wwPDB EM Validation Summary Report ⓘ

Oct 14, 2021 – 11:07 pm BST

PDB ID	:	7O1A
EMDB ID	:	EMD-12694
Title	:	Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome complex stalled in response to L-tryptophan
Authors	:	van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on	:	2021-03-29
Resolution	:	2.40 Å(reported)
Based on initial model	:	6TBV

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

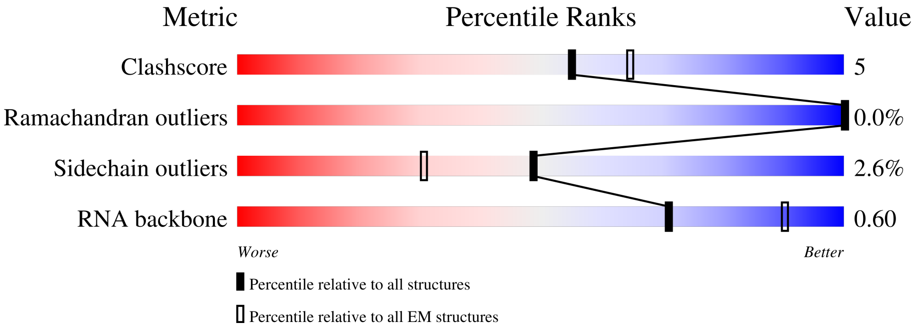
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

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

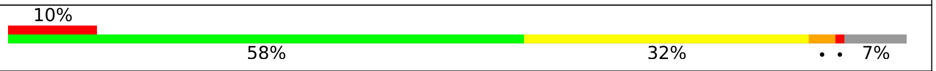
The reported resolution of this entry is 2.40 Å.

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 >=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 <=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	AA	1534	
2	AB	240	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	

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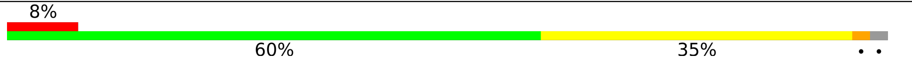
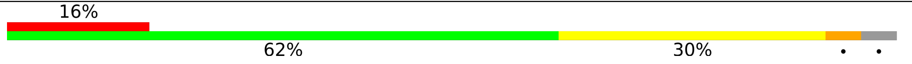
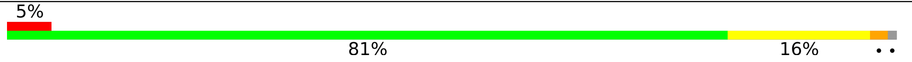
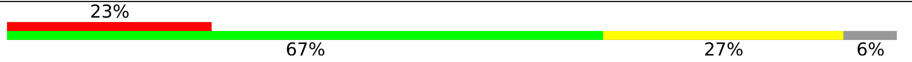
Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	

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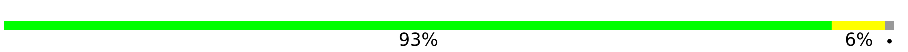
Mol	Chain	Length	Quality of chain
33	BL	144	
34	BM	136	
35	BN	127	
36	BO	117	
37	BP	115	
38	BQ	118	
39	BR	103	
40	BS	110	
41	BT	100	
42	BU	104	
43	BV	94	
44	BW	85	
45	BX	78	
46	BY	63	
47	BZ	59	
48	B0	57	
49	B1	55	
50	B2	46	
51	B3	65	
52	B4	38	
53	B5	17	
54	B7	9	
55	B8	77	

2 Entry composition ⓘ

There are 60 unique types of molecules in this entry. The entry contains 146602 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 Ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1534	32930	14694	6041	10661	1534	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AB	224	1753	1109	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AD	205	1643	1026	315	298	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	155	1144	711	216	211	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AF	106	862	545	156	154	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total 1181	C 735	N 227	O 215	S 4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total 979	C 616	N 173	O 184	S 6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	99	Total 795	C 498	N 152	O 144	S 1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total 877	C 540	N 174	O 160	S 3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total 957	C 591	N 196	O 165	S 5	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total 883	C 546	N 178	O 156	S 3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AN	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AO	88	714	439	144	130	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	AR	55	455	288	86	81	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	AS	82	656	419	125	110	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AT	86	670	414	138	115	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AU	56	465	290	96	78	1	0	0

- Molecule 22 is a RNA chain called Ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	BA	2897	62209	27759	11446	20107	2897	0	0

- Molecule 23 is a RNA chain called Ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	BB	120	2569	1144	468	837	120	0	0

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	BC	271	2082	1288	423	364	7	0	0

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BD	209	1566	980	288	294	4	0	0

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	BE	201	1552	974	283	290	5	0	0

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BF	177	1410	899	249	256	6	0	0

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BG	176	1323	832	243	246	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BH	149	1110	699	197	213	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BI	66	522	323	99	94	6	0	0

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BJ	142	1129	714	212	199	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BK	123	946	593	181	166	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	BL	144	1053	654	207	190	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	BM	136	1075	686	205	178	6	0	0

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BN	118	945	585	194	161	5	0	0

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BO	117	900	557	179	163	1	0	0

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BP	114	917	574	179	163	1	0	0

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	BQ	117	947	604	192	151	0	0

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	BR	103	816	516	153	145	2	0	0

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BS	110	857	532	166	156	3	0	0

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BT	93	738	466	139	131	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	BU	102	779	492	146	141	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BV	94	753	479	137	134	3	0	0

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BW	76	580	359	117	103	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BX	77	625	388	129	106	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BY	62	501	308	98	94	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BZ	58	449	281	87	79	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	B0	56	444	269	94	80	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	B1	51	414	266	76	72	0	0

- Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	B2	46	377	228	90	57	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	B3	64	504	323	105	74	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	B4	38	302	185	65	48	4	0	0

- Molecule 53 is a protein called TnaC - Tryptophanase leader peptide - R23F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	B5	17	146	97	24	25	0	0

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	B7	9	191	85	34	63	9	0	0

- Molecule 55 is a RNA chain called P-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total 1648	C 735	N 295	O 541	P 77	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AA	86	Total 86	Mg 86	0
56	BA	233	Total 233	Mg 233	0
56	BB	1	Total 1	Mg 1	0
56	BC	1	Total 1	Mg 1	0
56	BD	2	Total 2	Mg 2	0
56	BL	1	Total 1	Mg 1	0
56	B8	2	Total 2	Mg 2	0

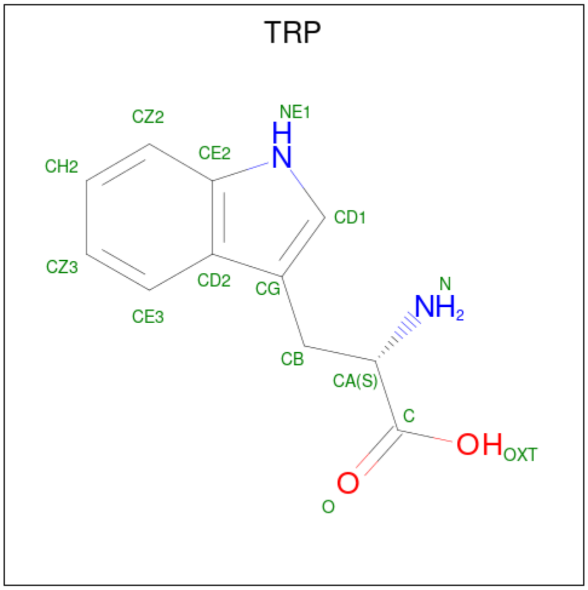
- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	AA	38	Total 38	K 38	0
57	AM	1	Total 1	K 1	0
57	BA	104	Total 104	K 104	0
57	BB	1	Total 1	K 1	0
57	BC	1	Total 1	K 1	0
57	BD	1	Total 1	K 1	0
57	BM	1	Total 1	K 1	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
58	AB	1	Total Zn 1 1	0
58	BI	1	Total Zn 1 1	0
58	B4	1	Total Zn 1 1	0

- Molecule 59 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms	AltConf
59	BA	1	Total C N O 15 11 2 2	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	AA	184	Total O 184 184	0
60	AK	1	Total O 1 1	0
60	AN	1	Total O 1 1	0
60	BA	1672	Total O 1672 1672	0
60	BB	2	Total O 2 2	0
60	BC	38	Total O 38 38	0

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Mol	Chain	Residues	Atoms	AltConf
60	BD	14	Total O 14 14	0
60	BE	21	Total O 21 21	0
60	BF	1	Total O 1 1	0
60	BJ	2	Total O 2 2	0
60	BK	3	Total O 3 3	0
60	BL	14	Total O 14 14	0
60	BM	2	Total O 2 2	0
60	BN	9	Total O 9 9	0
60	BO	1	Total O 1 1	0
60	BP	2	Total O 2 2	0
60	BQ	12	Total O 12 12	0
60	BR	4	Total O 4 4	0
60	BS	7	Total O 7 7	0
60	BT	3	Total O 3 3	0
60	BU	1	Total O 1 1	0
60	BW	5	Total O 5 5	0
60	BX	4	Total O 4 4	0
60	B0	4	Total O 4 4	0
60	B2	6	Total O 6 6	0
60	B3	7	Total O 7 7	0
60	B4	1	Total O 1 1	0

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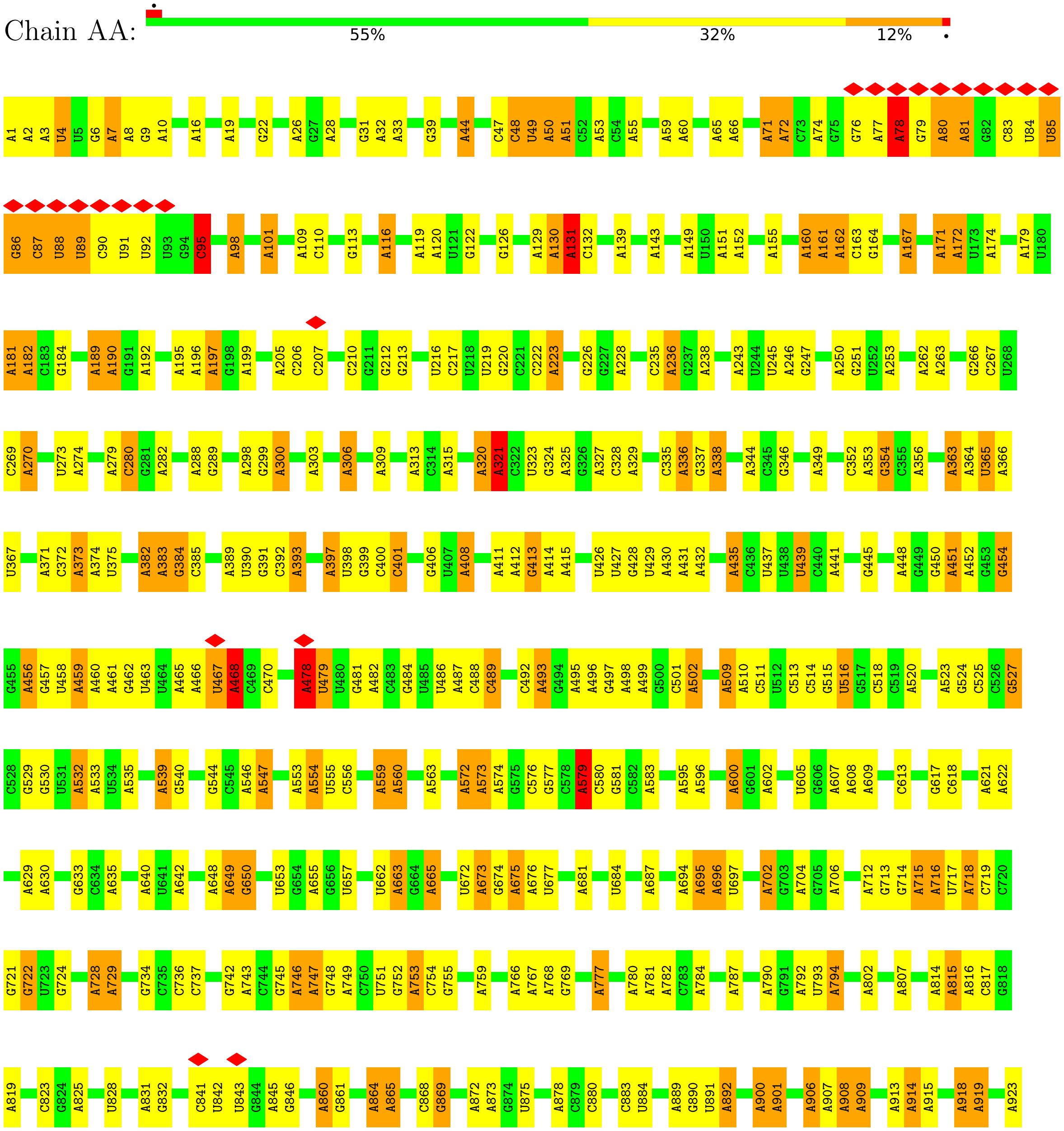
Mol	Chain	Residues	Atoms	AltConf
60	B5	2	Total O 2 2	0
60	B8	3	Total O 3 3	0

