	9875	0
2	C	1624	0	1699	140	0
3	D	1639	0	1699	150	0
4	E	1105	0	1148	96	0
5	F	817	0	808	120	0
6	G	1160	0	1207	90	0
7	H	975	0	1023	81	0
8	I	1022	0	1070	106	0
9	J	786	0	828	64	0
10	K	869	0	877	117	0
11	L	951	0	1008	131	0
12	M	845	0	900	138	0
13	N	759	0	789	187	0
14	O	700	0	723	66	0
15	P	649	0	665	54	0
16	Q	648	0	690	80	0
17	R	414	0	439	86	0
18	S	619	0	628	154	0
19	T	665	0	710	60	0
20	B	1830	0	1839	154	0
21	Z	2348	0	2104	564	0
22	Z	1	0	0	0	0
23	Z	32	0	12	33	0
All	All	53225	0	37397	11535	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 129.

The worst 5 of 11535 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)
1:A:1088:G:C2	1:A:1098:C:N3	1.67	1.59
1:A:714:G:H2'	1:A:715:A:C8	1.08	1.58
1:A:510:A:O3'	1:A:511:C:P	1.16	1.54
1:A:317:U:C4	1:A:337:G:C2	1.98	1.51
1:A:253:A:N6	1:A:274:A:C6	1.79	1.51

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	C	204/233 (88%)	149 (73%)	40 (20%)	15 (7%)	1	10
3	D	203/206 (98%)	162 (80%)	25 (12%)	16 (8%)	1	9
4	E	148/167 (89%)	119 (80%)	23 (16%)	6 (4%)	2	17
5	F	98/131 (75%)	76 (78%)	10 (10%)	12 (12%)	0	4
6	G	147/179 (82%)	115 (78%)	25 (17%)	7 (5%)	2	16
7	H	127/130 (98%)	104 (82%)	18 (14%)	5 (4%)	2	18
8	I	125/130 (96%)	93 (74%)	22 (18%)	10 (8%)	1	9
9	J	96/103 (93%)	70 (73%)	16 (17%)	10 (10%)	0	6
10	K	114/129 (88%)	86 (75%)	19 (17%)	9 (8%)	1	9
11	L	121/124 (98%)	81 (67%)	26 (22%)	14 (12%)	0	4
12	M	105/118 (89%)	78 (74%)	18 (17%)	9 (9%)	0	8
13	N	96/101 (95%)	61 (64%)	24 (25%)	11 (12%)	0	5
14	O	84/89 (94%)	68 (81%)	13 (16%)	3 (4%)	2	20
15	P	80/82 (98%)	64 (80%)	9 (11%)	7 (9%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	78/84 (93%)	50 (64%)	22 (28%)	6 (8%)	1	9
17	R	49/75 (65%)	35 (71%)	12 (24%)	2 (4%)	2	17
18	S	77/92 (84%)	55 (71%)	15 (20%)	7 (9%)	0	8
19	T	83/87 (95%)	72 (87%)	4 (5%)	7 (8%)	0	8
20	B	231/241 (96%)	218 (94%)	11 (5%)	2 (1%)	14	50
21	Z	319/334 (96%)	259 (81%)	41 (13%)	19 (6%)	1	12
All	All	2585/2835 (91%)	2015 (78%)	393 (15%)	177 (7%)	2	11

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	62	SER
2	C	158	GLY
2	C	174	LEU
2	C	178	ARG
2	C	195	ILE

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	C	170/190 (90%)	156 (92%)	14 (8%)	10	30
3	D	171/173 (99%)	138 (81%)	33 (19%)	1	8
4	E	113/126 (90%)	98 (87%)	15 (13%)	4	14
5	F	87/112 (78%)	80 (92%)	7 (8%)	11	31
6	G	121/147 (82%)	110 (91%)	11 (9%)	9	27
7	H	103/105 (98%)	90 (87%)	13 (13%)	4	16
8	I	105/107 (98%)	94 (90%)	11 (10%)	6	21
9	J	86/90 (96%)	75 (87%)	11 (13%)	4	15
10	K	89/99 (90%)	80 (90%)	9 (10%)	7	23
11	L	102/104 (98%)	90 (88%)	12 (12%)	5	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	88/96 (92%)	79 (90%)	9 (10%)	7	23
13	N	74/84 (88%)	69 (93%)	5 (7%)	14	36
14	O	74/77 (96%)	67 (90%)	7 (10%)	8	25
15	P	65/65 (100%)	54 (83%)	11 (17%)	2	10
16	Q	74/78 (95%)	66 (89%)	8 (11%)	6	21
17	R	43/65 (66%)	36 (84%)	7 (16%)	2	11
18	S	66/79 (84%)	62 (94%)	4 (6%)	17	38
19	T	65/66 (98%)	55 (85%)	10 (15%)	2	12
20	B	194/199 (98%)	186 (96%)	8 (4%)	27	48
21	Z	234/286 (82%)	202 (86%)	32 (14%)	3	14
All	All	2124/2348 (90%)	1887 (89%)	237 (11%)	8	19

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	23	HIS
21	Z	203	GLU
12	M	95	PRO
21	Z	186	ARG
21	Z	330	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
11	L	4	ASN
15	P	29	ASN
11	L	71	HIS
13	N	48	GLN
17	R	30	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1522/1527 (99%)	758 (49%)	90 (5%)

5 of 758 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	8	A
1	A	9	G
1	A	10	A
1	A	14	U

