



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 5UYQ / pdb_00005uyq
EMDB ID : EMD-8620
Title : 70S ribosome bound with near-cognate ternary complex base-paired to A site codon, closed 30S (Structure III-nc)
Authors : Loveland, A.B.; Demo, G.; Grigorieff, N.; Korostelev, A.A.
Deposited on : 2017-02-24
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

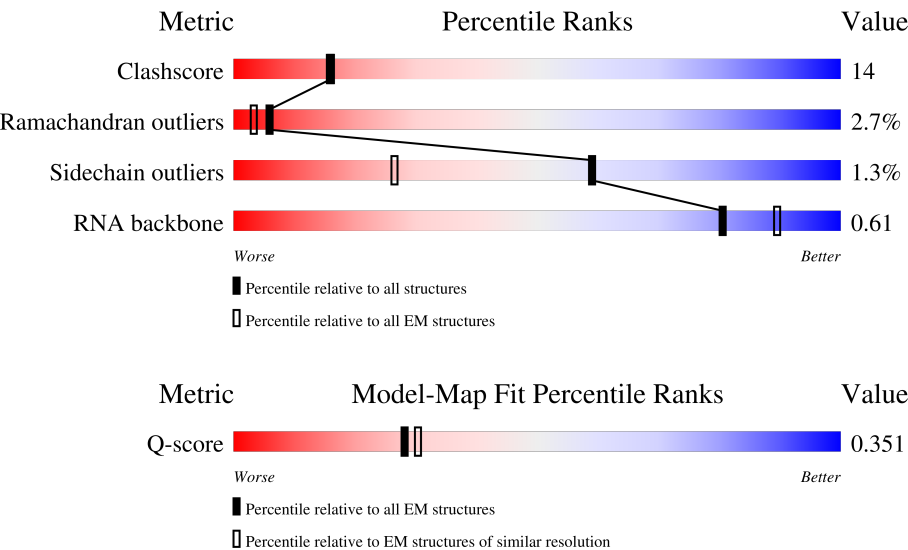
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



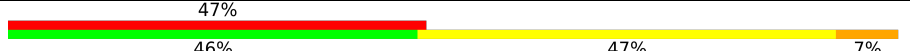
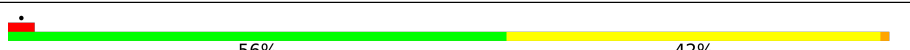
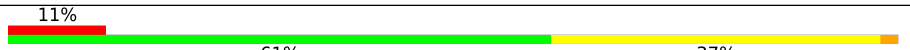
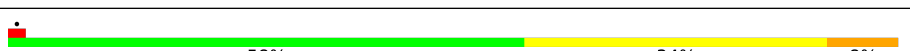
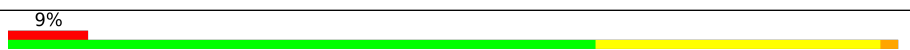
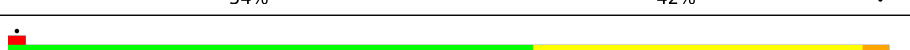
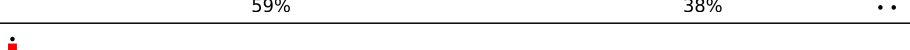
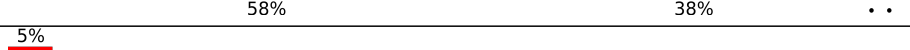
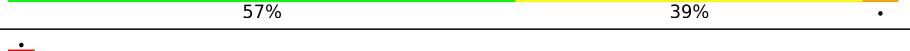
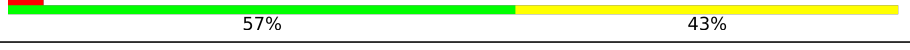
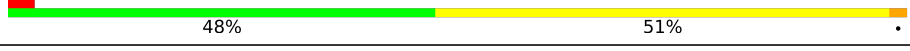
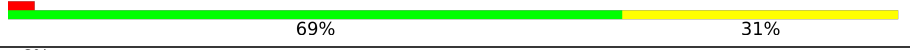
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	04	271	
2	05	209	
3	06	201	

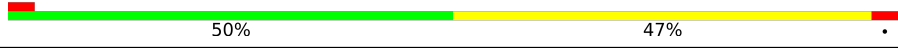
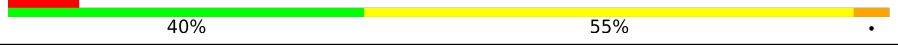
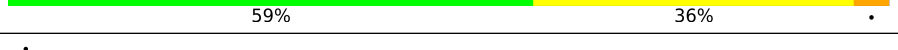
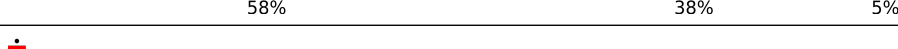
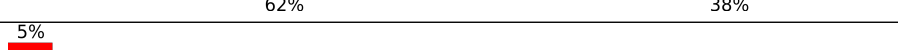
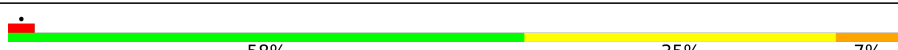
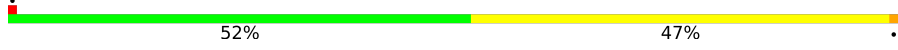
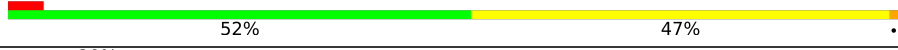
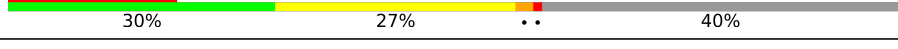
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	07	177	
5	08	176	
6	09	149	
7	10	131	
8	11	141	
9	12	142	
10	13	122	
11	14	143	
12	15	136	
13	16	120	
14	17	116	
15	18	114	
16	19	117	
17	20	103	
18	21	110	
19	22	93	
20	23	102	
21	24	94	
22	25	75	
23	26	77	
24	27	63	
25	28	58	
26	29	66	
27	30	56	
28	31	50	

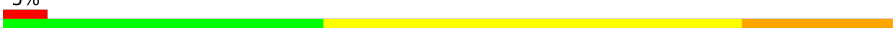
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	32	46	
30	33	64	
31	34	38	
32	B	218	
33	C	206	
34	D	205	
35	E	157	
36	F	100	
37	G	151	
38	H	129	
39	I	127	
40	J	98	
41	K	116	
42	L	123	
43	M	114	
44	N	100	
45	O	88	
46	P	82	
47	Q	80	
48	R	65	
49	S	79	
50	T	85	
51	U	65	
52	03	223	
53	A	1539	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	01	2903	
55	02	120	
56	W	77	
56	X	77	
57	V	18	
58	Y	76	
59	Z	392	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 153759 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	04	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	05	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	06	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	07	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	08	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	09	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	10	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	11	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	12	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	13	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	14	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	15	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	16	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	17	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	18	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	19	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	20	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	21	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	22	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	23	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	24	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	25	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	26	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	27	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	28	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	29	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	30	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	31	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	32	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	33	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	34	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	F	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	G	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	J	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	R	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

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

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	U	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	03	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	01	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
01	747	C	U	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	02	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

- Molecule 56 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
56	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	V	18	Total	C	N	O	P	0	0
			395	178	84	116	17		

- Molecule 58 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Y	76	Total	C	N	O	P	S	0	0
			1618	723	282	536	76	1		

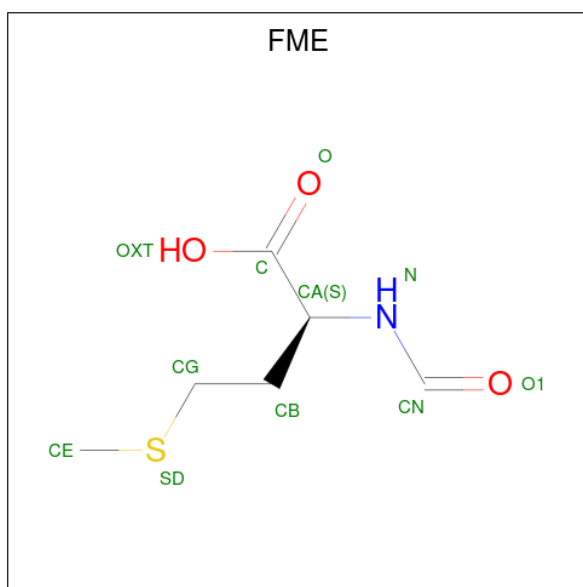
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	34	U8U	-	insertion	GB 558570689

- Molecule 59 is a protein called Elongation factor Tu 2.

