



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 05:40 am BST

PDB ID : 6SW9
EMDB ID : EMD-10320
Title : IC2A model of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in *P. abyssi*
Authors : Coureux, P.-D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2019-09-20
Resolution : 4.20 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

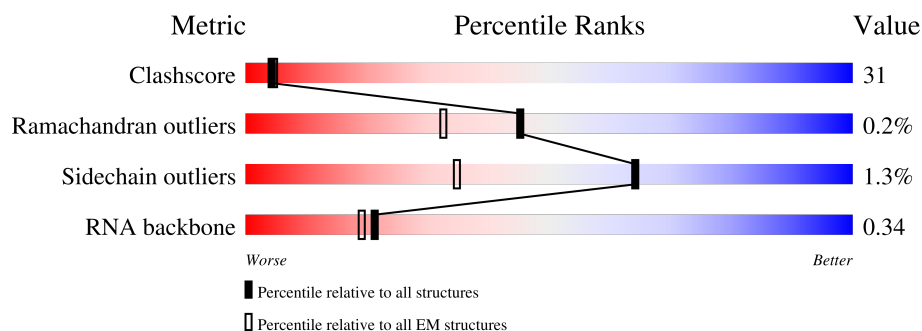
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.











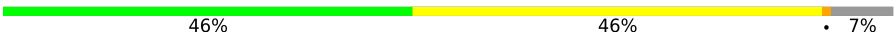
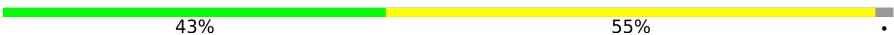



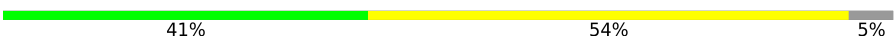











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1497	
2	A	199	
3	B	202	
4	C	63	
5	D	180	
6	E	243	
7	F	236	




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Mol	Chain	Length	Quality of chain
8	G	125	
9	H	215	
10	I	130	
11	J	127	
12	K	135	
13	L	102	
14	M	137	
15	N	147	
16	O	148	
17	P	56	
18	Q	158	
19	R	113	
20	S	67	
21	T	132	
22	U	150	
23	V	99	
24	W	65	
25	X	71	
26	Y	51	
27	Z	210	
28	0	36	
29	3	123	
30	5	20	
31	4	76	
32	6	113	

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Mol	Chain	Length	Quality of chain
33	7	414	 10% 36% 63%
34	8	129	 71% 65% 33%
35	9	254	 72% 66% 33%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70661 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	2	1497	Total	C	N	O	P	0	0
			32291	14394	5959	10441	1497		

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	188	Total	C	N	O	S	0	0
			1533	995	268	266	4		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	61	Total	C	N	O	S	0	0
			482	304	85	85	8		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	175	Total	C	N	O	S	0	0
			1470	924	284	258	4		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	213	Total	C	N	O	S	0	0
			1720	1092	322	299	7		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	126	Total	C	N	O	S	0	0
			996	617	206	173			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	134	Total	C	N	O	S	0	0
			1065	668	206	188	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			817	507	158	148	4		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	128	Total	C	N	O	S	0	0
			964	597	192	173	2		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	138	Total	C	N	O	S	0	0
			1116	700	221	190	5		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	152	Total	C	N	O	S	0	0
			1262	804	240	214	4		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	109	Total	C	N	O	S	0	0
			900	572	174	151	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	66	Total	C	N	O	S	0	0
			558	355	106	96	1		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	125	Total	C	N	O	S	0	0
			1018	647	195	169	7		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	149	Total	C	N	O		0	0
			1223	790	221	212			

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	63	Total	C	N	O	S	0	0
			481	303	93	80	5		

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	67	Total	C	N	O		0	0
			536	327	111	98			

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	50	Total	C	N	O	S	0	0
			408	262	77	63	6		

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	197	Total	C	N	O	S	0	0
			1550	989	286	271	4		

- Molecule 28 is a protein called 50S ribosomal protein L41e.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	123	Total	C	N	O	S	0	0
			941	599	157	181	4		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 31 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms					AltConf	Trace	
31	4	76	Total	C	N	O	P	S	0	0
			1622	724	291	530	76	1		

- Molecule 32 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 33 is a protein called Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	414	Total	C	N	O	S	0	0
			3213	2058	548	595	12		

- Molecule 34 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	129	Total	C	N	O	S	0	0
			1032	659	171	192	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	?	-	GLU	deletion	UNP Q97W59
8	?	-	LYS	deletion	UNP Q97W59
8	?	-	GLY	deletion	UNP Q97W59
8	?	-	ARG	deletion	UNP Q97W59
8	?	-	LYS	deletion	UNP Q97W59
8	?	-	GLU	deletion	UNP Q97W59
8	?	-	GLY	deletion	UNP Q97W59
8	?	-	THR	deletion	UNP Q97W59

- Molecule 35 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	253	Total	C	N	O	S	0	0
			2025	1296	345	383	1		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	?	-	SER	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	TRP	deletion	UNP Q97Z79
9	?	-	VAL	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	LYS	deletion	UNP Q97Z79
9	?	-	HIS	deletion	UNP Q97Z79
9	?	-	ALA	deletion	UNP Q97Z79
9	?	-	GLU	deletion	UNP Q97Z79
9	?	-	GLU	deletion	UNP Q97Z79

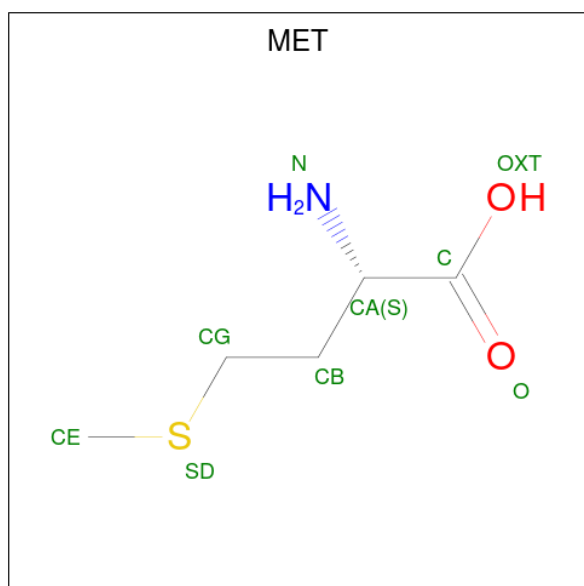
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	31	Total	Mg	0
			31	31	
36	5	1	Total	Mg	0
			1	1	
36	4	1	Total	Mg	0
			1	1	
36	7	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	C	2	Total 2	Zn 2	0
37	F	1	Total 1	Zn 1	0
37	P	1	Total 1	Zn 1	0
37	R	1	Total 1	Zn 1	0
37	W	1	Total 1	Zn 1	0

- Molecule 38 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
38	7	1	Total 8	C 5	N 1	O 1	S 1	0

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	N	O	P	0
			32	10	6	13	3	


- Molecule 40 is water.

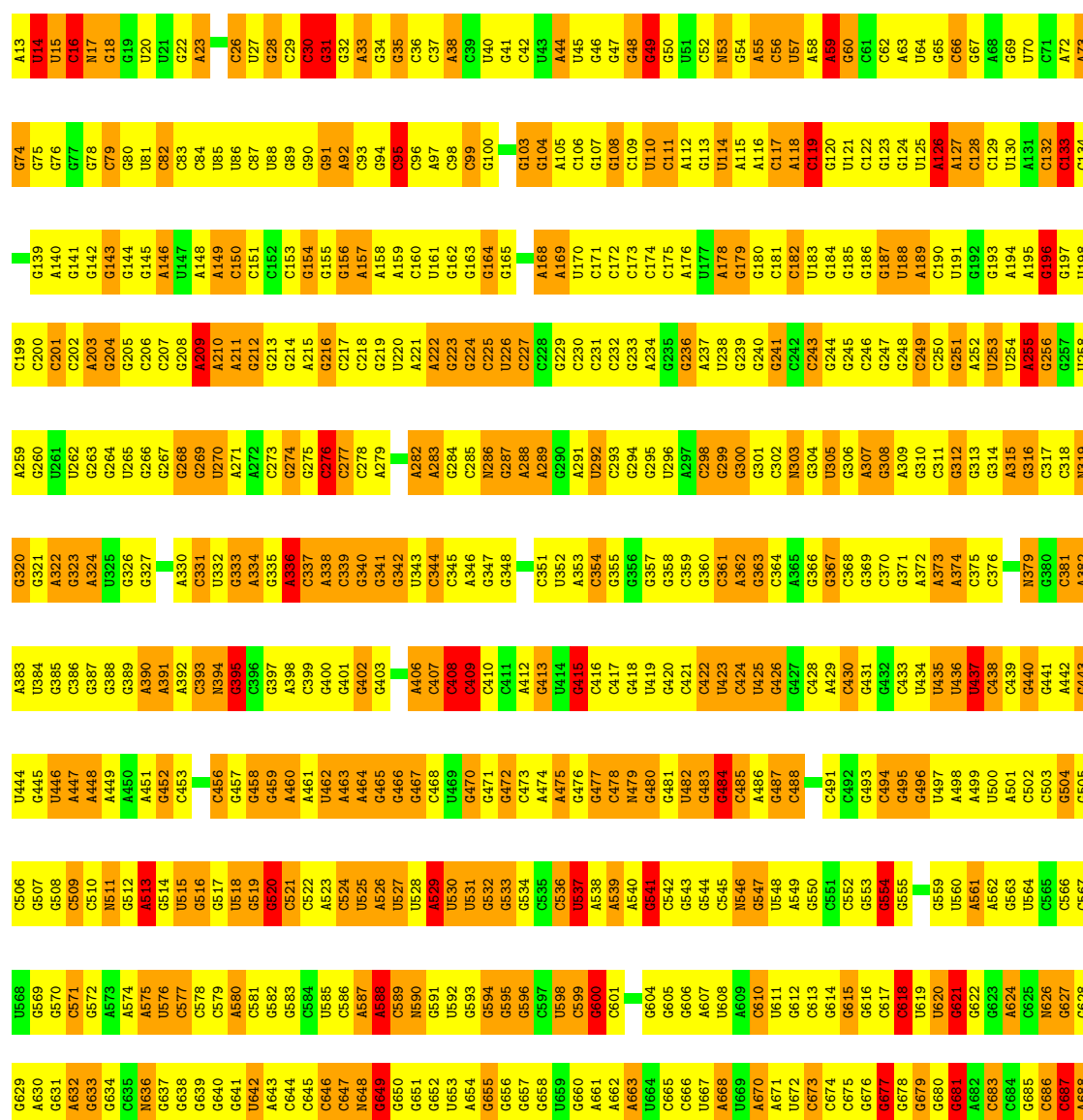
Mol	Chain	Residues	Atoms		AltConf
40	2	40	Total	O	0
			40	40	
40	K	1	Total	O	0
			1	1	
40	Q	1	Total	O	0
			1	1	

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

Chain 2: 