5 of 90 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	910	C
1	A	1300	G
1	A	953	G
1	A	1101	A
1	A	1369	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
23	GGM	Z	402	-	34,34,45	2.09	8 (23%)	47,54,69	2.78	20 (42%)

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
23	GGM	Z	402	-	-	4/18/38/48	0/3/3/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	402	GGM	PA-O3A	8.00	1.68	1.59
23	Z	402	GGM	C3'-C2'	-2.99	1.45	1.53
23	Z	402	GGM	O4'-C1'	2.86	1.48	1.42
23	Z	402	GGM	PG-O2G	2.34	1.63	1.56
23	Z	402	GGM	PG-N3B	2.15	1.69	1.63

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	402	GGM	C3'-C2'-C1'	11.47	123.17	101.46
23	Z	402	GGM	C2-N3-C4	5.30	121.43	112.30
23	Z	402	GGM	O4'-C1'-C2'	-4.55	96.87	106.62
23	Z	402	GGM	O1G-PG-N3B	-4.54	105.09	111.77
23	Z	402	GGM	C2'-C3'-C4'	-4.48	93.95	102.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Z	402	GGM	PG-N3B-PB-O2B
23	Z	402	GGM	PB-N3B-PG-O1G
23	Z	402	GGM	PG-N3B-PB-O3A
23	Z	402	GGM	PA-O3A-PB-O2B

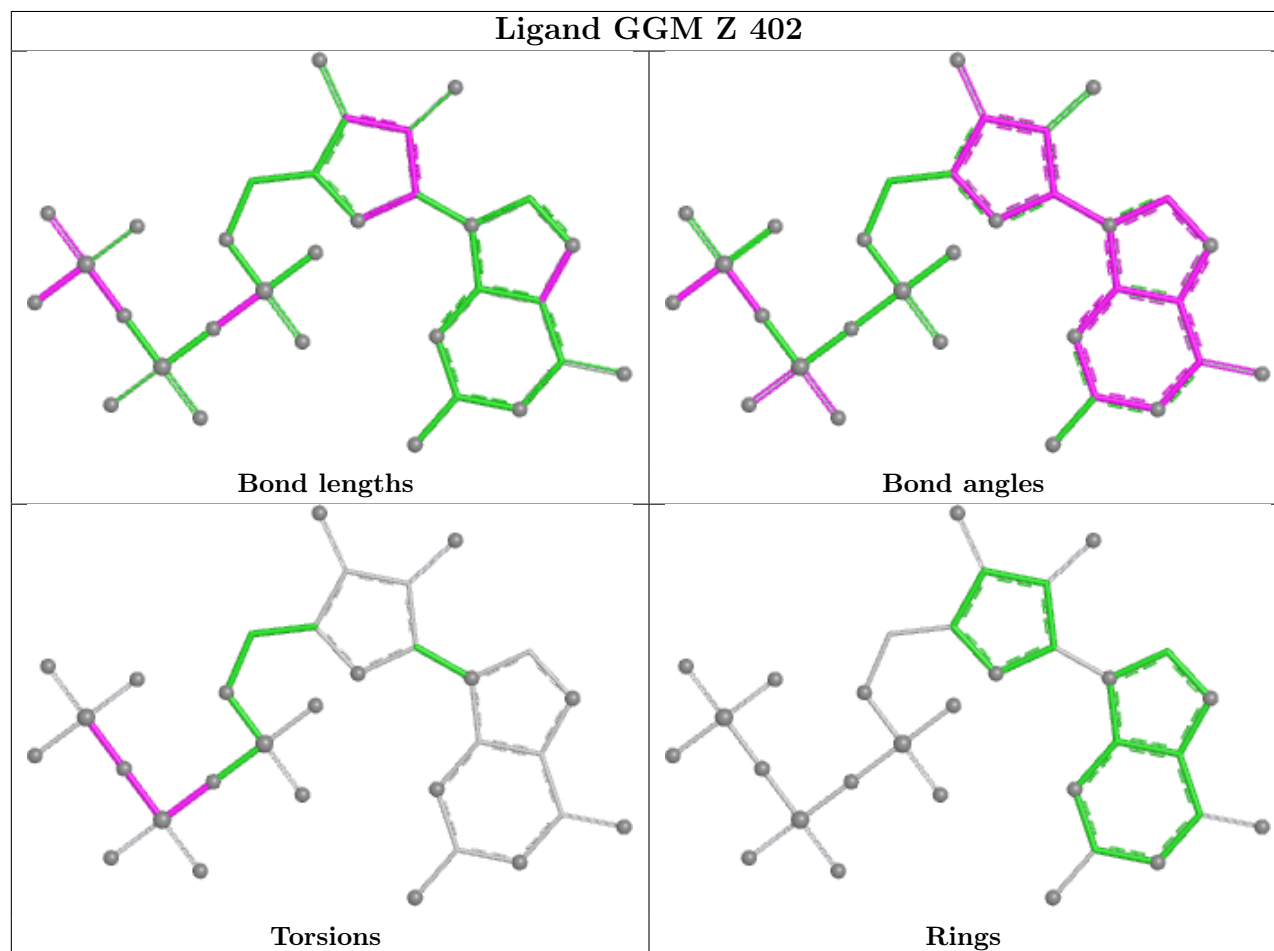
There are no ring outliers.