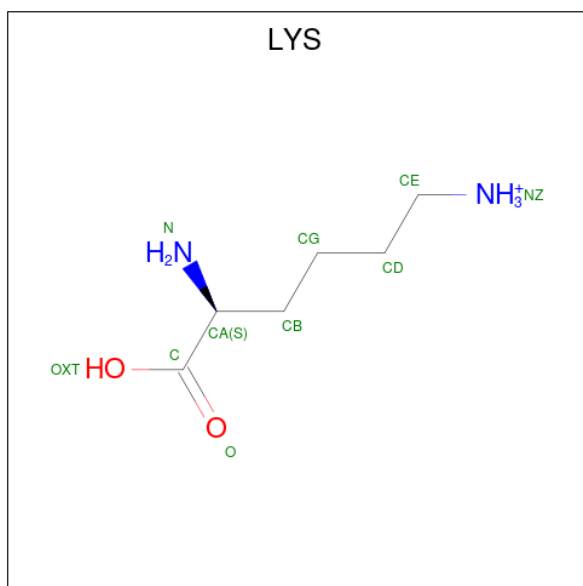
Mol	Chain	Residues	Atoms					AltConf	Trace
59	Z	392	Total	C	N	O	S	0	0
			3029	1915	521	580	13		

- Molecule 60 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	W	1	10	6	1	2	1	0

- Molecule 61 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).

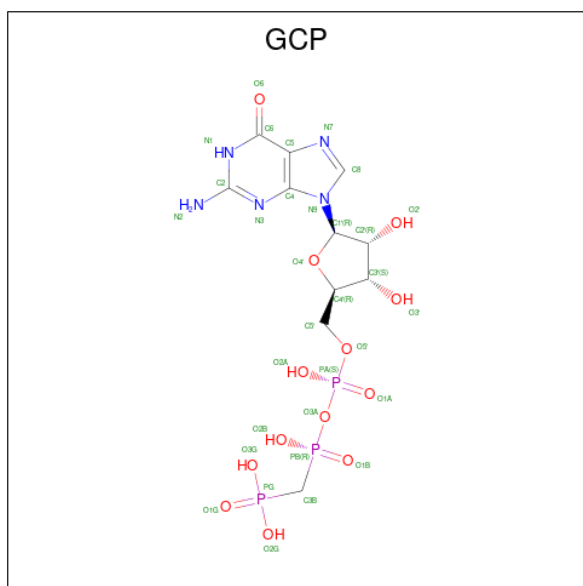


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
61	Y	1	9	6	2	1	0

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	Z	1	Total	Mg	0
			1	1	

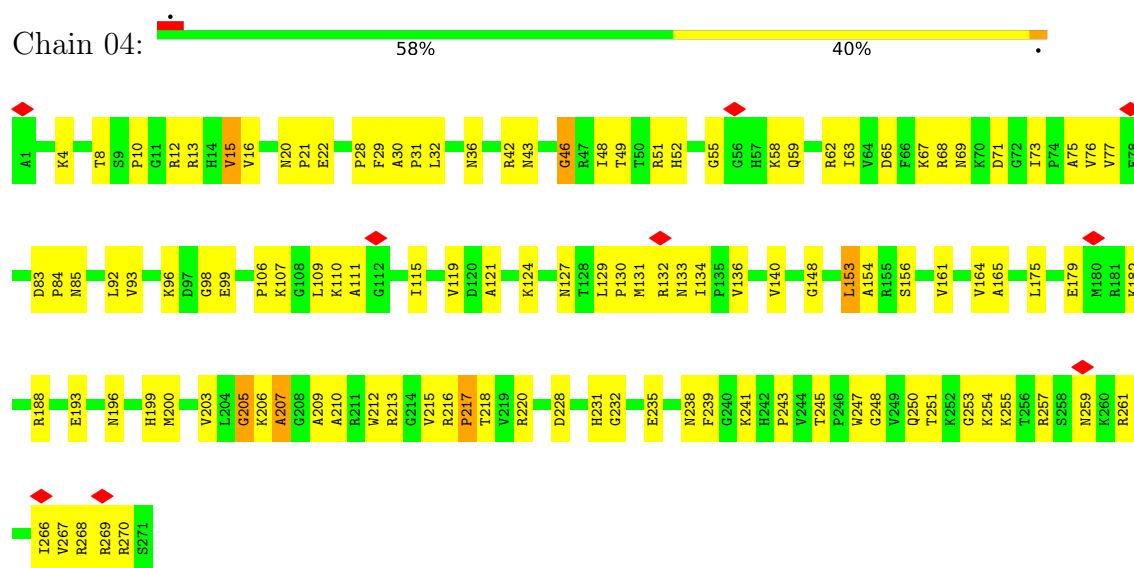
- Molecule 63 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