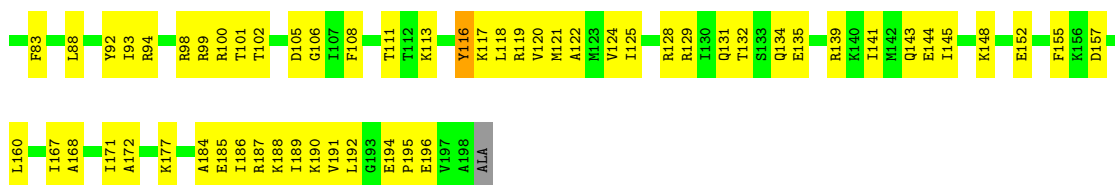


G1480	U1420	C1360	C1299	C1237	U1173	G1113	C1052	U992	U932	G869	C809	A749	G689
U1481	U1421	U1361	G1300	C1238	C1174	G1114	A1053	C993	U933	A871	U810	C750	U690
C1422	C1422	C1362	G1301	C1239	A1175	G1115	C1054	U994	G934	C870	U811	N751	G691
G1483	G1423	C1363	C1302	G1240	G1176	G1116	U1055	U995	G935	A872	C812	G752	G692
U1484	G1424	U1364	G1303	A1241	U1177	G1117	U1056	G996	A936	G873	G813	G753	C693
G1485	G1425	U1365	U1304	A1242	A1178	G1118	A1057	C997	U937	C874	A814	A754	G694
U1486	U1426	G1366	G1305	A1243	U1179	G1119	A1058	C998	U938	C875	G815	U755	A695
G1487	G1427	C1367	A1306	G1244	G1180	A1120	G1059	G999	C939	U876	C816	U756	A696
U1488	G1428	A1368	A1307	G1245	C1181	C1121	U1060	G1000	A940	G877	U817	A757	G697
C1489	U1429	C1369	G1308	G1246	C1182	U1122	G1061	A1001	A941	A878	C818	A758	G698
U1490	C1430	A1370	C1309	G1247	C1183	C1123	U1062	C1002	C942	A879	G819	A759	C699
U1491	G1431	C1371	U1310	G1248	C1184	U1124	G1063	G1003	C943	A880	C820	U760	G701
A1492	G1432	A1372	G1311	A1249	G1185	U1125	G1064	C1004	C944	C881	C821	A761	C701
C1493	C1433	C1373	A1312	G1250	G1186	G1126	U1065	G1005	C945	U882	C822	C762	C702
G1494	U1434	C1374	A1313	G1251	A1187	G1127	A1066	C1006	G946	U883	G823	C763	N703
G1495	C1435	G1375	C1314	U1252	A1188	G1128	A1067	C1007	G947	A884	G824	C764	G704
C1496	G1436	C1376	C1315	A1253	C1189	G1129	C1068	C1008	G948	A885	U825	G765	G705
U1497	A1437	C1377	C1317	A1254	C1190	G1130	G1069	A1009	A949	A886	G826	G766	C706
C1498	G1438	59H1378	C1318	C1257	C1191	A1131	A1070	G1010	A950	G887	C827	G767	U707
G1499	C1439	C1379	U1319	C1257	C1192	C1132	G1071	A1011	C951	G888	N828	U768	U708
A1500	U1440	C1380	A1320	C1257	N1193	U1133	C1072	G1012	C952	U891	G829	A769	G709
U1501	U1441	C1381	G1321	G1194	G1194	U1134	G1073	G1013	U953	U892	U830	G770	A710
C1502	A1442	A1382	U1322	A1261	G1195	C1135	A1074	G1014	C954	U893	A831	U771	A711
G1443	G1443	C1383	A1323	A1262	G1196	C1136	C1077	G1015	A955	G893	G832	C772	C712
U1504	G1444	U1384	C1324	A1263	C1197	G1137	C1078	G1016	C956	G894	G833	C773	G713
C1505	U1445	C1385	C1325	C1264	U1198	G1138	C1079	U1017	N957	C995	G834	U774	G714
U1506	U1446	C1386	C1326	C1265	A1199	C1139	C1079	G1018	G958	G896	A835	G775	G715
C1507	C1447	A1387	G1327	C1266	C1200	G1140	G1080	C1019	G959	G897	A836	G776	U716
C1448	C1448	C1388	C1328	G1267	A1201	A1141	C1081	A1020	G960	G898	G837	C777	C717
G1449	G1449	C1389	G1329	C1268	C1202	U1142	G1082	U1021	G961	G899	C838	U778	N718
U1450	C1390	C1390	C1330	C1269	G1203	A1143	C1083	G1022	G962	G900	N839	G779	G719
G1451	C1391	A1391	G1331	C1270	C1270	C1204	C1084	G1023	C963	A901	G840	U780	A720
A1452	A1392	A1392	U1332	U1271	G1205	G1145	C1085	C1024	G964	G902	U841	A781	G721
G1453	C1393	C1393	C1333	C1272	C1206	C1146	C1086	C1025	A965	C903	U842	A782	G722
U1454	C1394	A1394	A1334	A1273	G1207	N1147	C1087	G1026	C966	A904	A843	A783	G723
G1455	G1395	G1395	U1335	G1274	C1208	G1148	A1088	C1027	G967	C905	A844	G784	G724
G1456	C1396	G1396	C1336	C1275	U1209	G1149	G1089	G1028	G968	U906	G845	G785	U725
C1457	C1397	A1397	A1337	C1276	A1210	A1150	U1090	G1029	C969	A907	C846	A786	G726
G1458	C1398	C1398	U1338	C1277	C1211	G1151	U1091	U1030	A970	C908	C947	U787	A727
A1459	C1399	C1399	C1339	G1278	A1212	G1152	G1092	C1031	G971	A909	N848	G788	G728
U1460	C1400	C1400	G1340	C1279	A1213	A1153	C1093	A1032	G972	A910	G849	C789	G729
U1461	U1401	U1401	C1341	A1280	U1214	A1154	C1094	G1033	A973	C911	C850	G790	C730
A1462	A1402	G1402	G1342	U1281	G1215	G1155	A1095	C1034	U974	G912	N851	G791	N731
G1463	G1403	C1403	C1343	C1282	G1216	G1156	G1096	U1035	G975	G913	G852	G792	G732
U1464	U1404	G1404	G1344	G1283	G1217	G1157	U1097	C1036	A976	G914	C853	C793	G733
C1465	A1405	U1405	G1345	C1284	C1218	G1158	C1098	G1037	A977	U915	C854	U794	A734
G1466	G1406	G1406	C1346	G1285	G1219	C1159	C1099	U1038	G978	G916	U855	A795	G735
U1467	A1407	C1407	G1347	C1286	G1220	G1160	C1100	A1039	G979	C917	G856	G796	G736
A1468	G1408	A1408	A1348	G1287	G1221	G1161	U1101	C1040	C980	A918	G857	G797	C737
U1469	G1409	A1409	A1349	C1288	G1162	C1163	C1102	N1041	C981	G919	G858	U798	C738
C1470	C1410	C1410	U1350	C1289	G1163	C1103	G1103	G1042	A982	G923	G859	G799	A739
A1471	C1411	C1411	A1351	G1290	G1164	G1104	U1043	U1043	G983	C924	A860	U800	G740
U1472	C1412	C1412	C1352	C1291	A1165	G1105	G1044	G1044	G984	C924	G861	C801	G741
G1473	G1413	G1413	G1353	A1292	C1166	C1106	A1045	A1045	C985	G925	U862	G802	G742
U1474	A1414	A1414	U1354	C1293	G1167	U1107	G1046	U986	U986	G926	A863	G803	G743
U1475	U1415	U1415	C1355	A1294	G1168	C1108	G1047	C1048	A988	G927	G864	G804	A744
A1476	C1416	C1416	C1356	U1295	N1233	G1109	G1109	C1048	A989	U928	G865	C805	G745
G1477	U1417	U1417	C1357	C1296	G1234	A1170	G1110	G1049	A989	G929	G866	G806	G746
C1478	C1418	C1418	U1358	G1297	A1235	G1171	G1111	G1050	G990	A930	C867	A807	G747
N1479	N1479	C1419	C1359	C1298	C1236	C1172	A1112	C1051	C991	A931	G868	A808	A748

• Molecule 2: 30S ribosomal protein S3Ae

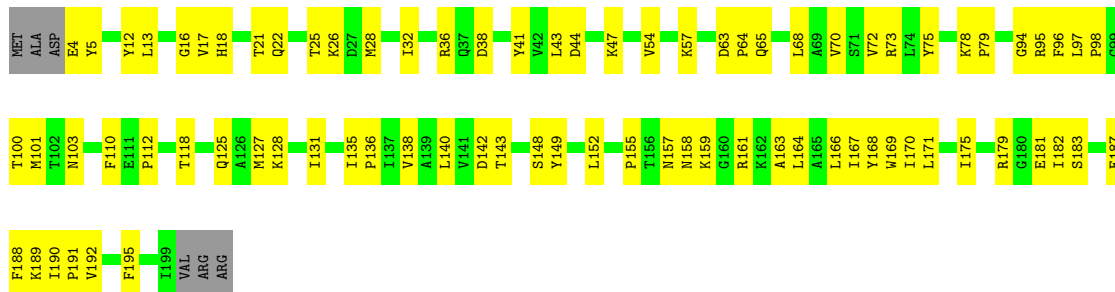
Chain A:  46% 48% 6%

MET	ALA	ALA	LYS	ARG	ARG	VAL	SER	ALA	ALA	K11	D12	K13	W14	K15	L16	K17	Q18	I22	Y23	A24	F27	V31	E32	V33	A38	D39	E42	K43	V44	L45	N46	R47	V48	V49	E50	V51	T52	L53	K54	D55	G58	D59	F60	H64	F69	Q70	Y71	Y72	D73	V74	K75
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



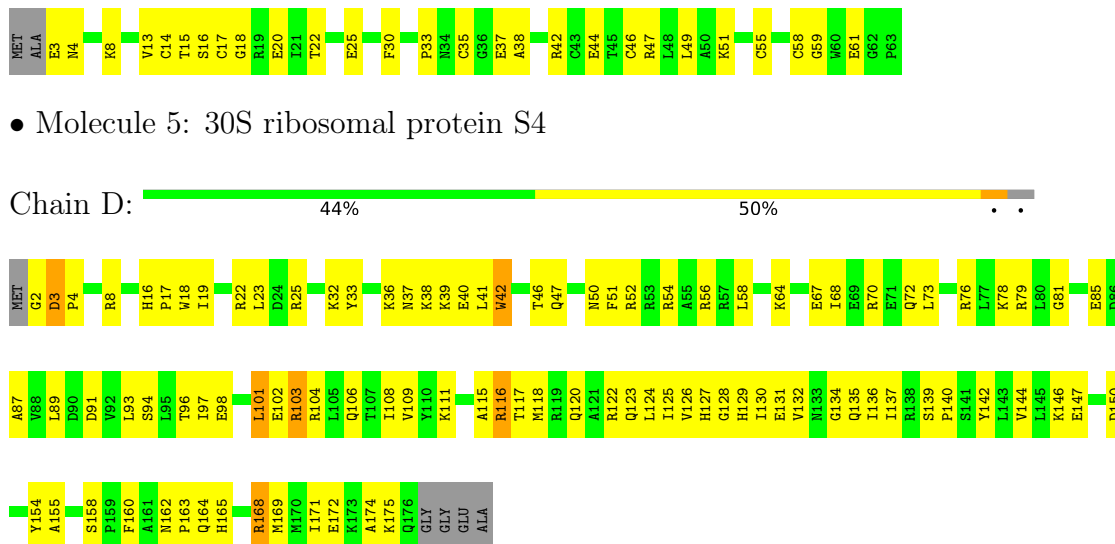
• Molecule 3: 30S ribosomal protein S2

Chain B: 57% 40%



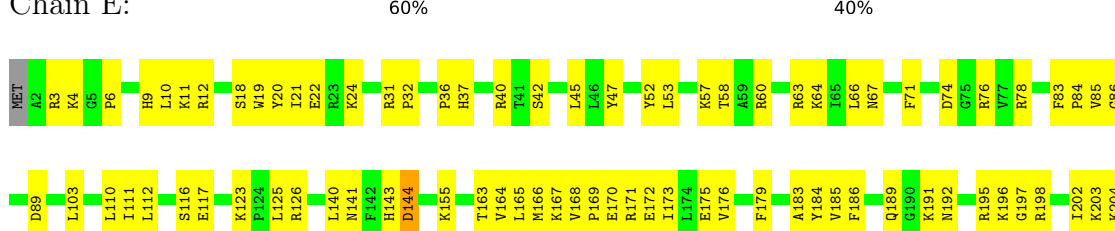
• Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C: 54% 43%



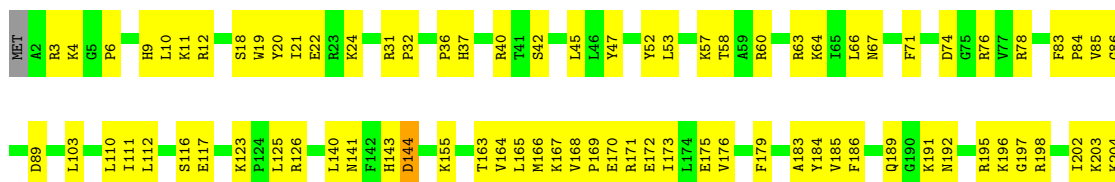
• Molecule 5: 30S ribosomal protein S4

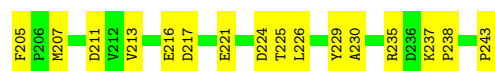
Chain D: 44% 50%



• Molecule 6: 30S ribosomal protein S4e

Chain E: 60% 40%





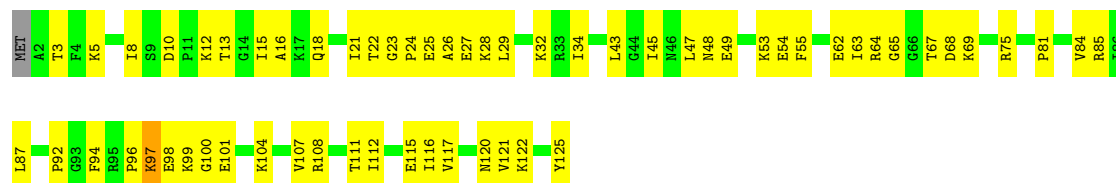
• Molecule 7: 30S ribosomal protein S5

Chain F: 53% 43% ..



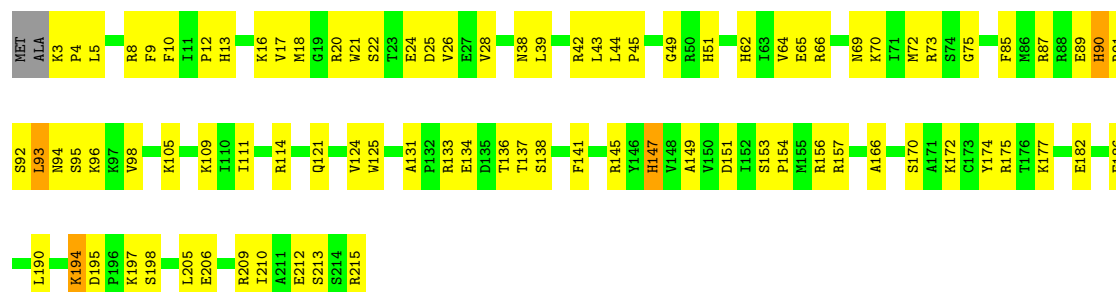
• Molecule 8: 30S ribosomal protein S6e

Chain G: 51% 47% ..



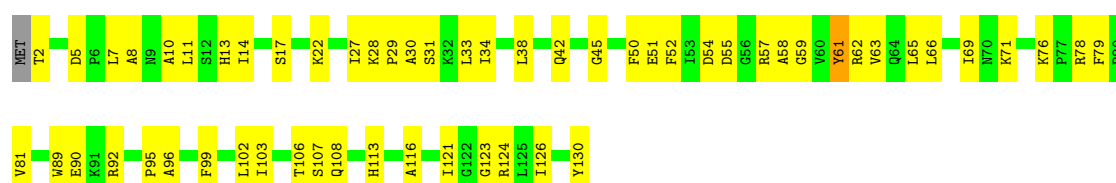
• Molecule 9: 30S ribosomal protein S7

Chain H: 58% 39% ..

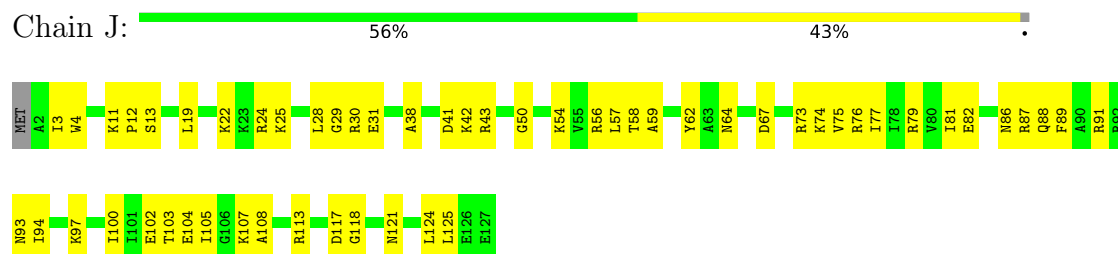


• Molecule 10: 30S ribosomal protein S8

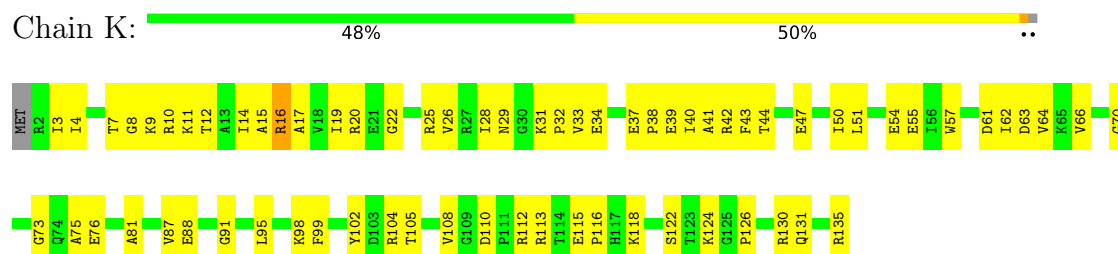
Chain I: 55% 43% ..