1 monomer is involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Z	402	GGM	33	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
1	A	195
21	Z	4

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Mol	Chain	Number of breaks
12	M	1
13	N	1
20	B	1

The worst 5 of 202 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1249:C	O3'	1250:A	P	3.76
1	A	646:G	O3'	647:C	P	3.66
1	A	886:G	O3'	887:G	P	3.56
1	A	1309:G	O3'	1310:G	P	3.30
1	A	317:U	O3'	318:G	P	3.28

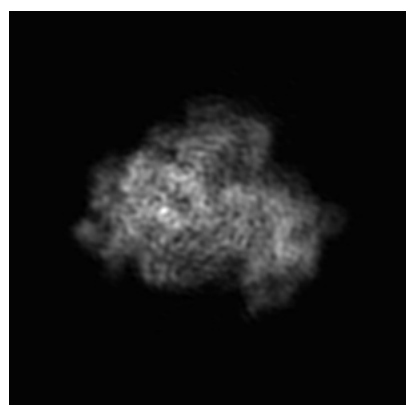
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8621. These allow visual inspection of the internal detail of the map and identification of artifacts.

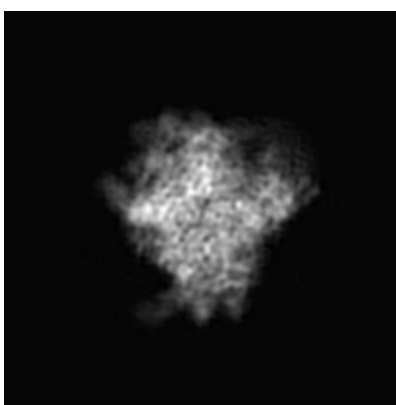
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

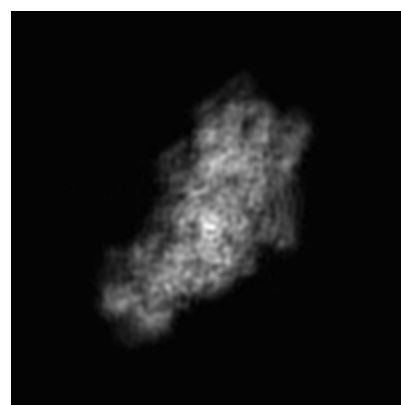
6.1.1 Primary map



X



Y

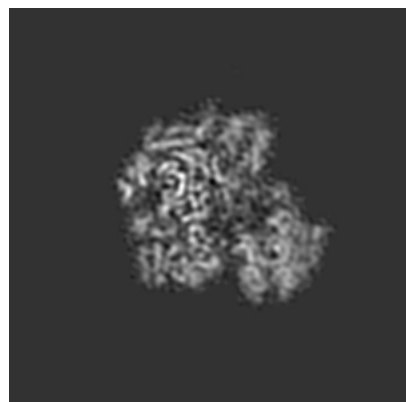


Z

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

6.2 Central slices [i](#)

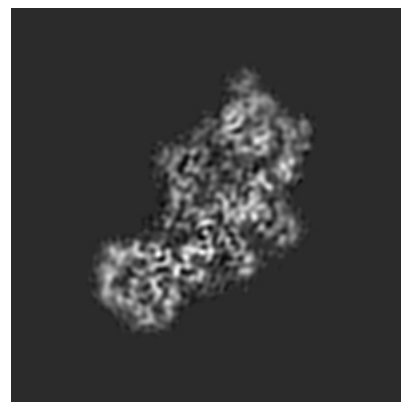
6.2.1 Primary map



X Index: 110



Y Index: 110

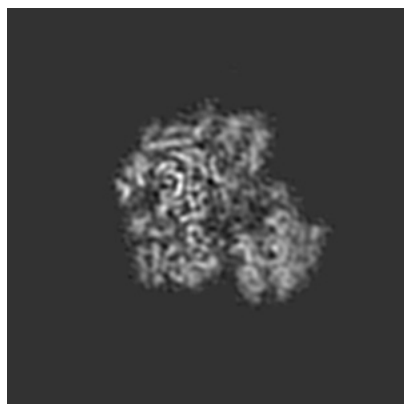


Z Index: 110

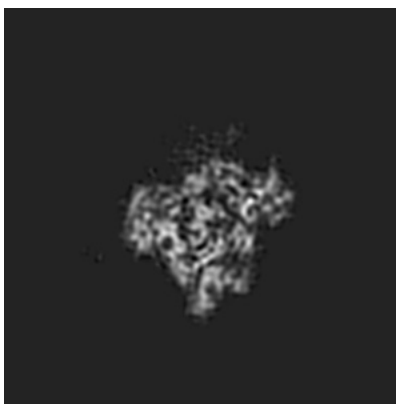
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