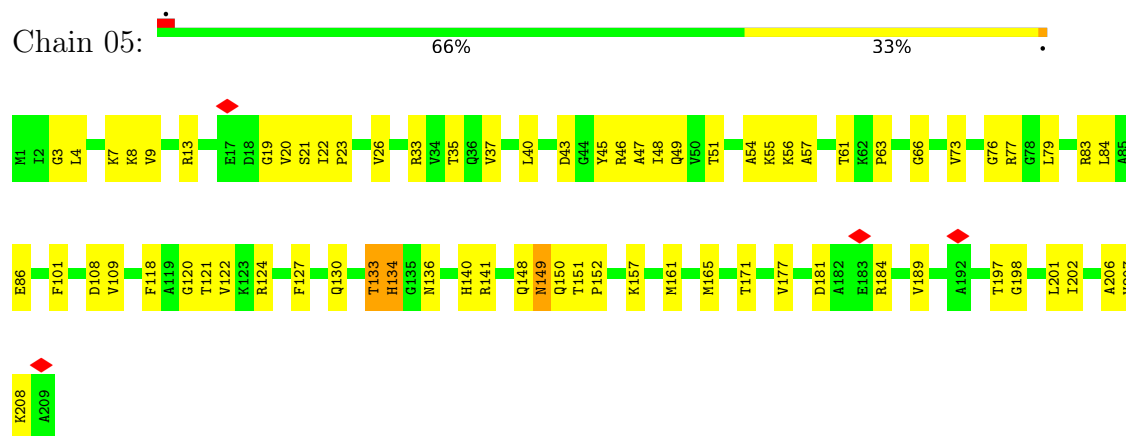
3 Residue-property plots

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

• Molecule 1: 50S ribosomal protein L2

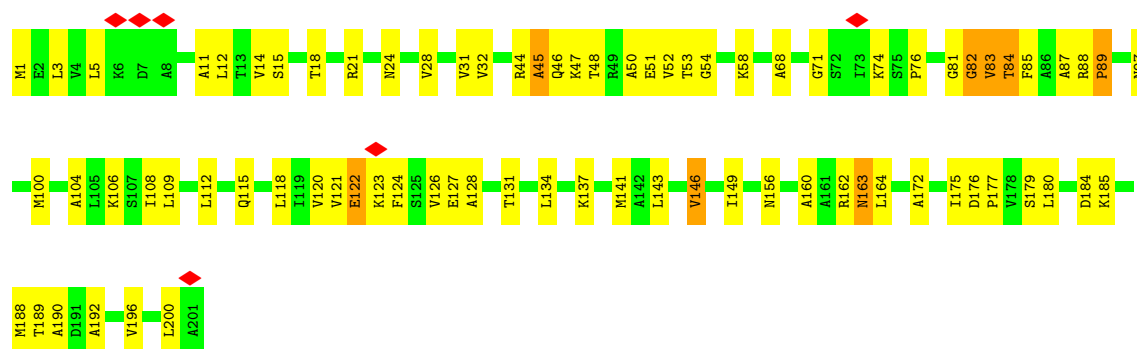


• Molecule 2: 50S ribosomal protein L3



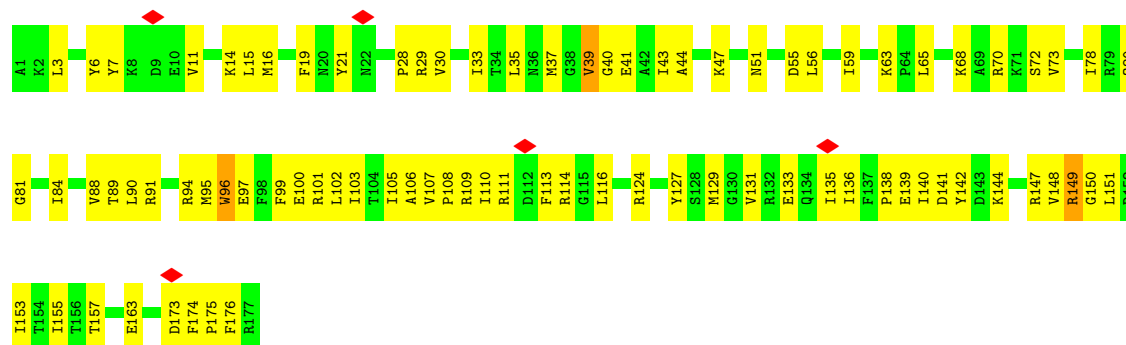
• Molecule 3: 50S ribosomal protein L4





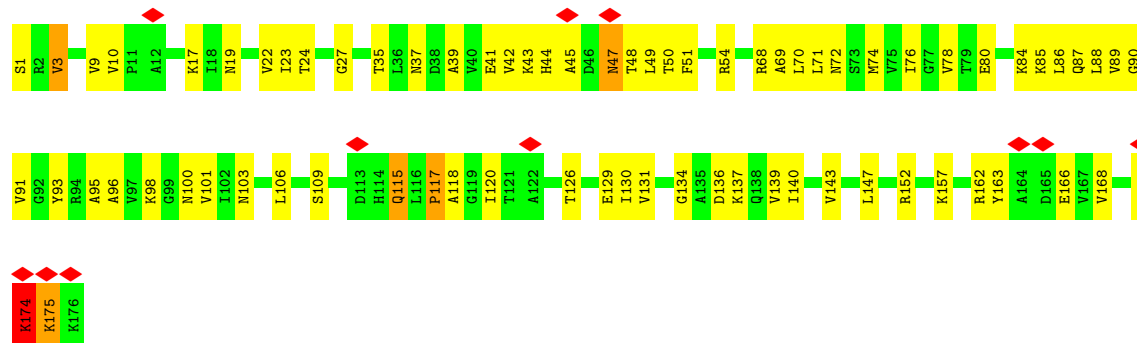
• Molecule 4: 50S ribosomal protein L5

Chain 07: 53% 46%



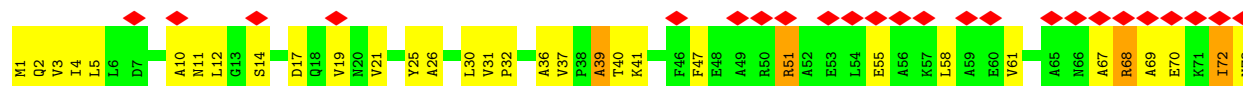
• Molecule 5: 50S ribosomal protein L6

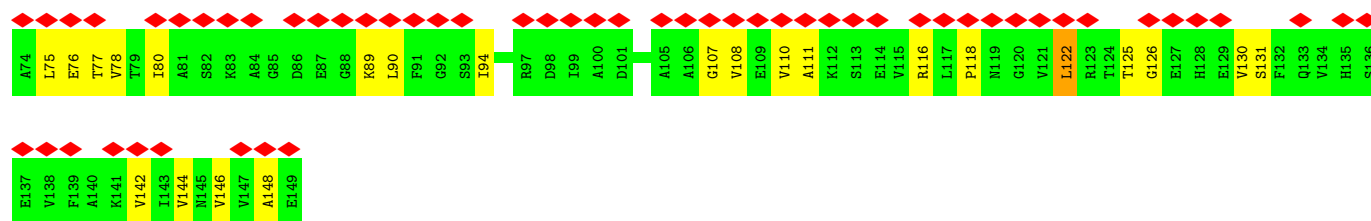
Chain 08: 6% 58% 39%



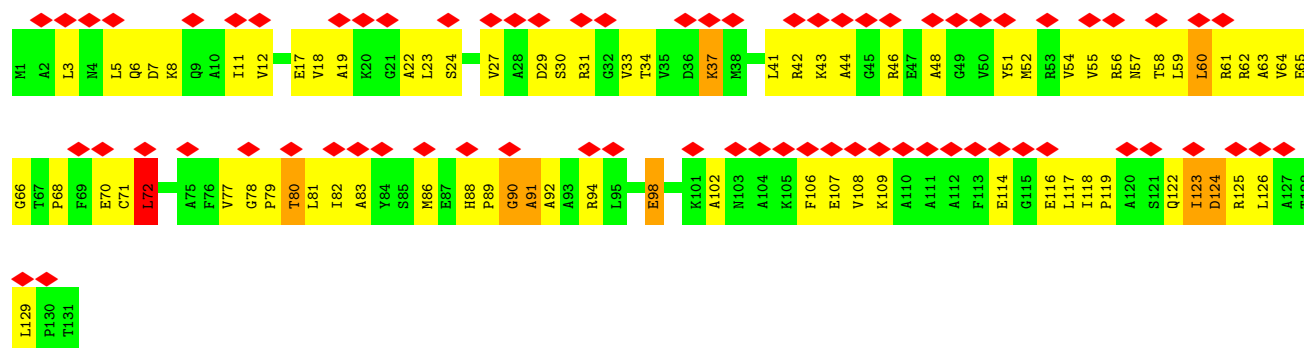
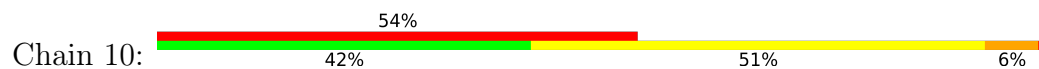
• Molecule 6: 50S ribosomal protein L9

