



## wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 05:07 pm GMT

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](mailto: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>.

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

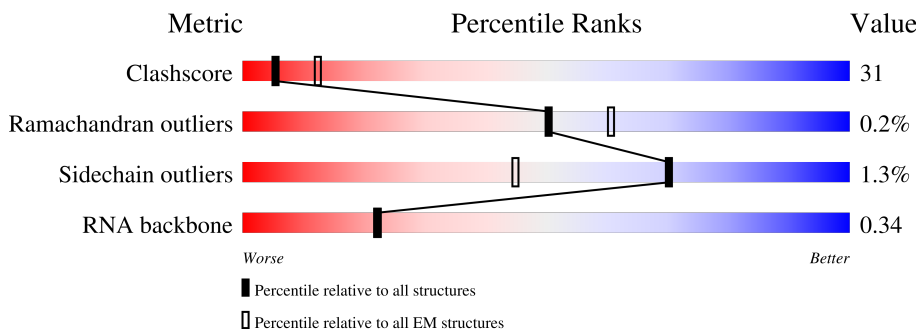
# 1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	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

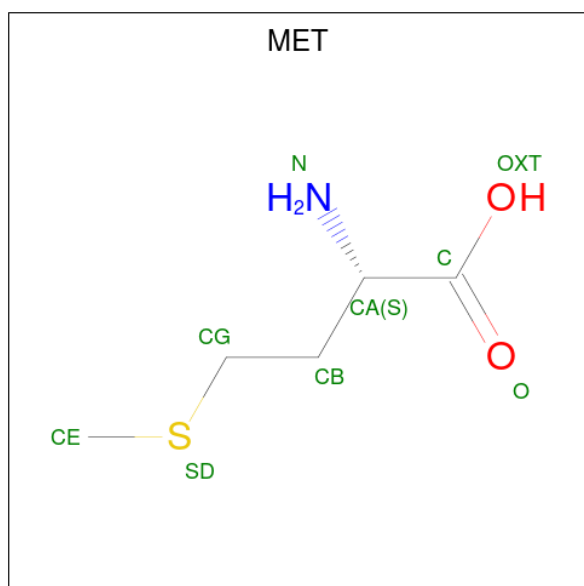
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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.

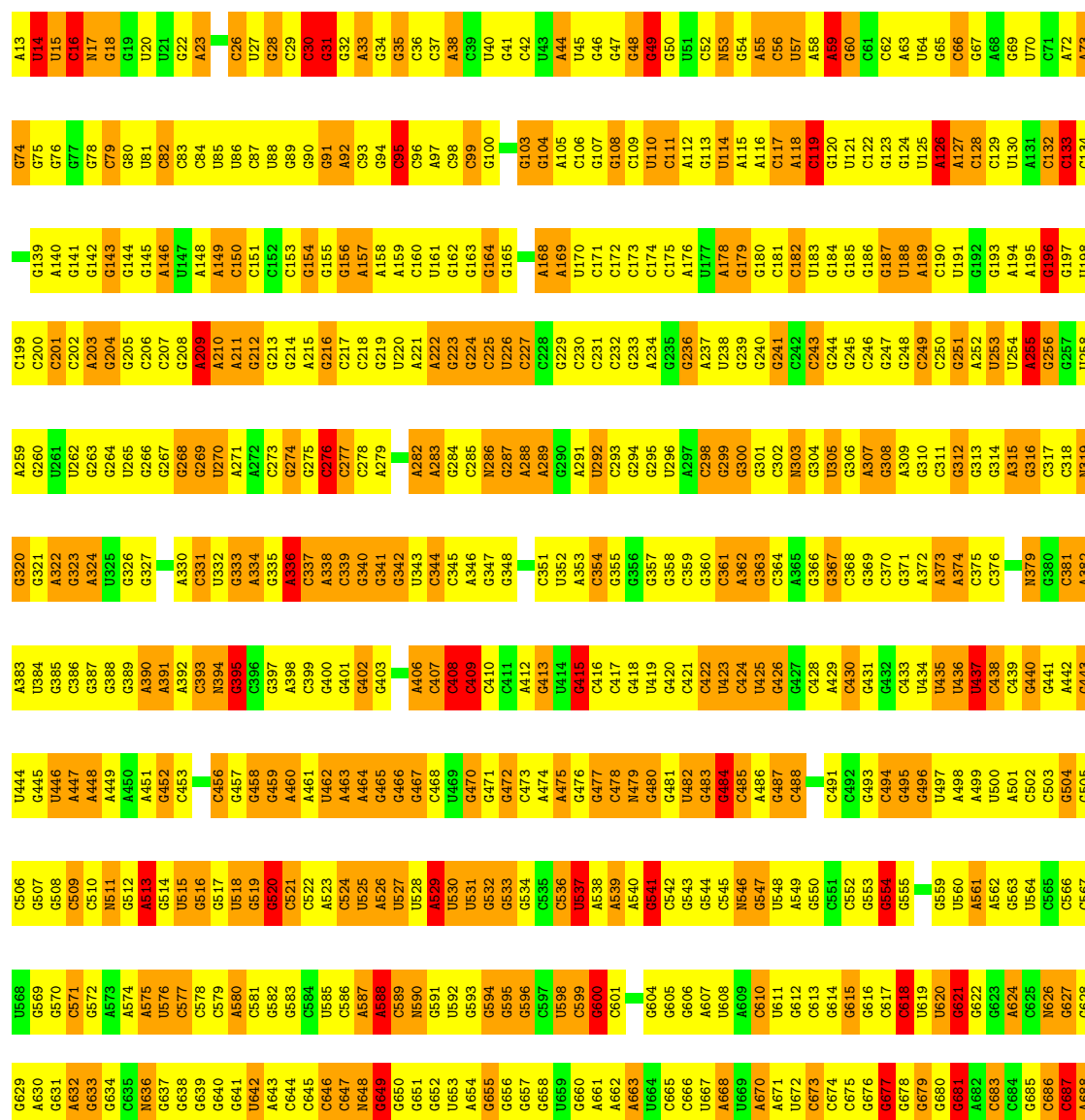
Mol	Chain	Residues	Atoms		AltConf
40	2	40	Total	O	0
			40	40	
40	K	1	Total	O	0
			1	1	
40	Q	1	Total	O	0
			1	1	

### 3 Residue-property plots

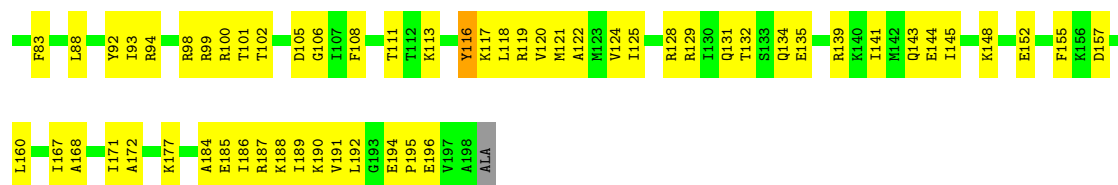
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 



G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A749	C750	N751	G752	G753	A754	G755	G756	A757	G758	A759	G760	A761	C762	G763	G764	G765	G766	G767	G768	A769	G770	U771	C772	G773	U774	G775	G776	G777	U778	C779	G780	A781	A782	A783	G784	G785	A786	G787	G788	C789	G790	G791	G792	C793	A794	A795	G796	G797	U798	G799	U800	C801	U802	G803	G804	C805	G806	A807	G808																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C809	U810	U811	C812	G813	G814	G815	C816	U817	G818	G819	C820	C821	G822	G823	G824	U825	G826	C827	U828	G829	A830	A831	G832	G833	G834	A835	A836	G837	C838	G839	G840	U841	U842	A843	A844	G845	G846	G847	U848	G849	C850	G851	G852	C853	U854	U855	U856	G857	G858	G859	A860	C861	U862	G863	C864	G865	G866	C867	U868																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G869	C870	A871	A872	G873	G874	C875	U876	G877	A878	A879	G880	C881	U882	U883	A884	A885	G886	G887	G888	U889	U890	U891	U892	G893	G894	C895	G896	G897	G898	G899	A900	G901	G902	A903	A904	C905	U906	A907	G908	A909	A910	G911	G912	G913	G914	U915	U916	G917	G918	G919	G920	C921	C922	G923	C924	G925	G926	U927	U928	U929	A930	A931																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
U932	U933	G934	G935	A936	U937	U938	C939	A940	A941	C942	G943	G944	C945	G946	G947	A948	A949	A950	C951	C952	U953	C954	A955	C956	U957	G958	G959	G960	G961	G962	C963	G964	A965	C966	G967	G968	C969	A970	G971	G972	A973	U974	G975	A976	A977	G978	G979	G980	C981	A982	G983	G984	C985	U986	U987	A988	A989	G990	G991																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U992	C993	U994	U995	G996	C997	C998	G999	U1000	U1001	C1002	G1003	C1004	G1005	C1006	C1007	G1008	A1009	G1010	A1011	G1012	G1013	A1014	G1015	G1016	U1017	G1018	C1019	G1020	G1021	G1022	C1023	G1024	A1025	C1026	G1027	N1028	G1029	U1030	C1031	A1032	G1033	U1034	U1035	C1036	U1037	U1038	A1039	C1040	N1041	U1042	G1043	G1044	A1045	C1046	U1047	C1048	G1049	U1050	C1051																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G1052	A1053	C1054	U1055	U1056	U1057	A1058	G1059	U1060	U1061	U1062	G1063	G1064	U1065	A1066	A1067	C1068	G1069	A1070	G1071	C1072	G1073	A1074	G1075	C1076	G1077	C1078	C1079	G1080	C1081	C1082	C1083	C1084	A1085	C1086	C1087	A1088	G1089	U1090	U1091	G1092	C1093	C1094	A1095	G1096	U1097	C1098	C1099	C1100	U1101	C1102	G1103	C1104	G1105	C1106	U1107	G1108	G1109	G1110	G1111	A1112																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G1113	G1114	G1115	U1116	U1117	G1118	G1119	A1120	C1121	U1122	C1123	U1124	G1125	G1126	G1127	G1128	C1129	G1130	A1131	C1132	U1133	G1134	C1135	C1136	G1137	G1138	C1139	G1140	C1141	C1142	C1143	A1144	G1145	C1146	N1147	G1148	G1149	A1150	G1151	G1152	A1153	A1154	G1155	G1156	G1157	C1158	C1159	G1160	G1161	G1162	C1163	G1164	A1165	U1166	G1167	G1168	U1169	A1170	G1171	G1172																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U1173	C1174	A1175	G1176	U1177	A1178	U1179	G1180	C1181	C1182	C1183	G1184	A1185	A1186	A1187	A1188	C1189	C1190	C1191	C1192	N1193	G1194	G1195	G1196	C1197	U1198	A1199	C1200	G1201	C1202	G1203	G1204	G1205	C1206	G1207	C1208	U1209	A1210	C1211	A1212	U1213	U1214	G1215	G1216	G1217	C1218	G1219	G1220	G1221	U1222	A1223	G1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
C1237	C1238	N1239	G1240	A1241	A1242	A1243	G1244	G1245	G1246	G1247	G1248	A1249	G1250	G1251	A1252	A1253	A1254	U1255	U1256	U1257	U1258	U1259	U1260	A1261	A1262	A1263	C1264	C1265	C1266	G1267	C1268	C1269	C1270	U1271	C1272	A1273	G1274	U1275	U1276	C1277	G1278	A1279	C1280	U1281	C1282	G1283	C1284	G1285	G1286	G1287	C1288	U1289	G1290	C1291	A1292	C1293	A1294	C1295	C1296	U1297	C1298																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C1299	C1300	G1301	C1302	U1303	U1304	G1305	A1306	A1307	G1308	C1309	U1310	G1311	G1312	A1313	C1316	C1317	C1318	U1319	A1320	G1321	U1322	A1323	C1324	C1325	C1326	G1327	C1328	C1329	C1330	G1331	U1332	C1333	A1334	U1335	C1336	A1337	U1338	C1339	C1340	U1341	G1342	C1343	G1344	C1345	C1346	G1347	A1348	U1349	A1350	A1351	C1352	G1353	U1354	C1355	C1356	C1357	U1358	G1359																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
C1360	U1361	C1362	C1363	U1364	U1365	G1366	C1367	A1368	C1369	A1370	C1371	A1372	C1373	C1374	C1375	C1376	C1377	U1378	G1379	C1380	C1381	A1382	C1383	U1384	C1385	C1386	A1387	C1388	C1389	C1390	A1391	C1392	C1393	C1394	G1395	G1396	G1397	C1398	C1399	C1400	U1401	A1402	G1403	G1404	U1405	G1406	A1407	G1408	G1409	C1410	C1411	C1412	G1413	A1414	U1415	C1416	U1417	C1418	U1419																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U1420	U1421	C1422	G1423	G1424	U1425	A1426	G1427	A1428	U1429	C1430	G1431	G1432	G1433	U1434	C1435	A1436	A1437	G1438	C1439	A1440	U1441	A1442	G1443	G1444	C1445	U1446	C1447	C1448	G1449	U1450	G1451	A1452	C1453	G1454	G1455	G1456	G1457	G1458	A1459	G1460	A1461	A1462	G1463	U1464	C1465	G1466	U1467	A1468	A1469	C1470	A1471	A1472	G1473	G1474	U1475	U1476	A1477	C1478	U1479																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G1480	U1481	A1482	G1483	U1484	G1485	G1486	A1487	A1488	U1489	C1490	U1491	G1492	C1493	G1494	G1495	C1496	U1497	G1498	A1499	G1500	U1501	C1502	A1503	U1504	C1505	U1506	C1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1927	U1928	U1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U20