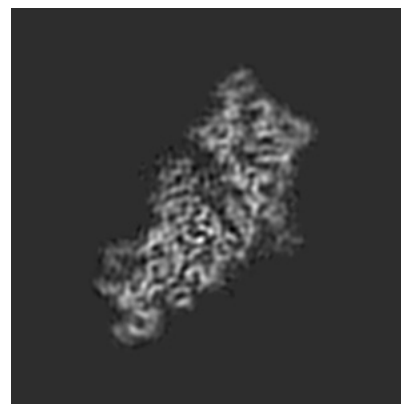
6.3.1 Primary map



X Index: 110



Y Index: 84

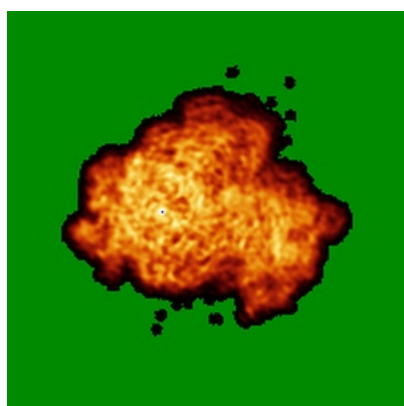


Z Index: 103

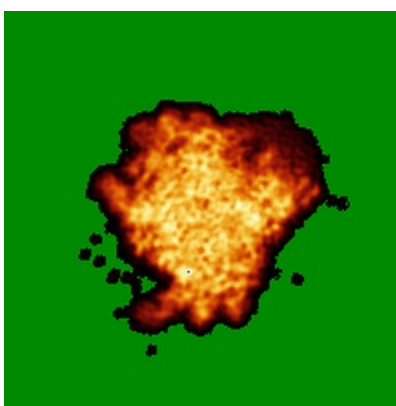
The images above show the largest variance slices of the map in three orthogonal directions.

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

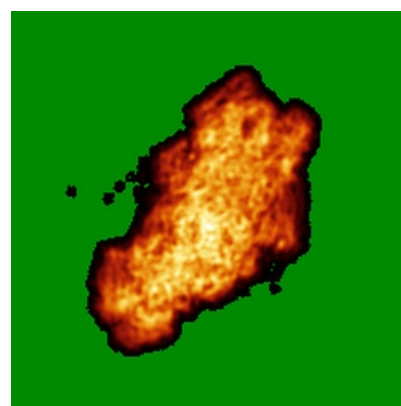
6.4.1 Primary map



X



Y



Z

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 0.0309. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

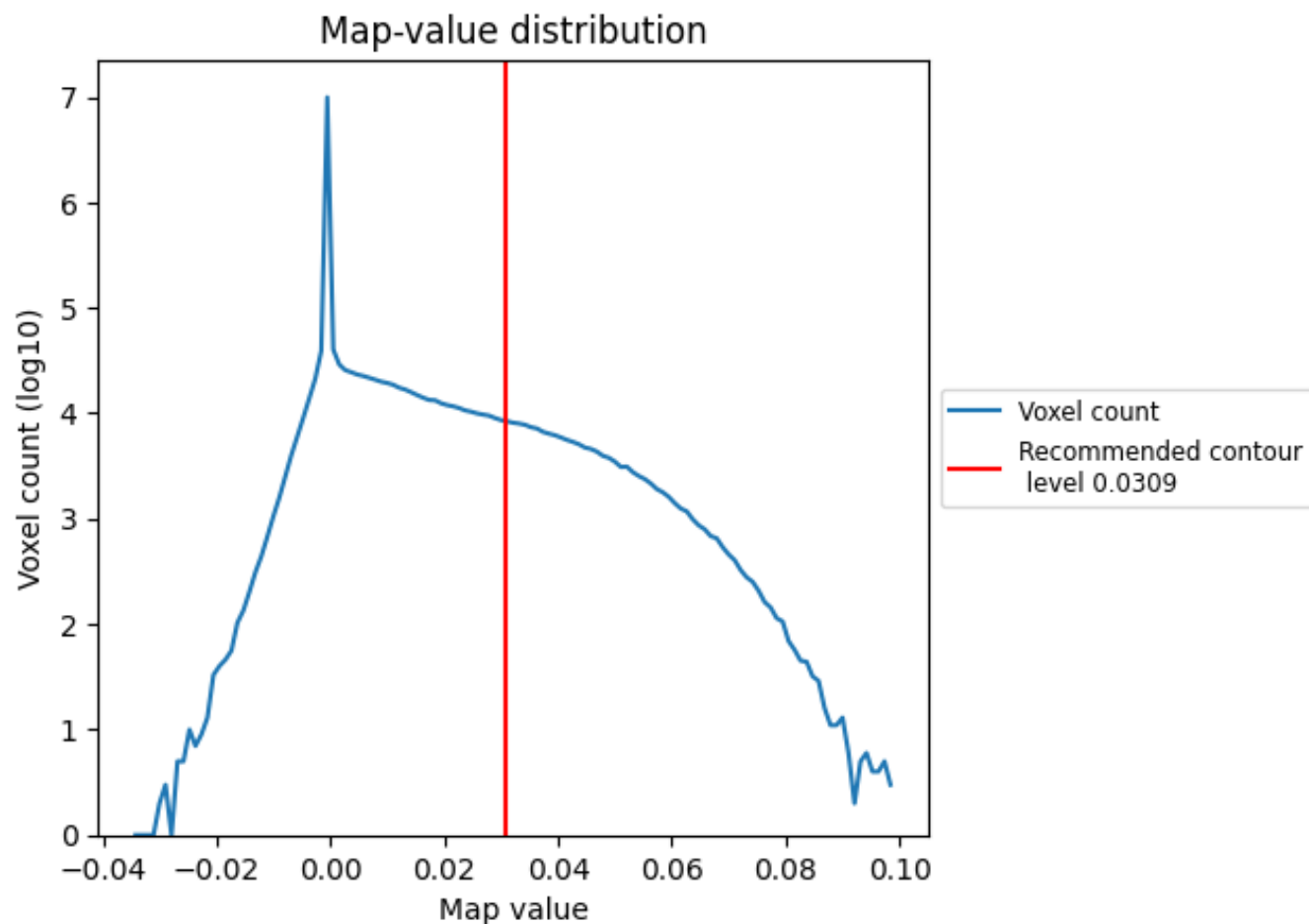
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