Chain 09: 54% 62% 34%





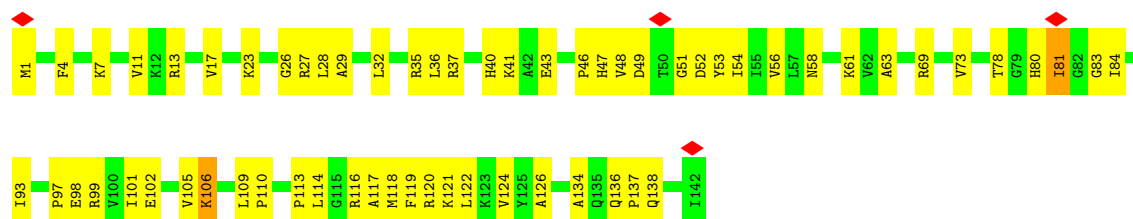
• Molecule 7: 50S ribosomal protein L10



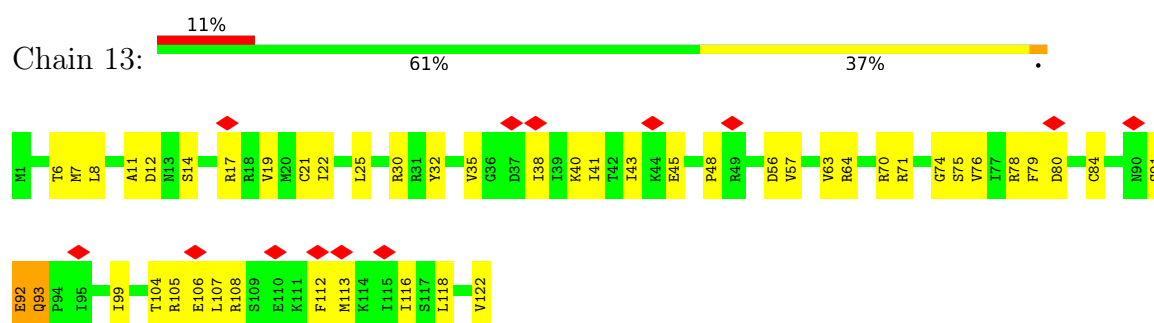
• Molecule 8: 50S ribosomal protein L11



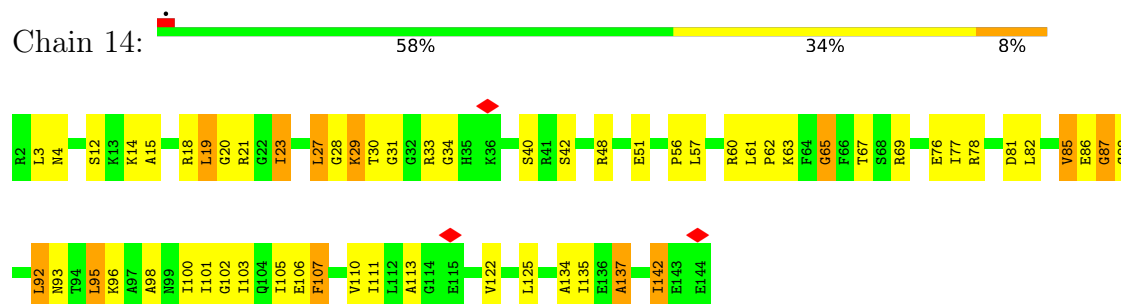
• Molecule 9: 50S ribosomal protein L13



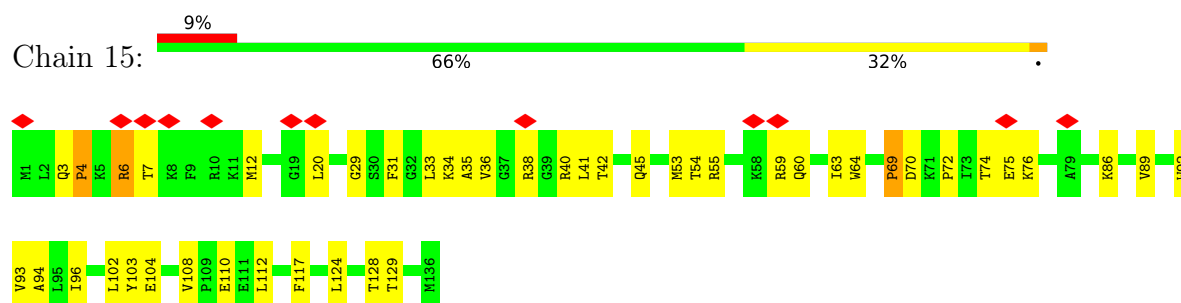
• Molecule 10: 50S ribosomal protein L14



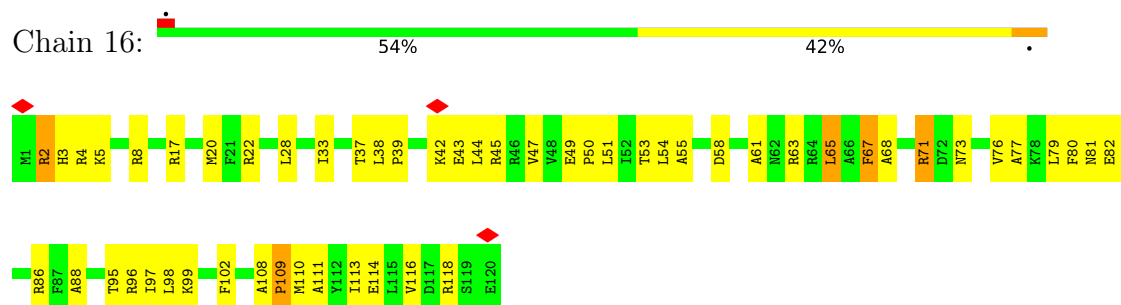
- Molecule 11: 50S ribosomal protein L15



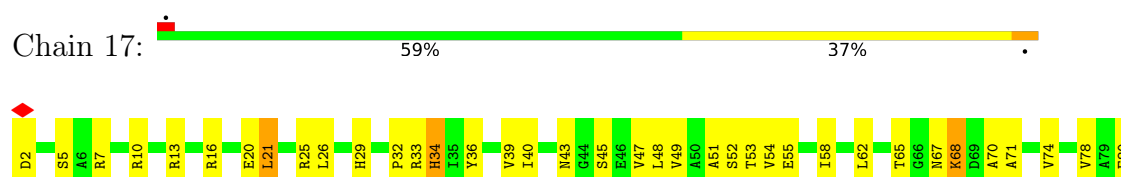
- Molecule 12: 50S ribosomal protein L16



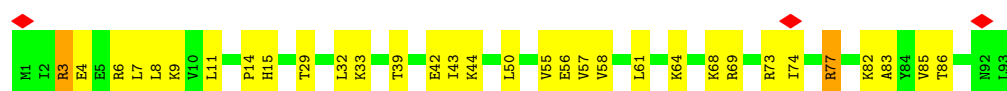
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