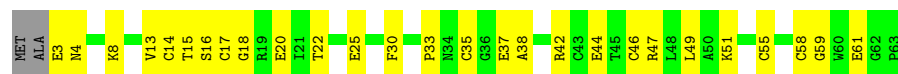
• Molecule 3: 30S ribosomal protein S2

Chain B: 57% 40%



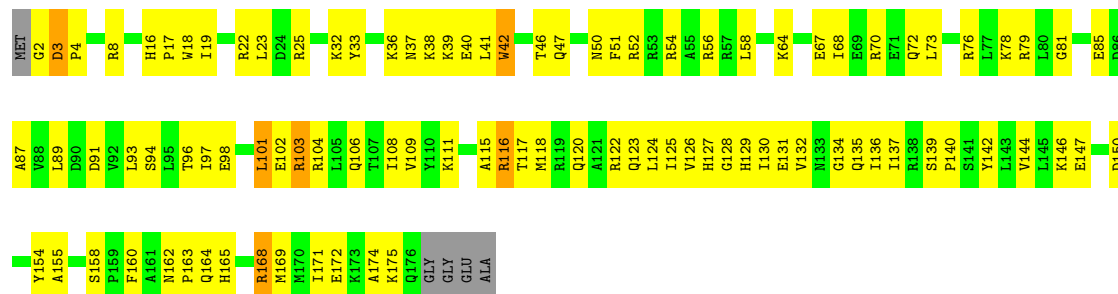
• Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C: 54% 43%



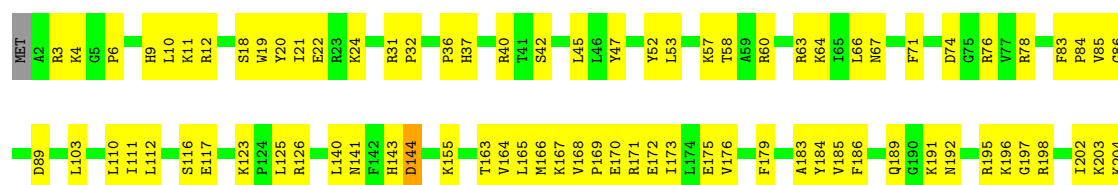
• Molecule 5: 30S ribosomal protein S4

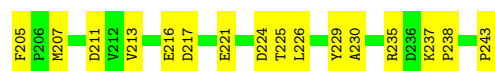
Chain D: 44% 50%



• Molecule 6: 30S ribosomal protein S4e

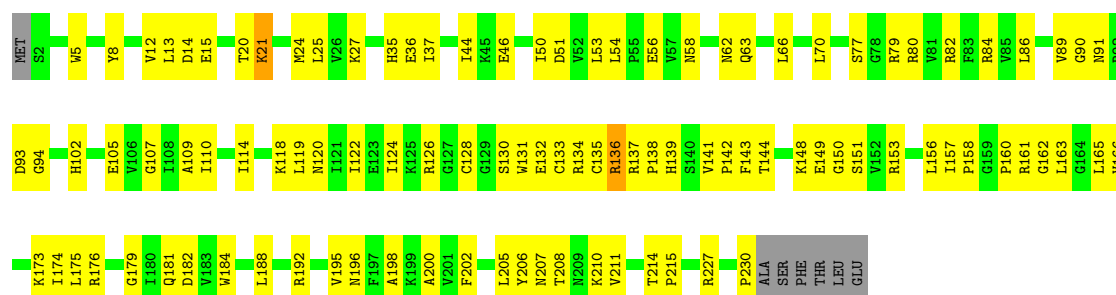
Chain E: 60% 40%





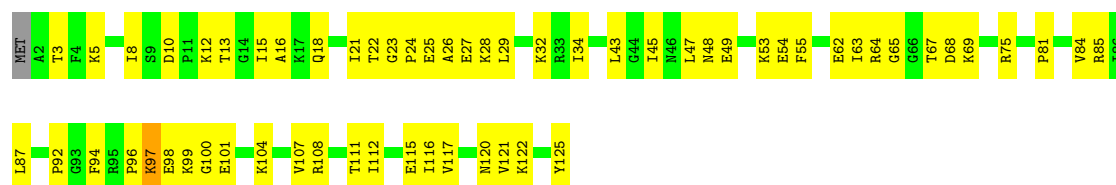
• Molecule 7: 30S ribosomal protein S5

Chain F: 53% 43% ..



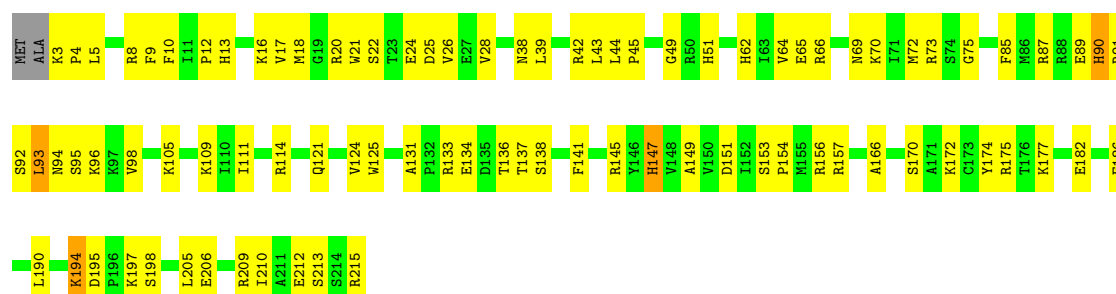
• Molecule 8: 30S ribosomal protein S6e

Chain G: 51% 47% ..



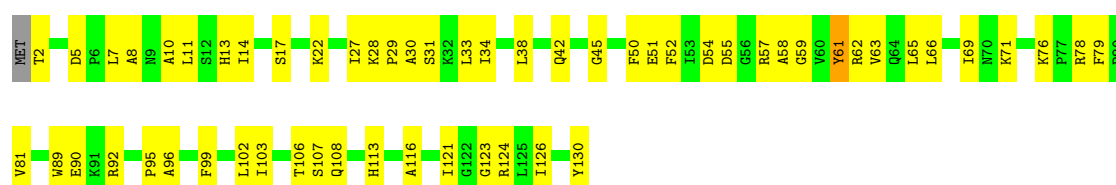
• Molecule 9: 30S ribosomal protein S7

Chain H: 58% 39% ..



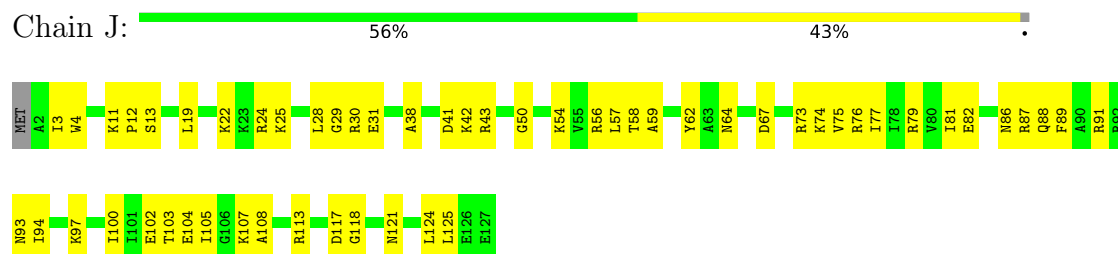
• Molecule 10: 30S ribosomal protein S8

Chain I: 55% 43% ..

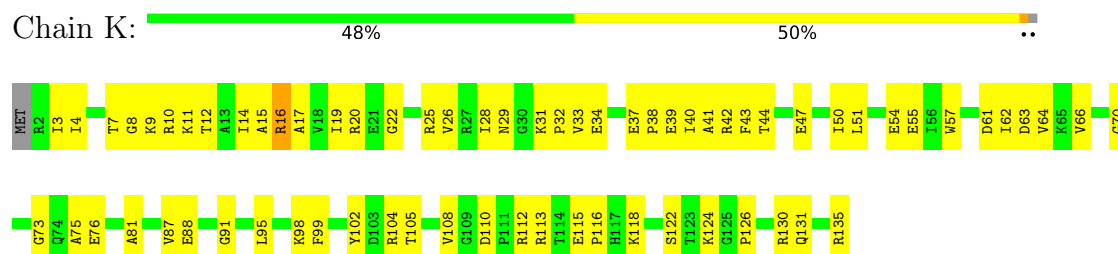




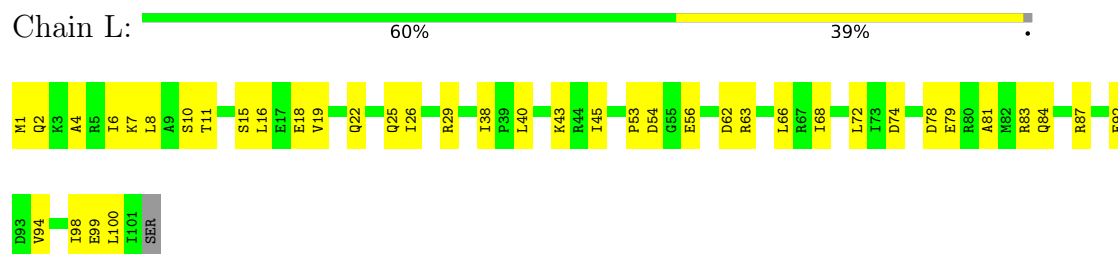
- Molecule 11: 30S ribosomal protein S8e