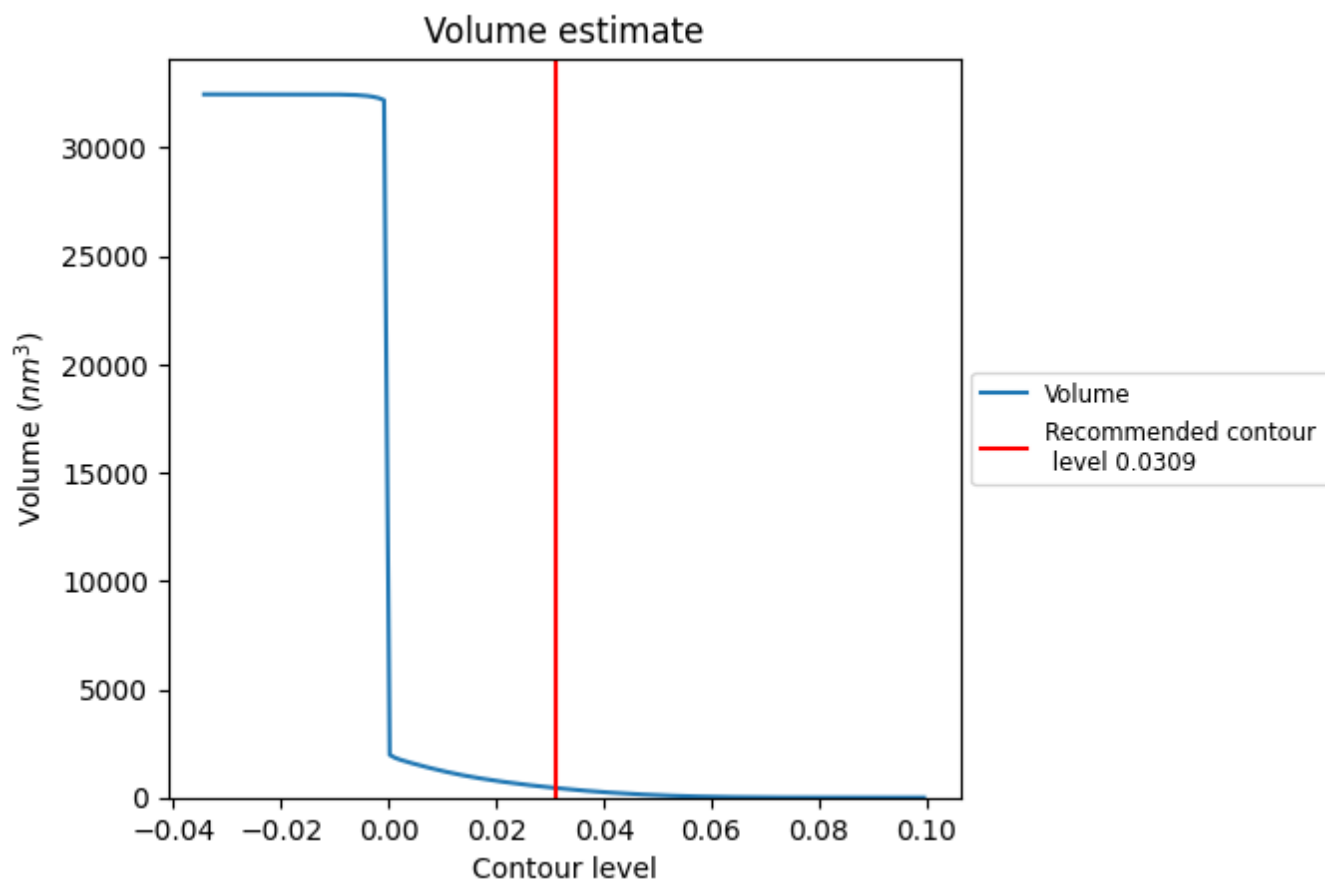
This section contains the results of statistical analysis of the map.

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.