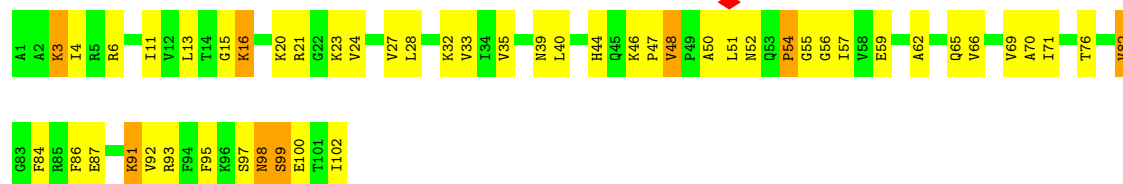


Chain 22:  66% 32%



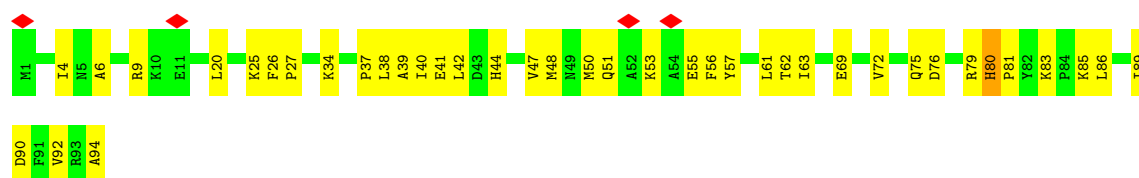
- Molecule 20: 50S ribosomal protein L24

Chain 23:  51% 41% 8%



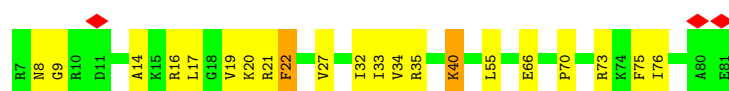
- Molecule 21: 50S ribosomal protein L25

Chain 24:  57% 41%



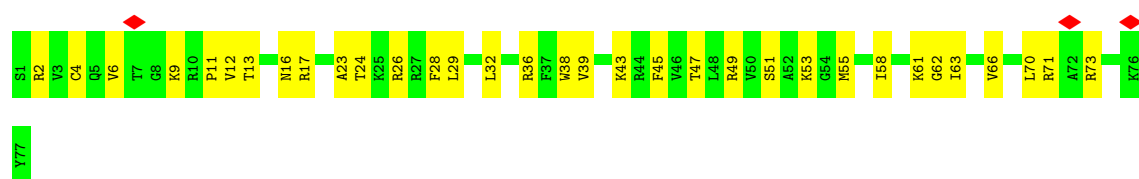
- Molecule 22: 50S ribosomal protein L27

Chain 25:  72% 25%



- Molecule 23: 50S ribosomal protein L28

Chain 26:  57% 43%



- Molecule 24: 50S ribosomal protein L29

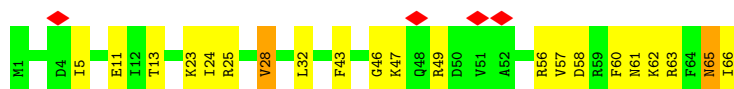
Chain 27:  48% 51%



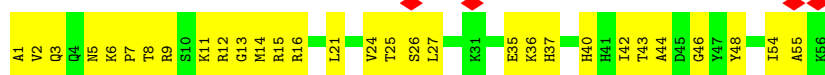
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



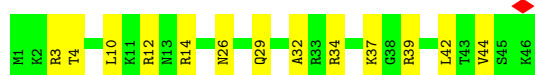
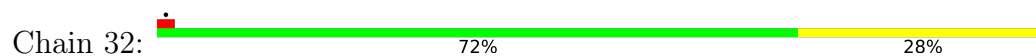
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

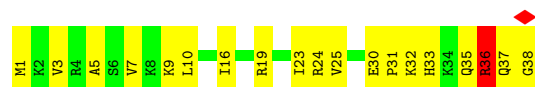


- Molecule 30: 50S ribosomal protein L35



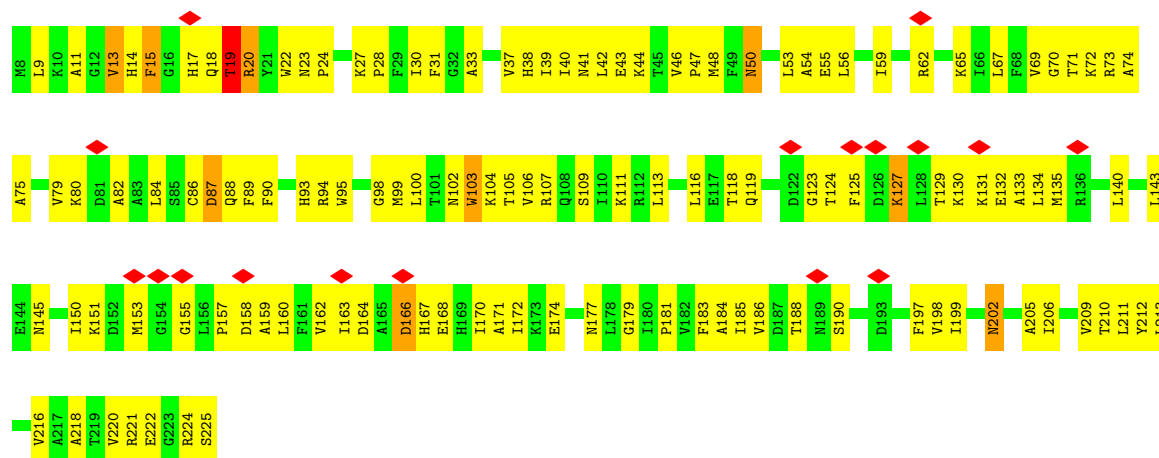
- Molecule 31: 50S ribosomal protein L36