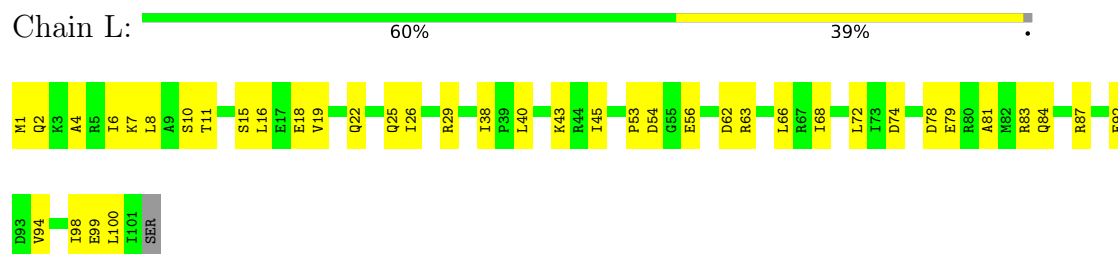
- Molecule 11: 30S ribosomal protein S8e



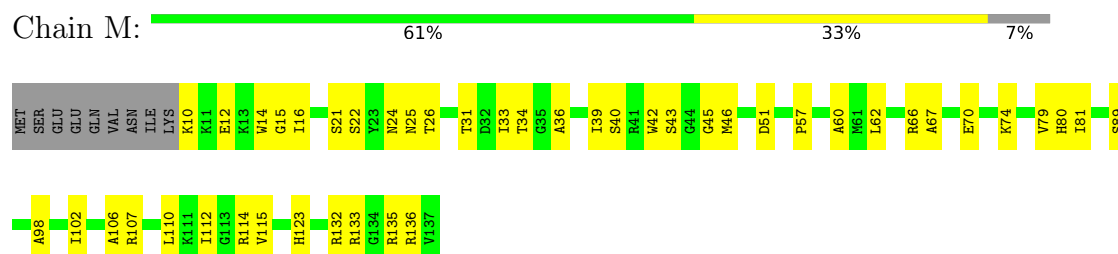
- Molecule 12: 30S ribosomal protein S9



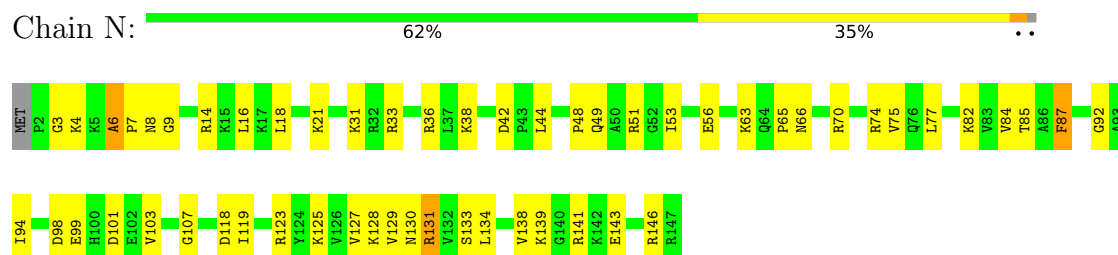
- Molecule 13: 30S ribosomal protein S10



- Molecule 14: 30S ribosomal protein S11

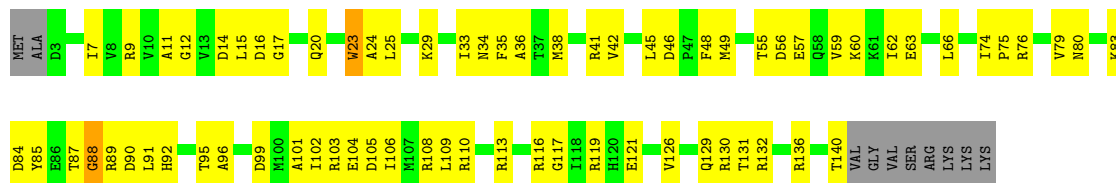


- Molecule 15: 30S ribosomal protein S12



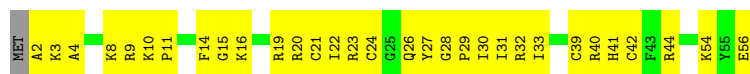
- Molecule 16: 30S ribosomal protein S13

Chain O:  46% 46% 7%



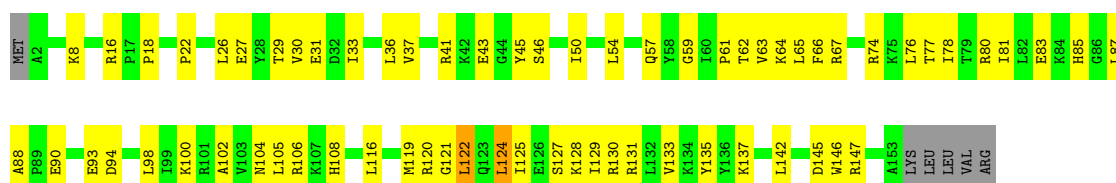
- Molecule 17: 30S ribosomal protein S14 type Z

Chain P:  43% 55%



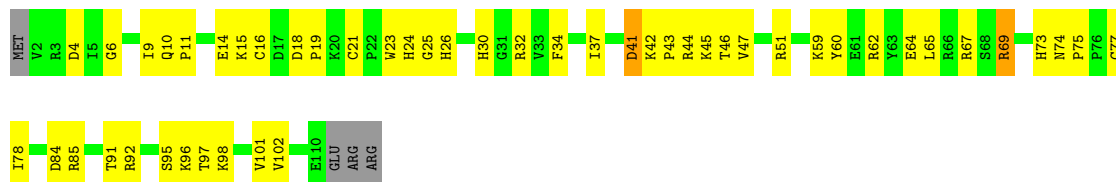
- Molecule 18: 30S ribosomal protein S15

Chain Q:  54% 41%



- Molecule 19: 30S ribosomal protein S17

Chain R:  53% 42%



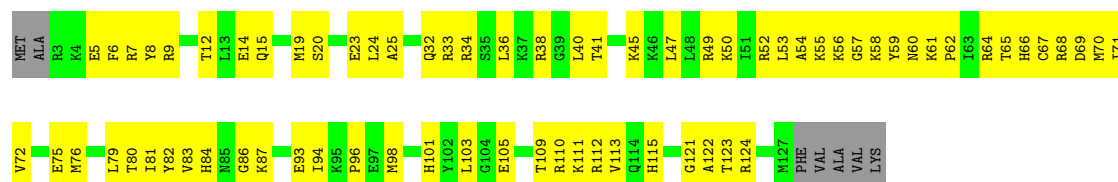
- Molecule 20: 30S ribosomal protein S17e

Chain S:  55% 43%



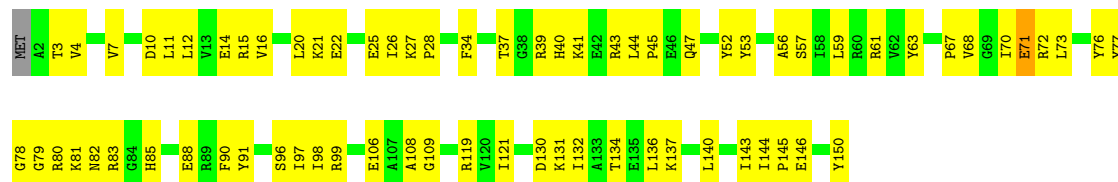
- Molecule 21: 30S ribosomal protein S19

Chain T:  41% 54% 5%



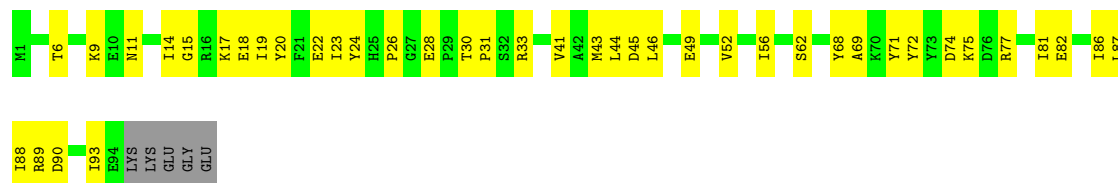
- Molecule 22: 30S ribosomal protein S19e

Chain U: 52% 47%



- Molecule 23: 30S ribosomal protein S24e

Chain V: 54% 41% 5%



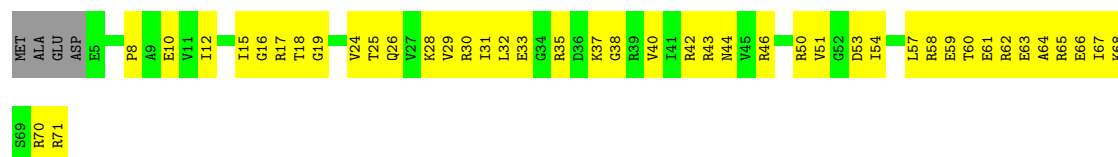
- Molecule 24: 30S ribosomal protein S27e

Chain W: 60% 37%



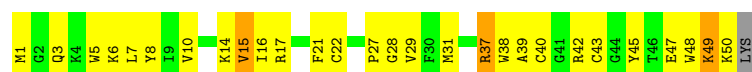
- Molecule 25: 30S ribosomal protein S28e

Chain X: 34% 61% 6%

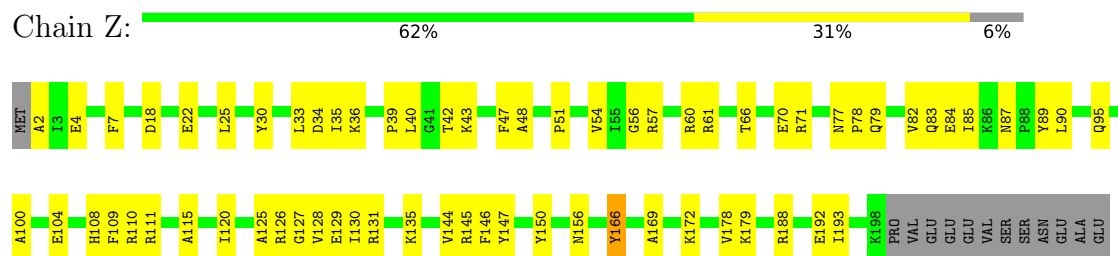


- Molecule 26: 30S ribosomal protein S27ae

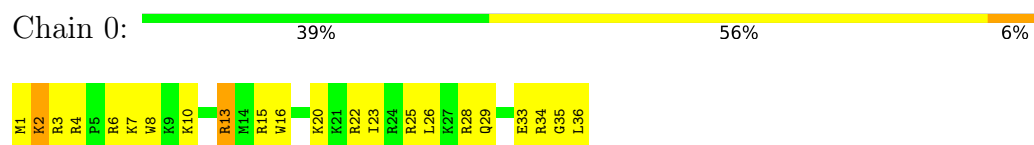
Chain Y: 43% 49% 6%



- Molecule 27: 30S ribosomal protein S3



- Molecule 28: 50S ribosomal protein L41e



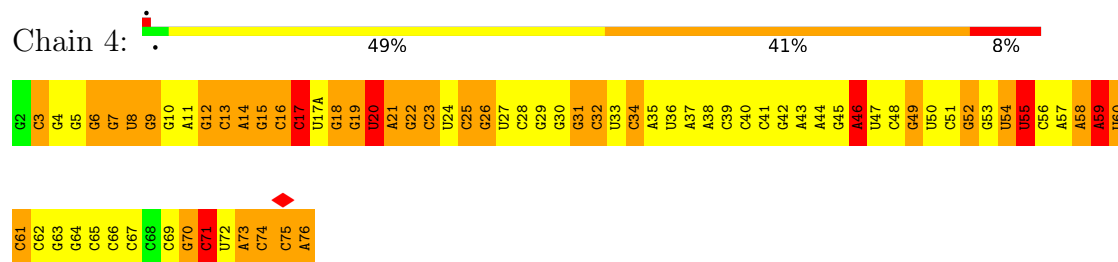
- Molecule 29: 50S ribosomal protein L7Ae



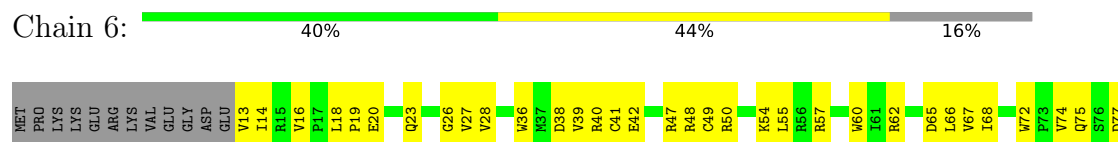
- Molecule 30: mRNA

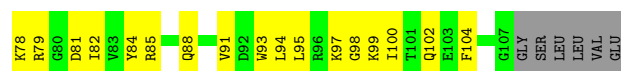


- Molecule 31: initiator Met-tRNA fMet from E. coli (A1U72 variant)