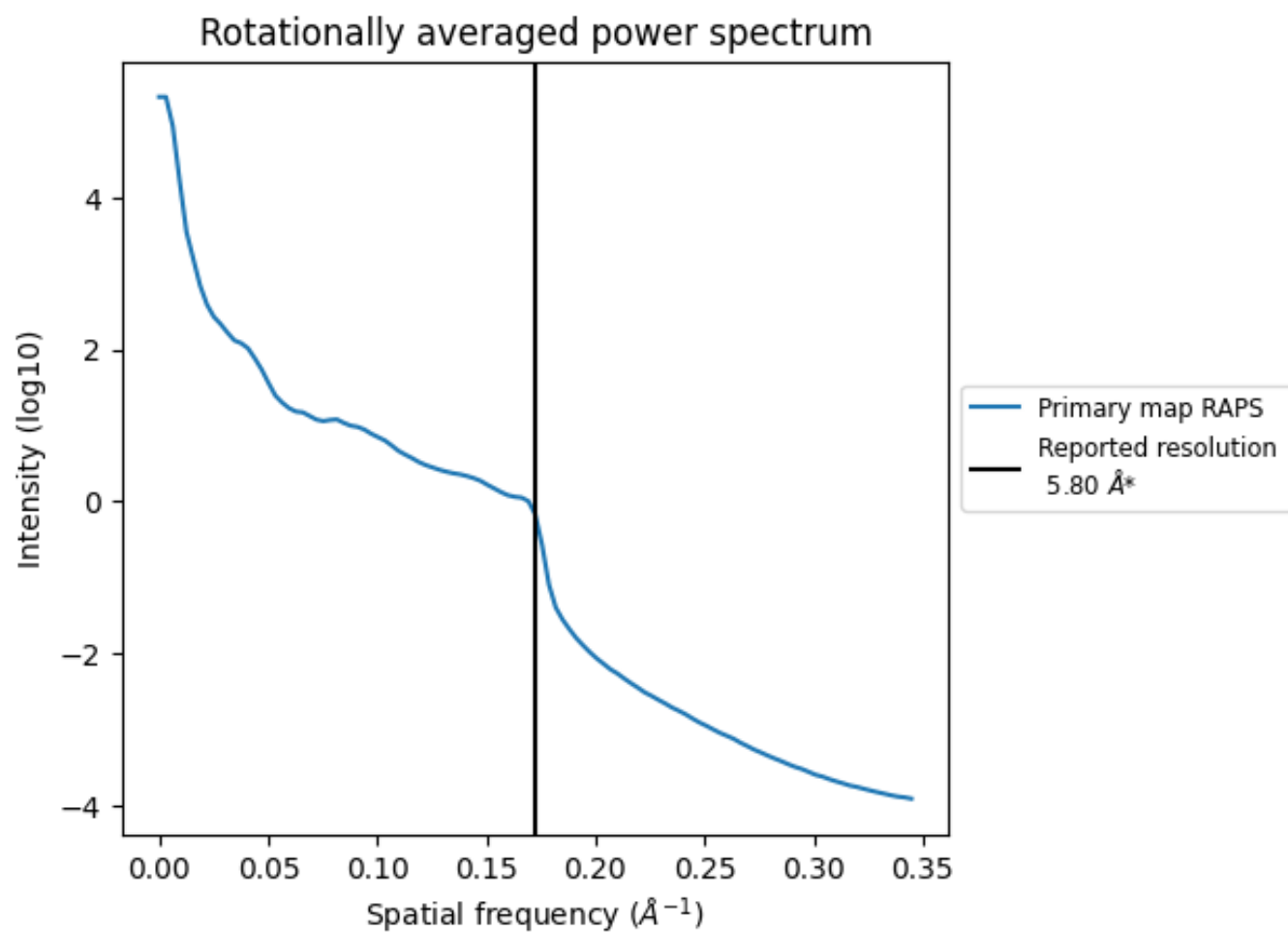
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 446 nm³; this corresponds to an approximate mass of 403 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 ⓘ