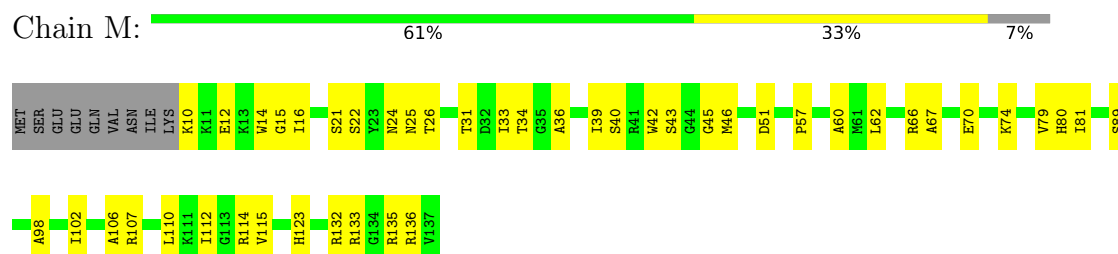
- Molecule 12: 30S ribosomal protein S9



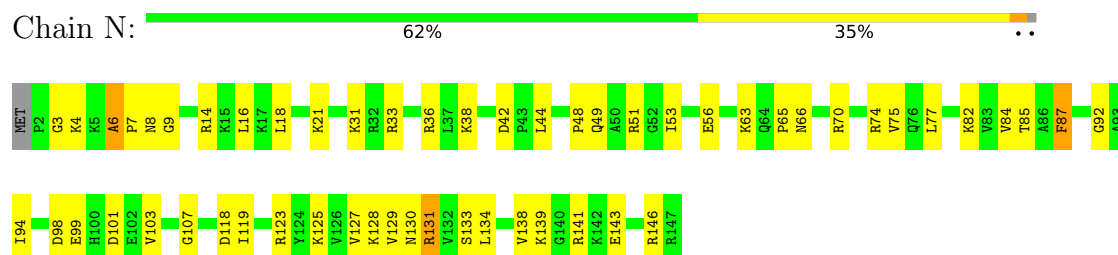
- Molecule 13: 30S ribosomal protein S10



- Molecule 14: 30S ribosomal protein S11

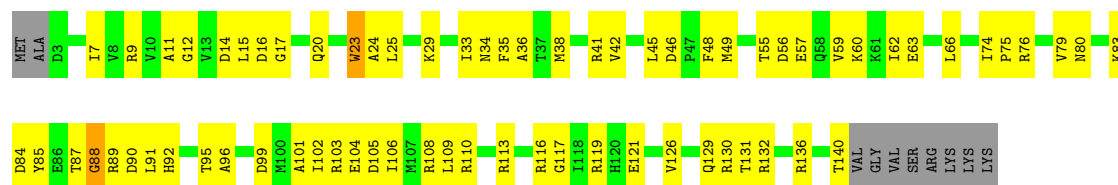


- Molecule 15: 30S ribosomal protein S12



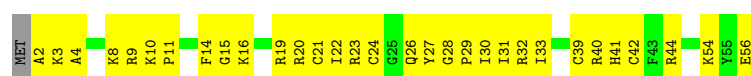
- Molecule 16: 30S ribosomal protein S13

Chain O:  46% 46% 7%



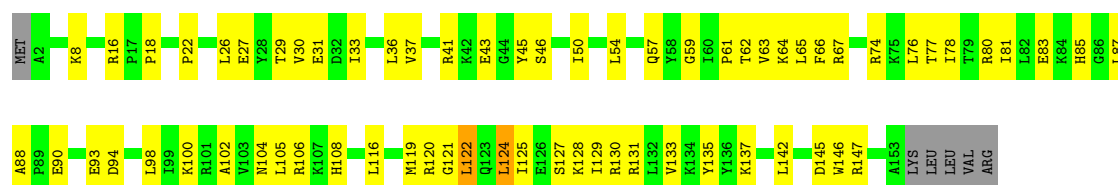
- Molecule 17: 30S ribosomal protein S14 type Z

Chain P:  43% 55%



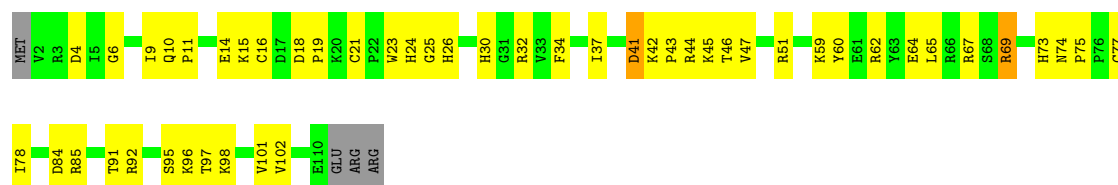
- Molecule 18: 30S ribosomal protein S15

Chain Q:  54% 41%



- Molecule 19: 30S ribosomal protein S17

Chain R:  53% 42%



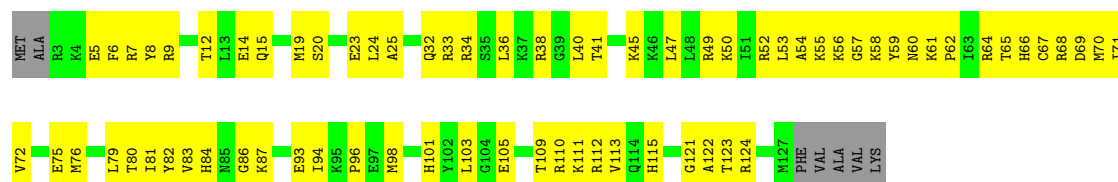
- Molecule 20: 30S ribosomal protein S17e

Chain S:  55% 43%



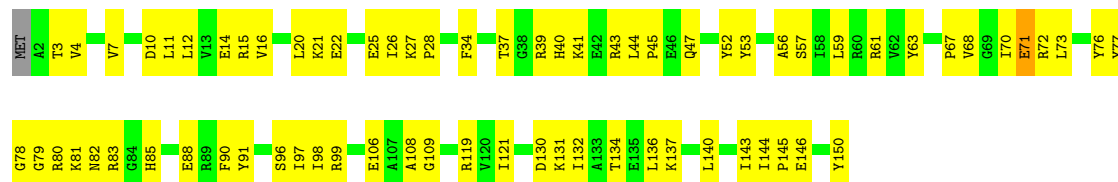
- Molecule 21: 30S ribosomal protein S19

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%



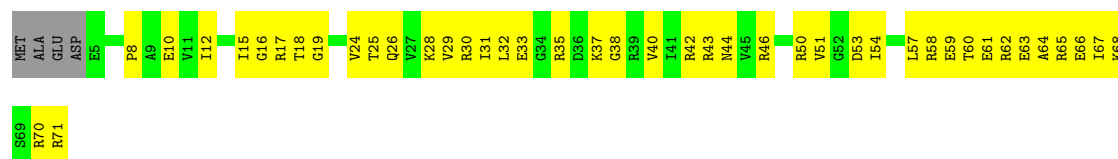
- Molecule 24: 30S ribosomal protein S27e

Chain W: 60% 37%



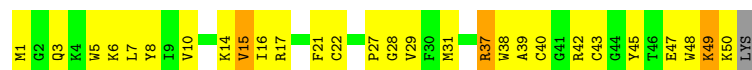
- Molecule 25: 30S ribosomal protein S28e

Chain X: 34% 61% 6%

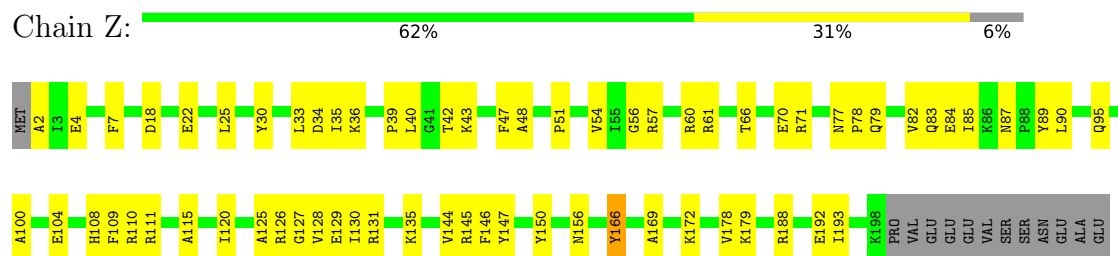


- Molecule 26: 30S ribosomal protein S27ae

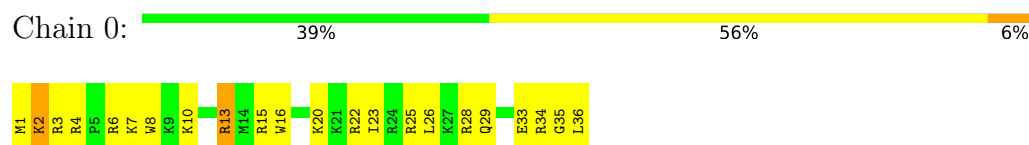
Chain Y: 43% 49% 6%



- Molecule 27: 30S ribosomal protein S3



- Molecule 28: 50S ribosomal protein L41e



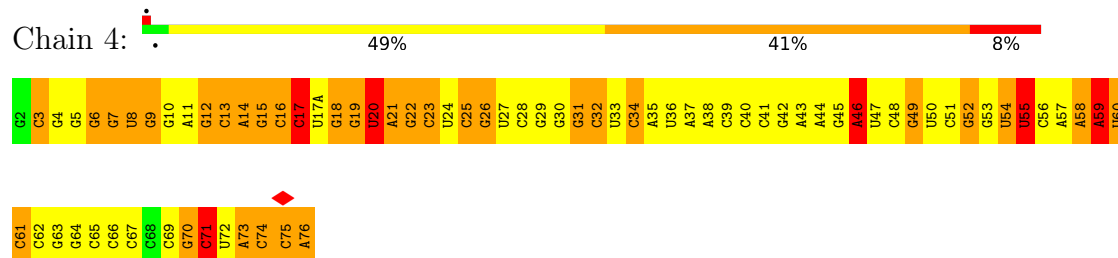
- Molecule 29: 50S ribosomal protein L7Ae



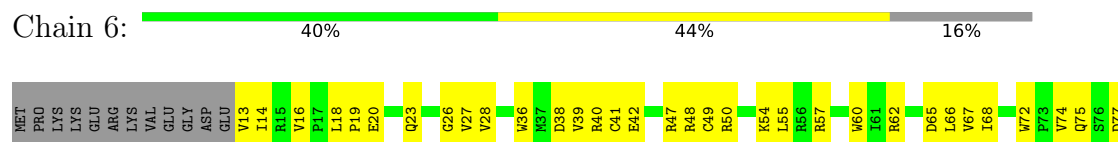
- Molecule 30: mRNA

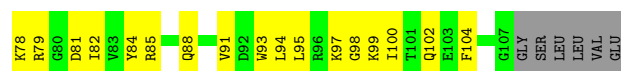


- Molecule 31: initiator Met-tRNA fMet from E. coli (A1U72 variant)