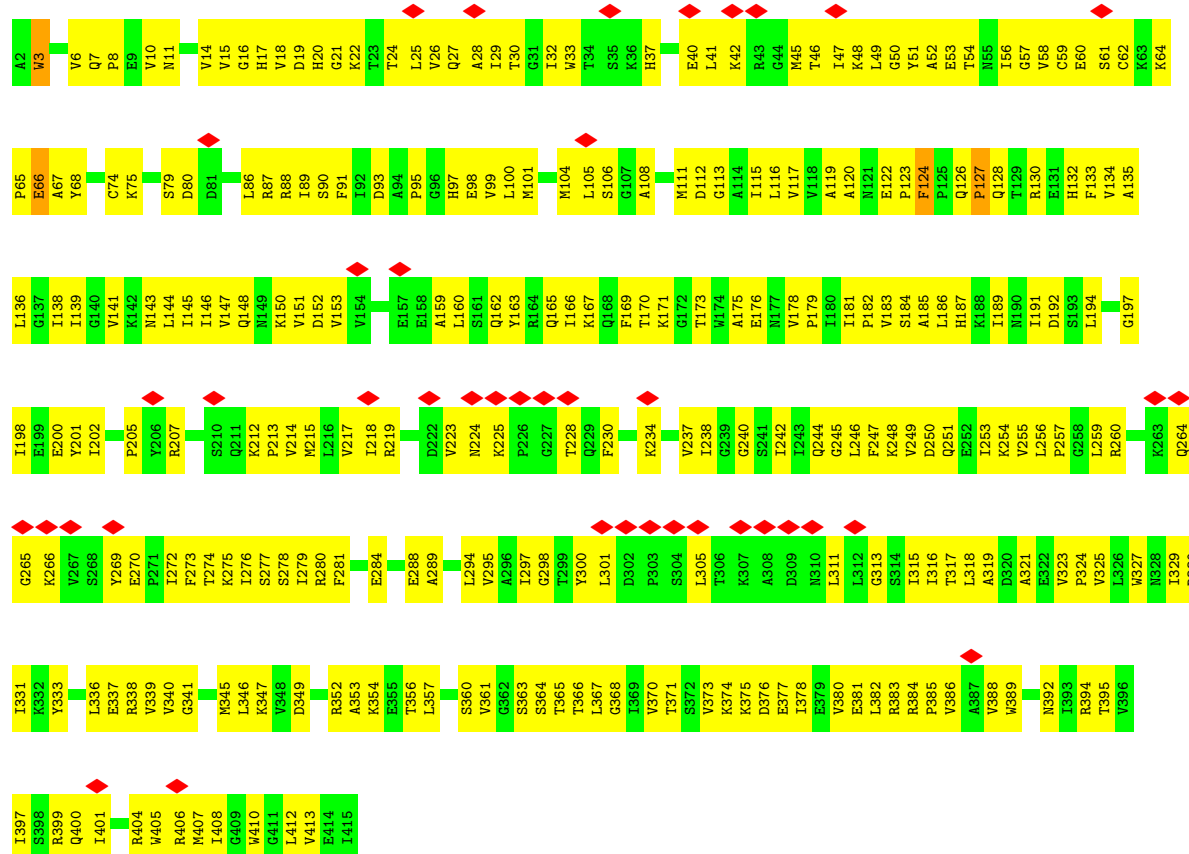


- Molecule 32: Translation initiation factor 1A

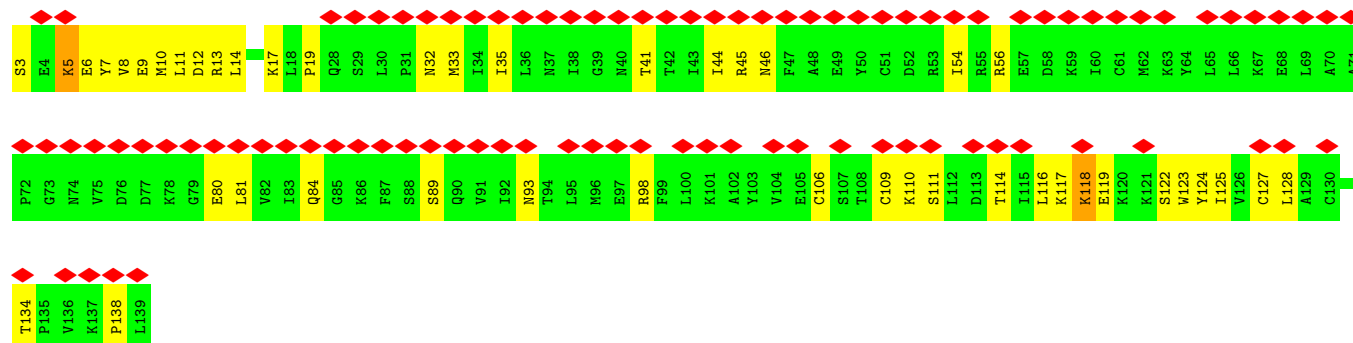




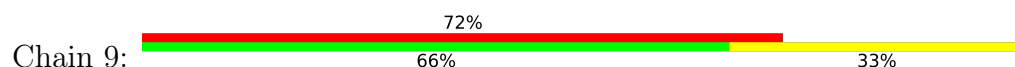
• Molecule 33: Translation initiation factor 2 subunit gamma

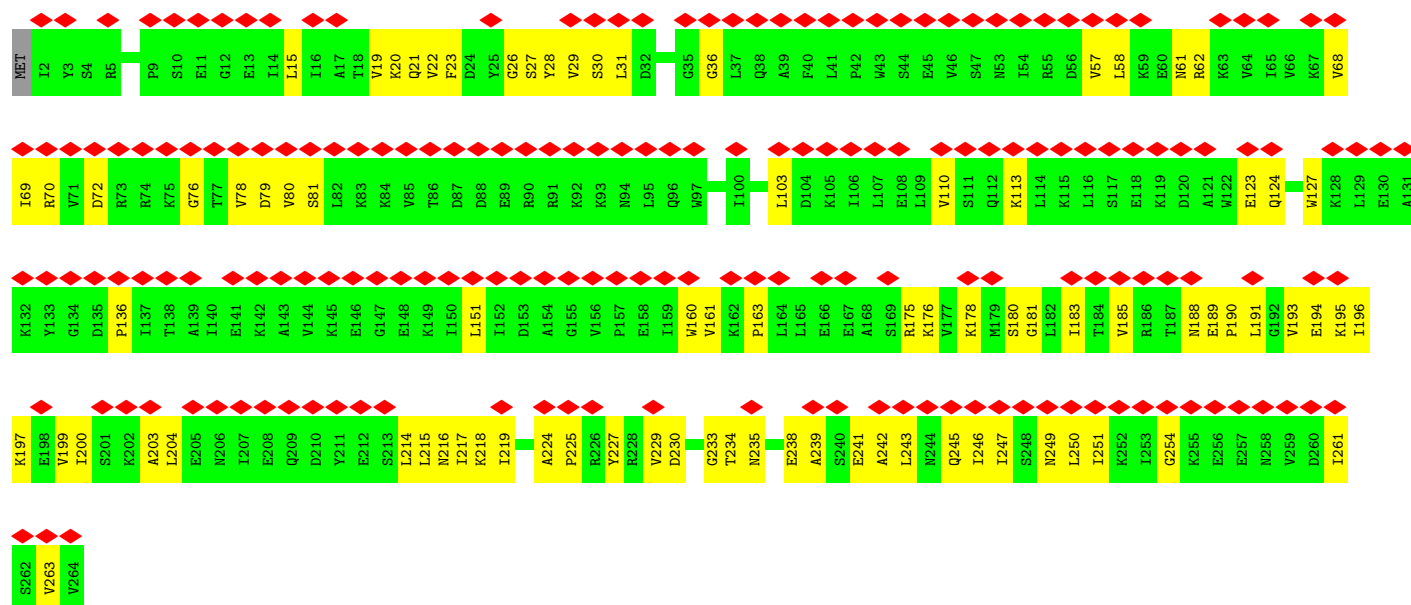


• Molecule 34: Translation initiation factor 2 subunit beta



• Molecule 35: Translation initiation factor 2 subunit alpha





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	379.32, 379.32, 379.32	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, UR3, B8H, MG, MA6, OMC, 4SU, 6MZ, 5MU, H2U, 5HM, PSU, LHH, 4AC, 5MC, ZN, GNP

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	1.32	33/35019 (0.1%)	1.41	329/54586 (0.6%)
2	A	0.61	0/1559	0.63	0/2090
3	B	0.56	0/1602	0.61	0/2165
4	C	0.57	0/496	0.60	0/673
5	D	0.63	1/1494 (0.1%)	0.64	1/2003 (0.0%)
6	E	0.62	0/2032	0.64	0/2742
7	F	0.67	0/1838	0.65	0/2478
8	G	0.46	0/993	0.56	0/1329
9	H	0.52	1/1757 (0.1%)	0.61	1/2359 (0.0%)
10	I	0.69	0/1055	0.72	0/1415
11	J	0.51	0/1005	0.65	0/1339
12	K	0.52	0/1081	0.61	0/1449
13	L	0.45	0/825	0.56	0/1107
14	M	0.51	0/982	0.61	0/1322
15	N	0.62	0/1165	0.67	1/1547 (0.1%)
16	O	0.52	1/1135 (0.1%)	0.60	0/1526
17	P	0.55	0/465	0.58	0/613
18	Q	0.54	0/1290	0.61	1/1734 (0.1%)
19	R	0.68	1/923 (0.1%)	0.64	0/1247
20	S	0.51	0/565	0.56	0/747
21	T	0.50	0/1037	0.63	0/1385
22	U	0.55	0/1253	0.60	0/1689
23	V	0.58	0/808	0.61	0/1086
24	W	0.45	0/488	0.60	0/659
25	X	0.49	0/538	0.62	0/719
26	Y	0.40	0/420	0.63	0/559
27	Z	0.50	0/1572	0.62	0/2110
28	0	0.62	0/349	0.65	0/451
29	3	0.37	0/953	0.59	0/1284
30	5	1.02	0/481	1.29	3/748 (0.4%)
31	4	0.90	1/1699 (0.1%)	1.29	15/2648 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	6	0.43	0/793	0.68	0/1072
33	7	0.37	0/3272	0.62	1/4430 (0.0%)
34	8	0.26	0/1045	0.48	0/1400
35	9	0.26	0/2050	0.44	0/2760
All	All	1.00	38/74039 (0.1%)	1.11	352/107471 (0.3%)

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
7	F	0	1
18	Q	0	1
All	All	0	2

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1453	G	C8-N7	-8.66	1.25	1.30
19	R	41	ASP	CA-CB	-8.15	1.36	1.53
1	2	955	A	N9-C4	-7.73	1.33	1.37
1	2	795	A	N9-C4	-7.69	1.33	1.37
1	2	126	A	N9-C4	-7.46	1.33	1.37

The worst 5 of 352 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	825	U	N3-C2-O2	-9.45	115.58	122.20
1	2	26	C	C6-N1-C2	-9.44	116.52	120.30
1	2	1383	C	C2-N1-C1'	9.44	129.18	118.80
1	2	494	C	N3-C2-O2	-9.26	115.42	121.90
1	2	683	C	N3-C4-N4	8.90	124.23	118.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	F	5	TRP	Peptide
18	Q	106	ARG	Peptide

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	32291	0	16316	2022	0
2	A	1533	0	1627	96	0
3	B	1571	0	1630	68	0
4	C	482	0	461	24	0
5	D	1470	0	1542	90	0
6	E	1983	0	2060	75	0
7	F	1808	0	1879	91	0
8	G	977	0	1037	59	0
9	H	1720	0	1775	87	0
10	I	1034	0	1069	57	0
11	J	996	0	1076	53	0
12	K	1065	0	1121	73	0
13	L	817	0	871	32	0
14	M	964	0	994	43	0
15	N	1148	0	1248	43	0
16	O	1116	0	1152	72	0
17	P	455	0	475	29	0
18	Q	1262	0	1331	53	0
19	R	900	0	921	52	0
20	S	558	0	595	31	0
21	T	1018	0	1086	72	0
22	U	1223	0	1263	64	0
23	V	790	0	806	35	0
24	W	481	0	512	20	0
25	X	536	0	571	43	0
26	Y	408	0	413	33	0
27	Z	1550	0	1637	55	0
28	0	343	0	407	24	0
29	3	941	0	994	86	0
30	5	430	0	215	41	0
31	4	1622	0	830	133	0
32	6	777	0	806	52	0
33	7	3213	0	3331	336	0
34	8	1032	0	1073	39	0
35	9	2025	0	2133	76	0
36	2	31	0	0	0	0
36	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5	1	0	0	0	0
36	7	1	0	0	0	0
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	W	1	0	0	0	0
38	7	8	0	8	2	0
39	7	32	0	13	4	0
40	2	40	0	0	18	0
40	K	1	0	0	0	0
40	Q	1	0	0	1	0
All	All	70661	0	55278	3872	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 31.

The worst 5 of 3872 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)
1:2:140:A:N6	1:2:229:G:H1	1.36	1.23
33:7:213:PRO:HA	33:7:244:GLN:O	1.39	1.22
33:7:240:GLY:O	33:7:294:LEU:HA	1.57	1.04
1:2:1300:C:OP1	22:U:39:ARG:NH2	1.96	0.97
1:2:465:G:O6	1:2:512:G:N2	1.99	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	186/199 (94%)	157 (84%)	29 (16%)	0	100	100
3	B	194/202 (96%)	162 (84%)	32 (16%)	0	100	100
4	C	59/63 (94%)	43 (73%)	16 (27%)	0	100	100
5	D	173/180 (96%)	140 (81%)	32 (18%)	1 (1%)	22	59
6	E	240/243 (99%)	179 (75%)	60 (25%)	1 (0%)	30	67
7	F	227/236 (96%)	172 (76%)	55 (24%)	0	100	100
8	G	122/125 (98%)	97 (80%)	25 (20%)	0	100	100
9	H	211/215 (98%)	171 (81%)	40 (19%)	0	100	100
10	I	127/130 (98%)	96 (76%)	31 (24%)	0	100	100
11	J	124/127 (98%)	91 (73%)	33 (27%)	0	100	100
12	K	132/135 (98%)	107 (81%)	25 (19%)	0	100	100
13	L	99/102 (97%)	86 (87%)	13 (13%)	0	100	100
14	M	126/137 (92%)	105 (83%)	21 (17%)	0	100	100
15	N	144/147 (98%)	104 (72%)	39 (27%)	1 (1%)	19	56
16	O	136/148 (92%)	107 (79%)	28 (21%)	1 (1%)	19	56
17	P	53/56 (95%)	40 (76%)	13 (24%)	0	100	100
18	Q	150/158 (95%)	127 (85%)	23 (15%)	0	100	100
19	R	107/113 (95%)	80 (75%)	27 (25%)	0	100	100
20	S	64/67 (96%)	54 (84%)	10 (16%)	0	100	100
21	T	123/132 (93%)	94 (76%)	29 (24%)	0	100	100
22	U	147/150 (98%)	125 (85%)	22 (15%)	0	100	100
23	V	92/99 (93%)	69 (75%)	23 (25%)	0	100	100
24	W	61/65 (94%)	45 (74%)	16 (26%)	0	100	100
25	X	65/71 (92%)	48 (74%)	17 (26%)	0	100	100
26	Y	48/51 (94%)	28 (58%)	20 (42%)	0	100	100
27	Z	195/210 (93%)	152 (78%)	43 (22%)	0	100	100
28	0	34/36 (94%)	22 (65%)	12 (35%)	0	100	100
29	3	121/123 (98%)	96 (79%)	25 (21%)	0	100	100
32	6	93/113 (82%)	78 (84%)	15 (16%)	0	100	100
33	7	412/414 (100%)	363 (88%)	46 (11%)	3 (1%)	19	56
34	8	125/129 (97%)	113 (90%)	12 (10%)	0	100	100
35	9	247/254 (97%)	234 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4437/4630 (96%)	3585 (81%)	845 (19%)	7 (0%)	45	77