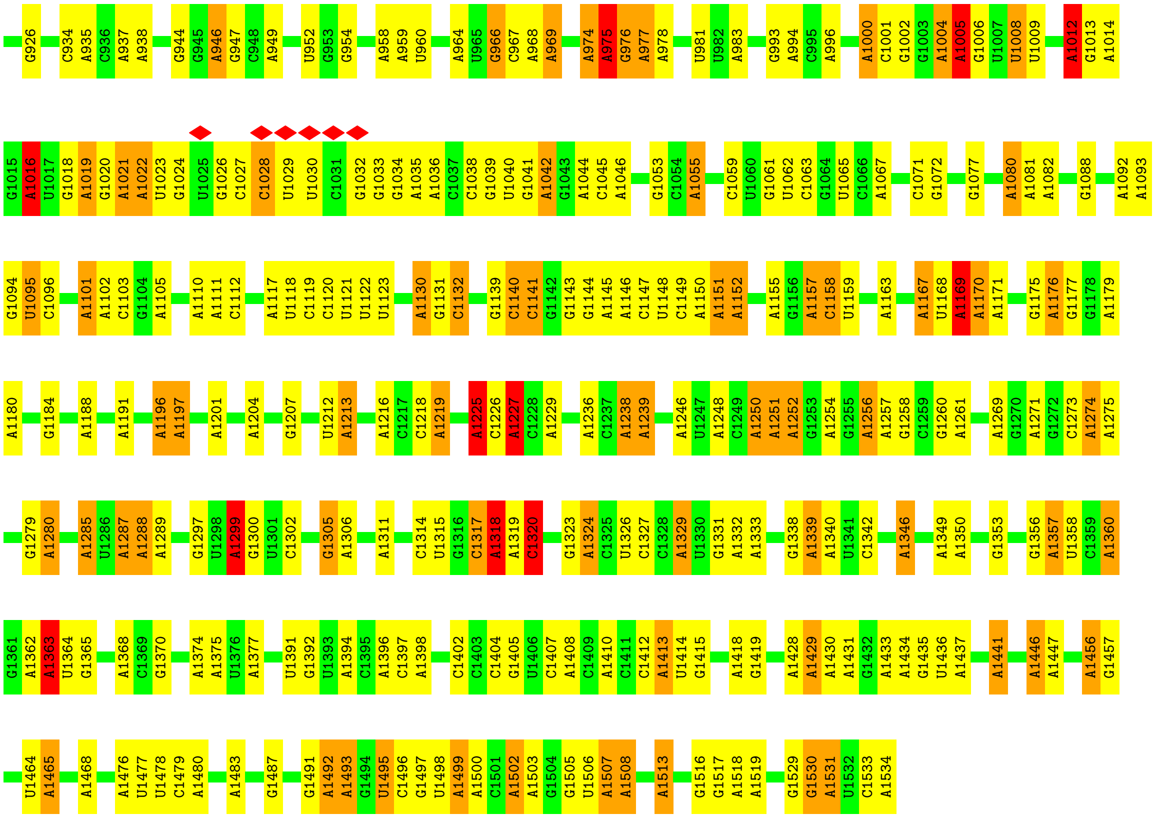
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ribosomal RNA 16S

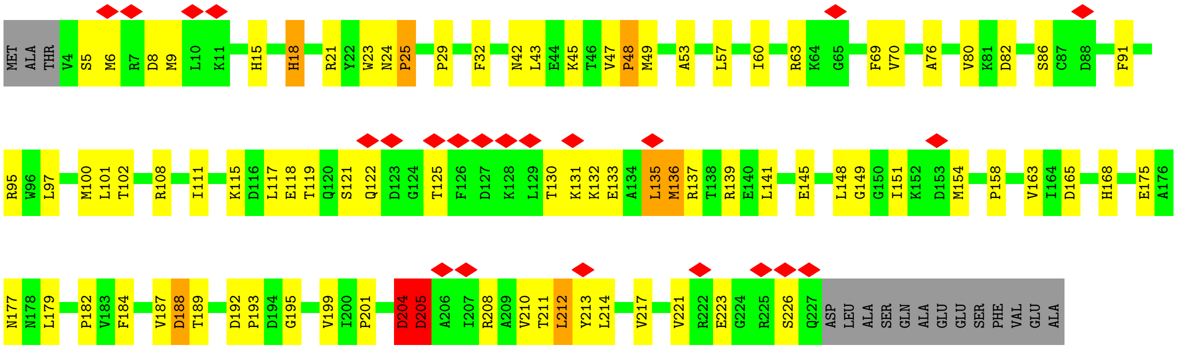
Chain AA:





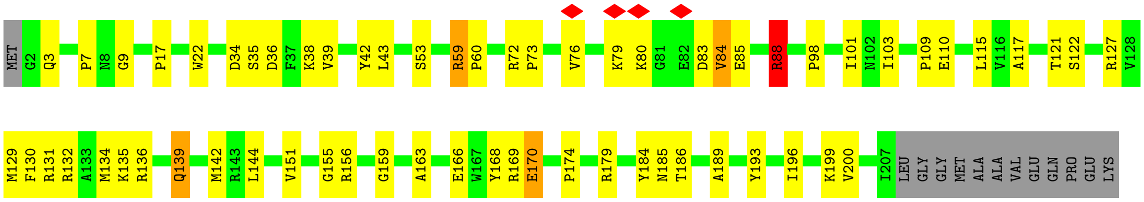
- Molecule 2: 30S ribosomal protein S2

Chain AB:



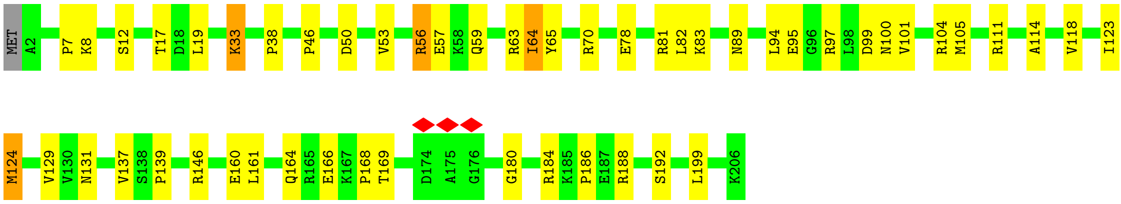
- Molecule 3: 30S ribosomal protein S3

Chain AC:



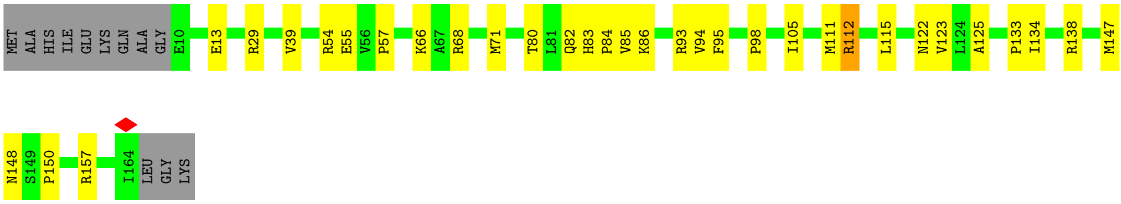
- Molecule 4: 30S ribosomal protein S4

Chain AD:



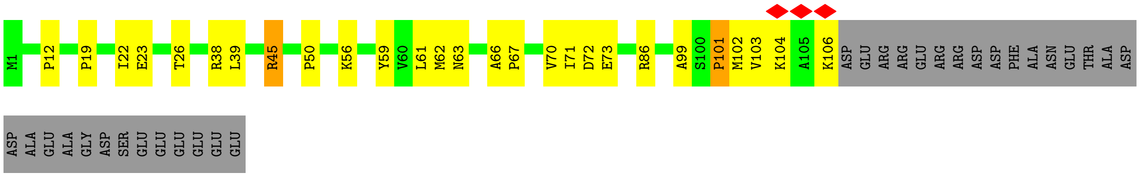
- Molecule 5: 30S ribosomal protein S5

Chain AE:



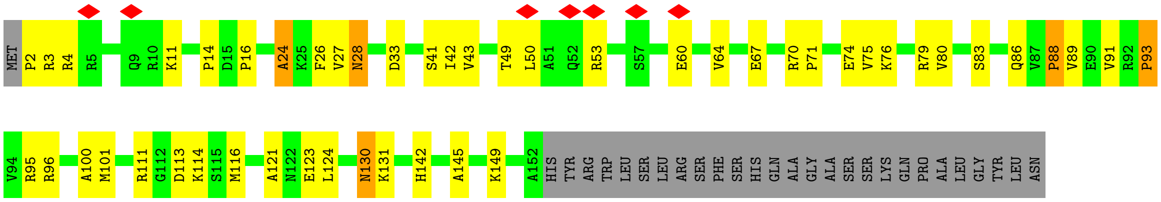
- Molecule 6: 30S ribosomal protein S6

Chain AF:



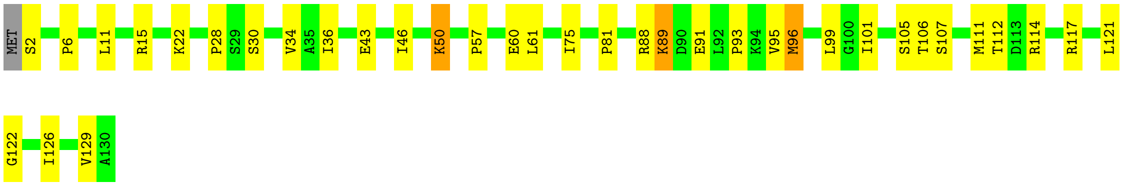
- Molecule 7: 30S ribosomal protein S7

Chain AG:



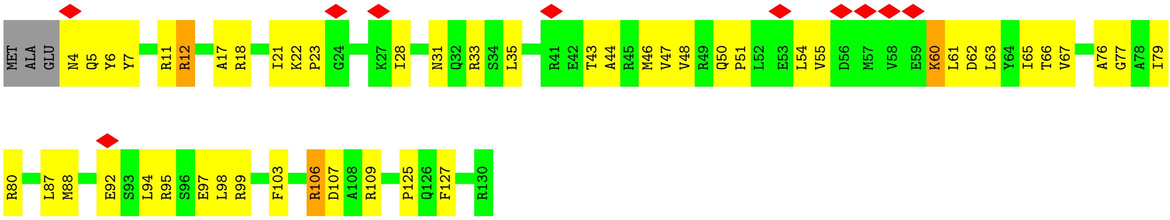
- Molecule 8: 30S ribosomal protein S8

Chain AH:



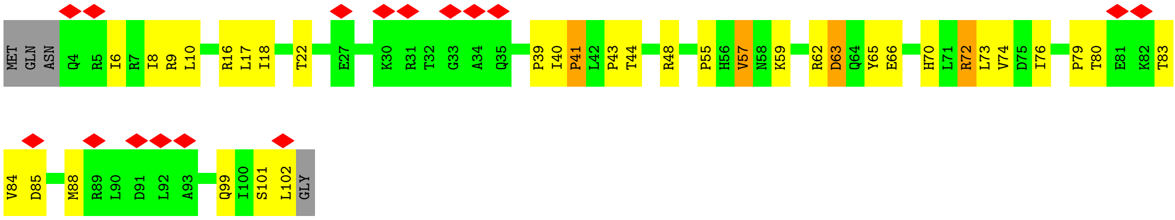
- Molecule 9: 30S ribosomal protein S9

Chain AI:



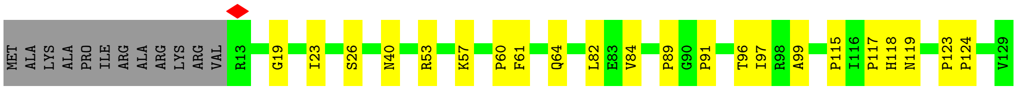
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



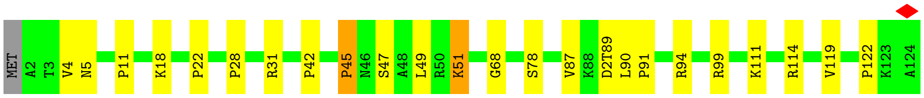
- Molecule 11: 30S ribosomal protein S11

Chain AK:



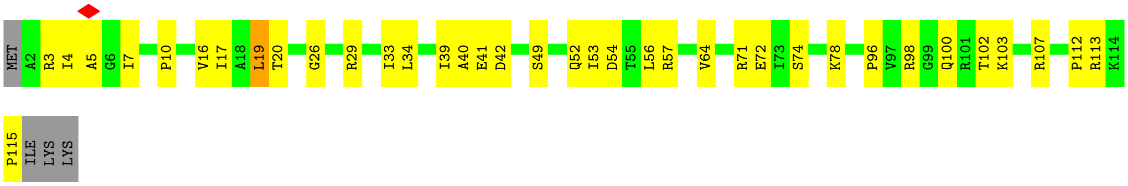
- Molecule 12: 30S ribosomal protein S12

Chain AL:



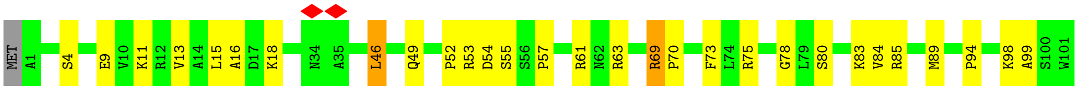
- Molecule 13: 30S ribosomal protein S13

Chain AM:



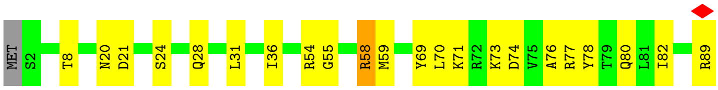
- Molecule 14: 30S ribosomal protein S14

Chain AN:



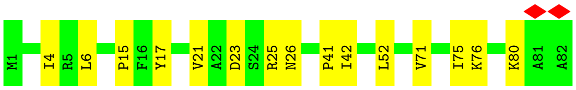
- Molecule 15: 30S ribosomal protein S15

Chain AO:



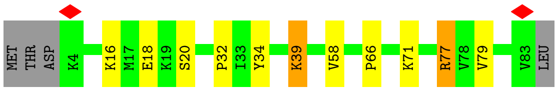
- Molecule 16: 30S ribosomal protein S16

Chain AP:



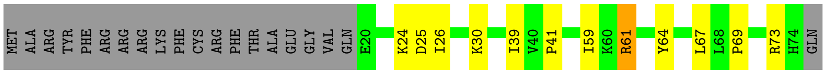
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



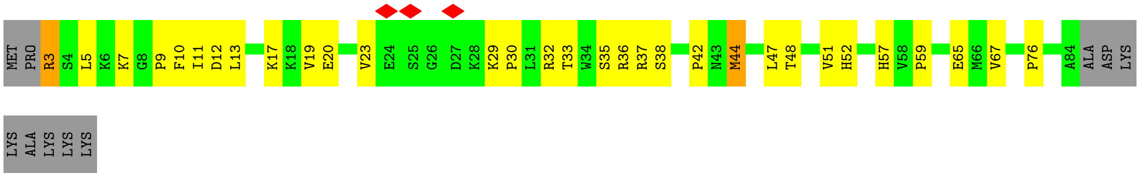
- Molecule 18: 30S ribosomal protein S18

Chain AR:



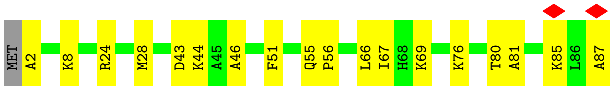
- Molecule 19: 30S ribosomal protein S19

Chain AS:



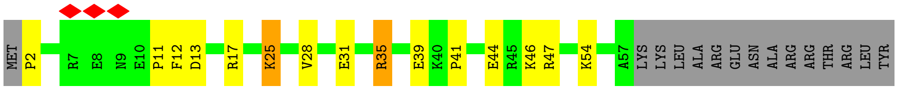
- Molecule 20: 30S ribosomal protein S20

Chain AT:



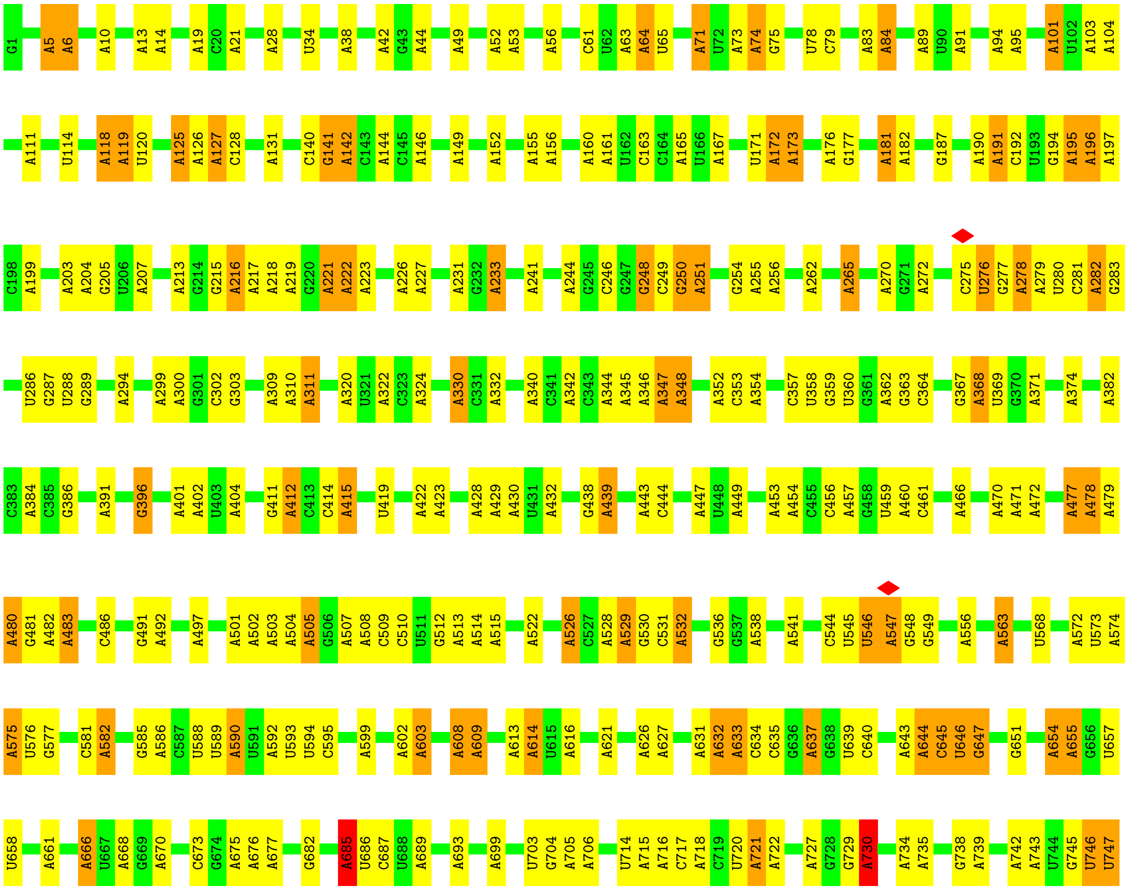
- Molecule 21: 30S ribosomal protein S21

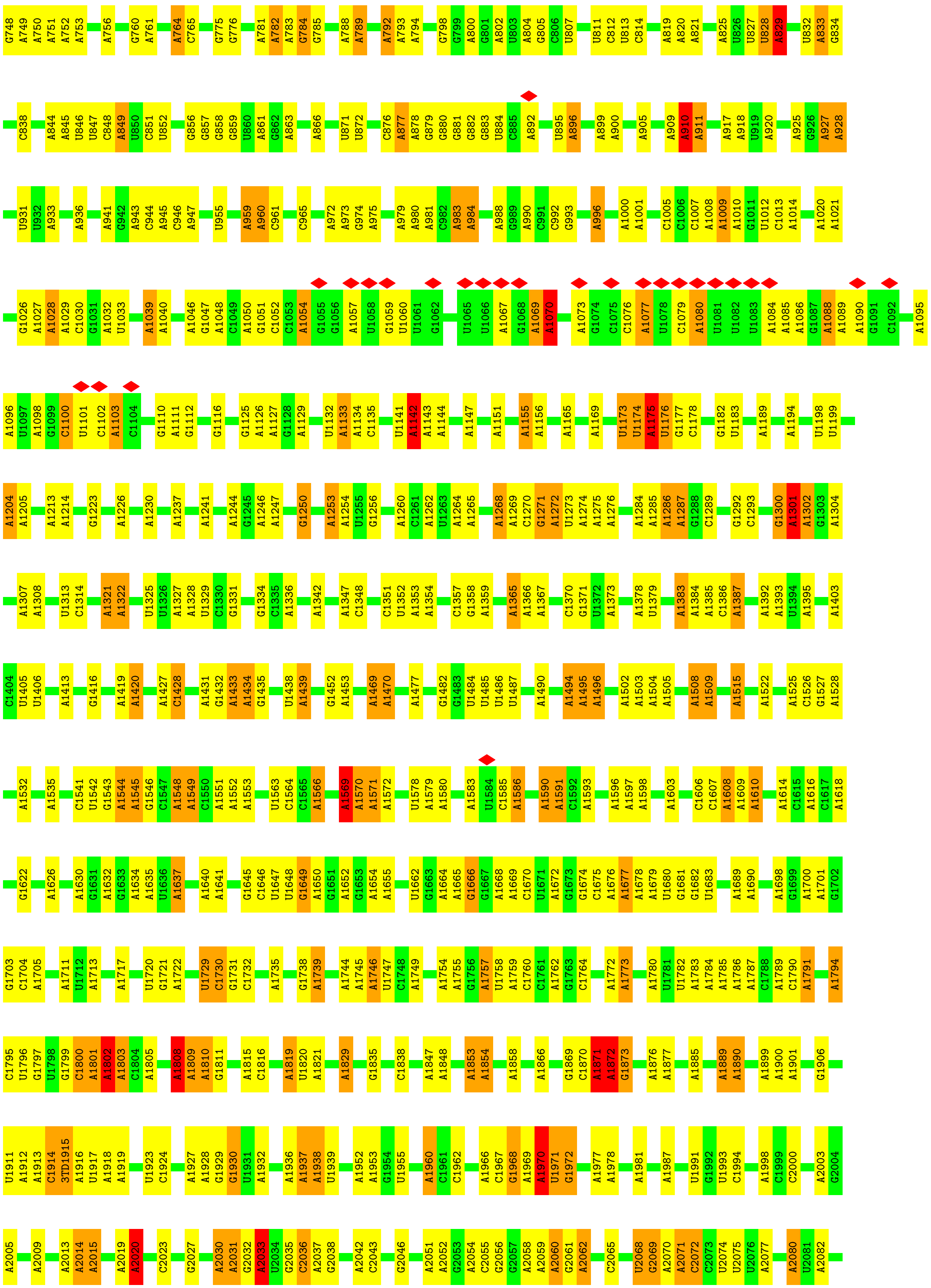
Chain AU:



- Molecule 22: Ribosomal RNA 23S

Chain BA:

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C838 A844 A845 U846 U847 C848 A849 U850 C851 U852 G856 G857 G858 G859 U860 A861 G862 A863 A866 U871 U872 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A892 U895 A896 A899 A900 A905 A909 A910 A911 A917 A918 U919 A920 A925 G926 A927 A928
U931 U932 A933 A936 A941 G942 A943 C944 A945 C946 A947 U955 A959 A960 C961 C965 A972 A973 G974 A975 A979 A980 A981 C982 A983 A984 A988 G989 A990 C991 C992 G993 A996 A1000 A1001 C1005 C1006 C1007 A1008 A1009 A1010 G1011 U1012 C1013 A1014 A1020 A1021
G1026 A1027 A1028 A1029 C1030 G1031 A1032 U1033 A1039 A1040 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 U1065 U1066 A1067 G1068 A1069 A1070 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 A1095
A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 G1110 A1111 G1112 G1116 G1125 A1126 A1127 G1128 A1129 U1132 A1133 A1134 C1135 U1141 A1142 A1143 A1144 A1147 A1151 A1155 A1156 A1165 A1169 U1173 U1174 A1175 U1176 G1177 C1178 G1182 U1183 A1189 A1194 U1198 U1199
A1204 A1205 A1213 A1214 G1223 A1226 A1230 A1237 A1241 A1244 G1245 A1246 A1247 G1250 A1253 A1254 U1255 G1256 A1260 C1261 A1262 U1263 A1264 A1265 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 A1284 A1285 A1286 A1287 G1288 C1289 G1292 C1293 G1300 A1301 A1302 G1303 A1304
A1307 A1308 U1313 C1314 A1321 A1322 U1325 U1326 A1327 A1328 U1329 C1330 G1331 G1334 C1335 A1336 A1342 A1347 C1348 C1351 U1352 A1353 A1354 C1357 G1358 A1359 A1365 A1366 A1367 C1370 G1371 U1372 A1373 A1378 U1379 A1383 A1384 A1385 C1386 A1387 A1392 A1393 U1394 A1395 A1403
C1404 U1405 U1406 A1413 G1416 A1419 A1420 A1427 C1428 A1431 G1432 A1433 A1434 G1435 U1438 A1439 G1452 A1453 A1469 A1470 A1477 G1482 G1483 U1484 U1485 U1486 U1487 A1490 A1494 A1495 A1496 A1502 A1503 A1504 A1505 A1508 A1509 A1515 A1522 A1525 C1526 G1527 A1528
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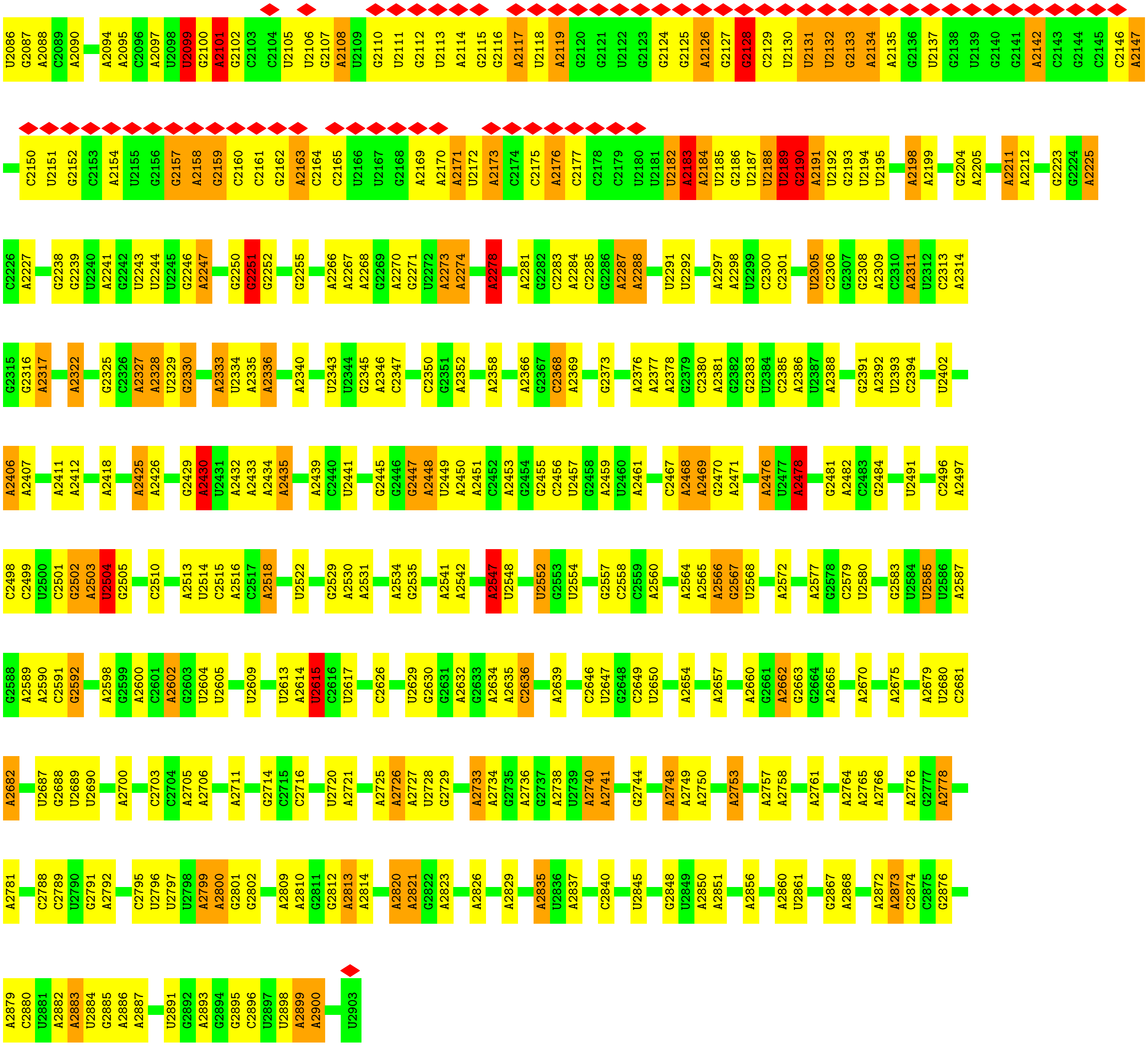
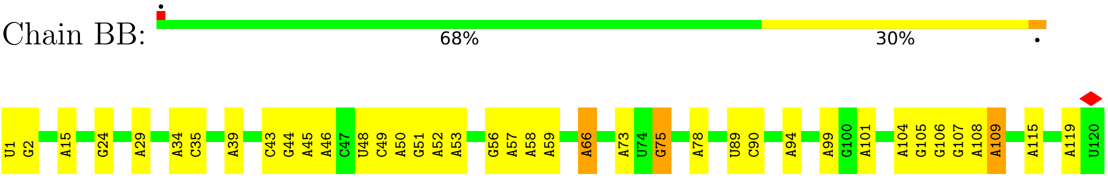
G1622 A1626 A1630 G1631 A1632 G1633 A1634 A1635 U1636 A1637 A1640 A1641 G1645 C1646 U1647 U1648 G1649 A1650 G1651 A1652 G1653 A1654 A1655 U1662 G1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 A1672 G1673 G1674 C1675 A1676 A1677 A1678 A1679 U1680 G1681 G1682 U1683 A1689 A1690 A1698 G1699 A1700 A1701 G1702
G1703 C1704 A1705 A1711 U1712 A1713 A1717 U1720 G1721 A1722 U1729 C1730 G1731 C1732 A1735 G1738 A1739 A1744 A1745 A1746 U1747 C1748 A1749 A1754 A1755 G1756 A1757 U1758 A1759 C1760 C1761 A1762 G1763 C1764 A1772 A1773 A1780 U1781 U1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 A1794
C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 C1804 A1805 A1808 A1809 A1810 G1811 A1815 C1816 A1819 U1820 A1821 A1829 G1835 C1838 A1847 A1848 A1853 A1854 A1858 A1866 G1869 C1870 A1871 A1872 G1873 A1876 A1877 A1885 A1889 A1890 A1899 A1900 A1901 G1906
U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1918 A1919 U1923 C1924 A1927 A1928 G1929 G1930 U1931 A1932 A1936 A1937 A1938 U1939 A1952 A1953 G1954 U1955 A1960 C1961 C1962 A1966 C1967 G1968 A1969 A1970 U1971 G1972 A1977 A1978 A1981 A1987 U1991 G1992 U1993 C1994 A1998 C1999 C2000 A2003 G2004
A2005 A2009 A2013 A2014 A2015 A2019 A2020 C2023 G2027 A2030 A2031 G2032 A2033 U2034 G2035 C2036 A2037 G2038 A2042 C2043 G2046 A2051 A2052 G2053 A2054 C2055 G2056 G2057 A2058 A2059 A2060 G2061 A2062 C2065 U2068 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2076 A2077 A2080 U2081 A2082