Chain 34:  50% 47%



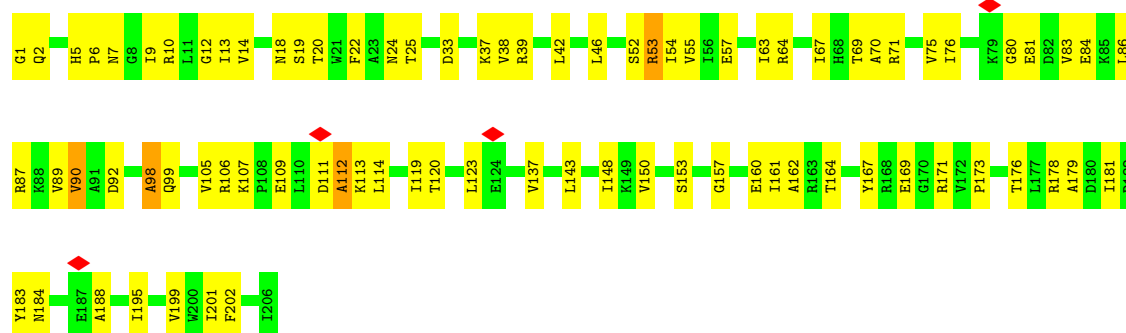
• Molecule 32: 30S ribosomal protein S2

Chain B:  8% 40% 55%



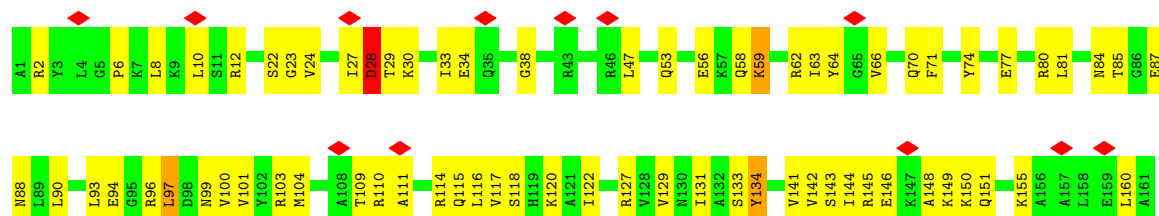
• Molecule 33: 30S ribosomal protein S3

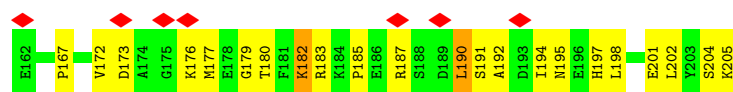
Chain C:  60% 38%



• Molecule 34: 30S ribosomal protein S4

Chain D:  9% 55% 42%

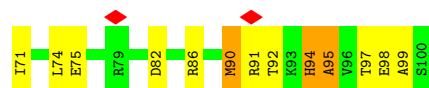




- Molecule 35: 30S ribosomal protein S5



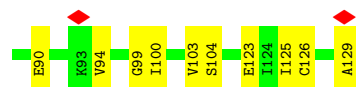
- Molecule 36: 30S ribosomal protein S6



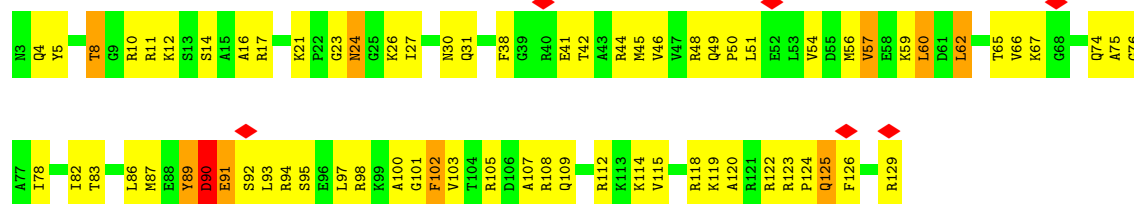
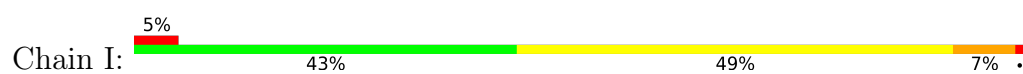
- Molecule 37: 30S ribosomal protein S7



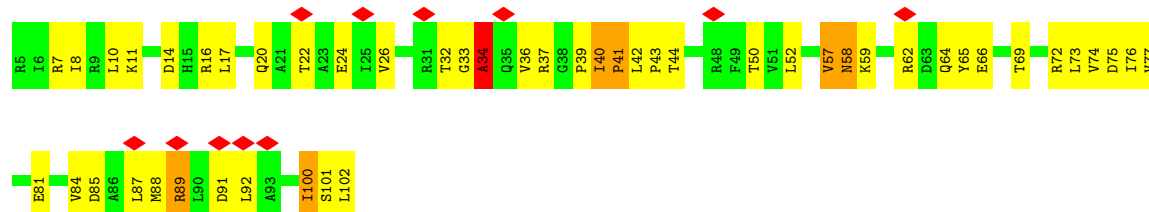
- Molecule 38: 30S ribosomal protein S8



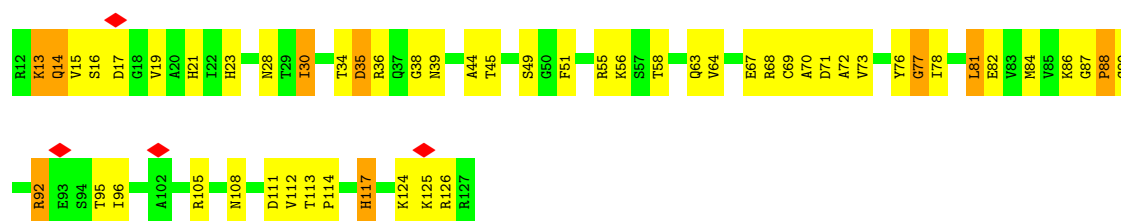
- Molecule 39: 30S ribosomal protein S9



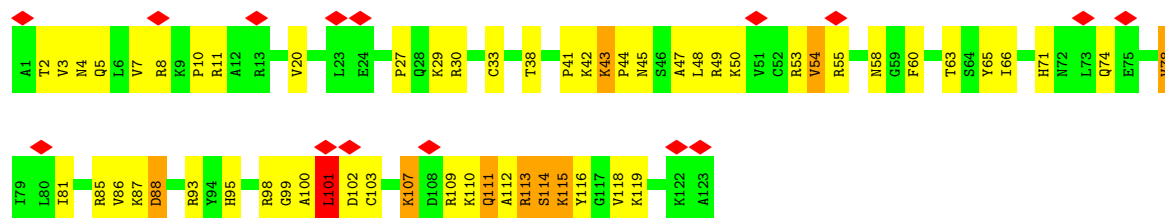
- Molecule 40: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S13





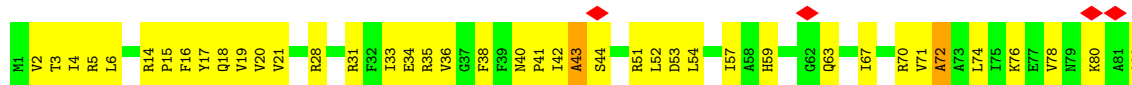
- Molecule 44: 30S ribosomal protein S14



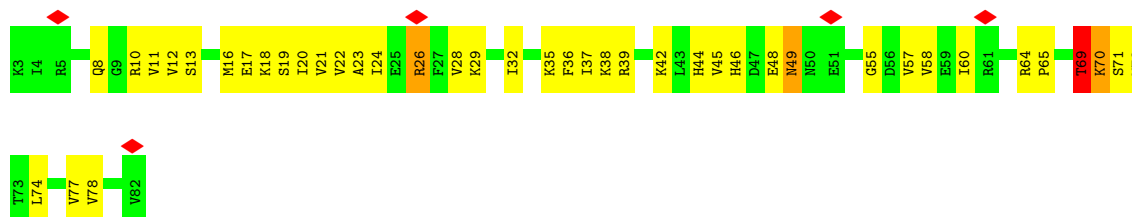
- Molecule 45: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S16



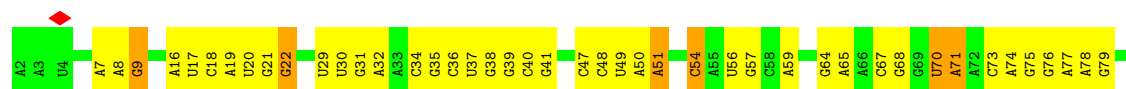
- Molecule 47: 30S ribosomal protein S17



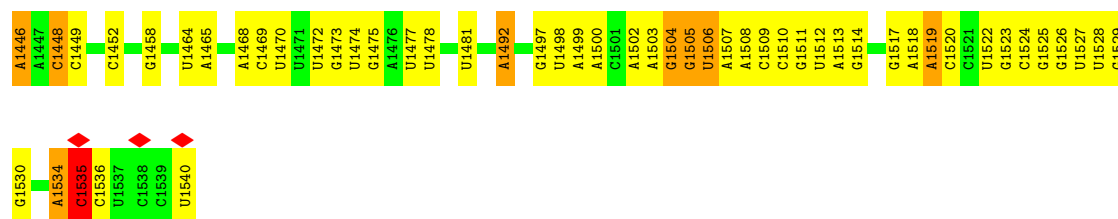
- Molecule 48: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S19