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	88	GLY
33	7	66	GLU
5	D	103	ARG
33	7	265	GLY
15	N	6	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	161/167 (96%)	159 (99%)	2 (1%)	67	78
3	B	168/173 (97%)	167 (99%)	1 (1%)	84	88
4	C	54/55 (98%)	53 (98%)	1 (2%)	52	69
5	D	158/160 (99%)	154 (98%)	4 (2%)	42	62
6	E	213/214 (100%)	212 (100%)	1 (0%)	86	90
7	F	192/198 (97%)	187 (97%)	5 (3%)	41	61
8	G	107/108 (99%)	106 (99%)	1 (1%)	75	83
9	H	183/184 (100%)	180 (98%)	3 (2%)	58	73
10	I	106/107 (99%)	105 (99%)	1 (1%)	75	83
11	J	102/103 (99%)	101 (99%)	1 (1%)	73	81
12	K	110/111 (99%)	109 (99%)	1 (1%)	75	83
13	L	90/91 (99%)	89 (99%)	1 (1%)	70	79
14	M	95/104 (91%)	95 (100%)	0	100	100
15	N	120/121 (99%)	118 (98%)	2 (2%)	56	72
16	O	115/123 (94%)	115 (100%)	0	100	100
17	P	45/46 (98%)	44 (98%)	1 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Q	137/143 (96%)	135 (98%)	2 (2%)	60	74
19	R	98/102 (96%)	97 (99%)	1 (1%)	73	81
20	S	60/61 (98%)	60 (100%)	0	100	100
21	T	109/114 (96%)	109 (100%)	0	100	100
22	U	126/127 (99%)	124 (98%)	2 (2%)	58	73
23	V	86/90 (96%)	86 (100%)	0	100	100
24	W	54/56 (96%)	54 (100%)	0	100	100
25	X	57/60 (95%)	56 (98%)	1 (2%)	54	71
26	Y	41/42 (98%)	38 (93%)	3 (7%)	11	34
27	Z	156/168 (93%)	154 (99%)	2 (1%)	65	76
28	0	34/34 (100%)	32 (94%)	2 (6%)	16	40
29	3	99/99 (100%)	97 (98%)	2 (2%)	50	68
32	6	83/99 (84%)	83 (100%)	0	100	100
33	7	356/356 (100%)	352 (99%)	4 (1%)	70	79
34	8	117/118 (99%)	113 (97%)	4 (3%)	32	53
35	9	226/228 (99%)	225 (100%)	1 (0%)	89	91
All	All	3858/3962 (97%)	3809 (99%)	49 (1%)	64	76

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	U	71	GLU
27	Z	178	VAL
22	U	85	HIS
26	Y	37	ARG
28	0	13	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	66	ASN
21	T	66	HIS
33	7	224	ASN
16	O	6	HIS
19	R	26	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1458/1497 (97%)	501 (34%)	19 (1%)
30	5	19/20 (95%)	9 (47%)	0
31	4	75/76 (98%)	32 (42%)	1 (1%)
All	All	1552/1593 (97%)	542 (34%)	20 (1%)

5 of 542 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	14	U
1	2	15	U
1	2	16	C
1	2	23	A
1	2	30	C

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1155	G
1	2	1435	C
31	4	73	A
1	2	1448	C
1	2	599	C

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

48 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
1	4AC	2	868	1	21,24,25	1.23	3 (14%)	29,34,37	1.37	4 (13%)
1	4AC	2	1479	1	21,24,25	1.10	3 (14%)	29,34,37	1.50	4 (13%)
1	LHH	2	250	1	22,25,26	2.45	8 (36%)	29,35,38	1.20	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5HM	2	1378	1	19,23,24	2.94	7 (36%)	25,33,36	0.64	0
1	MA6	2	1488	1	18,26,27	0.95	1 (5%)	19,38,41	1.18	2 (10%)
1	B8H	2	938	1	19,22,23	0.82	0	22,32,35	1.52	3 (13%)
1	4AC	2	17	1	21,24,25	1.06	2 (9%)	29,34,37	1.77	5 (17%)
1	4AC	2	479	1	21,24,25	1.13	3 (14%)	29,34,37	1.59	5 (17%)
1	4AC	2	1028	1	21,24,25	1.05	3 (14%)	29,34,37	1.62	4 (13%)
1	4AC	2	1239	1	21,24,25	1.15	2 (9%)	29,34,37	1.87	4 (13%)
1	OMC	2	1376	1	19,22,23	0.90	2 (10%)	26,31,34	0.76	0
1	4AC	2	751	1	21,24,25	1.13	3 (14%)	29,34,37	1.26	4 (13%)
1	UR3	2	1467	1	19,22,23	1.10	2 (10%)	26,32,35	1.50	5 (19%)
1	4AC	2	303	1	21,24,25	1.16	3 (14%)	29,34,37	1.44	3 (10%)
1	4AC	2	703	1	21,24,25	1.07	2 (9%)	29,34,37	1.82	6 (20%)
1	5MC	2	939	1	18,22,23	1.05	2 (11%)	26,32,35	1.25	3 (11%)
1	4AC	2	546	1	21,24,25	1.03	2 (9%)	29,34,37	1.44	3 (10%)
31	H2U	4	20	31	18,21,22	1.10	2 (11%)	21,30,33	2.24	1 (4%)
1	4AC	2	394	1	21,24,25	1.02	2 (9%)	29,34,37	1.66	5 (17%)
1	5MC	2	1202	1	18,22,23	1.00	1 (5%)	26,32,35	1.21	1 (3%)
1	4AC	2	718	1	21,24,25	1.08	2 (9%)	29,34,37	1.18	3 (10%)
1	4AC	2	731	1	21,24,25	1.16	3 (14%)	29,34,37	1.37	5 (17%)
1	4AC	2	1147	1	21,24,25	1.12	3 (14%)	29,34,37	2.24	6 (20%)
1	4AC	2	957	1	21,24,25	1.12	1 (4%)	29,34,37	2.29	7 (24%)
31	OMC	4	32	31	19,22,23	0.99	2 (10%)	26,31,34	1.13	2 (7%)
1	4AC	2	828	1	21,24,25	1.01	1 (4%)	29,34,37	1.64	4 (13%)
1	4AC	2	1233	1	21,24,25	1.09	2 (9%)	29,34,37	1.53	4 (13%)
1	4AC	2	286	1	21,24,25	1.11	2 (9%)	29,34,37	1.64	7 (24%)
1	4AC	2	636	1	21,24,25	1.12	3 (14%)	29,34,37	1.60	4 (13%)
1	4AC	2	1184	1	21,24,25	1.06	3 (14%)	29,34,37	1.39	4 (13%)
1	4AC	2	851	1	21,24,25	1.24	3 (14%)	29,34,37	1.57	4 (13%)
31	4SU	4	8	31	18,21,22	1.79	5 (27%)	26,30,33	2.15	4 (15%)
31	5MU	4	54	31	19,22,23	1.44	6 (31%)	28,32,35	2.05	8 (28%)
1	4AC	2	648	1	21,24,25	1.20	3 (14%)	29,34,37	1.85	7 (24%)
1	4AC	2	848	1	21,24,25	1.12	2 (9%)	29,34,37	1.75	4 (13%)
1	4AC	2	53	1	21,24,25	1.06	2 (9%)	29,34,37	1.48	5 (17%)
1	6MZ	2	1469	36,1	18,25,26	0.76	1 (5%)	16,36,39	2.10	3 (18%)
1	A2M	2	373	1	18,25,26	1.06	1 (5%)	18,36,39	1.39	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	2	511	1	21,24,25	1.15	3 (14%)	29,34,37	1.87	6 (20%)
1	4AC	2	590	36,1	21,24,25	1.15	3 (14%)	29,34,37	1.47	4 (13%)
1	MA6	2	1487	1	18,26,27	0.92	1 (5%)	19,38,41	1.28	3 (15%)
31	PSU	4	55	31	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
1	4AC	2	626	1	21,24,25	1.05	3 (14%)	29,34,37	1.41	4 (13%)
1	4AC	2	1041	1	21,24,25	1.01	2 (9%)	29,34,37	1.98	4 (13%)
1	4AC	2	319	1	21,24,25	1.20	3 (14%)	29,34,37	1.48	4 (13%)
1	4AC	2	379	1	21,24,25	1.08	3 (14%)	29,34,37	1.55	5 (17%)
1	4AC	2	1193	1	21,24,25	1.13	2 (9%)	29,34,37	2.00	5 (17%)
1	4AC	2	839	1	21,24,25	1.13	2 (9%)	29,34,37	1.80	6 (20%)

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
1	4AC	2	868	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	LHH	2	250	1	-	1/13/31/32	0/2/2/2
1	5HM	2	1378	1	-	2/9/27/28	0/2/2/2
1	MA6	2	1488	1	-	0/7/29/30	0/3/3/3
1	B8H	2	938	1	-	3/7/25/26	0/2/2/2
1	4AC	2	17	1	-	0/11/29/30	0/2/2/2
1	4AC	2	479	1	-	3/11/29/30	0/2/2/2
1	4AC	2	1028	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1239	1	-	2/11/29/30	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	UR3	2	1467	1	-	6/7/25/26	0/2/2/2
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	5MC	2	939	1	-	0/7/25/26	0/2/2/2
1	4AC	2	546	1	-	2/11/29/30	0/2/2/2
31	H2U	4	20	31	-	4/7/38/39	0/2/2/2
1	4AC	2	394	1	-	2/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
1	4AC	2	731	1	-	3/11/29/30	0/2/2/2
1	4AC	2	1147	1	-	2/11/29/30	0/2/2/2
1	4AC	2	957	1	-	1/11/29/30	0/2/2/2
31	OMC	4	32	31	-	2/9/27/28	0/2/2/2
1	4AC	2	828	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
1	4AC	2	286	1	-	5/11/29/30	0/2/2/2
1	4AC	2	636	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1184	1	-	2/11/29/30	0/2/2/2
1	4AC	2	851	1	-	4/11/29/30	0/2/2/2
31	4SU	4	8	31	-	5/7/25/26	0/2/2/2
31	5MU	4	54	31	-	1/7/25/26	0/2/2/2
1	4AC	2	648	1	-	2/11/29/30	0/2/2/2
1	4AC	2	848	1	-	2/11/29/30	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	6MZ	2	1469	36,1	-	0/5/27/28	0/3/3/3
1	A2M	2	373	1	-	1/5/27/28	0/3/3/3
1	4AC	2	511	1	-	2/11/29/30	0/2/2/2
1	4AC	2	590	36,1	-	2/11/29/30	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
31	PSU	4	55	31	-	0/7/25/26	0/2/2/2
1	4AC	2	626	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1041	1	-	0/11/29/30	0/2/2/2
1	4AC	2	319	1	-	4/11/29/30	0/2/2/2
1	4AC	2	379	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1193	1	-	0/11/29/30	0/2/2/2
1	4AC	2	839	1	-	1/11/29/30	0/2/2/2

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1378	5HM	C4-N3	6.29	1.44	1.34
1	2	250	LHH	C4-N4	6.05	1.48	1.39
1	2	250	LHH	C7-N4	5.67	1.47	1.37
1	2	1378	5HM	C2-N3	5.46	1.47	1.36
1	2	1378	5HM	C4-N4	5.36	1.48	1.34

The worst 5 of 193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	20	H2U	C4-N3-C2	-9.61	117.82	125.79
31	4	8	4SU	C4-N3-C2	-6.85	120.68	127.34
1	2	1469	6MZ	C2-N1-C6	6.51	122.17	116.59
1	2	1147	4AC	C5-C4-N4	-6.34	111.91	122.92
1	2	957	4AC	N4-C4-N3	6.19	124.24	113.85

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	250	LHH	C1'-C2'-O2'-C1
1	2	286	4AC	C3'-C4'-C5'-O5'
1	2	373	A2M	C1'-C2'-O2'-CM'
1	2	379	4AC	C3'-C4'-C5'-O5'
1	2	511	4AC	O4'-C4'-C5'-O5'

There are no ring outliers.

47 monomers are involved in 149 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	868	4AC	3	0
1	2	1479	4AC	5	0
1	2	1378	5HM	4	0
1	2	1488	MA6	3	0
1	2	938	B8H	1	0
1	2	17	4AC	3	0
1	2	479	4AC	4	0
1	2	1028	4AC	2	0
1	2	1239	4AC	5	0
1	2	1376	OMC	2	0
1	2	751	4AC	1	0
1	2	1467	UR3	4	0
1	2	303	4AC	3	0
1	2	703	4AC	6	0
1	2	939	5MC	1	0
1	2	546	4AC	2	0
31	4	20	H2U	1	0
1	2	394	4AC	4	0
1	2	1202	5MC	3	0
1	2	718	4AC	4	0
1	2	731	4AC	4	0
1	2	1147	4AC	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	957	4AC	4	0
31	4	32	OMC	3	0
1	2	828	4AC	3	0
1	2	1233	4AC	6	0
1	2	286	4AC	1	0
1	2	636	4AC	2	0
1	2	1184	4AC	4	0
1	2	851	4AC	6	0
31	4	8	4SU	2	0
31	4	54	5MU	3	0
1	2	648	4AC	5	0
1	2	848	4AC	2	0
1	2	53	4AC	1	0
1	2	1469	6MZ	2	0
1	2	373	A2M	7	0
1	2	511	4AC	1	0
1	2	590	4AC	2	0
1	2	1487	MA6	4	0
31	4	55	PSU	3	0
1	2	626	4AC	1	0
1	2	1041	4AC	4	0
1	2	319	4AC	3	0
1	2	379	4AC	2	0
1	2	1193	4AC	3	0
1	2	839	4AC	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 40 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
38	MET	7	501	-	6,7,8	0.50	0	2,7,9	0.39	0
39	GNP	7	502	36	29,34,34	1.58	7 (24%)	33,54,54	2.14	7 (21%)

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	MET	7	501	-	-	2/5/6/8	-
39	GNP	7	502	36	-	7/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	502	GNP	PB-O3A	4.26	1.64	1.59
39	7	502	GNP	PB-O1B	3.18	1.51	1.46
39	7	502	GNP	C6-N1	2.97	1.38	1.33
39	7	502	GNP	PG-N3B	2.80	1.70	1.63
39	7	502	GNP	PG-O1G	2.60	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	7	502	GNP	C5-C6-N1	-8.34	112.03	123.43
39	7	502	GNP	C2-N1-C6	5.83	125.19	115.93
39	7	502	GNP	PB-O3A-PA	-2.95	122.22	132.62
39	7	502	GNP	N3-C2-N1	-2.85	123.42	127.22
39	7	502	GNP	C4-C5-C6	-2.70	118.22	120.80