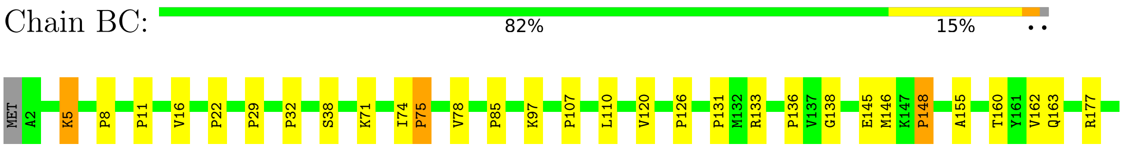
- Molecule 23: Ribosomal RNA 5S

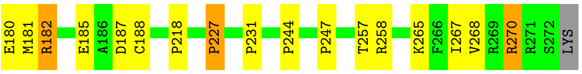
Chain BB:



- Molecule 24: 50S ribosomal protein L2

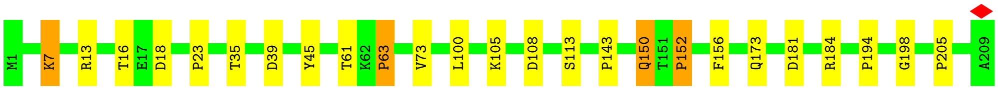
Chain BC:





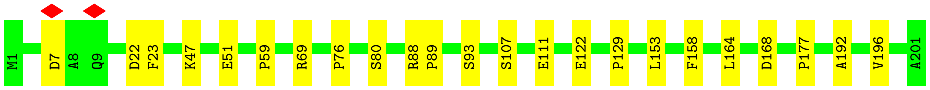
- Molecule 25: 50S ribosomal protein L3

Chain BD:



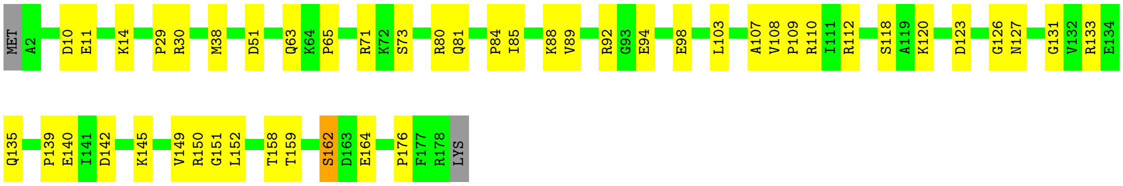
- Molecule 26: 50S ribosomal protein L4

Chain BE:



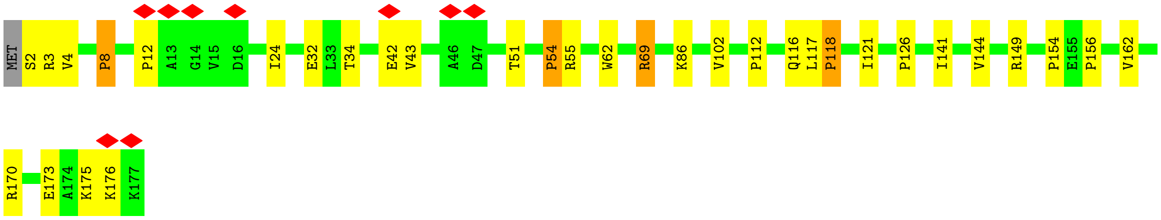
- Molecule 27: 50S ribosomal protein L5

Chain BF:



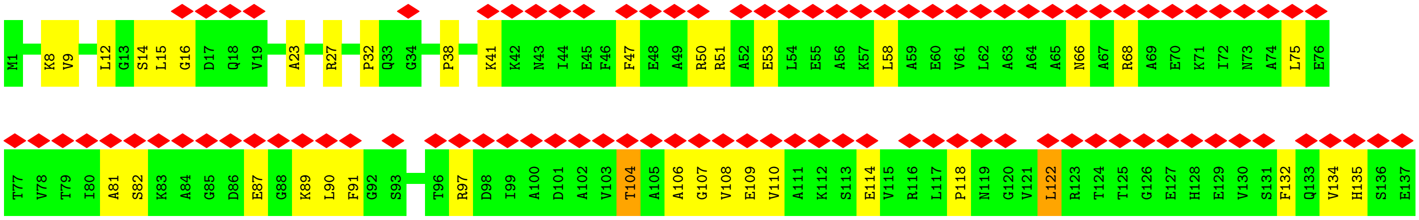
- Molecule 28: 50S ribosomal protein L6

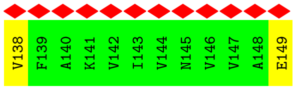
Chain BG:



- Molecule 29: 50S ribosomal protein L9

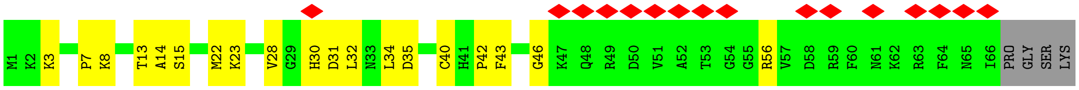
Chain BH:





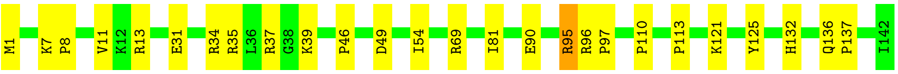
- Molecule 30: 50S ribosomal protein L31

Chain BI:

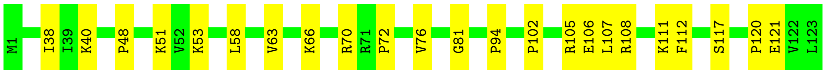
- Molecule 31: 50S ribosomal protein L13

Chain BJ:

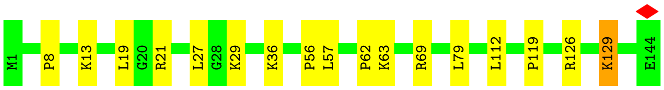
- Molecule 32: 50S ribosomal protein L14

Chain BK:

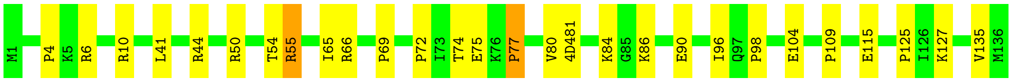
- Molecule 33: 50S ribosomal protein L15

Chain BL:

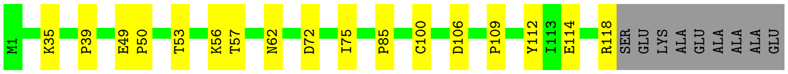
- Molecule 34: 50S ribosomal protein L16

Chain BM:

- Molecule 35: 50S ribosomal protein L17

Chain BN:

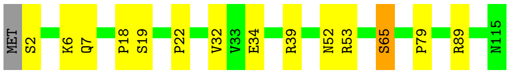



- Molecule 36: 50S ribosomal protein L18

Chain BO:

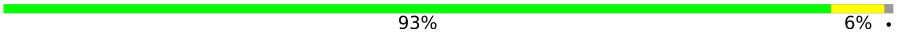

- Molecule 37: 50S ribosomal protein L19

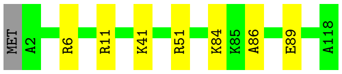
Chain BP:



- Molecule 38: 50S ribosomal protein L20

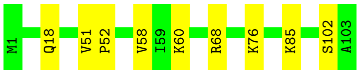
Chain BQ:





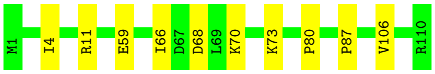
- Molecule 39: 50S ribosomal protein L21

Chain BR:



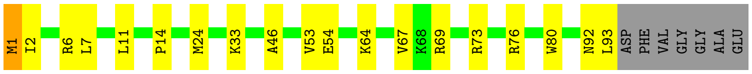
- Molecule 40: 50S ribosomal protein L22

Chain BS:



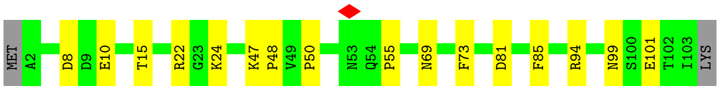
- Molecule 41: 50S ribosomal protein L23

Chain BT:



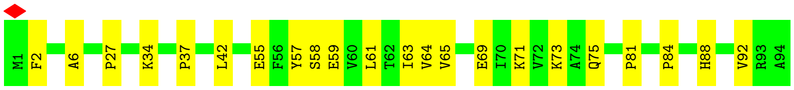
- Molecule 42: 50S ribosomal protein L24

Chain BU:



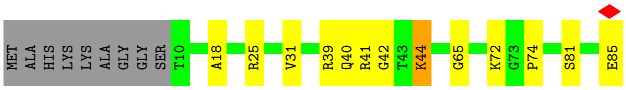
- Molecule 43: 50S ribosomal protein L25

Chain BV:



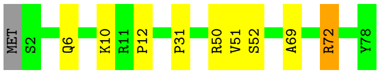
- Molecule 44: 50S ribosomal protein L27

Chain BW:



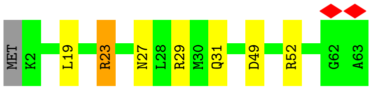
- Molecule 45: 50S ribosomal protein L28

Chain BX:



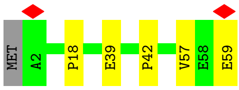
- Molecule 46: 50S ribosomal protein L29

Chain BY:



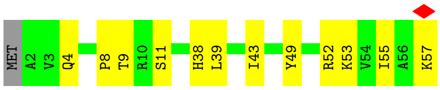
- Molecule 47: 50S ribosomal protein L30

Chain BZ:



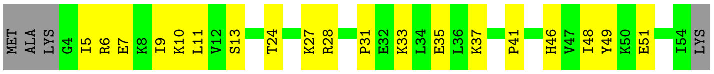
- Molecule 48: 50S ribosomal protein L32

Chain B0:



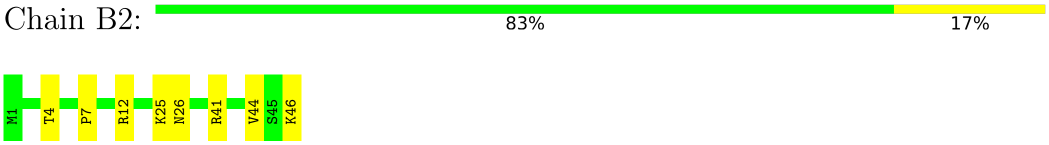
- Molecule 49: 50S ribosomal protein L33

Chain B1:



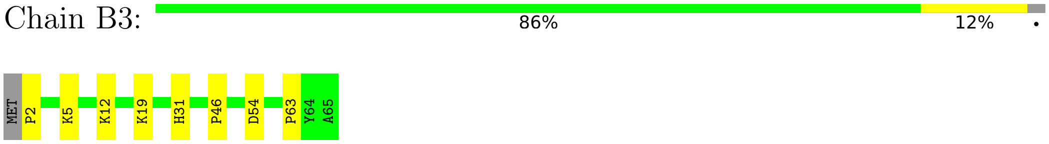
- Molecule 50: 50S ribosomal protein L34

Chain B2:



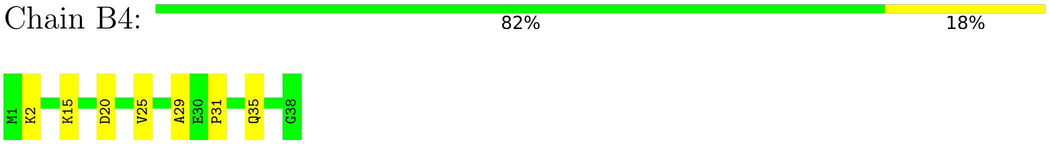
- Molecule 51: 50S ribosomal protein L35

Chain B3:



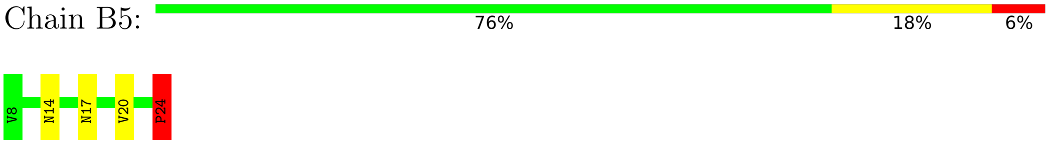
- Molecule 52: 50S ribosomal protein L36

Chain B4:



- Molecule 53: TnaC - Tryptophanase leader peptide - R23F

Chain B5:

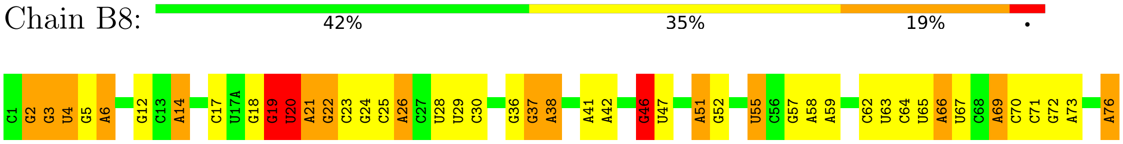


- Molecule 54: mRNA

Chain B7:

- Molecule 55: P-site tRNA-Pro

Chain B8:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	191230	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 $(e^-/\text{Å}^2)$	44	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-1600	Depositor
Magnification	59880	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	271.375, 271.375, 271.375	wwPDB
Map dimensions	325, 325, 325	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, G7M, 6MZ, ZN, 2MG, 5MU, MEQ, K, OMC, 2MA, D2T, 1MG, MA6, 4D4, 3TD, 5MC, 4OC, MG, PSU, OMU, OMG

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	AA	1.48	1296/36593 (3.5%)	3.33	3996/57081 (7.0%)
2	AB	0.90	9/1784 (0.5%)	1.10	13/2403 (0.5%)
3	AC	0.86	7/1651 (0.4%)	0.69	3/2225 (0.1%)
4	AD	0.80	6/1665 (0.4%)	0.65	2/2227 (0.1%)
5	AE	0.87	5/1157 (0.4%)	0.61	1/1557 (0.1%)
6	AF	0.94	5/881 (0.6%)	0.58	0/1189
7	AG	0.99	8/1195 (0.7%)	0.70	1/1602 (0.1%)
8	AH	0.96	6/989 (0.6%)	0.69	2/1326 (0.2%)
9	AI	0.73	3/1034 (0.3%)	0.72	2/1375 (0.1%)
10	AJ	1.08	6/805 (0.7%)	0.74	0/1089
11	AK	1.12	7/893 (0.8%)	0.67	0/1205
12	AL	1.09	8/960 (0.8%)	0.62	0/1286
13	AM	0.91	5/892 (0.6%)	0.74	2/1193 (0.2%)
14	AN	0.90	4/811 (0.5%)	0.63	1/1081 (0.1%)
15	AO	0.32	0/722	0.53	0/964
16	AP	0.73	2/659 (0.3%)	0.57	0/884
17	AQ	0.73	2/657 (0.3%)	0.77	2/881 (0.2%)
18	AR	0.84	2/462 (0.4%)	0.58	0/621
19	AS	1.08	5/672 (0.7%)	0.78	2/904 (0.2%)
20	AT	0.56	1/676 (0.1%)	0.47	0/895
21	AU	1.15	5/472 (1.1%)	0.62	0/627
22	BA	1.57	2305/69121 (3.3%)	3.43	7802/107828 (7.2%)
23	BB	1.34	75/2872 (2.6%)	2.95	243/4478 (5.4%)
24	BC	1.14	17/2121 (0.8%)	0.65	0/2852
25	BD	0.86	8/1576 (0.5%)	0.56	0/2119
26	BE	0.76	5/1571 (0.3%)	0.55	0/2113
27	BF	0.84	6/1434 (0.4%)	0.63	2/1926 (0.1%)
28	BG	0.98	8/1343 (0.6%)	0.59	0/1816
29	BH	0.71	3/1121 (0.3%)	0.67	2/1515 (0.1%)
30	BI	0.82	2/531 (0.4%)	0.70	1/709 (0.1%)
31	BJ	0.92	6/1152 (0.5%)	0.55	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BK	0.93	5/955 (0.5%)	0.63	0/1279
33	BL	0.83	4/1062 (0.4%)	0.58	0/1413
34	BM	1.02	7/1081 (0.6%)	0.59	0/1443
35	BN	0.86	4/958 (0.4%)	0.61	0/1281
36	BO	0.65	2/910 (0.2%)	0.50	0/1219
37	BP	0.80	3/929 (0.3%)	0.56	0/1242
38	BQ	0.38	0/960	0.50	0/1278
39	BR	0.63	2/829 (0.2%)	0.56	0/1107
40	BS	0.69	2/864 (0.2%)	0.59	0/1156
41	BT	0.64	1/744 (0.1%)	0.78	4/994 (0.4%)
42	BU	0.82	3/787 (0.4%)	0.58	0/1051
43	BV	0.92	4/766 (0.5%)	0.56	0/1025
44	BW	0.64	1/587 (0.2%)	0.55	0/776
45	BX	0.77	2/635 (0.3%)	0.55	0/848
46	BY	0.30	0/502	0.45	0/667
47	BZ	0.84	2/453 (0.4%)	0.54	0/605
48	B0	0.65	1/450 (0.2%)	0.58	0/599
49	B1	0.92	2/421 (0.5%)	0.60	0/561
50	B2	0.75	1/380 (0.3%)	0.56	0/498
51	B3	1.13	4/513 (0.8%)	0.61	0/676
52	B4	0.79	1/303 (0.3%)	0.55	0/397
53	B5	1.33	2/151 (1.3%)	0.90	1/205 (0.5%)
54	B7	1.51	6/212 (2.8%)	2.52	12/328 (3.7%)
55	B8	1.53	41/1765 (2.3%)	3.06	169/2750 (6.1%)
All	All	1.38	3927/155689 (2.5%)	2.93	12263/232920 (5.3%)

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
2	AB	0	2
7	AG	0	1
29	BH	0	2
43	BV	0	1
All	All	0	6

The worst 5 of 3927 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2449	U	C5-C6	23.39	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B8	20	U	C5-C6	22.49	1.54	1.34
10	AJ	41	PRO	N-CD	12.96	1.66	1.47
7	AG	2	PRO	N-CD	12.92	1.66	1.47
21	AU	2	PRO	N-CD	12.52	1.65	1.47

The worst 5 of 12263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2872	A	N1-C6-N6	-26.13	102.92	118.60
22	BA	1848	A	N1-C6-N6	-22.75	104.95	118.60
22	BA	1285	A	N1-C6-N6	-22.74	104.95	118.60
22	BA	1253	A	N1-C6-N6	-22.72	104.97	118.60
1	AA	1299	A	N1-C6-N6	-22.71	104.97	118.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	204	ASP	Sidechain
2	AB	205	ASP	Sidechain
7	AG	24	ALA	Mainchain
29	BH	104	THR	Peptide
29	BH	66	ASN	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	AA	32930	0	16580	240	0
2	AB	1753	0	1780	60	0
3	AC	1624	0	1696	41	0
4	AD	1643	0	1707	38	0
5	AE	1144	0	1185	25	0
6	AF	862	0	864	34	0
7	AG	1181	0	1238	31	0
8	AH	979	0	1031	29	0
9	AI	1022	0	1070	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	836	26	0
11	AK	877	0	887	16	0
12	AL	957	0	1017	12	0
13	AM	883	0	941	25	0
14	AN	799	0	841	23	0
15	AO	714	0	734	18	0
16	AP	649	0	666	10	0
17	AQ	648	0	691	12	0
18	AR	455	0	478	13	0
19	AS	656	0	680	25	0
20	AT	670	0	719	10	0
21	AU	465	0	491	9	0
22	BA	62209	0	31290	320	0
23	BB	2569	0	1301	7	0
24	BC	2082	0	2154	27	0
25	BD	1566	0	1617	12	0
26	BE	1552	0	1619	10	0
27	BF	1410	0	1444	26	0
28	BG	1323	0	1371	18	0
29	BH	1110	0	1148	28	0
30	BI	522	0	520	13	0
31	BJ	1129	0	1162	14	0
32	BK	946	0	1023	13	0
33	BL	1053	0	1128	12	0
34	BM	1075	0	1155	14	0
35	BN	945	0	989	9	0
36	BO	900	0	935	8	0
37	BP	917	0	962	9	0
38	BQ	947	0	1019	7	0
39	BR	816	0	839	7	0
40	BS	857	0	922	7	0
41	BT	738	0	807	10	0
42	BU	779	0	831	11	0
43	BV	753	0	780	9	0
44	BW	580	0	594	21	0
45	BX	625	0	652	4	0
46	BY	501	0	531	5	0
47	BZ	449	0	488	1	0
48	B0	444	0	458	5	0
49	B1	414	0	442	12	0
50	B2	377	0	418	5	0
51	B3	504	0	572	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B4	302	0	340	4	0
53	B5	146	0	139	3	0
54	B7	191	0	99	0	0
55	B8	1648	0	833	27	0
56	AA	86	0	0	0	0
56	B8	2	0	0	0	0
56	BA	233	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	2	0	0	0	0
56	BL	1	0	0	0	0
57	AA	38	0	0	0	0
57	AM	1	0	0	0	0
57	BA	104	0	0	1	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	1	0	0	0	0
57	BM	1	0	0	0	0
58	AB	1	0	0	0	0
58	B4	1	0	0	0	0
58	BI	1	0	0	0	0
59	BA	15	0	9	0	0
60	AA	184	0	0	1	0
60	AK	1	0	0	0	0
60	AN	1	0	0	0	0
60	B0	4	0	0	0	0
60	B2	6	0	0	0	0
60	B3	7	0	0	0	0
60	B4	1	0	0	0	0
60	B5	2	0	0	1	0
60	B8	3	0	0	1	0
60	BA	1672	0	0	25	0
60	BB	2	0	0	0	0
60	BC	38	0	0	1	0
60	BD	14	0	0	0	0
60	BE	21	0	0	2	0
60	BF	1	0	0	0	0
60	BJ	2	0	0	0	0
60	BK	3	0	0	0	0
60	BL	14	0	0	0	0
60	BM	2	0	0	0	0
60	BN	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BO	1	0	0	0	0
60	BP	2	0	0	0	0
60	BQ	12	0	0	0	0
60	BR	4	0	0	0	0
60	BS	7	0	0	0	0
60	BT	3	0	0	0	0
60	BU	1	0	0	0	0
60	BW	5	0	0	3	0
60	BX	4	0	0	0	0
All	All	146602	0	96723	1260	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 5.

The worst 5 of 1260 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)
6:AF:39:LEU:HD11	6:AF:62:MET:CE	1.55	1.34
6:AF:39:LEU:CD1	6:AF:62:MET:CE	2.07	1.33
42:BU:10:GLU:OE2	42:BU:73:PHE:HB3	1.34	1.23
6:AF:39:LEU:CD1	6:AF:62:MET:HE2	1.65	1.19
6:AF:39:LEU:HD12	6:AF:62:MET:HG2	1.27	1.14

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	AB	222/240 (92%)	211 (95%)	11 (5%)	0	100	100
3	AC	204/233 (88%)	193 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	AE	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
6	AF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	AG	149/179 (83%)	136 (91%)	13 (9%)	0	100	100
8	AH	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	AI	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
10	AJ	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	15	23
11	AK	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	AL	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	AM	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
14	AN	99/102 (97%)	91 (92%)	8 (8%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
17	AQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	80/92 (87%)	74 (92%)	6 (8%)	0	100	100
20	AT	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
25	BD	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
26	BE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	BF	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
28	BG	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
33	BL	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
34	BM	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
35	BN	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
36	BO	115/117 (98%)	114 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BP	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
40	BS	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	BT	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
42	BU	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
43	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
44	BW	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	BX	75/78 (96%)	75 (100%)	0	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	B0	54/57 (95%)	54 (100%)	0	0	100	100
49	B1	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
All	All	5590/5930 (94%)	5381 (96%)	208 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AJ	57	VAL

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	AB	186/198 (94%)	182 (98%)	4 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	170/190 (90%)	163 (96%)	7 (4%)	30	48
4	AD	172/173 (99%)	167 (97%)	5 (3%)	42	62
5	AE	118/126 (94%)	115 (98%)	3 (2%)	47	67
6	AF	92/116 (79%)	91 (99%)	1 (1%)	73	87
7	AG	124/147 (84%)	115 (93%)	9 (7%)	14	22
8	AH	104/105 (99%)	101 (97%)	3 (3%)	42	62
9	AI	105/107 (98%)	101 (96%)	4 (4%)	33	51
10	AJ	87/90 (97%)	82 (94%)	5 (6%)	20	33
11	AK	90/99 (91%)	89 (99%)	1 (1%)	73	87
12	AL	102/103 (99%)	97 (95%)	5 (5%)	25	40
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	76 (96%)	3 (4%)	33	51
15	AO	76/77 (99%)	74 (97%)	2 (3%)	46	66
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	72 (97%)	2 (3%)	44	65
18	AR	48/65 (74%)	46 (96%)	2 (4%)	30	47
19	AS	71/79 (90%)	70 (99%)	1 (1%)	67	82
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	48/61 (79%)	45 (94%)	3 (6%)	18	28
24	BC	216/218 (99%)	213 (99%)	3 (1%)	67	82
25	BD	163/163 (100%)	157 (96%)	6 (4%)	34	53
26	BE	165/165 (100%)	162 (98%)	3 (2%)	59	76
27	BF	148/150 (99%)	142 (96%)	6 (4%)	30	48
28	BG	137/138 (99%)	134 (98%)	3 (2%)	52	71
29	BH	114/114 (100%)	112 (98%)	2 (2%)	59	76
30	BI	59/62 (95%)	57 (97%)	2 (3%)	37	56
31	BJ	116/116 (100%)	114 (98%)	2 (2%)	60	78
32	BK	104/104 (100%)	101 (97%)	3 (3%)	42	62
33	BL	103/103 (100%)	102 (99%)	1 (1%)	76	88
34	BM	108/108 (100%)	104 (96%)	4 (4%)	34	53
35	BN	98/103 (95%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BO	87/87 (100%)	84 (97%)	3 (3%)	37	56
37	BP	99/100 (99%)	96 (97%)	3 (3%)	41	61
38	BQ	89/90 (99%)	88 (99%)	1 (1%)	73	87
39	BR	84/84 (100%)	82 (98%)	2 (2%)	49	68
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	78 (98%)	2 (2%)	47	67
42	BU	83/85 (98%)	82 (99%)	1 (1%)	71	85
43	BV	78/78 (100%)	76 (97%)	2 (3%)	46	66
44	BW	57/63 (90%)	55 (96%)	2 (4%)	36	55
45	BX	67/68 (98%)	66 (98%)	1 (2%)	65	80
46	BY	54/55 (98%)	53 (98%)	1 (2%)	57	75
47	BZ	48/49 (98%)	47 (98%)	1 (2%)	53	72
48	B0	47/48 (98%)	44 (94%)	3 (6%)	17	28
49	B1	45/49 (92%)	44 (98%)	1 (2%)	52	71
50	B2	38/38 (100%)	36 (95%)	2 (5%)	22	37
51	B3	51/52 (98%)	50 (98%)	1 (2%)	55	74
52	B4	34/34 (100%)	33 (97%)	1 (3%)	42	62
53	B5	17/17 (100%)	16 (94%)	1 (6%)	19	32
All	All	4650/4843 (96%)	4527 (97%)	123 (3%)	49	66