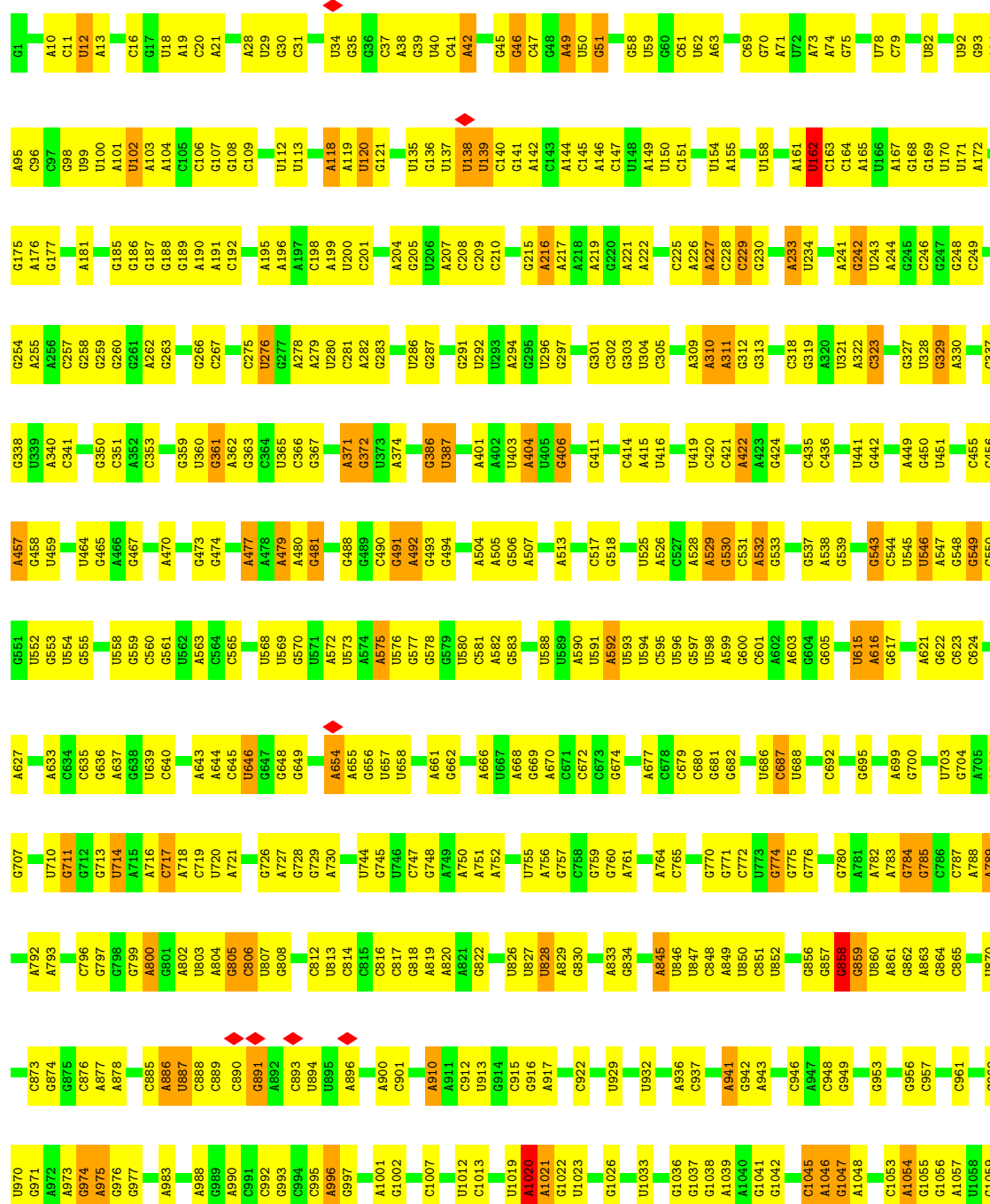


G368	C1369	G1370	G1371	U1372	G1373	A1377	C1378	G1379	U1380	U1381	C1384	G1385	C1389	U1390	U1391	G1392	U1393	A1394	C1395	A1398	C1399	C1400	G1401	C1402	C1403	G1405	C1412	A1413	U1414	G1415	A1418	G1419	G1422	G1423	U1424	U1425	A1429	A1430	A1431	G1432	A1433	G1434	U1436	A1437	A1441	G1442					
U1291	G1292	U1298	U1299	A1299	G1300	C1302	G1206	G1207	C1210	U1211	U1212	A1213	G1216	C1217	C1218	A1219	G1220	G1221	A1225	C1226	A1236	C1237	A1238	A1239	U1240	G1241	A1248	C1249	A1250	A1251	A1252	G1253	A1256	A1257	G1258	C1259	G1260	A1271	G1272	C1273	A1274	A1275	G1276	C1277	G1278	A1280	C1281	C1282	A1285	U1286	A1287
U1196	A1197	U1201	A1202	G1206	G1207	C1210	U1211	U1212	A1213	G1216	C1217	C1218	A1219	G1220	G1221	A1225	C1226	A1236	C1237	A1238	A1239	U1240	G1241	A1248	C1249	A1250	A1251	A1252	G1253	A1256	A1257	G1258	C1259	G1260	A1271	G1272	C1273	A1274	A1275	G1276	C1277	G1278	A1280	C1281	C1282	A1285	U1286	A1287			
G1100	A1101	C1111	C1112	U1121	U1122	G1127	C1128	C1129	A1130	G1134	U1135	C1136	C1137	G1138	G1139	G1144	A1145	C1146	C1147	U1148	C1149	A1150	A1151	A1157	C1158	U1159	C1162	A1163	U1168	A1169	A1170	A1171	U1070	C1071	G1072	U1073	G1074	U1075	U1078	A1081	A1082	U1083	U1086	G1087	G1094	C1098	G1099				
G1006	U1010	C1011	A1022	U1023	G1024	U1025	C1028	A1029	U1030	C1031	G1032	G1033	G1034	U1040	G1041	A1042	G1043	G1047	U1048	U1049	G1053	U1056	C1059	U1060	G1061	U1062	C1063	G1064	U1065	C1069	U1070	C1071	G1072	U1073	G1074	U1075	U1078	A1081	A1082	U1083	U1086	G1087	G1094	C1098	G1099						
A918	A919	U920	U921	C924	G925	G926	G927	G928	G929	C934	A935	G939	C940	G941	A946	G947	C948	A949	U955	A958	A959	U960	U961	G966	A969	A974	A975	G976	A977	A978	C979	U980	U981	U982	U986	G987	U992	G993	A994	C999	A1000	C1001	G1002	A1004	A1005						
C810	C811	G812	U813	A814	A815	A816	G818	A819	U820	G821	A831	G832	G833	U837	G838	U842	U843	G844	A845	G846	C853	U854	U855	C856	A860	G861	A865	C868	U869	U870	U871	A872	C876	G877	A878	C879	C880	G881	C886	U891	A892	G893	G894	A900	A901	G902	G903				
G698	C699	G700	U701	A702	G703	U709	G710	A715	A716	G722	U723	G724	G733	G734	G735	G736	C737	C738	C739	U740	G741	G742	A746	A747	G748	A749	U750	G751	G754	G755	A759	G760	A766	A767	A768	G769	A777	G778	C779	A780	A784	G785	G786	C796	C797	A802	G803				
U605	G606	A607	A608	A609	C613	G614	G616	G617	U618	C620	A621	U625	G626	G627	C631	U632	G633	C634	A635	A640	U641	A642	C643	U644	U645	U646	C651	U652	U653	G657	G661	U662	A663	G664	A665	G666	G667	A673	G674	A675	A687	G688	G689	G690	G691	A694	A695	A696	U697		
A520	G521	C522	A523	C528	A532	A533	G537	G538	A539	G540	G541	G542	U543	G544	A547	G548	C549	A553	A554	U555	C556	G557	A560	U561	U562	A563	C564	U565	G566	G570	U571	A572	A573	A574	G575	C576	G577	C578	A579	C580	G581	C582	A583	G584	U591	G592	G597	U598	G604		
A432	G433	U434	A435	C436	U437	U438	U439	C440	A441	G442	C443	G444	A448	G449	A450	A451	A452	G453	G454	A455	A456	G457	U458	A459	A460	A461	A466	U467	U476	A477	A478	U479	C483	G484	U485	U486	A487	C488	C489	G497	C501	A502	C503	C504	G505	G506	U509	G592	G597	U598	G604
U245	A246	G247	G255	G258	G259	C264	G265	G266	C267	A279	G280	G281	A288	G289	C290	U291	C295	U296	G297	A298	G299	A300	G301	G302	G305	A306	C312	A313	C314	A315	A321	C322	A327	C328	A329	C330	G331	G332	U333	C334	C335	A336	G337	A338	C339	A344	C345				
G350	G351	C352	A353	G354	U358	A363	A364	U367	U368	G369	C372	G376	C381	A382	A383	U387	U390	G391	G392	A393	G394	U398	G399	C400	C403	A404	U405	G406	U407	A408	U409	G410	A411	A412	G413	C418	C419	G420	U421	C422	G423	U426	U427	U428	A429	A430	A431				
A432	G433	U434	A435	C436	U437	U438	U439	C440	A441	G442	C443	G444	A448	G449	A450	A451	A452	G453	G454	A455	A456	G457	U458	A459	A460	A461	A466	U467	U476	A477	A478	U479	C483	G484	U485	U486	A487	C488	C489	G497	C501	A502	C503	C504	G505	G506	U509	G592	G597	U598	G604