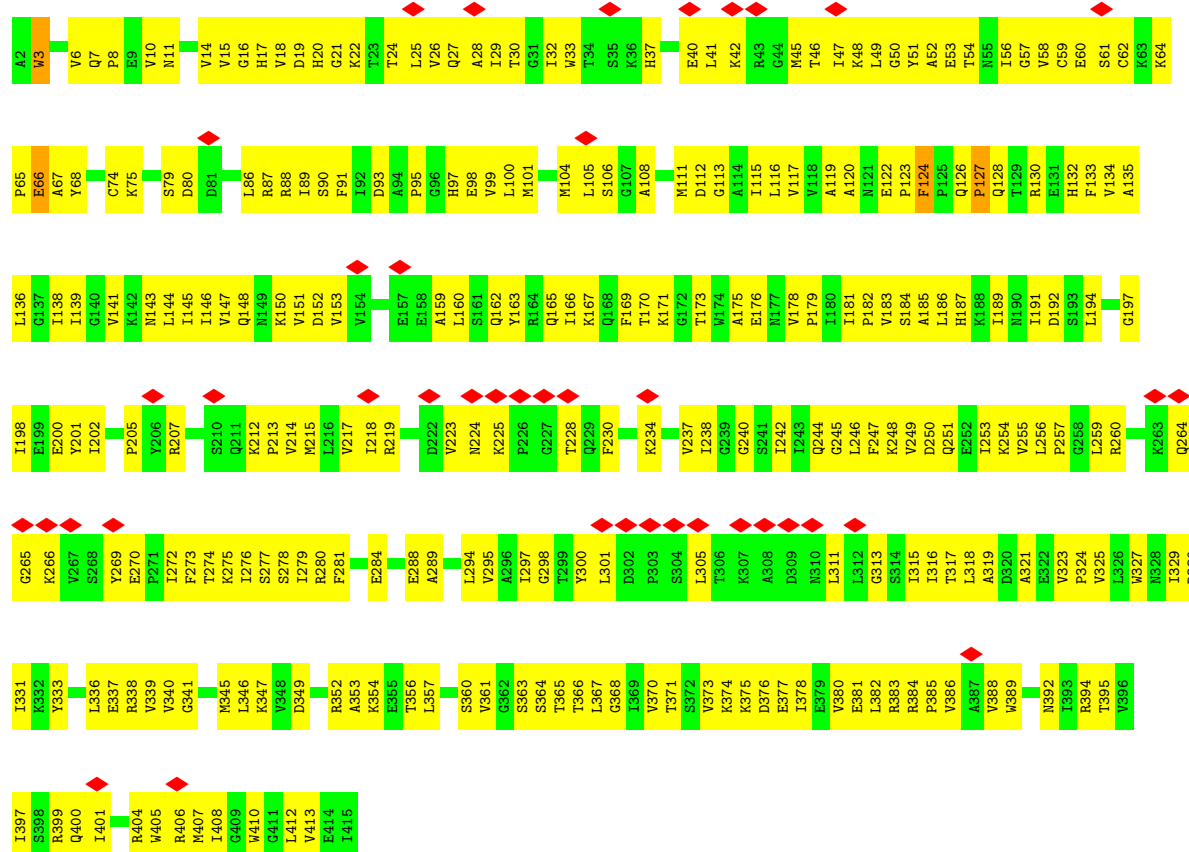


- Molecule 32: Translation initiation factor 1A

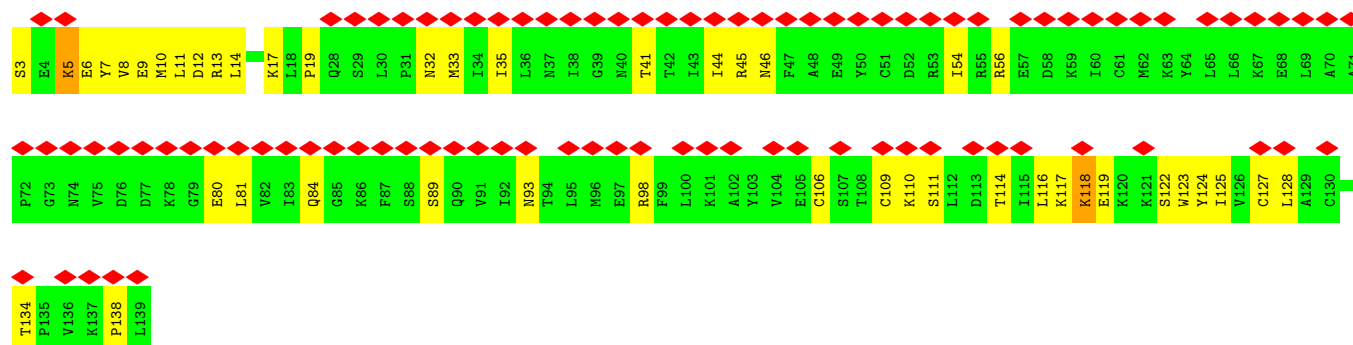




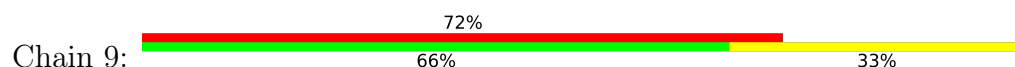
• Molecule 33: Translation initiation factor 2 subunit gamma

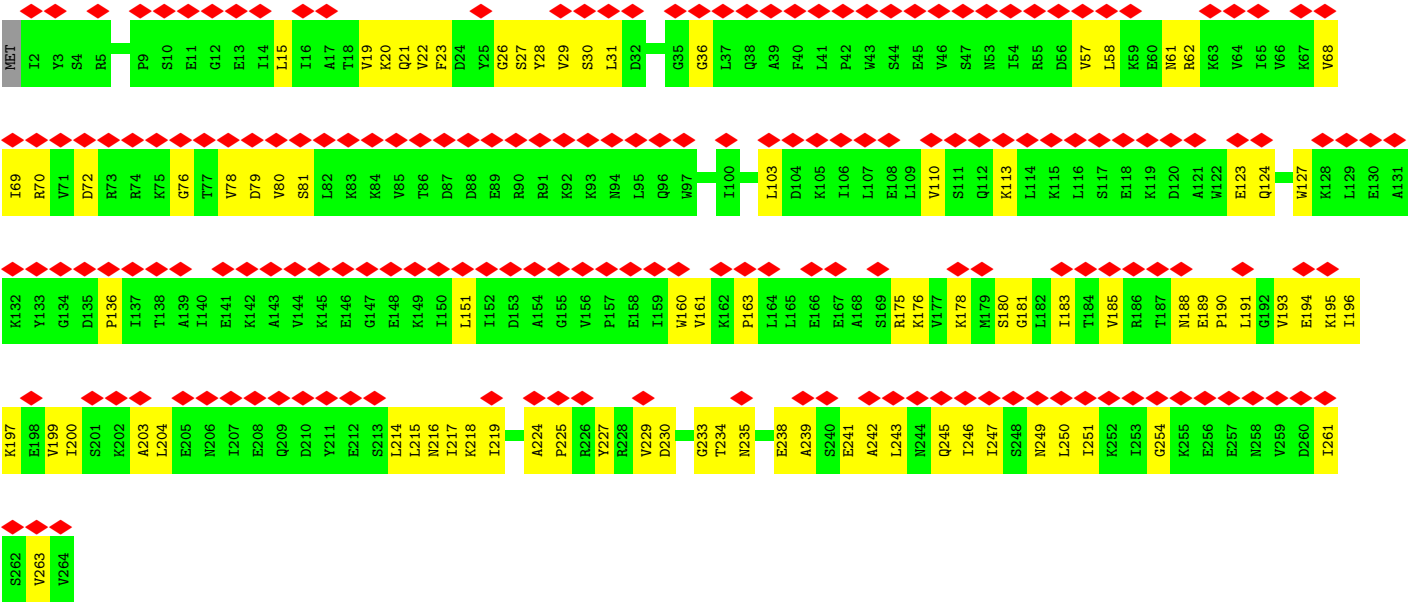


• Molecule 34: Translation initiation factor 2 subunit beta



• 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: B8H, MA6, PSU, 4SU, LHH, 5MU, A2M, GNP, ZN, 4AC, 6MZ, 5MC, 5HM, H2U, UR3, MG, OMC

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%)	25	64
6	E	240/243 (99%)	179 (75%)	60 (25%)	1 (0%)	34	72
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%)	22	62
16	O	136/148 (92%)	107 (79%)	28 (21%)	1 (1%)	22	62
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%)	22	62
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%)	50	80

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%)	71	83
3	B	168/173 (97%)	167 (99%)	1 (1%)	86	92
4	C	54/55 (98%)	53 (98%)	1 (2%)	57	74
5	D	158/160 (99%)	154 (98%)	4 (2%)	47	68
6	E	213/214 (100%)	212 (100%)	1 (0%)	88	93
7	F	192/198 (97%)	187 (97%)	5 (3%)	46	67
8	G	107/108 (99%)	106 (99%)	1 (1%)	78	87
9	H	183/184 (100%)	180 (98%)	3 (2%)	62	79
10	I	106/107 (99%)	105 (99%)	1 (1%)	78	87
11	J	102/103 (99%)	101 (99%)	1 (1%)	76	86
12	K	110/111 (99%)	109 (99%)	1 (1%)	78	87
13	L	90/91 (99%)	89 (99%)	1 (1%)	73	84
14	M	95/104 (91%)	95 (100%)	0	100	100
15	N	120/121 (99%)	118 (98%)	2 (2%)	60	78
16	O	115/123 (94%)	115 (100%)	0	100	100
17	P	45/46 (98%)	44 (98%)	1 (2%)	52	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Q	137/143 (96%)	135 (98%)	2 (2%)	65	80
19	R	98/102 (96%)	97 (99%)	1 (1%)	76	86
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%)	62	79
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%)	59	76
26	Y	41/42 (98%)	38 (93%)	3 (7%)	14	41
27	Z	156/168 (93%)	154 (99%)	2 (1%)	69	82
28	0	34/34 (100%)	32 (94%)	2 (6%)	19	47
29	3	99/99 (100%)	97 (98%)	2 (2%)	55	73
32	6	83/99 (84%)	83 (100%)	0	100	100
33	7	356/356 (100%)	352 (99%)	4 (1%)	73	84
34	8	117/118 (99%)	113 (97%)	4 (3%)	37	61
35	9	226/228 (99%)	225 (100%)	1 (0%)	91	94
All	All	3858/3962 (97%)	3809 (99%)	49 (1%)	70	82