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	AU	25	LYS
44	BW	81	SER
26	BE	168	ASP
44	BW	44	LYS
50	B2	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
28	BG	38	ASN
50	B2	26	ASN
50	B2	29	GLN

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Mol	Chain	Res	Type
9	AI	50	GLN
5	AE	135	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	180 (11%)	1 (0%)
22	BA	2891/2897 (99%)	295 (10%)	15 (0%)
23	BB	119/120 (99%)	7 (5%)	0
54	B7	8/9 (88%)	4 (50%)	0
55	B8	76/77 (98%)	14 (18%)	4 (5%)
All	All	4624/4637 (99%)	500 (10%)	20 (0%)

5 of 500 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	22	G
1	AA	39	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2518	A
55	B8	3	G
55	B8	20	U
55	B8	19	G
22	BA	1608	A

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

40 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	$\#\|Z\|>2$
22	6MZ	BA	1618	22	18,25,26	2.91	4 (22%)	16,36,39	1.95	3 (18%)
34	4D4	BM	81	34	9,11,12	2.52	3 (33%)	8,13,15	1.06	0
22	OMC	BA	2498	22,56	15,22,23	3.26	6 (40%)	17,31,34	1.41	3 (17%)
1	2MG	AA	1207	57,1	19,26,27	4.54	7 (36%)	21,38,41	2.36	8 (38%)
1	UR3	AA	1498	1	14,22,23	2.74	4 (28%)	15,32,35	0.77	1 (6%)
22	2MG	BA	1835	22	19,26,27	4.08	8 (42%)	21,38,41	2.30	8 (38%)
22	5MU	BA	747	22	15,22,23	1.30	2 (13%)	16,32,35	2.76	1 (6%)
22	OMG	BA	2251	22,57,55	18,26,27	3.47	8 (44%)	20,38,41	2.24	9 (45%)
55	G7M	B8	46	55	20,26,27	3.32	7 (35%)	20,39,42	3.02	7 (35%)
1	5MC	AA	967	1	15,22,23	2.96	5 (33%)	19,32,35	1.31	2 (10%)
22	PSU	BA	1917	22	17,21,22	3.66	9 (52%)	20,30,33	3.15	6 (30%)
22	2MG	BA	2445	22	19,26,27	4.23	7 (36%)	21,38,41	2.45	8 (38%)
22	5MC	BA	1962	22,57	15,22,23	2.93	5 (33%)	19,32,35	1.17	2 (10%)
25	MEQ	BD	150	25	8,9,10	1.64	2 (25%)	5,10,12	1.76	2 (40%)
1	5MC	AA	1407	1	15,22,23	2.94	5 (33%)	19,32,35	1.35	2 (10%)
1	G7M	AA	527	1	20,26,27	3.64	6 (30%)	20,39,42	3.16	6 (30%)
22	PSU	BA	2504	22,57	17,21,22	3.63	8 (47%)	20,30,33	3.26	7 (35%)
22	PSU	BA	955	22	17,21,22	3.69	8 (47%)	20,30,33	3.43	6 (30%)
1	2MG	AA	1516	1	19,26,27	4.37	7 (36%)	21,38,41	2.24	8 (38%)
55	1MG	B8	37	55	18,26,27	3.62	7 (38%)	19,39,42	1.43	2 (10%)
22	PSU	BA	2604	22	17,21,22	3.46	8 (47%)	20,30,33	3.16	6 (30%)
22	PSU	BA	2605	22	17,21,22	3.50	8 (47%)	20,30,33	3.25	6 (30%)
22	6MZ	BA	2030	22	18,25,26	2.75	5 (27%)	16,36,39	2.70	4 (25%)
22	5MU	BA	1939	22,57	15,22,23	1.12	1 (6%)	16,32,35	2.67	1 (6%)
22	3TD	BA	1915	22	17,22,23	4.77	8 (47%)	19,32,35	1.23	3 (15%)
12	D2T	AL	89	12	4,9,10	1.11	0	3,11,13	2.71	1 (33%)
1	MA6	AA	1519	1	19,26,27	1.18	1 (5%)	18,38,41	3.59	2 (11%)
22	OMU	BA	2552	22,56	14,22,23	3.37	5 (35%)	14,31,34	0.63	0
1	PSU	AA	516	1,56	17,21,22	3.75	9 (52%)	20,30,33	3.25	6 (30%)
22	PSU	BA	2580	22,57	17,21,22	3.56	9 (52%)	20,30,33	3.18	6 (30%)
22	PSU	BA	2457	22	17,21,22	3.61	9 (52%)	20,30,33	3.15	6 (30%)
22	PSU	BA	1911	22	17,21,22	3.63	8 (47%)	20,30,33	3.04	6 (30%)
22	2MA	BA	2503	22,57,56	17,25,26	3.77	5 (29%)	19,37,40	1.86	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MA6	AA	1518	1	19,26,27	1.21	1 (5%)	18,38,41	3.51	2 (11%)
1	2MG	AA	966	1	19,26,27	4.40	7 (36%)	21,38,41	2.22	8 (38%)
22	G7M	BA	2069	22,57	20,26,27	3.48	7 (35%)	20,39,42	2.99	7 (35%)
1	4OC	AA	1402	1,56	16,23,24	3.41	6 (37%)	17,32,35	1.18	2 (11%)
22	1MG	BA	745	22	18,26,27	3.69	7 (38%)	19,39,42	1.86	4 (21%)
22	PSU	BA	746	22,56	17,21,22	3.62	9 (52%)	20,30,33	3.09	7 (35%)
55	PSU	B8	55	55	17,21,22	3.59	9 (52%)	20,30,33	2.98	7 (35%)

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
22	6MZ	BA	1618	22	-	0/5/27/28	0/3/3/3
34	4D4	BM	81	34	-	3/11/12/14	-
22	OMC	BA	2498	22,56	-	0/7/27/28	0/2/2/2
1	2MG	AA	1207	57,1	-	0/5/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
22	5MU	BA	747	22	-	1/5/25/26	0/2/2/2
22	OMG	BA	2251	22,57,55	-	3/5/27/28	0/3/3/3
55	G7M	B8	46	55	-	0/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
22	2MG	BA	2445	22	-	1/5/27/28	0/3/3/3
22	5MC	BA	1962	22,57	-	2/5/25/26	0/2/2/2
25	MEQ	BD	150	25	-	3/8/9/11	-
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
22	PSU	BA	2504	22,57	-	2/7/25/26	0/2/2/2
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
55	1MG	B8	37	55	-	0/3/25/26	0/3/3/3
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
22	5MU	BA	1939	22,57	-	0/5/25/26	0/2/2/2
22	3TD	BA	1915	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	D2T	AL	89	12	-	1/3/12/14	-
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
22	OMU	BA	2552	22,56	-	1/7/27/28	0/2/2/2
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
22	PSU	BA	2580	22,57	-	0/7/25/26	0/2/2/2
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
22	2MA	BA	2503	22,57,56	-	2/3/25/26	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
22	G7M	BA	2069	22,57	-	2/3/25/26	0/3/3/3
1	4OC	AA	1402	1,56	-	2/9/29/30	0/2/2/2
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
22	PSU	BA	746	22,56	-	3/7/25/26	0/2/2/2
55	PSU	B8	55	55	-	2/7/25/26	0/2/2/2

The worst 5 of 240 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C5-C1’	-15.10	1.39	1.52
1	AA	1207	2MG	C2-N2	13.60	1.45	1.34
1	AA	966	2MG	C2-N2	13.45	1.45	1.34
1	AA	1516	2MG	C2-N2	13.18	1.45	1.34
22	BA	2445	2MG	C2-N2	12.32	1.44	1.34

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1519	MA6	N1-C6-N6	-13.93	102.40	117.06
1	AA	1518	MA6	N1-C6-N6	-13.60	102.74	117.06
22	BA	955	PSU	N1-C2-N3	-12.16	118.76	128.43
1	AA	527	G7M	C1’-N9-C4	11.40	146.68	126.64
1	AA	516	PSU	N1-C2-N3	-11.37	119.39	128.43

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	C3’-C4’-C5’-O5’
1	AA	966	2MG	O4’-C4’-C5’-O5’

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Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	BA	2251	OMG	1	0
55	B8	46	G7M	3	0
25	BD	150	MEQ	1	0
22	BA	2504	PSU	1	0
55	B8	37	1MG	2	0
22	BA	2030	6MZ	2	0
22	BA	1915	3TD	1	0
22	BA	2552	OMU	1	0
22	BA	2503	2MA	1	0
22	BA	746	PSU	1	0
55	B8	55	PSU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 477 ligands modelled in this entry, 476 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	TRP	BA	3001	-	12,16,16	0.91	0	12,22,22	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	TRP	BA	3001	-	-	0/3/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
22	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.28

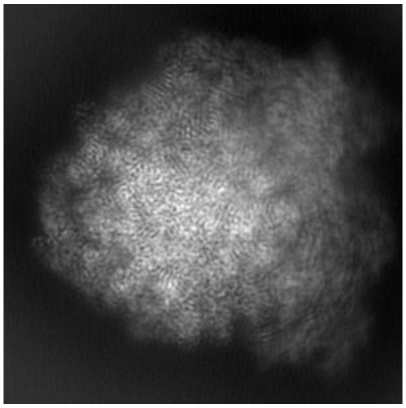
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-12694. These allow visual inspection of the internal detail of the map and identification of artifacts.

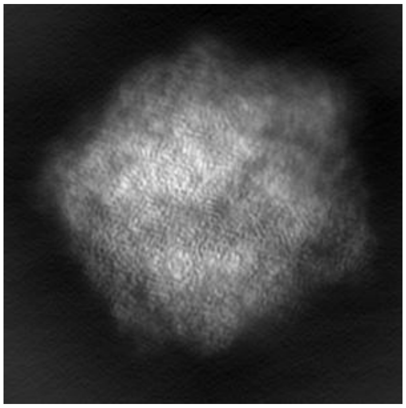
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

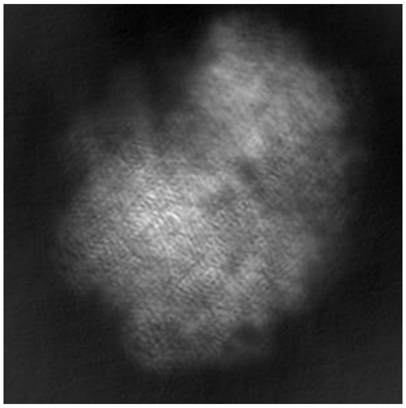
6.1.1 Primary map



X

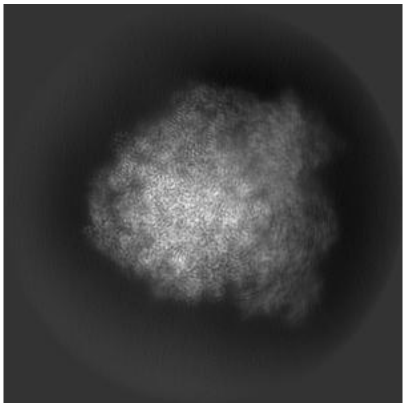


Y

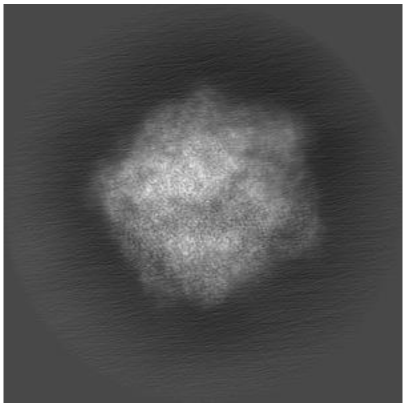


Z

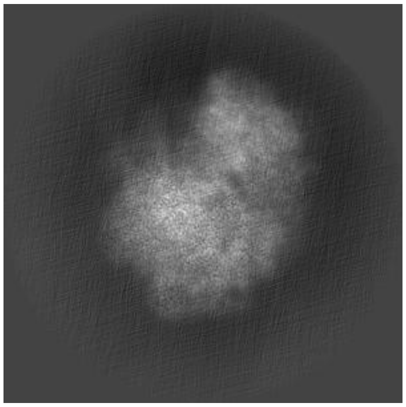
6.1.2 Raw map



X



Y

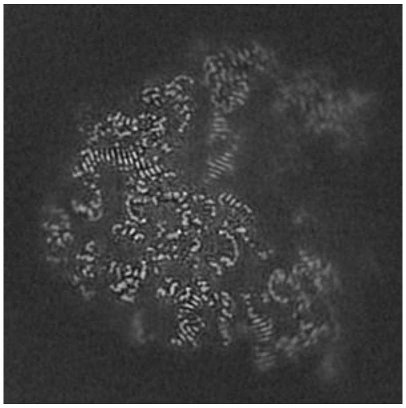


Z

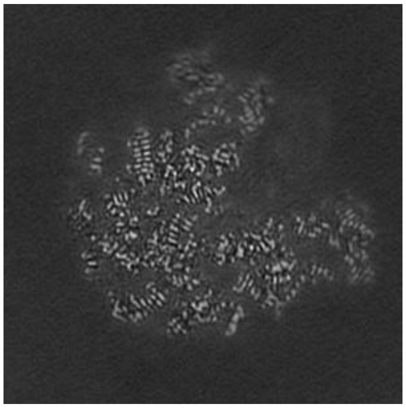
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