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

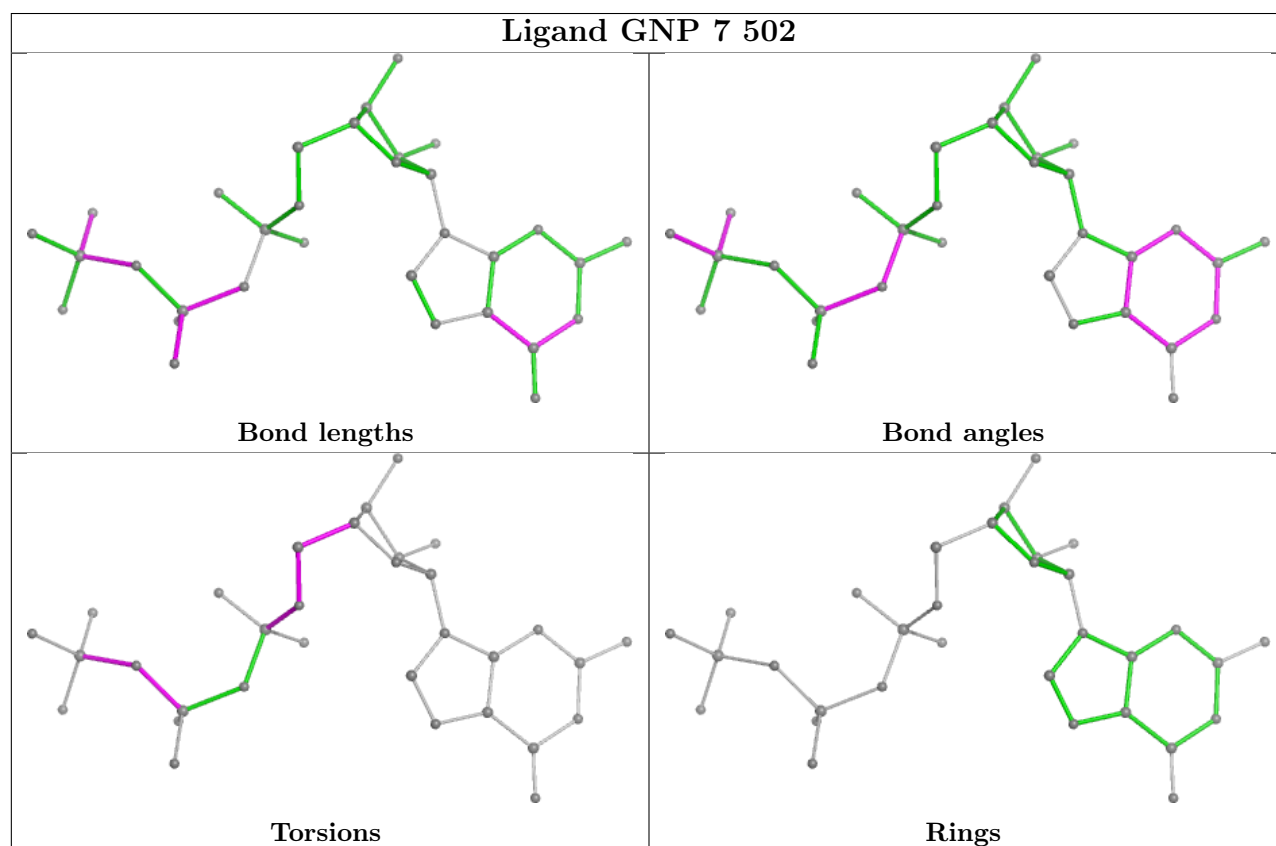
Mol	Chain	Res	Type	Atoms
39	7	502	GNP	PB-N3B-PG-O1G
39	7	502	GNP	PG-N3B-PB-O1B
39	7	502	GNP	C5'-O5'-PA-O3A
39	7	502	GNP	O4'-C4'-C5'-O5'
38	7	501	MET	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	7	501	MET	2	0
39	7	502	GNP	4	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	9	2
34	8	1
9	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	19:PRO	C	28:GLN	N	14.63
1	9	47:SER	C	53:ASN	N	11.57
1	9	169:SER	C	175:ARG	N	8.00
1	H	194:LYS	C	195:ASP	N	1.20

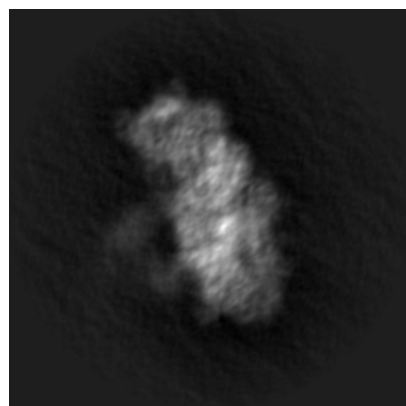
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10320. These allow visual inspection of the internal detail of the map and identification of artifacts.

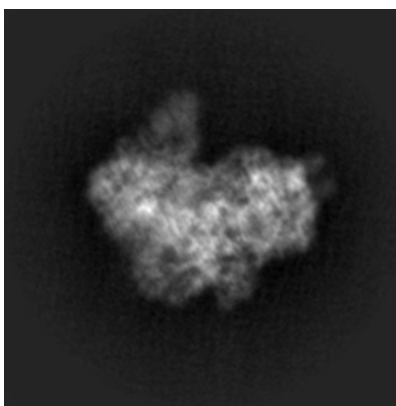
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

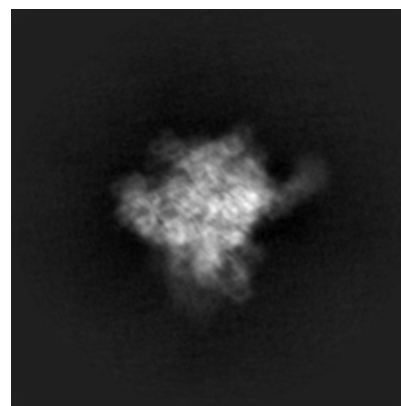
6.1.1 Primary map



X

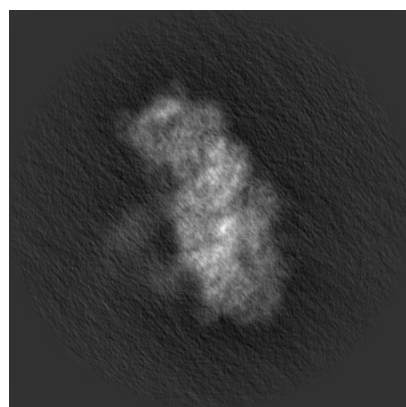


Y

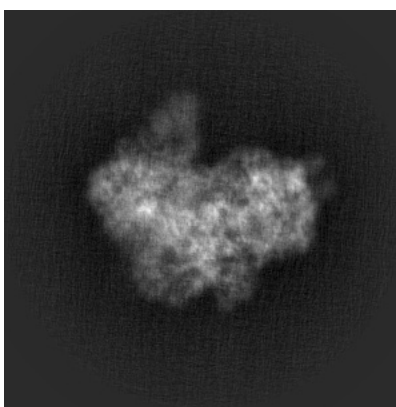


Z

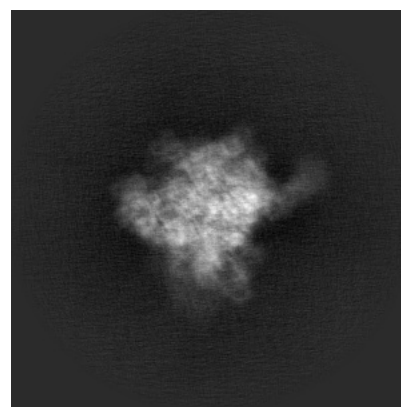
6.1.2 Raw map



X



Y

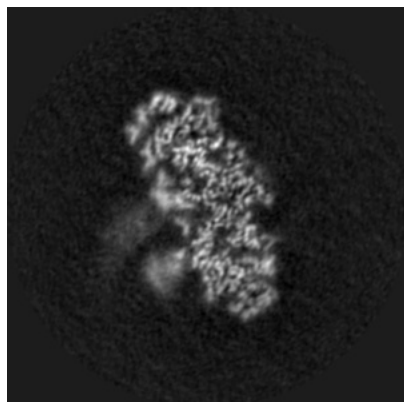


Z

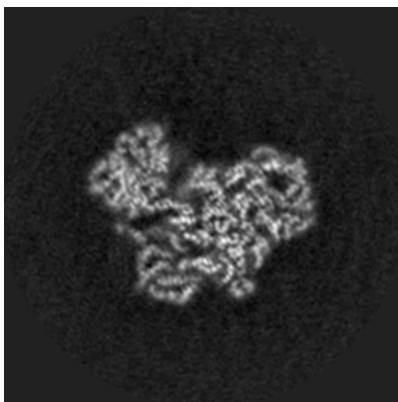
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

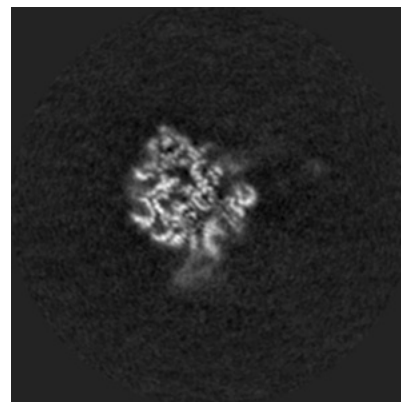
6.2.1 Primary map



X Index: 174

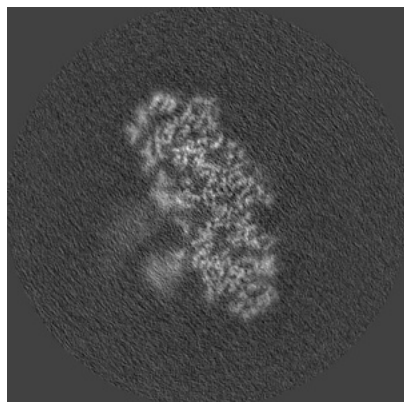


Y Index: 174

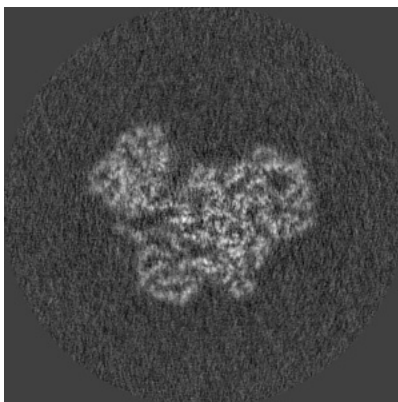


Z Index: 174

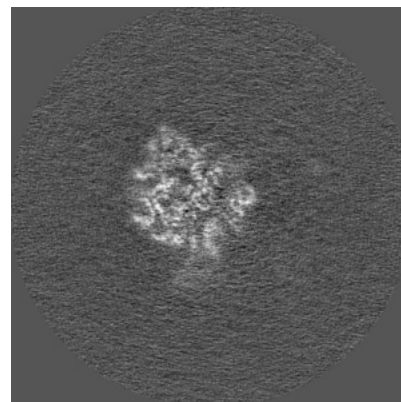
6.2.2 Raw map



X Index: 174



Y Index: 174

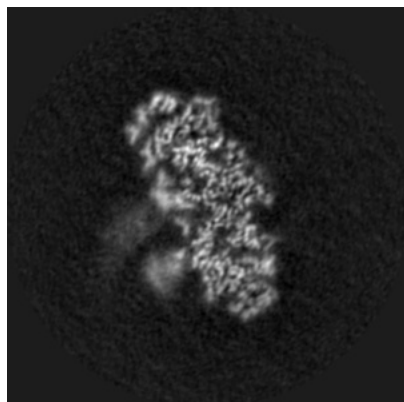


Z Index: 174

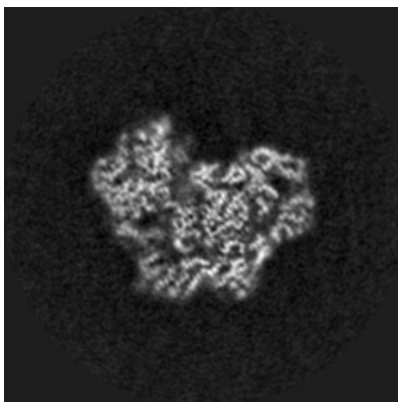
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

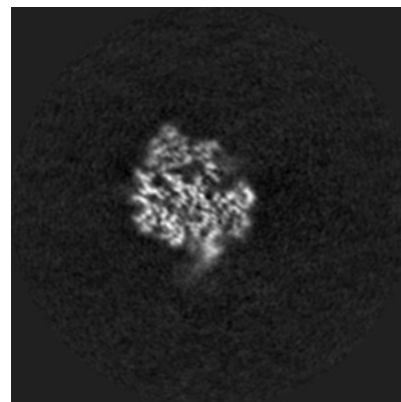
6.3.1 Primary map



X Index: 174

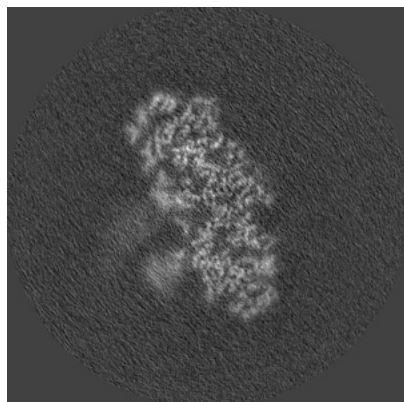


Y Index: 178

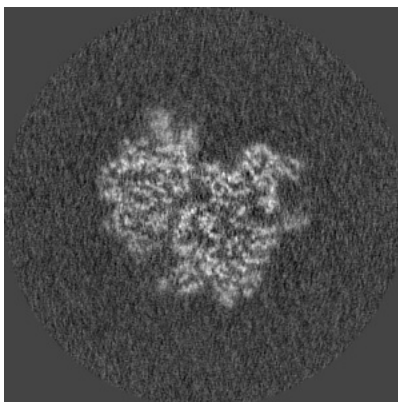


Z Index: 180

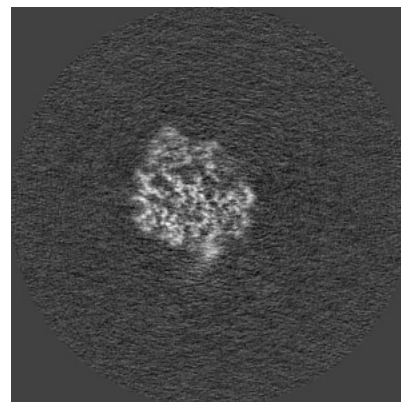
6.3.2 Raw map



X Index: 174



Y Index: 185

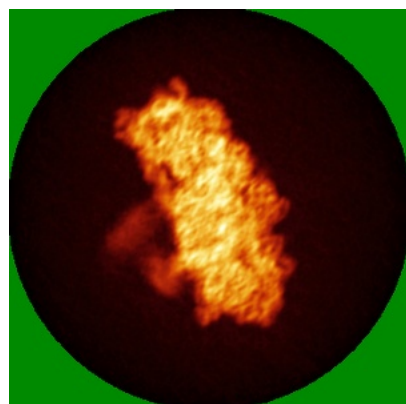


Z Index: 180

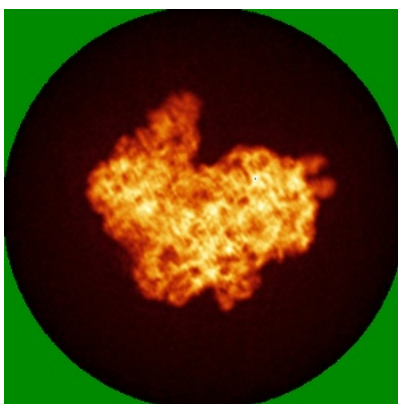
The images above show the largest variance slices of the map in three orthogonal directions.