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	590	36,1	21,24,25	1.15	3 (14%)	29,34,37	1.47	4 (13%)
1	4AC	2	718	1	21,24,25	1.08	2 (9%)	29,34,37	1.18	3 (10%)
31	5MU	4	54	31	19,22,23	1.44	6 (31%)	28,32,35	2.05	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	6MZ	2	1469	36,1	18,25,26	0.76	1 (5%)	16,36,39	2.10	3 (18%)
1	4AC	2	1028	1	21,24,25	1.05	3 (14%)	29,34,37	1.62	4 (13%)
31	4SU	4	8	31	18,21,22	1.79	5 (27%)	26,30,33	2.15	4 (15%)
1	4AC	2	319	1	21,24,25	1.20	3 (14%)	29,34,37	1.48	4 (13%)
1	4AC	2	851	1	21,24,25	1.24	3 (14%)	29,34,37	1.57	4 (13%)
1	4AC	2	731	1	21,24,25	1.16	3 (14%)	29,34,37	1.37	5 (17%)
1	4AC	2	868	1	21,24,25	1.23	3 (14%)	29,34,37	1.37	4 (13%)
1	MA6	2	1487	1	19,26,27	0.95	1 (5%)	18,38,41	1.32	3 (16%)
1	5HM	2	1378	1	19,23,24	2.94	7 (36%)	25,33,36	0.64	0
1	4AC	2	511	1	21,24,25	1.15	3 (14%)	29,34,37	1.87	6 (20%)
1	4AC	2	703	1	21,24,25	1.07	2 (9%)	29,34,37	1.82	6 (20%)
1	4AC	2	848	1	21,24,25	1.12	2 (9%)	29,34,37	1.75	4 (13%)
1	4AC	2	1147	1	21,24,25	1.12	3 (14%)	29,34,37	2.24	6 (20%)
1	4AC	2	1233	1	21,24,25	1.09	2 (9%)	29,34,37	1.53	4 (13%)
31	PSU	4	55	31	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
1	4AC	2	286	1	21,24,25	1.11	2 (9%)	29,34,37	1.64	7 (24%)
1	4AC	2	394	1	21,24,25	1.02	2 (9%)	29,34,37	1.66	5 (17%)
1	4AC	2	1184	1	21,24,25	1.06	3 (14%)	29,34,37	1.39	4 (13%)
1	4AC	2	546	1	21,24,25	1.03	2 (9%)	29,34,37	1.44	3 (10%)
1	4AC	2	957	1	21,24,25	1.12	1 (4%)	29,34,37	2.29	7 (24%)
1	5MC	2	1202	1	18,22,23	1.00	1 (5%)	26,32,35	1.21	1 (3%)
1	B8H	2	938	1	19,22,23	0.82	0	22,32,35	1.52	3 (13%)
1	4AC	2	1479	1	21,24,25	1.10	3 (14%)	29,34,37	1.50	4 (13%)
1	4AC	2	479	1	21,24,25	1.13	3 (14%)	29,34,37	1.59	5 (17%)
1	4AC	2	636	1	21,24,25	1.12	3 (14%)	29,34,37	1.60	4 (13%)
1	4AC	2	751	1	21,24,25	1.13	3 (14%)	29,34,37	1.26	4 (13%)
1	LHH	2	250	1	22,25,26	2.45	8 (36%)	29,35,38	1.20	2 (6%)
31	H2U	4	20	31	18,21,22	1.10	2 (11%)	21,30,33	2.24	1 (4%)
1	4AC	2	303	1	21,24,25	1.16	3 (14%)	29,34,37	1.44	3 (10%)
1	4AC	2	1193	1	21,24,25	1.13	2 (9%)	29,34,37	2.00	5 (17%)
1	4AC	2	1239	1	21,24,25	1.15	2 (9%)	29,34,37	1.87	4 (13%)
1	4AC	2	1041	1	21,24,25	1.01	2 (9%)	29,34,37	1.98	4 (13%)
1	UR3	2	1467	1	19,22,23	1.10	2 (10%)	26,32,35	1.50	5 (19%)
1	A2M	2	373	1	18,25,26	1.06	1 (5%)	18,36,39	1.39	4 (22%)
1	OMC	2	1376	1	19,22,23	0.90	2 (10%)	26,31,34	0.76	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4AC	2	17	1	21,24,25	1.06	2 (9%)	29,34,37	1.77	5 (17%)
1	4AC	2	379	1	21,24,25	1.08	3 (14%)	29,34,37	1.55	5 (17%)
1	4AC	2	828	1	21,24,25	1.01	1 (4%)	29,34,37	1.64	4 (13%)
31	OMC	4	32	31	19,22,23	0.99	2 (10%)	26,31,34	1.13	2 (7%)
1	5MC	2	939	1	18,22,23	1.05	2 (11%)	26,32,35	1.25	3 (11%)
1	MA6	2	1488	1	19,26,27	0.98	1 (5%)	18,38,41	1.21	2 (11%)
1	4AC	2	648	1	21,24,25	1.20	3 (14%)	29,34,37	1.85	7 (24%)
1	4AC	2	626	1	21,24,25	1.05	3 (14%)	29,34,37	1.41	4 (13%)
1	4AC	2	53	1	21,24,25	1.06	2 (9%)	29,34,37	1.48	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	590	36,1	-	2/11/29/30	0/2/2/2
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
31	5MU	4	54	31	-	1/7/25/26	0/2/2/2
1	6MZ	2	1469	36,1	-	0/5/27/28	0/3/3/3
1	4AC	2	1028	1	-	2/11/29/30	0/2/2/2
31	4SU	4	8	31	-	5/7/25/26	0/2/2/2
1	4AC	2	319	1	-	4/11/29/30	0/2/2/2
1	4AC	2	851	1	-	4/11/29/30	0/2/2/2
1	4AC	2	731	1	-	3/11/29/30	0/2/2/2
1	4AC	2	868	1	-	2/11/29/30	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	5HM	2	1378	1	-	2/9/27/28	0/2/2/2
1	4AC	2	511	1	-	2/11/29/30	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	4AC	2	848	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1147	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
31	PSU	4	55	31	-	0/7/25/26	0/2/2/2
1	4AC	2	286	1	-	5/11/29/30	0/2/2/2
1	4AC	2	394	1	-	2/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	1184	1	-	2/11/29/30	0/2/2/2
1	4AC	2	546	1	-	2/11/29/30	0/2/2/2
1	4AC	2	957	1	-	1/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	2/7/25/26	0/2/2/2
1	B8H	2	938	1	-	3/7/25/26	0/2/2/2
1	4AC	2	1479	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	636	1	-	0/11/29/30	0/2/2/2
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	LHH	2	250	1	-	1/13/31/32	0/2/2/2
31	H2U	4	20	31	-	4/7/38/39	0/2/2/2
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1193	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1239	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1041	1	-	0/11/29/30	0/2/2/2
1	UR3	2	1467	1	-	6/7/25/26	0/2/2/2
1	A2M	2	373	1	-	1/5/27/28	0/3/3/3
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
1	4AC	2	17	1	-	0/11/29/30	0/2/2/2
1	4AC	2	379	1	-	2/11/29/30	0/2/2/2
1	4AC	2	828	1	-	0/11/29/30	0/2/2/2
31	OMC	4	32	31	-	2/9/27/28	0/2/2/2
1	5MC	2	939	1	-	0/7/25/26	0/2/2/2
1	MA6	2	1488	1	-	0/7/29/30	0/3/3/3
1	4AC	2	648	1	-	2/11/29/30	0/2/2/2
1	4AC	2	626	1	-	2/11/29/30	0/2/2/2
1	4AC	2	53	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	590	4AC	2	0
1	2	718	4AC	4	0
31	4	54	5MU	3	0
1	2	1469	6MZ	2	0
1	2	1028	4AC	2	0
31	4	8	4SU	2	0
1	2	319	4AC	3	0
1	2	851	4AC	6	0
1	2	731	4AC	4	0
1	2	868	4AC	3	0
1	2	1487	MA6	4	0
1	2	1378	5HM	4	0
1	2	511	4AC	1	0
1	2	703	4AC	6	0
1	2	848	4AC	2	0
1	2	1147	4AC	5	0
1	2	1233	4AC	6	0
31	4	55	PSU	3	0
1	2	286	4AC	1	0
1	2	394	4AC	4	0
1	2	1184	4AC	4	0
1	2	546	4AC	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	957	4AC	4	0
1	2	1202	5MC	3	0
1	2	938	B8H	1	0
1	2	1479	4AC	5	0
1	2	479	4AC	4	0
1	2	636	4AC	2	0
1	2	751	4AC	1	0
31	4	20	H2U	1	0
1	2	303	4AC	3	0
1	2	1193	4AC	3	0
1	2	1239	4AC	5	0
1	2	1041	4AC	4	0
1	2	1467	UR3	4	0
1	2	373	A2M	7	0
1	2	1376	OMC	2	0
1	2	17	4AC	3	0
1	2	379	4AC	2	0
1	2	828	4AC	3	0
31	4	32	OMC	3	0
1	2	939	5MC	1	0
1	2	1488	MA6	3	0
1	2	648	4AC	5	0
1	2	626	4AC	1	0
1	2	53	4AC	1	0
1	2	839	4AC	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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:

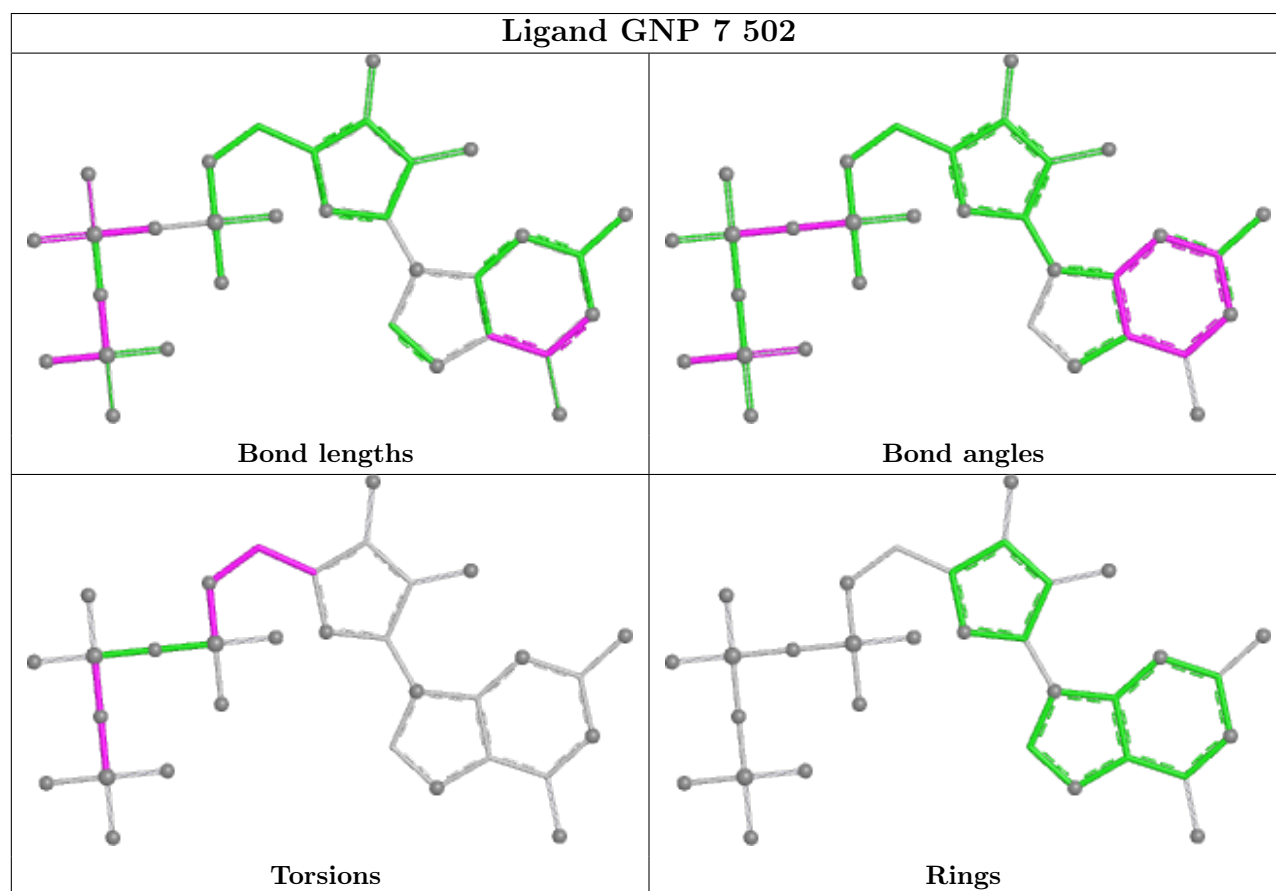
Mol	Chain	Res	Type	Atoms
39	7	502	GNP	PB-N3B-PG-O1G
39	7	502	GNP	PG-N3B-PB-O1B
39	7	502	GNP	C5'-O5'-PA-O3A
39	7	502	GNP	O4'-C4'-C5'-O5'
38	7	501	MET	CA-CB-CG-SD

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 [i](#)

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

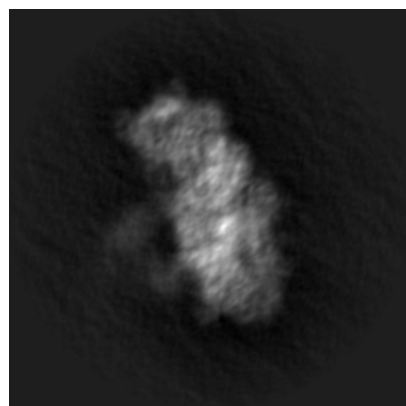
## 6 Map visualisation [i](#)

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.