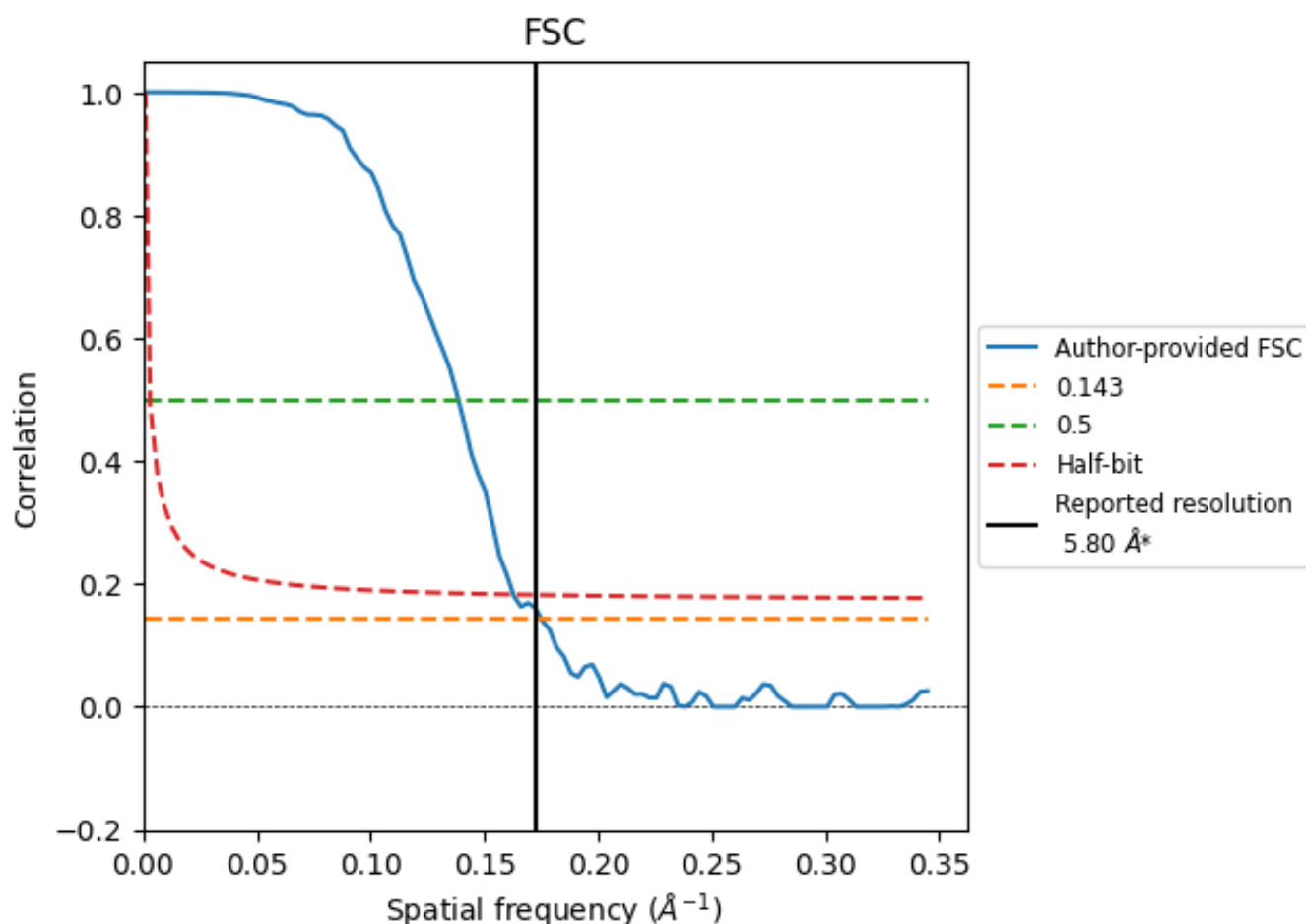


*Reported resolution corresponds to spatial frequency of 0.172 Å⁻¹

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 0.172 Å⁻¹

8.2 Resolution estimates [i](#)

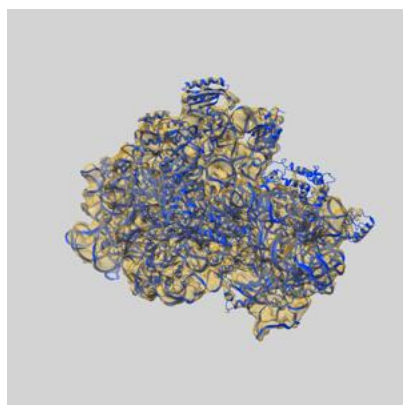
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	5.71	7.22	6.14
Unmasked-calculated*	-	-	-

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

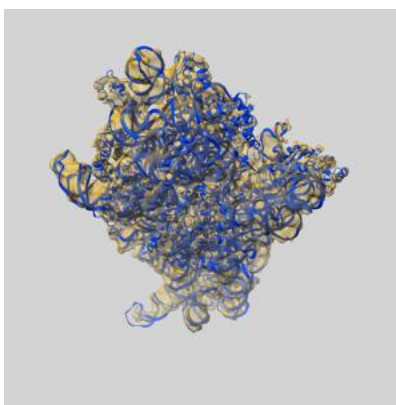
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8621 and PDB model 5UZ4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

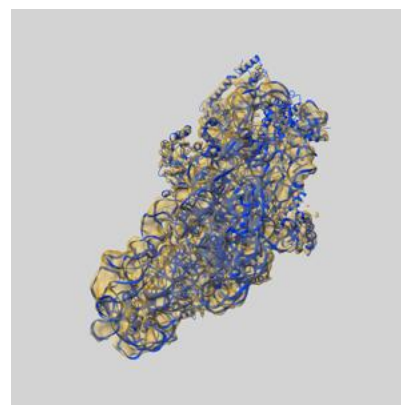
9.1 Map-model overlay [i](#)



X



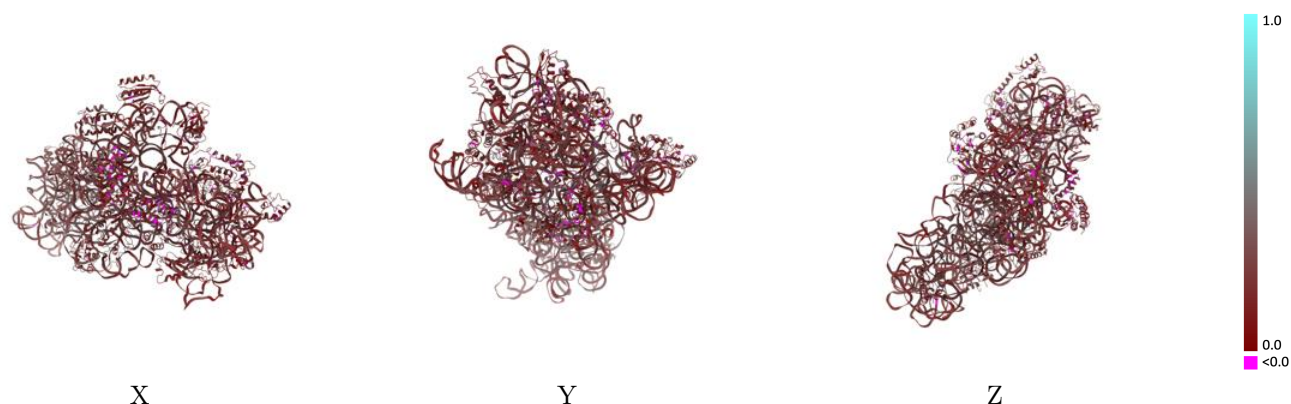
Y



Z

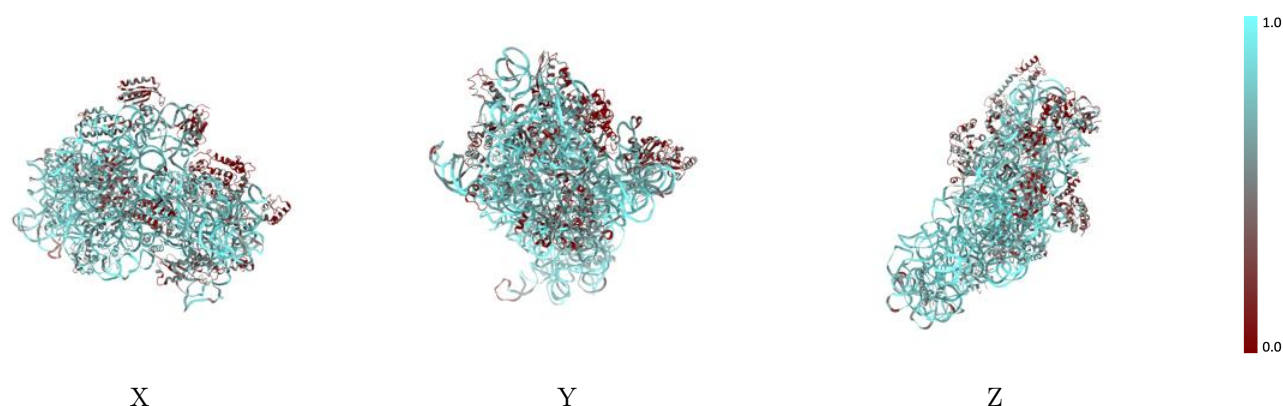
The images above show the 3D surface view of the map at the recommended contour level 0.0309 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