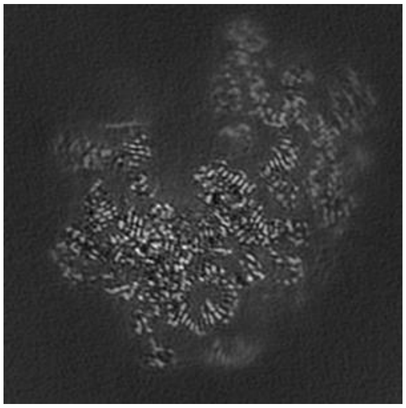
6.2.1 Primary map



X Index: 162

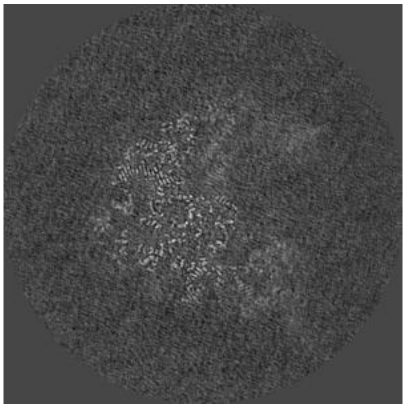


Y Index: 162

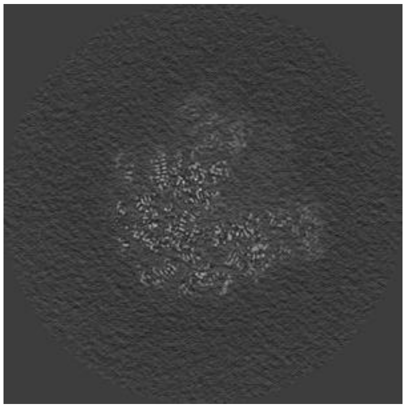


Z Index: 162

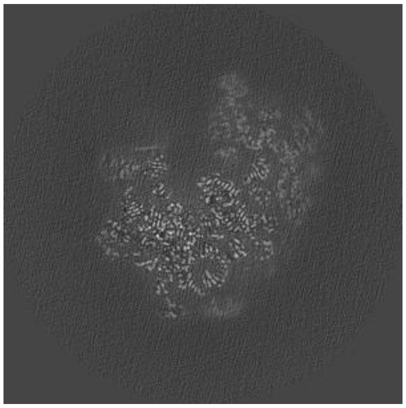
6.2.2 Raw map



X Index: 232



Y Index: 232

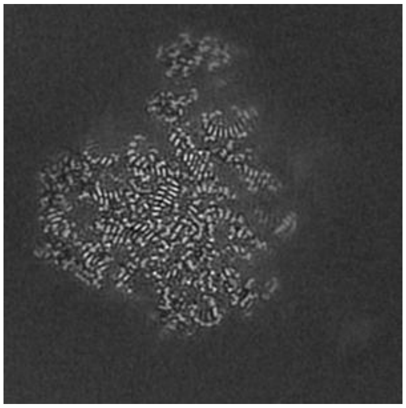


Z Index: 232

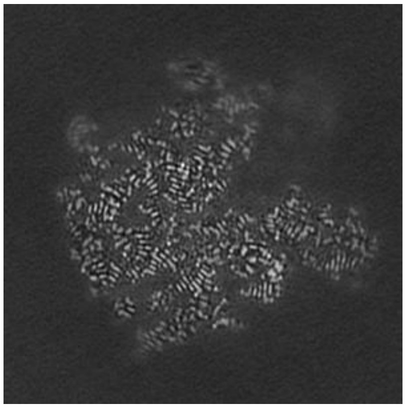
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

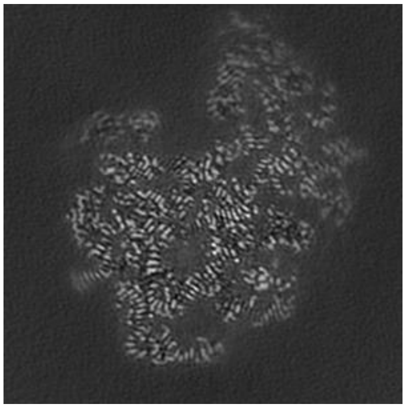
6.3.1 Primary map



X Index: 121

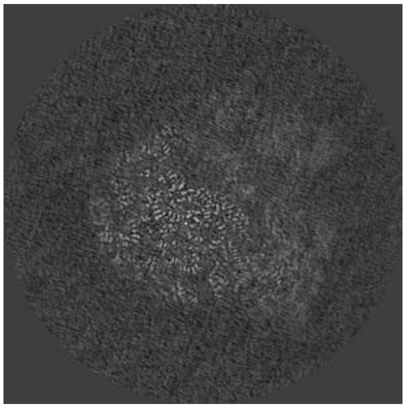


Y Index: 150

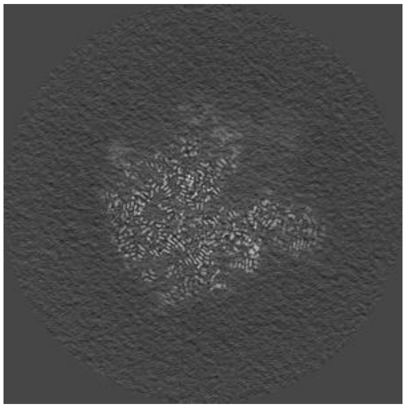


Z Index: 143

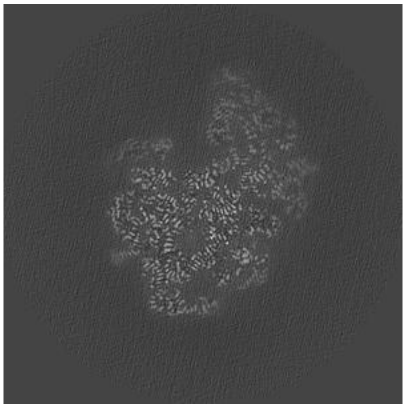
6.3.2 Raw map



X Index: 244



Y Index: 220



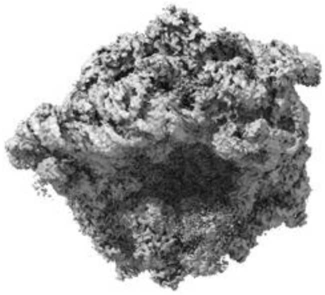
Z Index: 213

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

6.4 Orthogonal surface views

6.4.1 Primary map

X

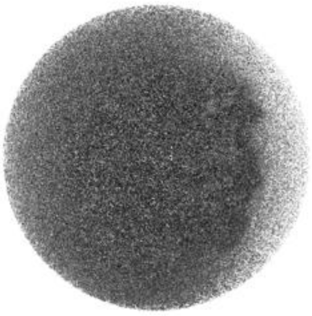


Y

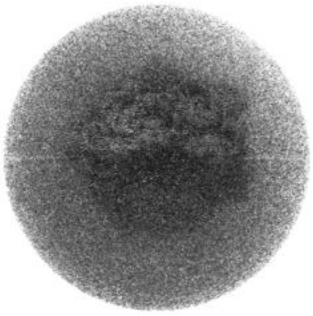
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

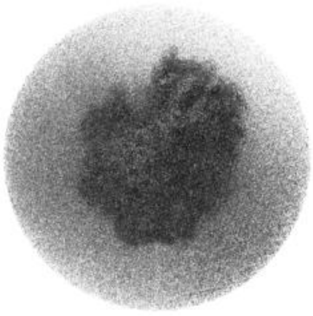
6.4.2 Raw map



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.

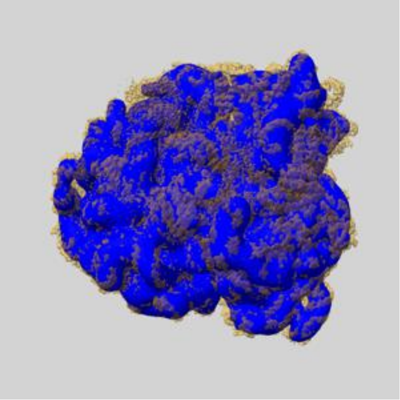
6.5 Mask visualisation

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

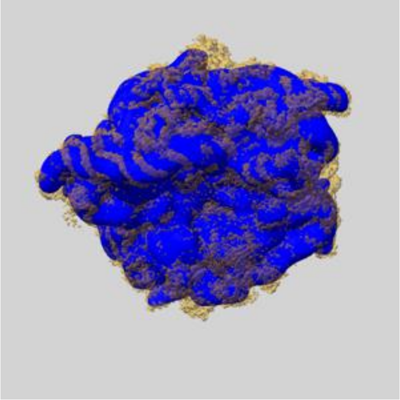
A mask typically either:

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

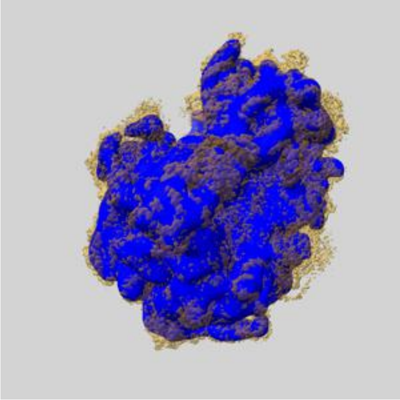
6.5.1 emd_12694_msk_1.map



X



Y

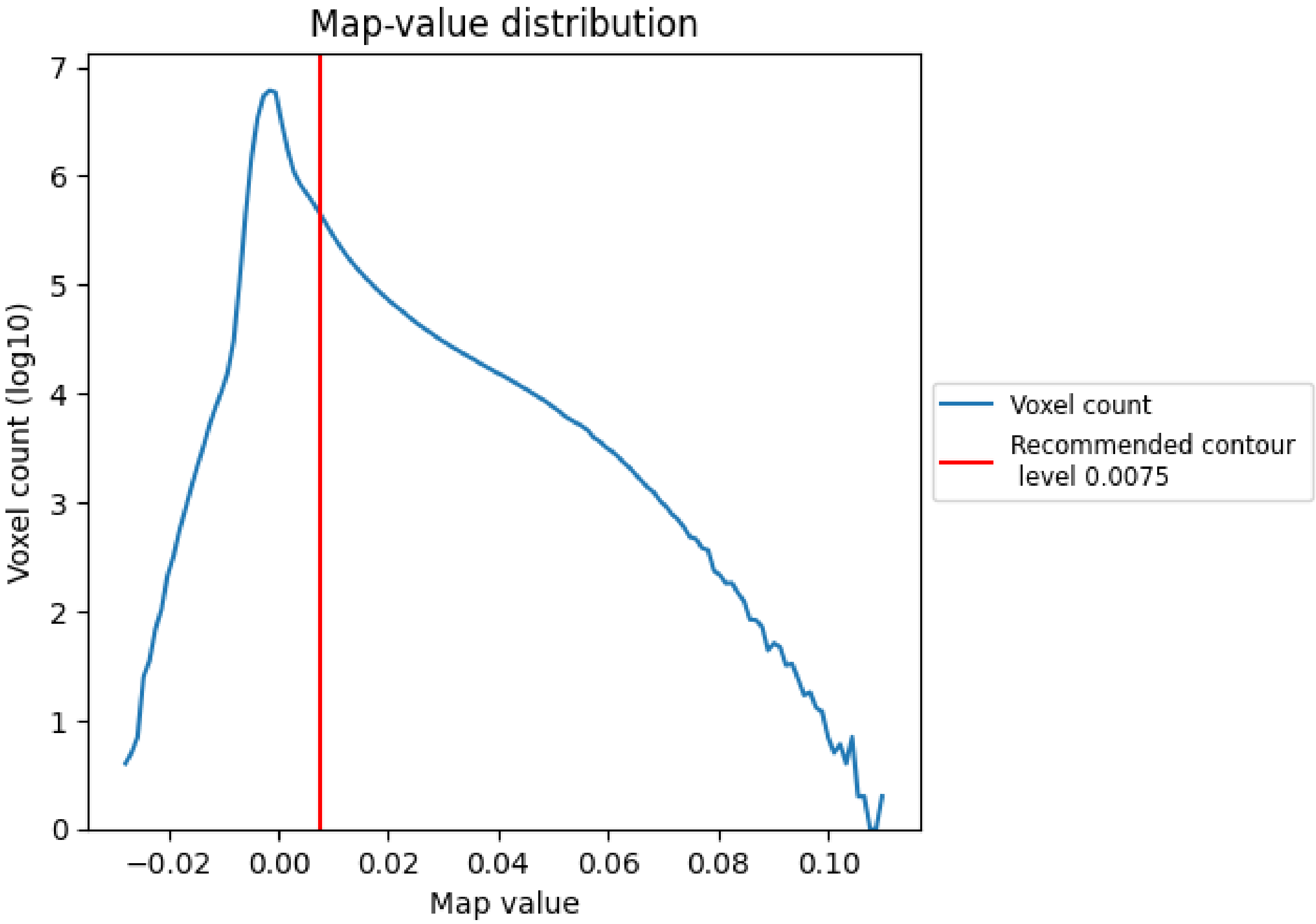


Z

7 Map analysis ⓘ

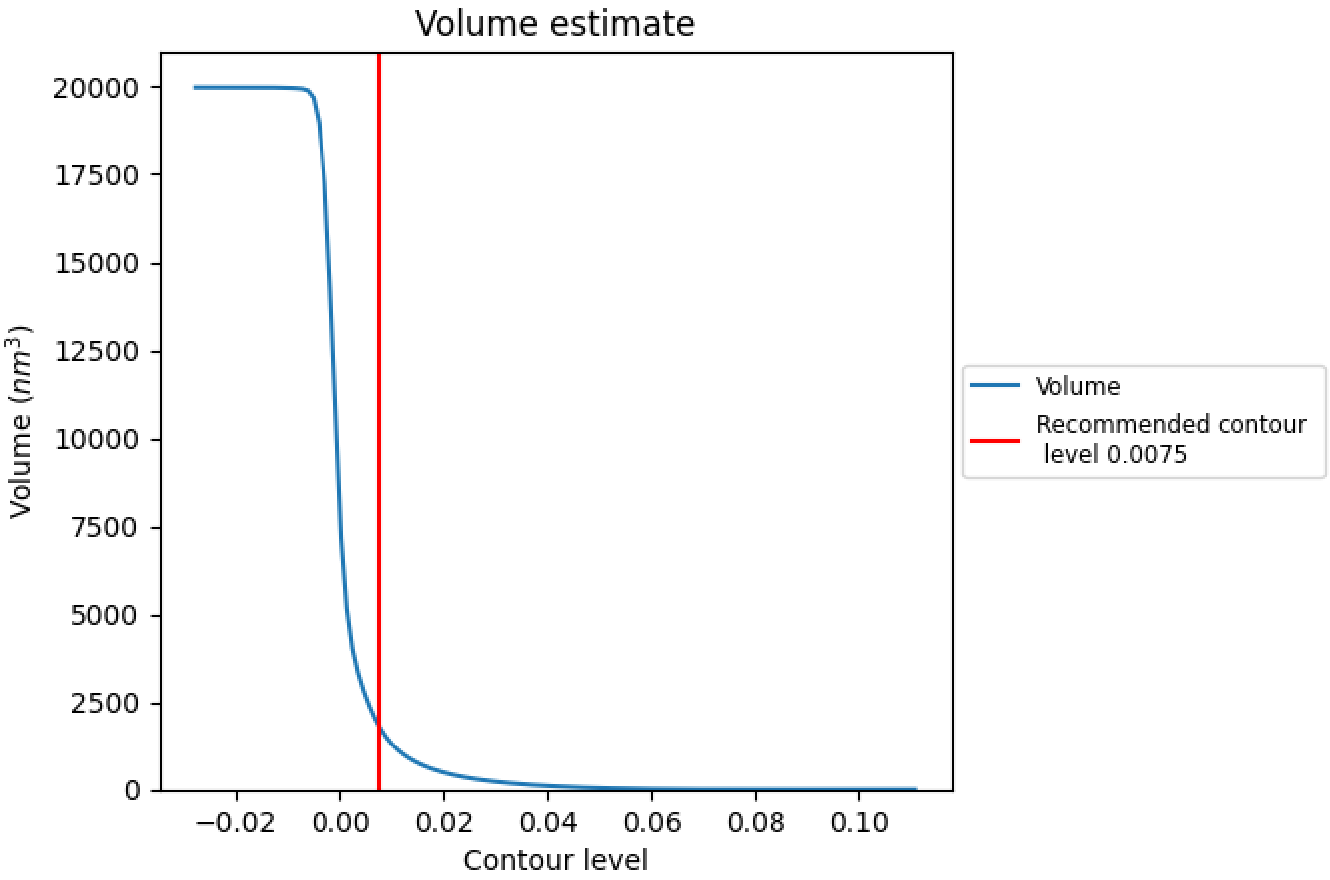
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