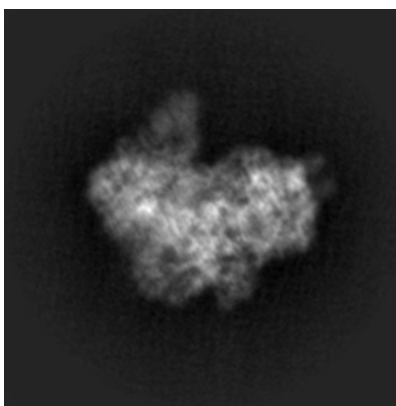
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

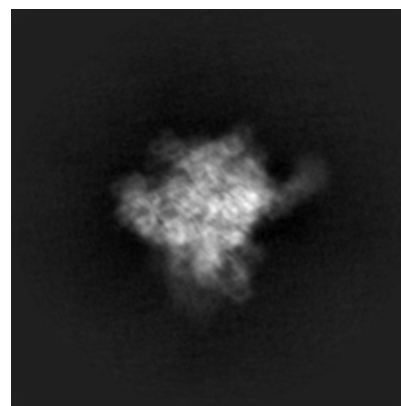
#### 6.1.1 Primary map



X

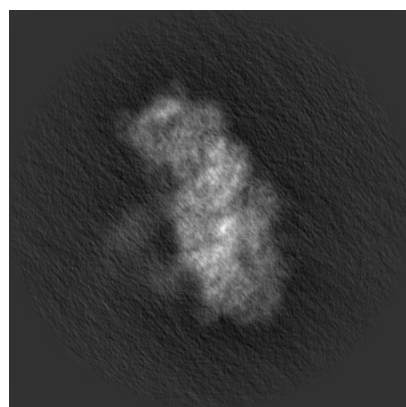


Y

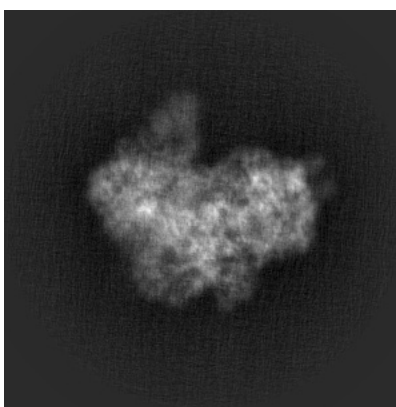


Z

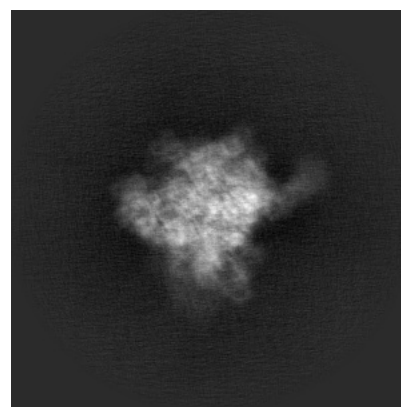
#### 6.1.2 Raw map



X



Y



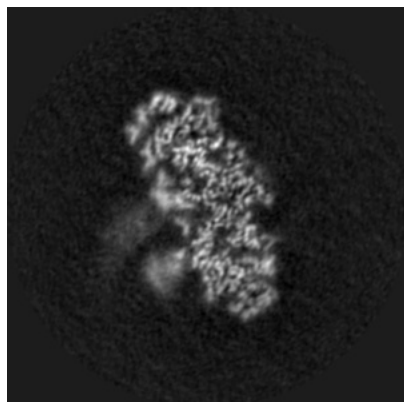
Z

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

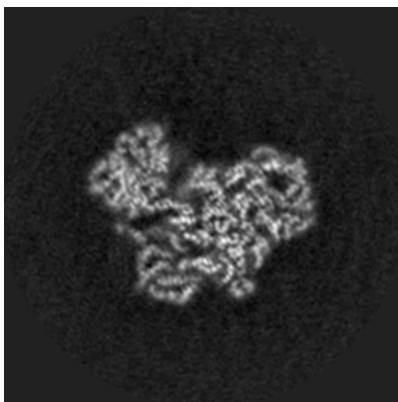


## 6.2 Central slices [i](#)

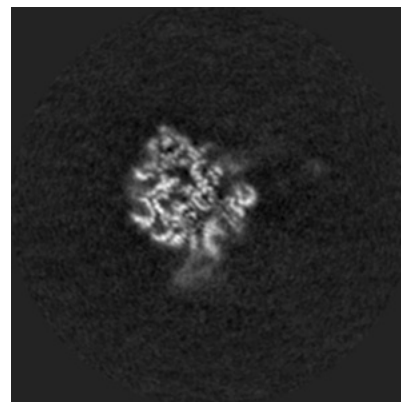
### 6.2.1 Primary map



X Index: 174

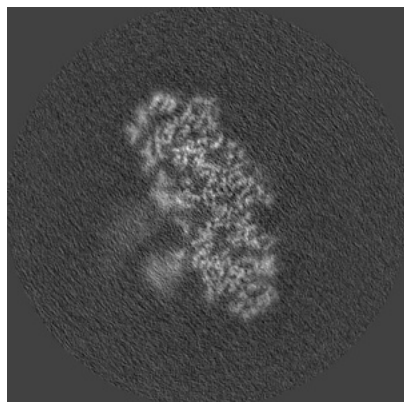


Y Index: 174

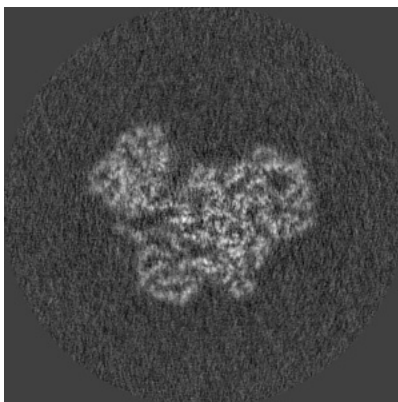


Z Index: 174

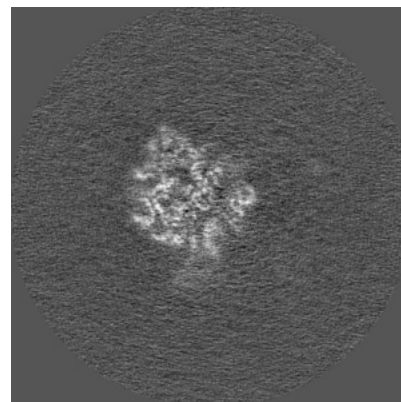
### 6.2.2 Raw map



X Index: 174



Y Index: 174

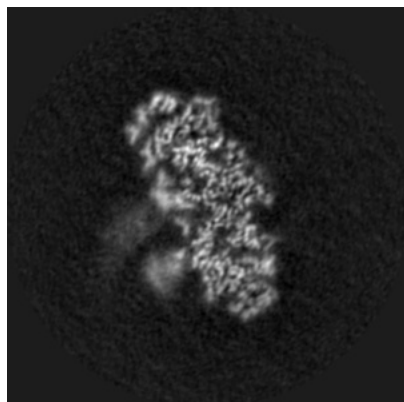


Z Index: 174

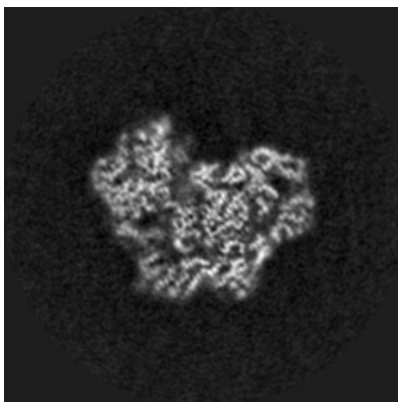
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

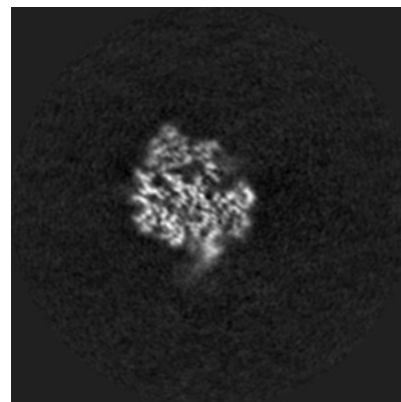
### 6.3.1 Primary map



X Index: 174

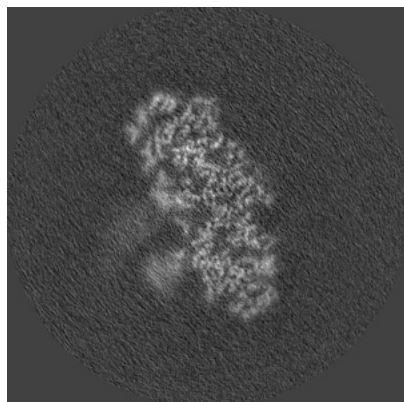


Y Index: 178

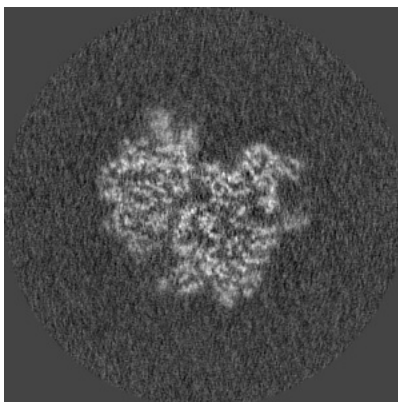


Z Index: 180

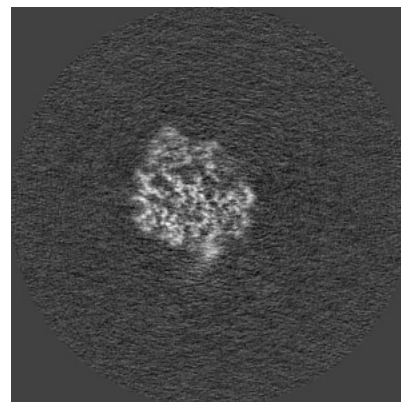
### 6.3.2 Raw map



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 surface views [i](#)

### 6.4.1 Primary map



X



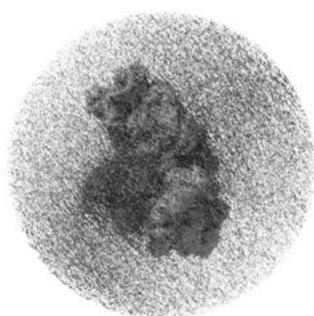
Y



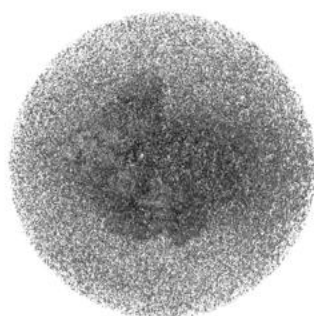
Z

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.

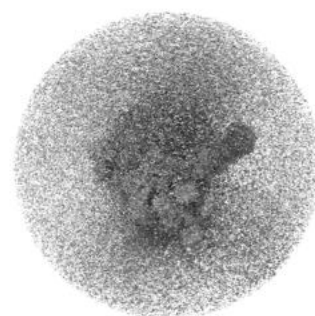
### 6.4.2 Raw map



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.