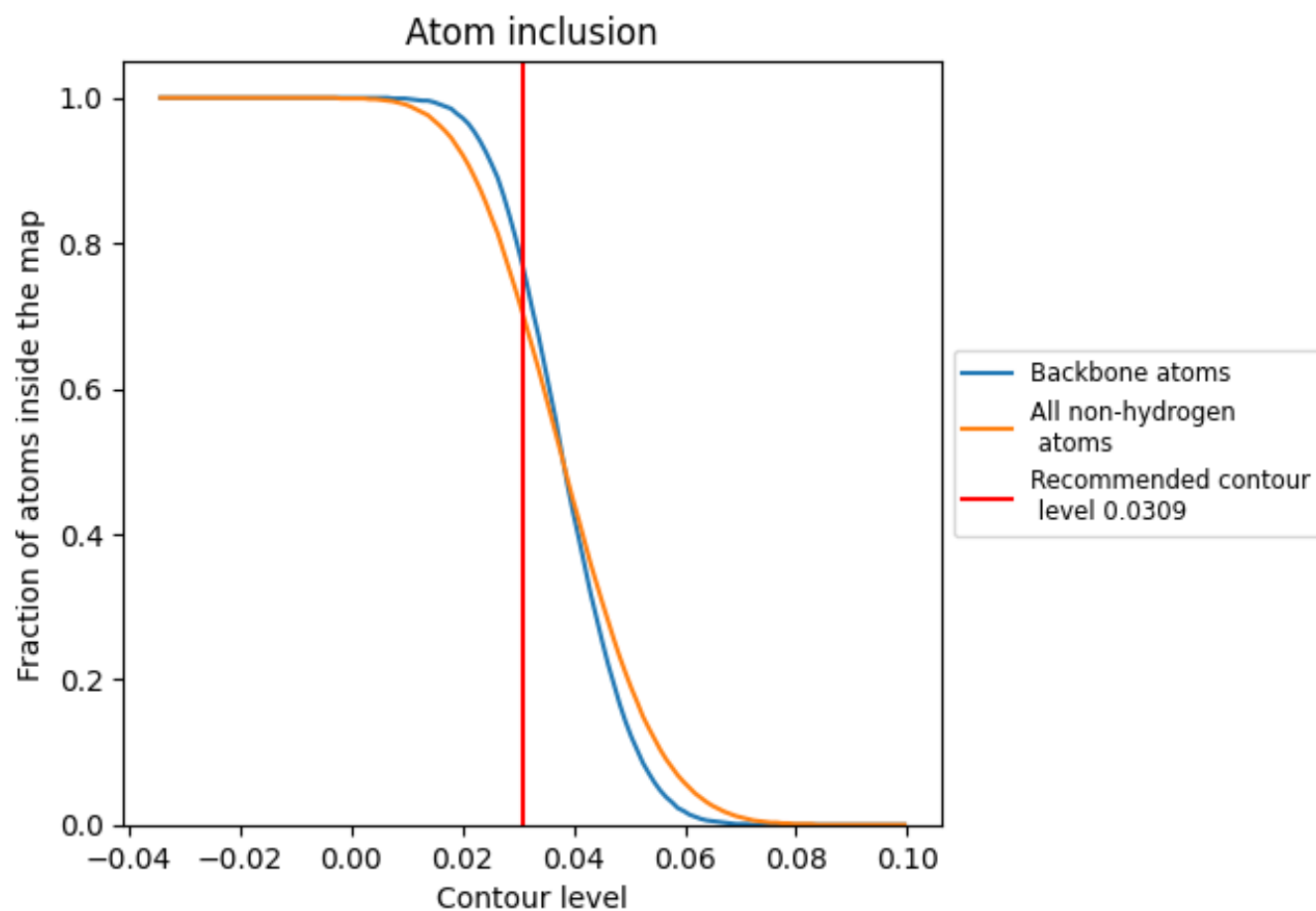
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0309).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.0309) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7020	 0.2320
A	 0.8420	 0.2390
B	 0.3460	 0.1380
C	 0.5470	 0.2460
D	 0.6270	 0.2430
E	 0.6630	 0.2670
F	 0.3200	 0.2100
G	 0.1600	 0.2100
H	 0.6410	 0.2650
I	 0.4560	 0.2130
J	 0.4070	 0.2360
K	 0.3230	 0.2140
L	 0.6850	 0.2930
M	 0.3640	 0.2070
N	 0.5180	 0.1930
O	 0.5520	 0.2220
P	 0.6680	 0.2600
Q	 0.6360	 0.2610
R	 0.4160	 0.1950
S	 0.4930	 0.2000
T	 0.6310	 0.2190
Z	 0.3290	 0.1930