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

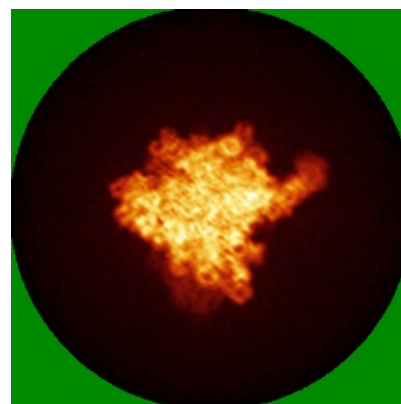
6.4.1 Primary map



X

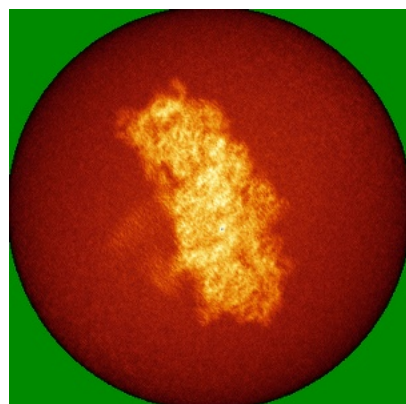


Y

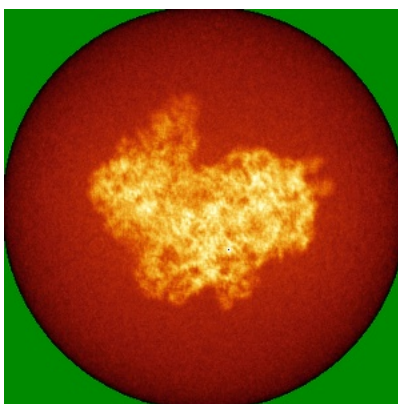


Z

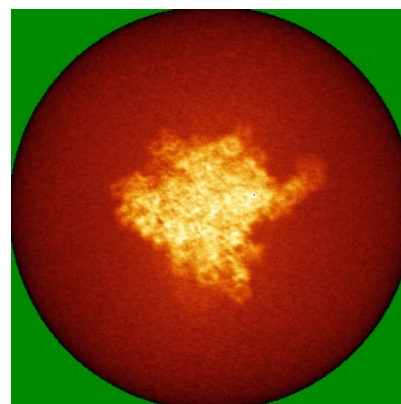
6.4.2 Raw map



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



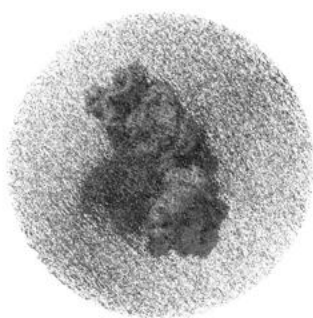
Y



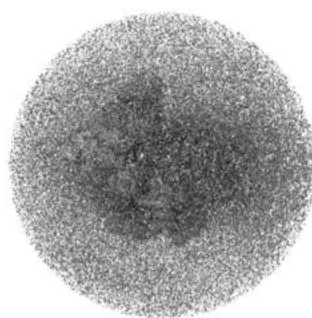
Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

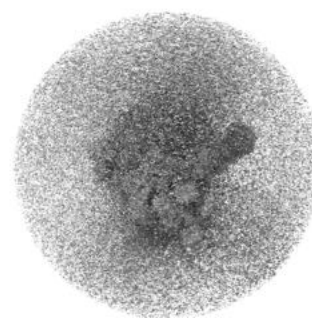
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

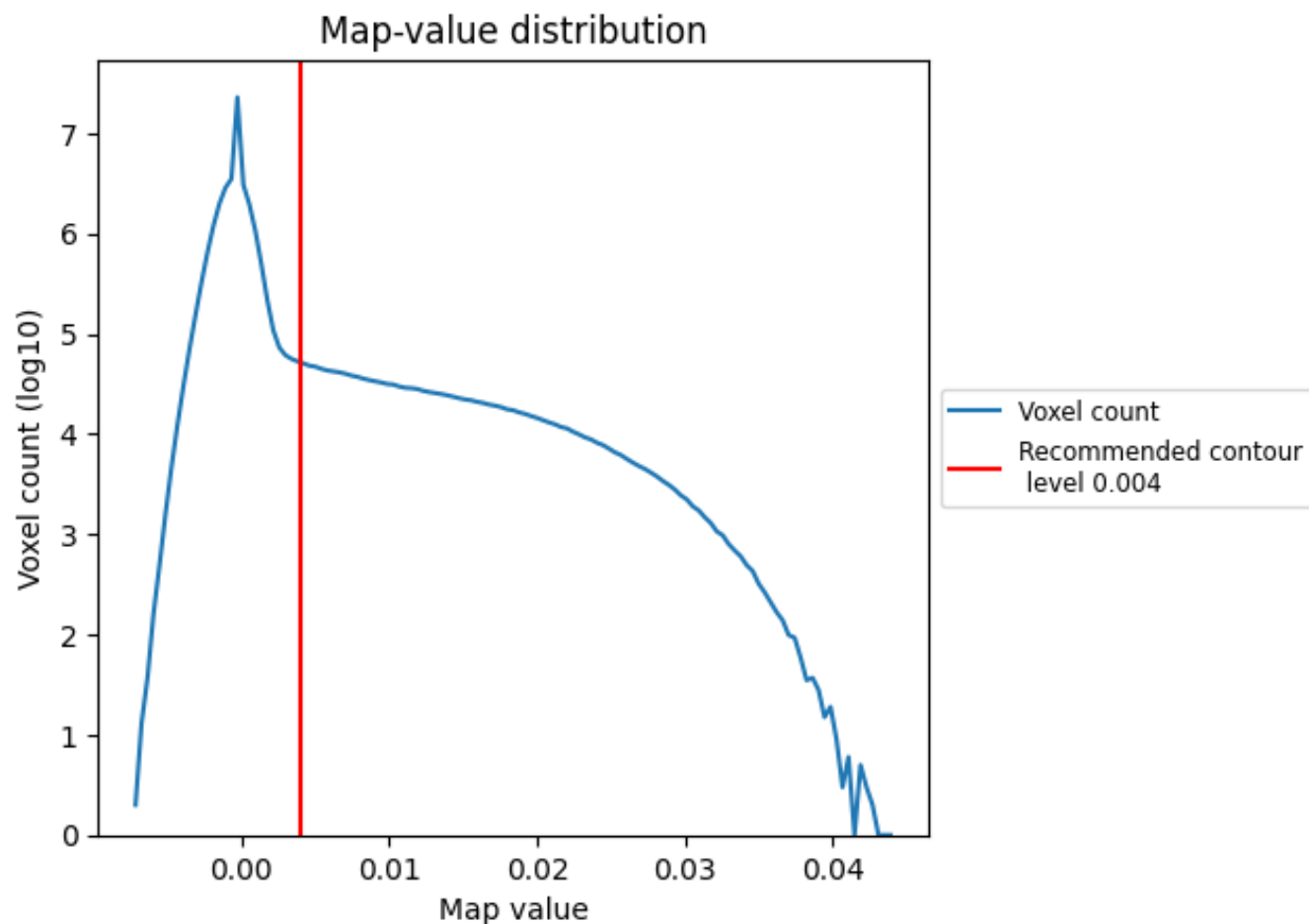
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

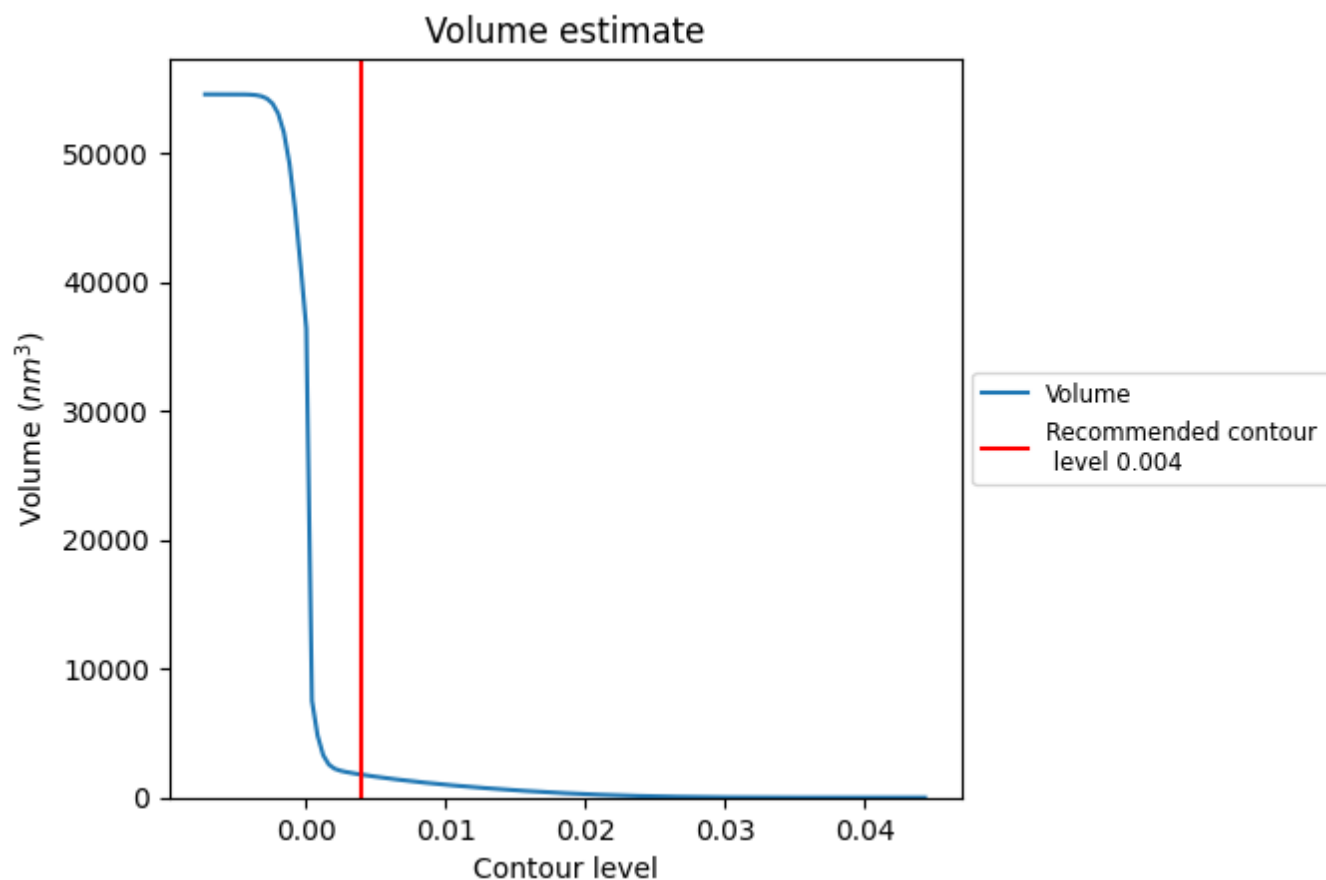
This section contains the results of statistical analysis of the map.

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.

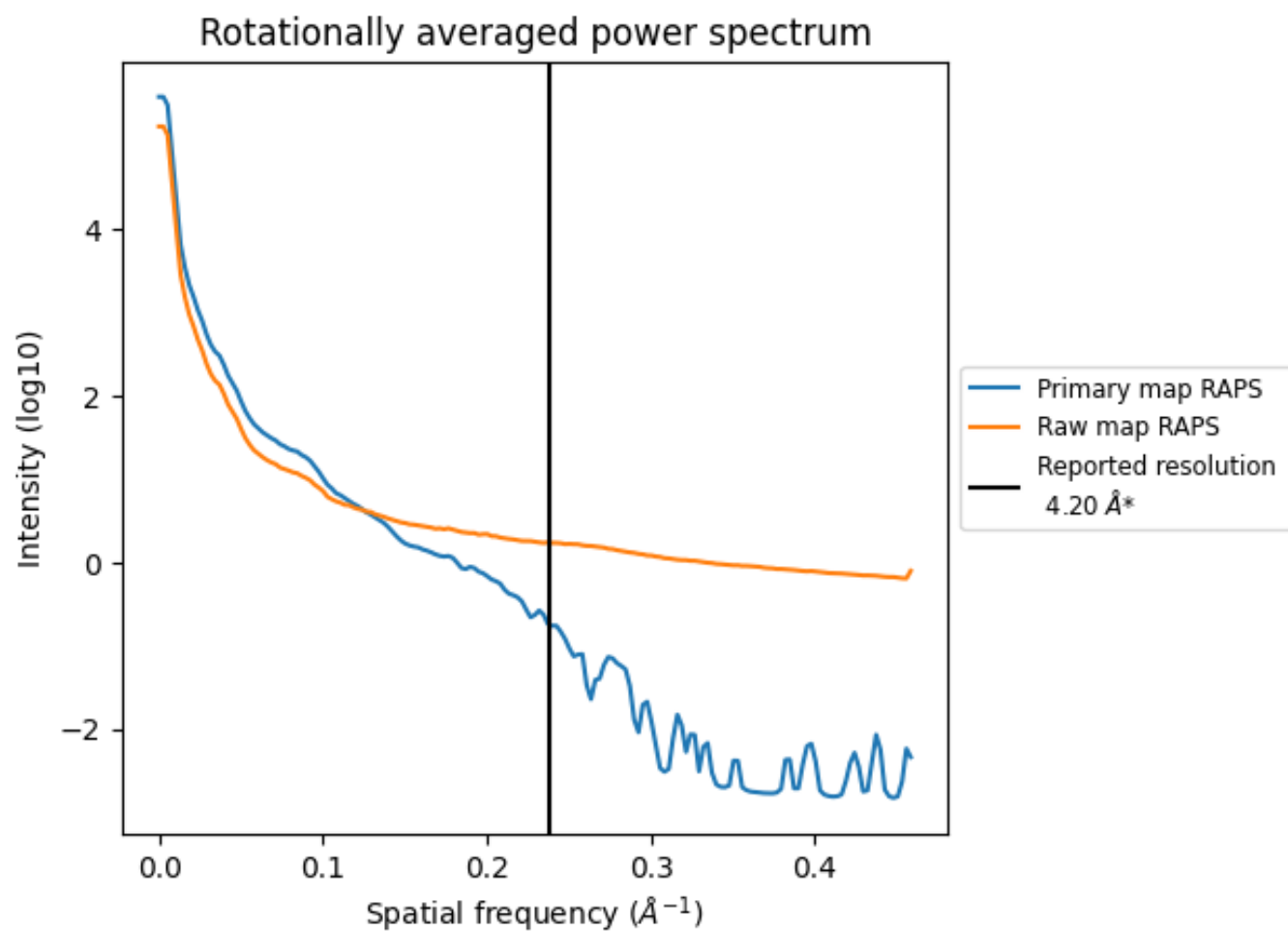
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1784 nm^3 ; this corresponds to an approximate mass of 1611 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 ⓘ