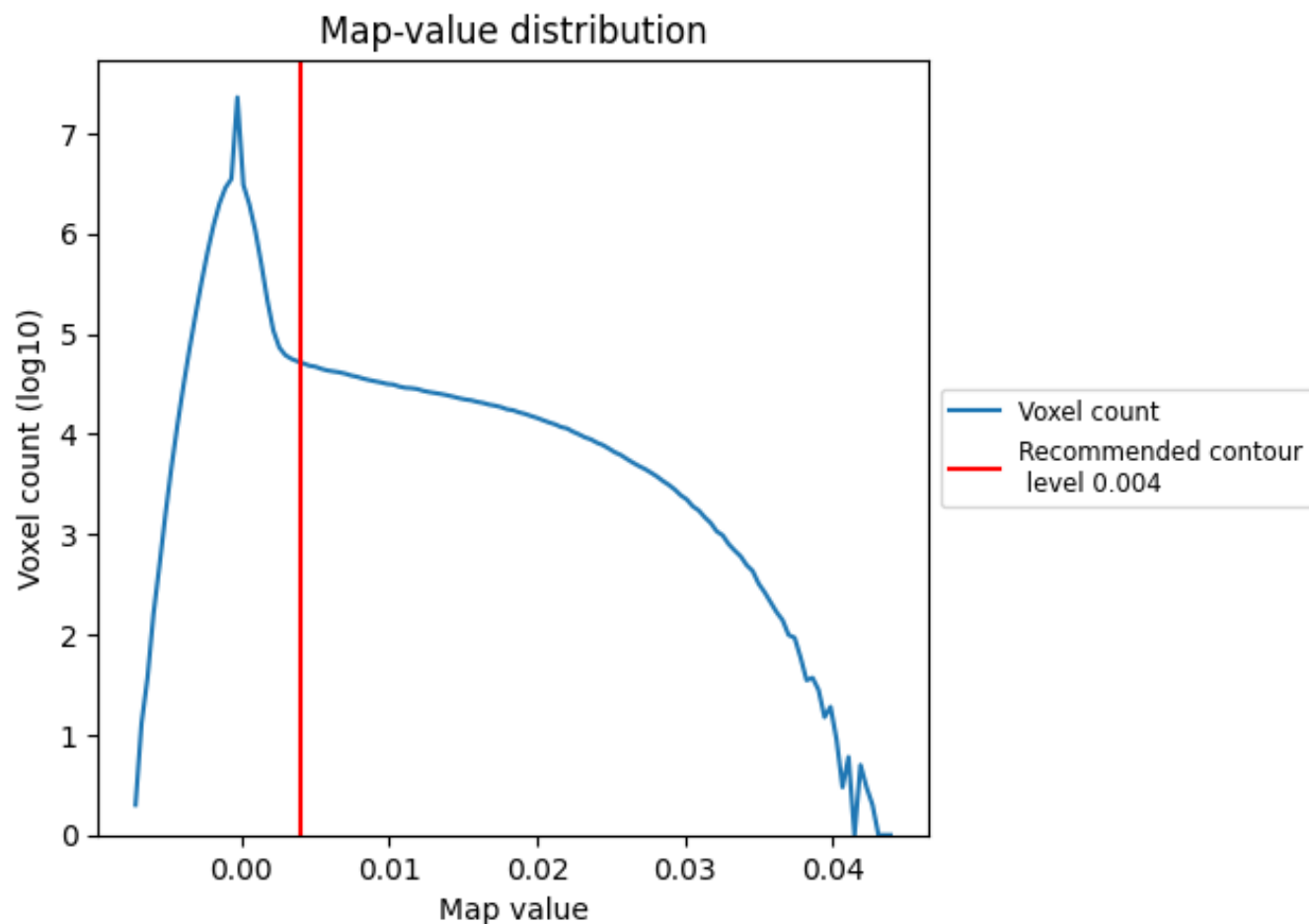
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

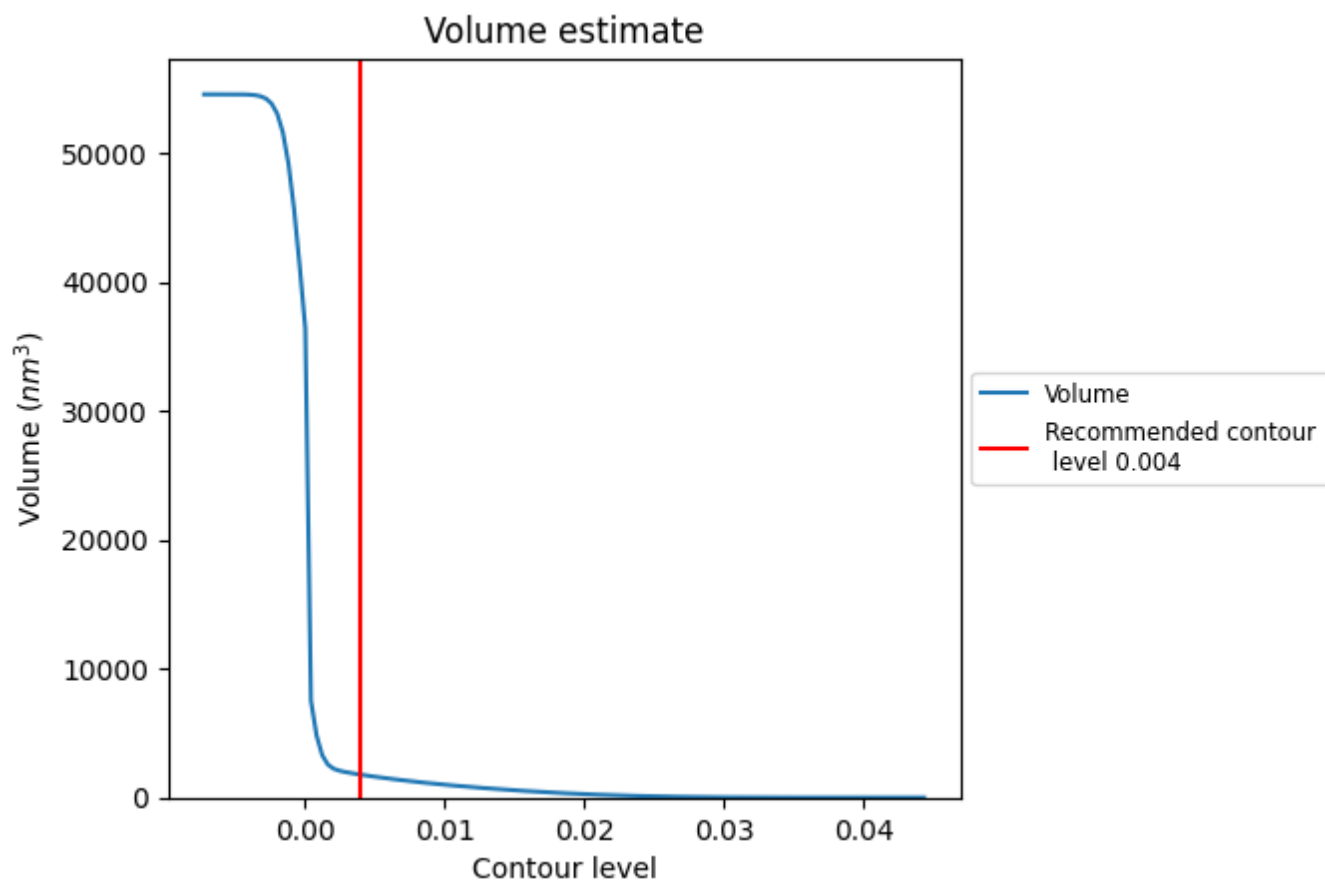
This section contains the results of statistical analysis of the map.

### 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.

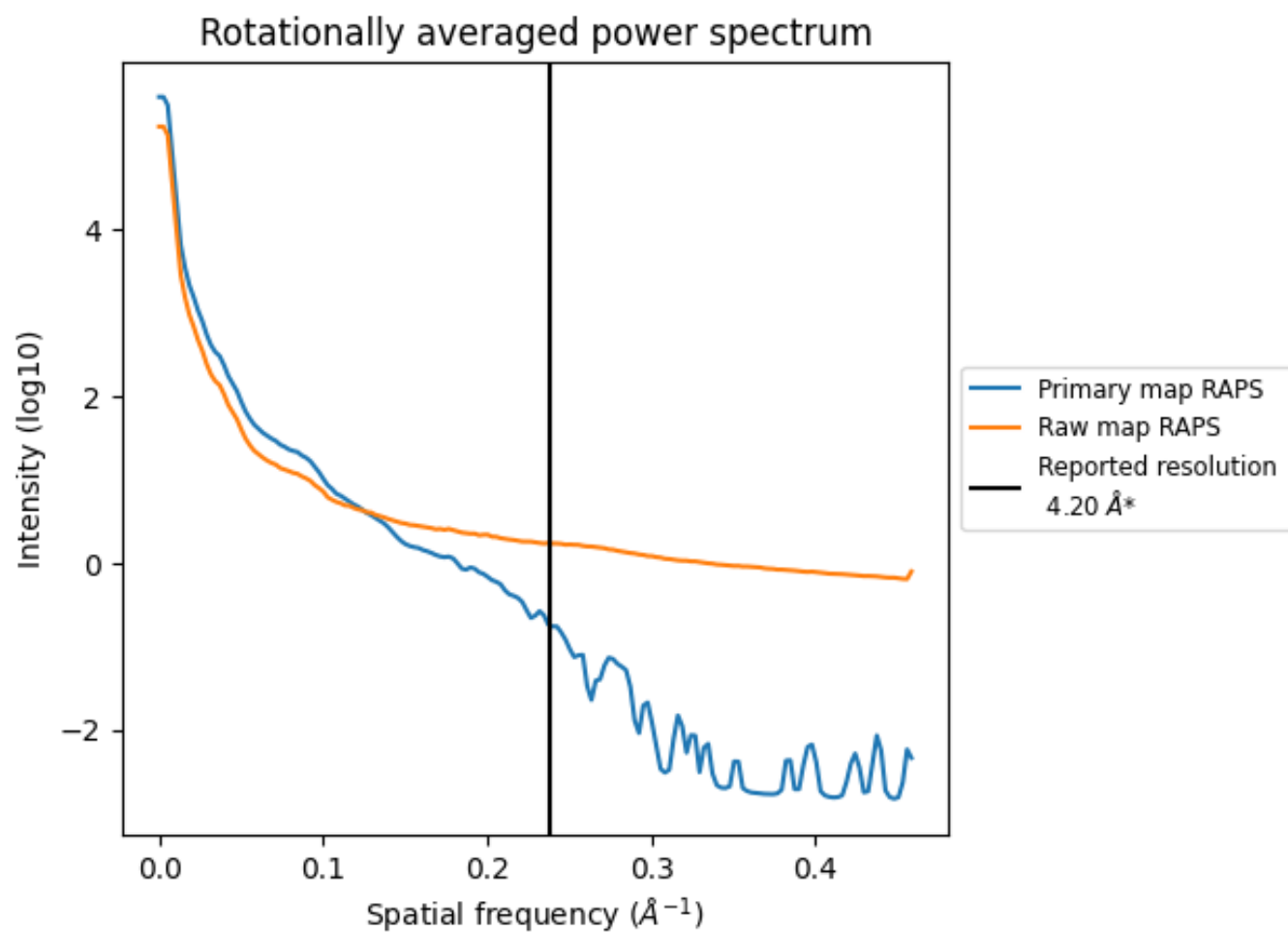
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1784  $\text{nm}^3$ ; 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 ⓘ

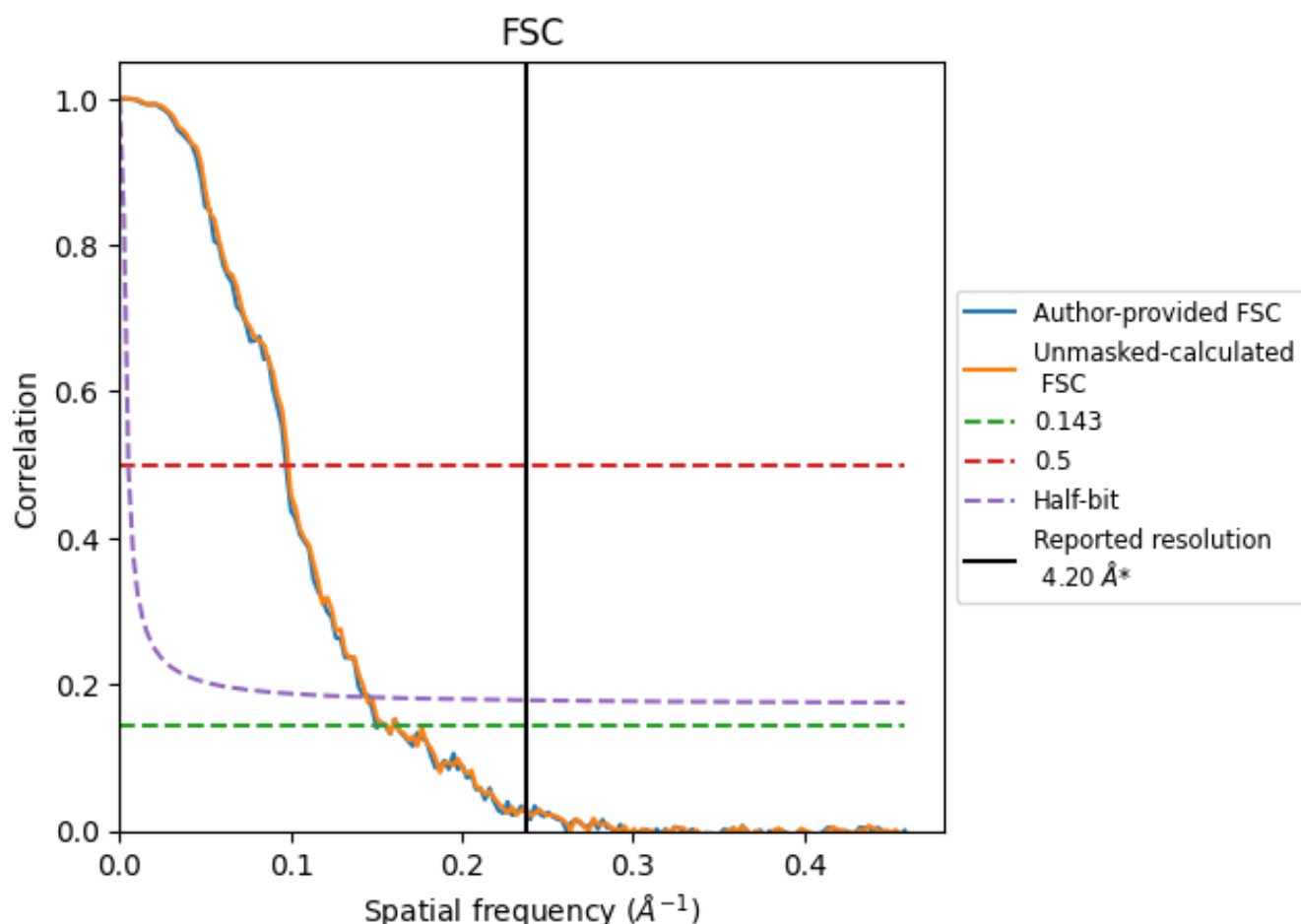


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 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 %