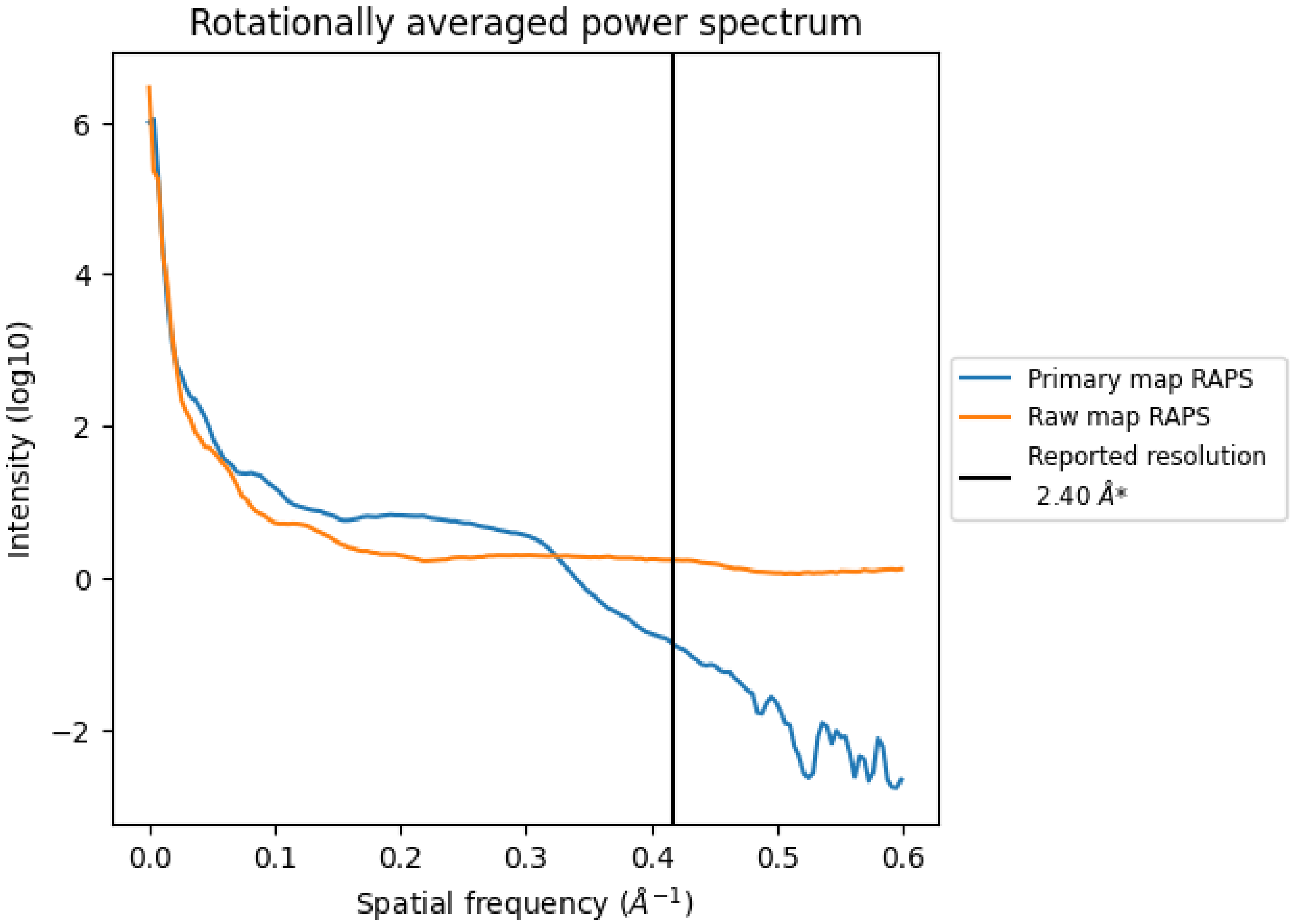
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1859 nm^3; this corresponds to an approximate mass of 1680 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 ⓘ

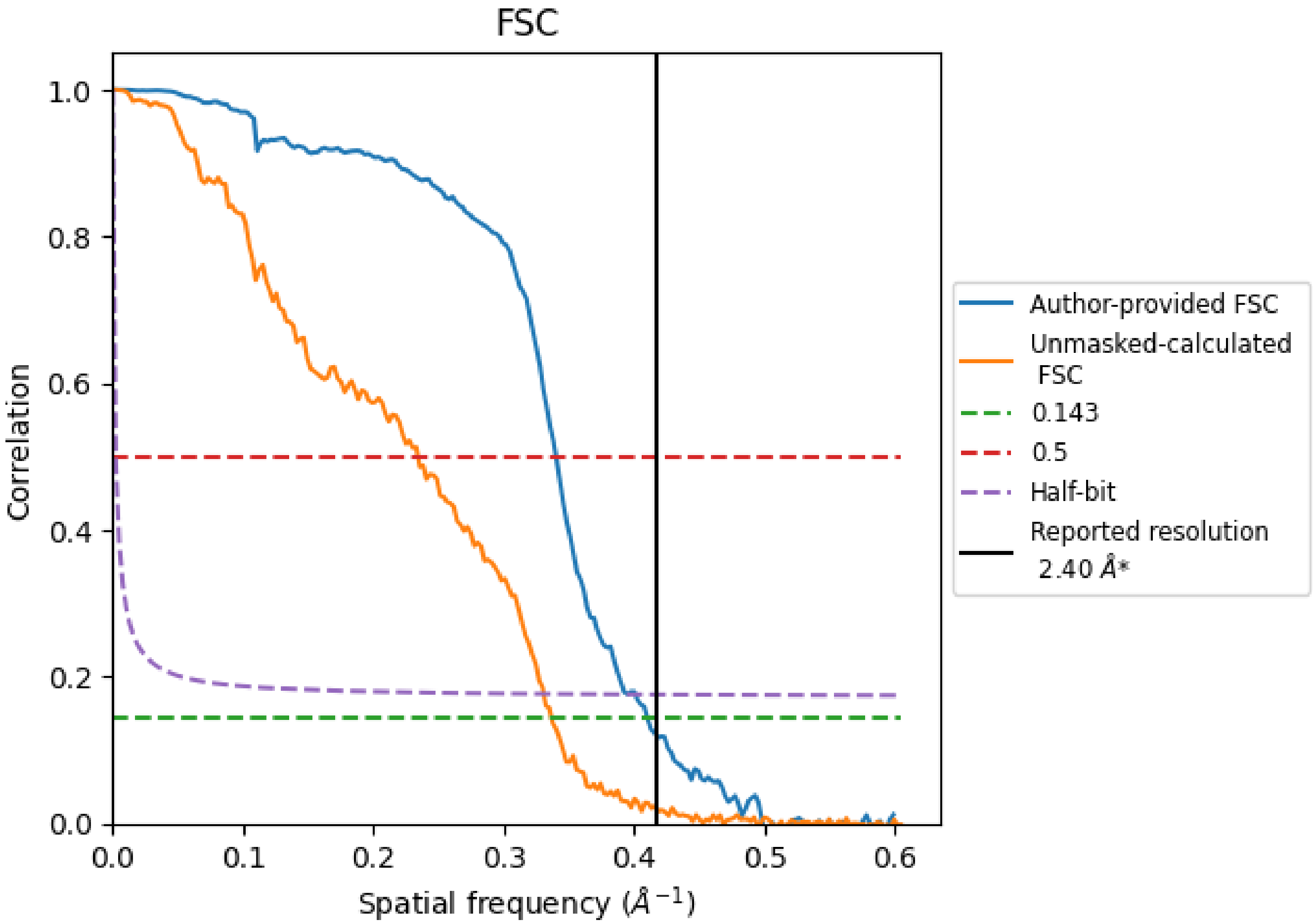


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.417 $Å^{-1}$

8.2 Resolution estimates ⓘ

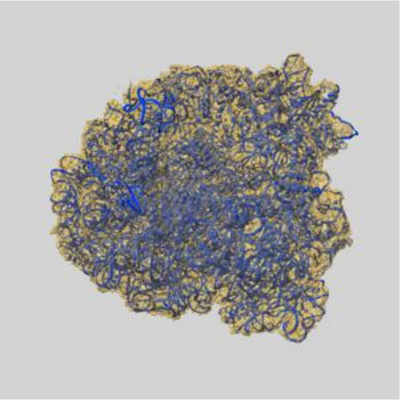
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.94	2.49
Unmasked-calculated*	2.97	4.27	3.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.97 differs from the reported value 2.4 by more than 10 %

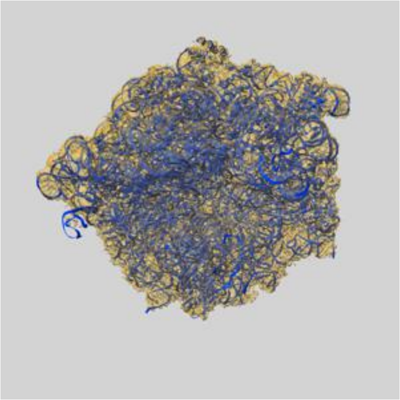
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12694 and PDB model 7O1A. Per-residue inclusion information can be found in section 3 on page 17.

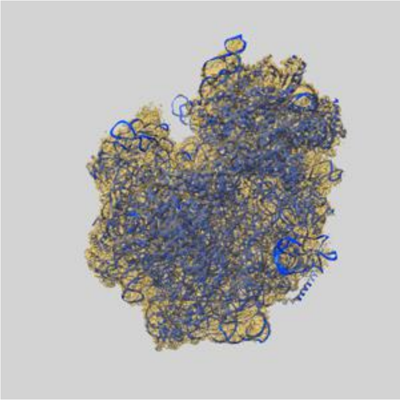
9.1 Map-model overlay



X



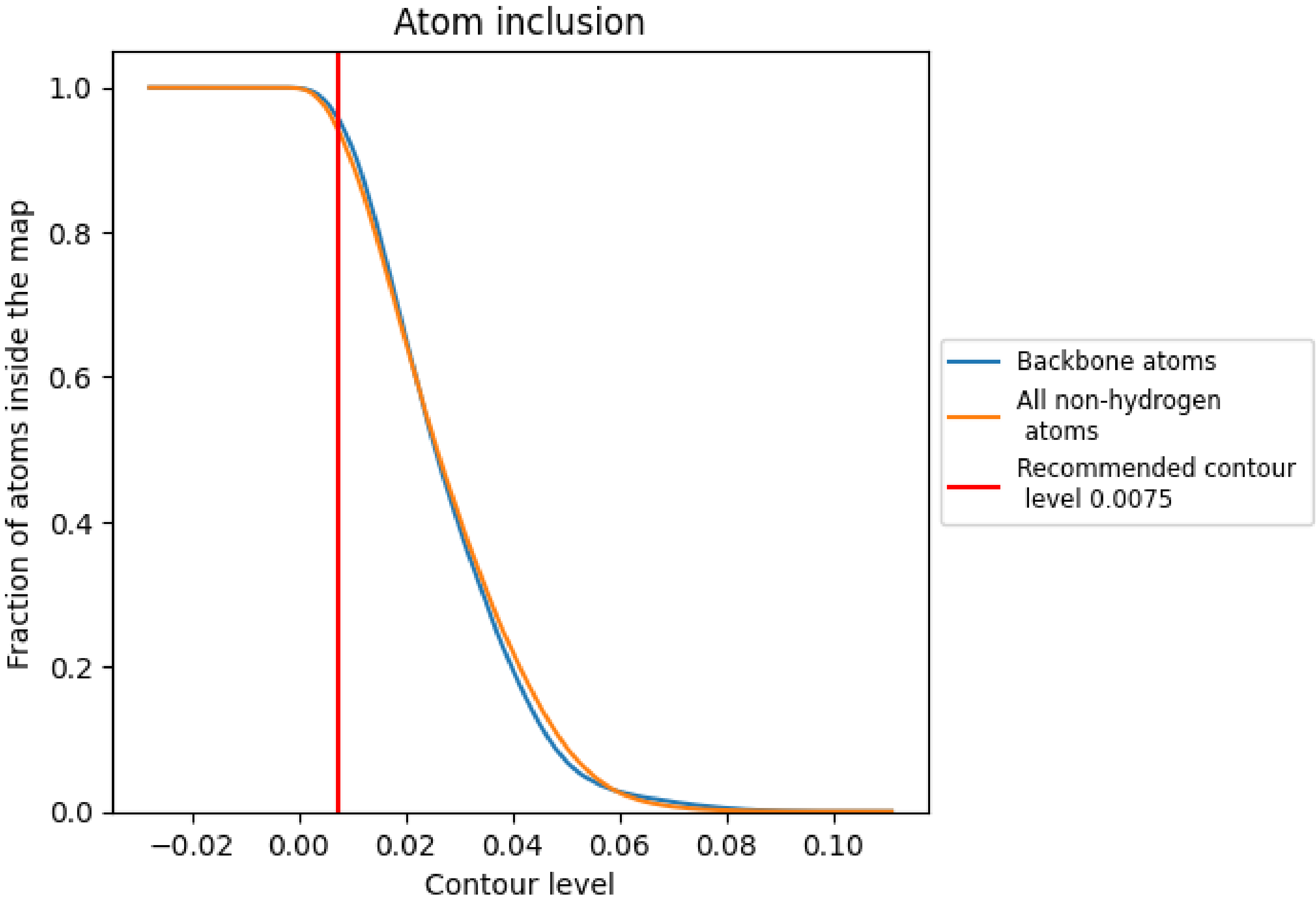
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075 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 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.