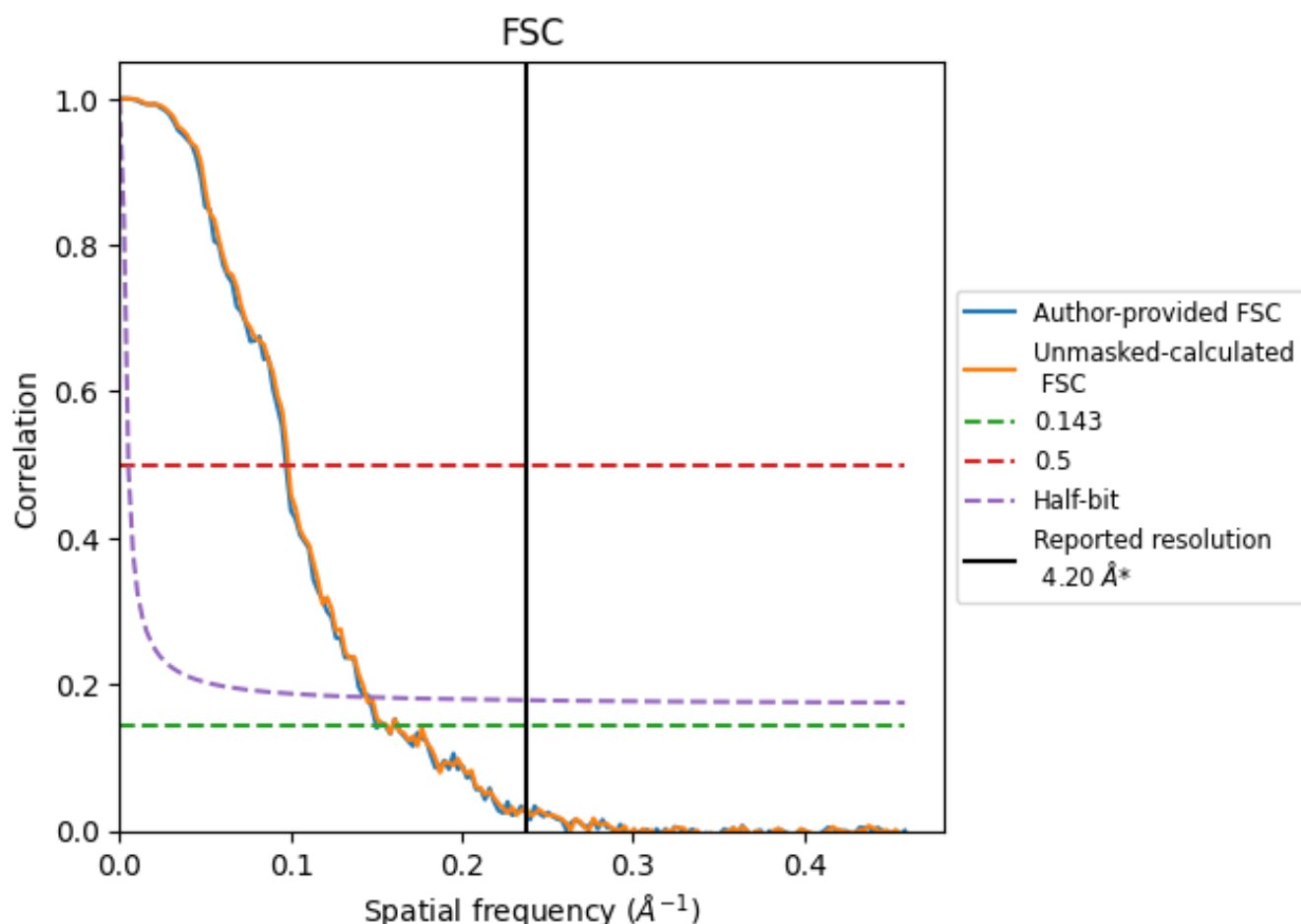


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	6.67	10.29	6.87
Unmasked-calculated*	6.41	10.14	6.93

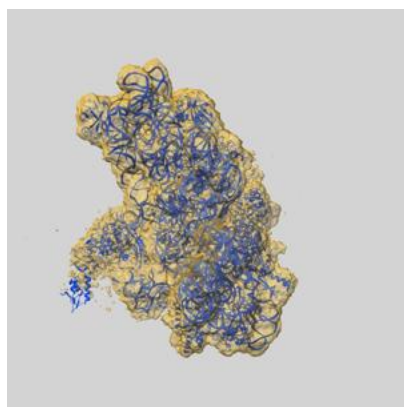
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.67 differs from the reported value 4.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 4.2 by more than 10 %

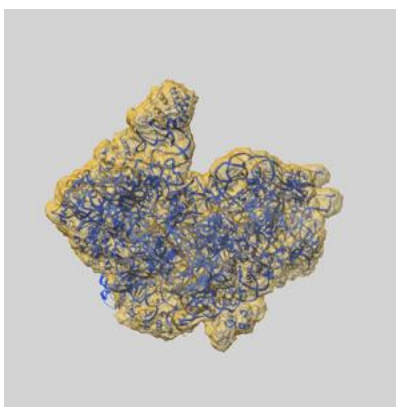
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10320 and PDB model 6SW9. Per-residue inclusion information can be found in section 3 on page 13.

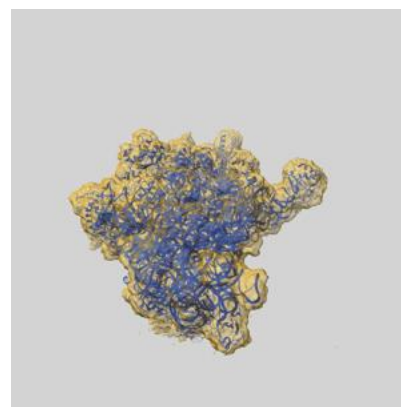
9.1 Map-model overlay [i](#)



X



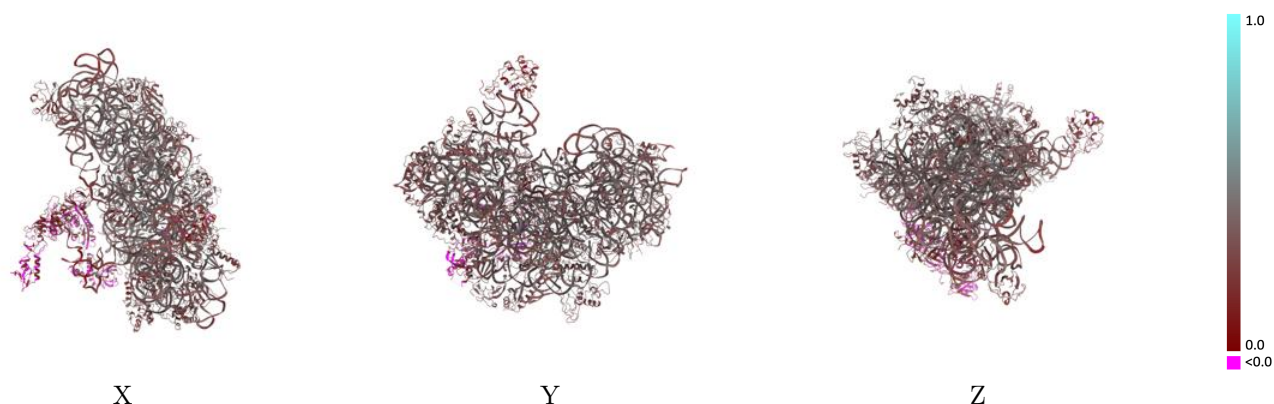
Y



Z

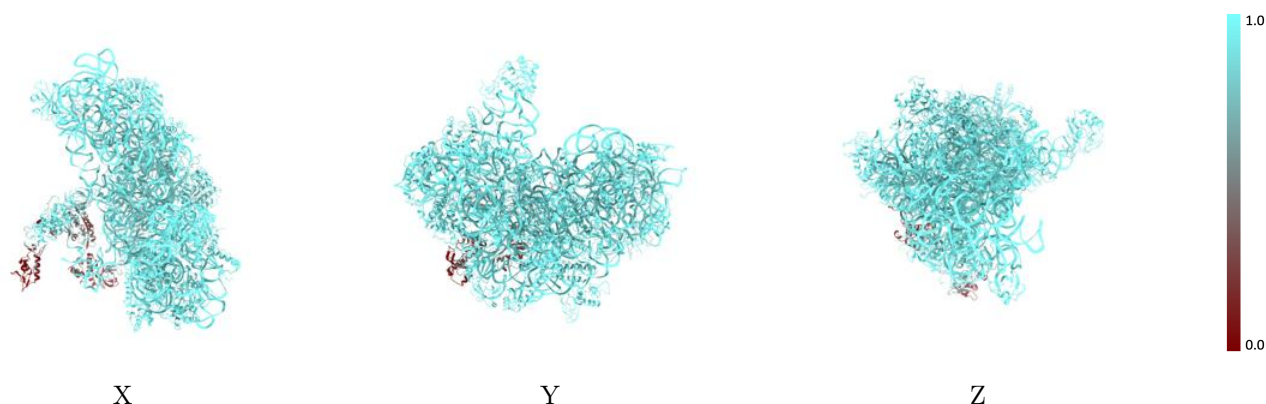
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



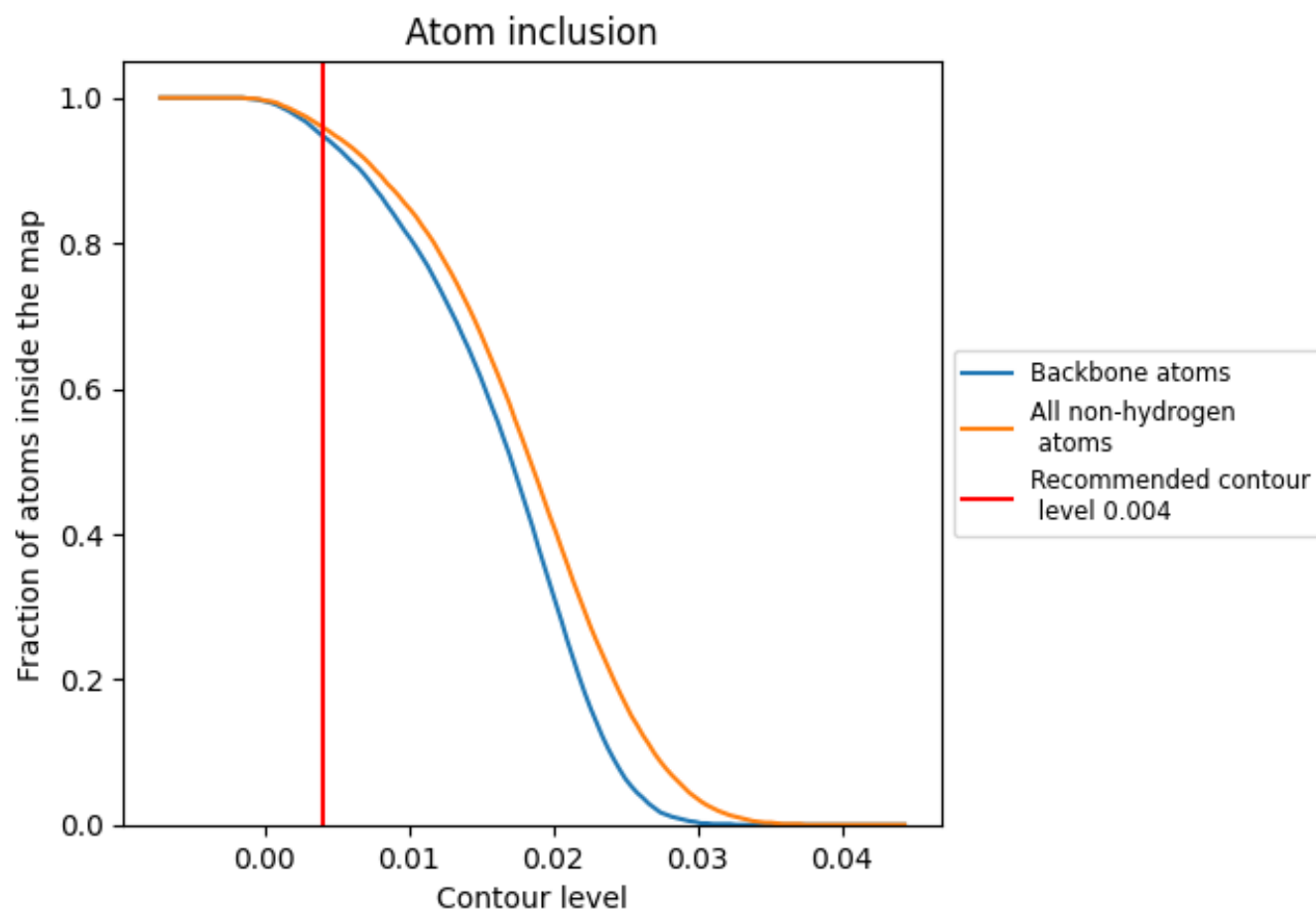
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.3370
0	 0.9970	 0.3730
2	 1.0000	 0.3830
3	 1.0000	 0.2200
4	 0.9870	 0.2310
5	 0.9980	 0.3390
6	 1.0000	 0.2490
7	 0.8600	 0.1420
8	 0.2740	 0.0540
9	 0.2580	 0.0380
A	 0.9960	 0.3430
B	 0.9970	 0.3580
C	 0.9940	 0.3660
D	 1.0000	 0.3580
E	 0.9990	 0.3700
F	 0.9930	 0.3750
G	 0.9980	 0.3170
H	 0.9960	 0.3410
I	 0.9980	 0.3770
J	 0.9980	 0.3550
K	 0.9980	 0.3510
L	 0.9980	 0.3520
M	 1.0000	 0.3570
N	 0.9980	 0.3830
O	 0.9980	 0.3280
P	 1.0000	 0.3630
Q	 0.9980	 0.3450
R	 0.9990	 0.3900
S	 0.9850	 0.3060
T	 0.9930	 0.3340
U	 0.9980	 0.3410
V	 0.9990	 0.3440
W	 0.9960	 0.3620
X	 1.0000	 0.3480
Y	 0.9900	 0.2050
Z	 0.9950	 0.3530