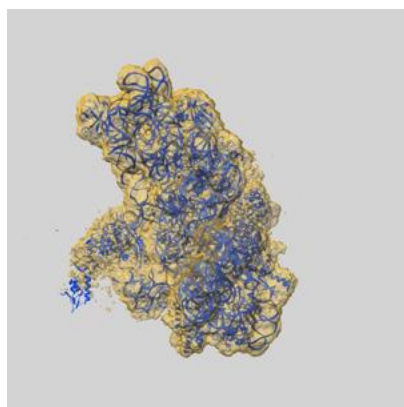
The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 4.2 by more than 10 %



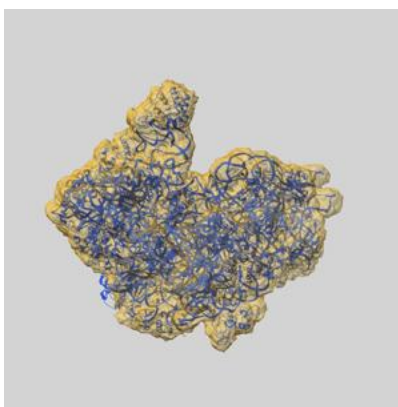
## 9 Map-model fit [i](#)

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.

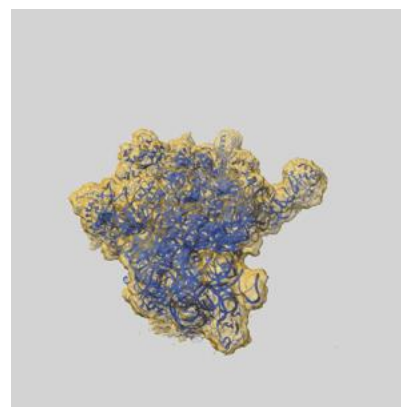
### 9.1 Map-model overlay [i](#)



X



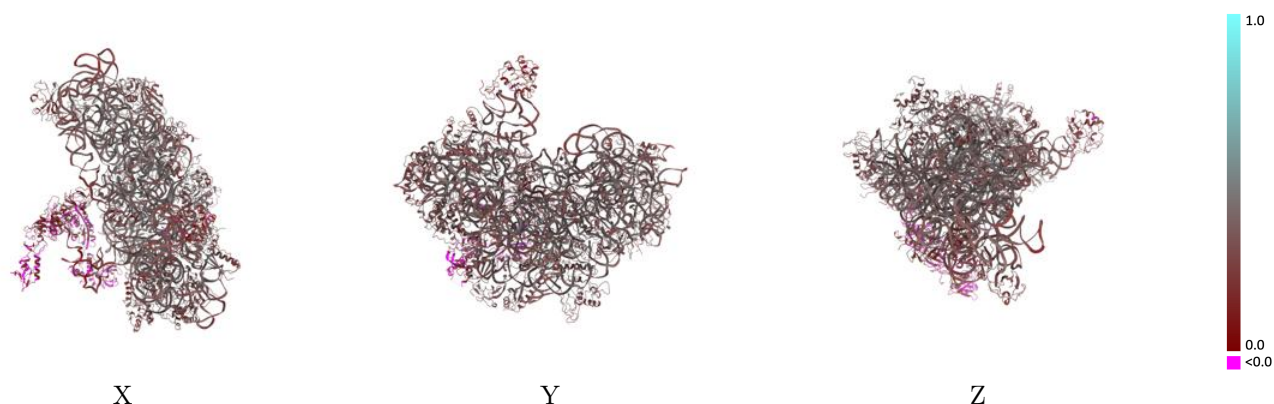
Y



Z

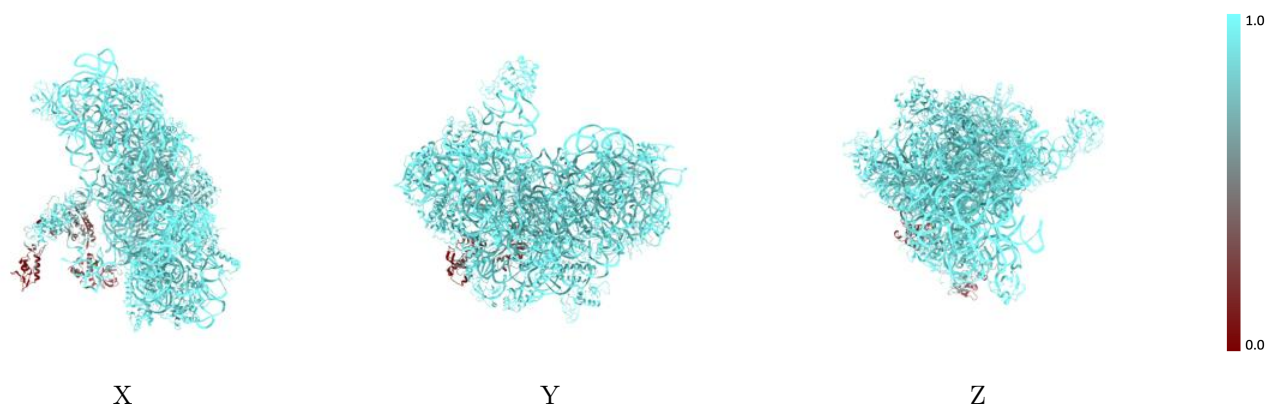
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



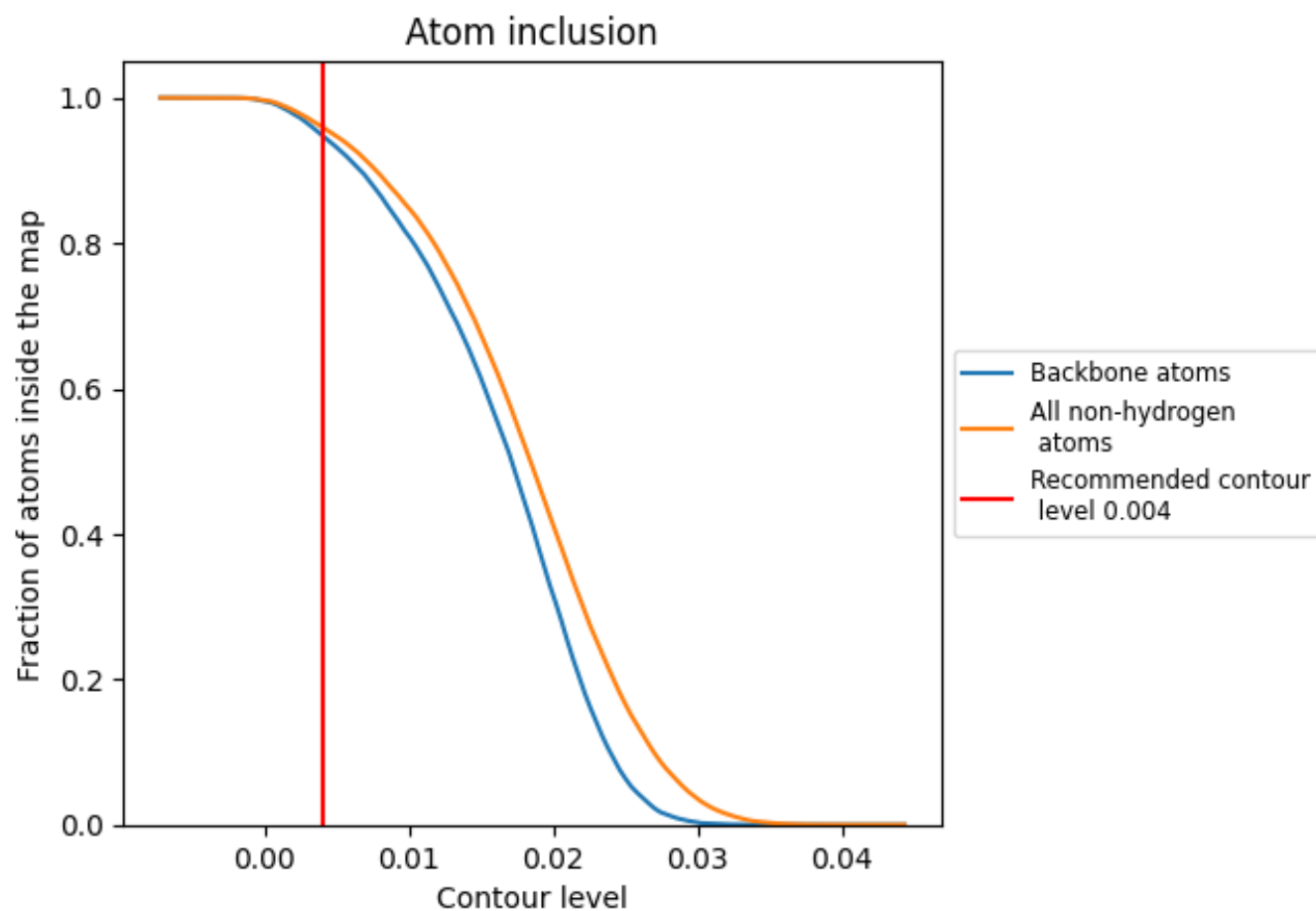
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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









































































## 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	 0.9969	 0.3730
2	 1.0000	 0.3830
3	 1.0000	 0.2200
4	 0.9871	 0.2310
5	 0.9977	 0.3390
6	 1.0000	 0.2490
7	 0.8601	 0.1420
8	 0.2744	 0.0540
9	 0.2583	 0.0380
A	 0.9960	 0.3430
B	 0.9967	 0.3580
C	 0.9937	 0.3660
D	 1.0000	 0.3580
E	 0.9990	 0.3700
F	 0.9932	 0.3750
G	 0.9979	 0.3170
H	 0.9964	 0.3410
I	 0.9980	 0.3770
J	 0.9979	 0.3550
K	 0.9981	 0.3510
L	 0.9975	 0.3520
M	 1.0000	 0.3570
N	 0.9982	 0.3830
O	 0.9981	 0.3280
P	 1.0000	 0.3620
Q	 0.9975	 0.3450
R	 0.9989	 0.3900
S	 0.9852	 0.3060
T	 0.9929	 0.3340
U	 0.9975	 0.3410
V	 0.9987	 0.3440
W	 0.9957	 0.3620
X	 1.0000	 0.3480
Y	 0.9899	 0.2050
Z	 0.9953	 0.3530