U245	A246	G247	G255	G258	G259	C264	G265	G266	C267	A279	G280	G281	A288	G289	C290	U291	C295	U296	G297	A298	G299	A300	G301	G302	G305	A306	C312	A313	C314	A315	A321	C322	A327	C328	A329	C330	G331	G332	U333	C334	C335	A336	G337	A338	C339	A344	C345				
G350	G351	C352	A353	G354	U358	A363	A364	U367	U368	G369	C372	G376	C381	A382	A383	U387	U390	G391	G392	A393	G394	U398	G399	C400	C403	A404	U405	G406	U407	A408	U409	G410	A411	A412	G413	C418	C419	G420	U421	C422	G423	U426	U427	U428	A429	A430	A431				
A432	G433	U434	A435	C436	U437	U438	U439	C440	A441	G442	C443	G444	A448	G449	A450	A451	A452	G453	G454	A455	A456	G457	U458	A459	A460	A461	A466	U467	U476	A477	A478	U479	C483	G484	U485	U486	A487	C488	C489	G497	C501	A502	C503	C504	G505	G506	U509	G592	G597	U598	G604
U245	A246	G247	G255	G258	G259	C264	G265	G266	C267	A279	G280	G281	A288	G289	C290	U291	C295	U296	G297	A298	G299	A300	G301	G302	G305	A306	C312	A313	C314	A315	A321	C322	A327	C328	A329	C330	G331	G332	U333	C334	C335	A336	G337	A338	C339	A344	C345				
G350	G351	C352	A353	G354	U358	A363	A364	U367	U368	G369	C372	G376	C381	A382	A383	U387	U390	G391	G392	A393	G394	U398	G399	C400	C403	A404	U405	G406	U407	A408	U409	G410	A411	A412	G413	C418	C419	G420	U421	C422	G423	U426	U427	U428	A429	A430	A431				
A432	G433	U434	A435	C436	U437	U438	U439	C440	A441	G442	C443	G444	A448	G449	A450	A451	A452	G453	G454	A455	A456	G457	U458	A459	A460	A461	A466	U467	U476	A477	A478	U479	C483	G484	U485	U486	A487	C488	C489	G497	C501	A502	C503	C504	G505	G506	U509	G592	G597	U598	G604
U245	A246	G247	G255	G258	G259	C264	G265	G266	C267	A279	G280	G281	A288	G289	C290	U291	C295	U296	G297	A298	G299	A300	G301	G302	G305	A306	C312	A313	C314	A315	A321	C322	A327	C328	A329	C330	G331	G332	U333	C334	C335	A336	G337	A338	C339	A344	C345				
G350	G351	C352	A353	G354	U358	A363	A364	U367	U368	G369	C372	G376	C381	A382	A383	U387	U390	G391	G392	A393	G394	U398	G399	C400	C403	A404	U405	G406	U407	A408	U409	G410	A411	A412	G413	C418	C419	G420	U421	C422	G423	U426	U427	U428	A429	A430	A431				
A432	G433	U434	A435	C436	U437	U438	U439	C440	A441	G442	C443	G444	A448	G449	A450	A451	A452	G453	G454	A455	A456	G457	U458	A459	A460	A461	A466	U467	U476	A477	A478	U479	C483	G484	U485	U486	A487	C488	C489	G497	C501	A502	C503	C504	G505	G506	U509	G592	G597	U598	G604
U245	A246	G247	G255	G258	G259	C264	G265	G266	C267	A279	G280	G281	A288	G289	C290	U291	C295	U296	G297	A298	G299	A300	G301	G302	G305	A306	C312	A313	C314	A315	A321	C322	A327	C328	A329	C330	G331	G332	U333	C334	C335	A336	G337	A338	C339	A344	C345				
G350	G351	C352	A353	G354	U358	A363	A364	U367	U368	G369	C372	G376	C381	A382	A383	U387	U390	G391	G392	A393	G394	U398	G399	C400	C403	A404	U405	G406	U407	A408	U409	G410	A411	A412	G413	C418	C419	G420	U421	C422	G423	U426	U427	U428	A429	A430	A431				
A432	G433	U434	A435	C436	U437	U438	U439	C440	A441	G442	C443	G444	A448	G449	A450	A451	A452	G453	G454	A455	A456	G457	U458	A459	A460	A461	A466	U467	U476	A477	A478	U479	C483	G484	U485	U486	A487	C488	C489	G497	C501	A502	C503	C504	G505	G506	U509	G592	G597	U598	G604
U245	A246	G247	G255	G258	G259	C264	G265	G266	C267	A279	G280	G281	A288	G289	C290	U291	C295	U296	G297	A298	G299	A300	G301	G302	G305	A306	C312	A313	C314	A315	A321	C322	A327	C328	A329	C330	G331	G332	U333	C334	C335	A336	G337	A338	C339	A344	C345				
G350	G351	C352	A353	G354	U358	A363	A364	U367	U368	G369	C372	G376	C381	A382	A383	U387	U390	G391	G392	A393	G394	U398	G399	C400	C403	A404	U405	G406	U407	A408	U409	G410	A411	A412	G413	C418	C419	G420	U421	C422	G423	U426	U427	U428	A429	A430	A431				
A432	G433	U434	A435	C436	U437	U438	U439	C440	A441	G442	C443	G444	A448	G449	A450	A451	A452	G453	G454	A455	A456	G457	U458	A459	A460	A461	A466	U467	U476	A477	A478	U479	C483	G484	U485	U486	A487	C488	C489	G497	C501	A502	C503	C504	G505	G506	U509	G592	G597	U598	G604
U245	A246	G247	G255	G258	G259	C264	G265	G266	C267	A279	G280	G281	A288	G289	C290	U291	C295	U296	G297	A298	G299	A300	G301	G302	G305	A306	C312	A313	C314	A315	A321	C322	A327	C328	A329	C330	G331	G332	U												

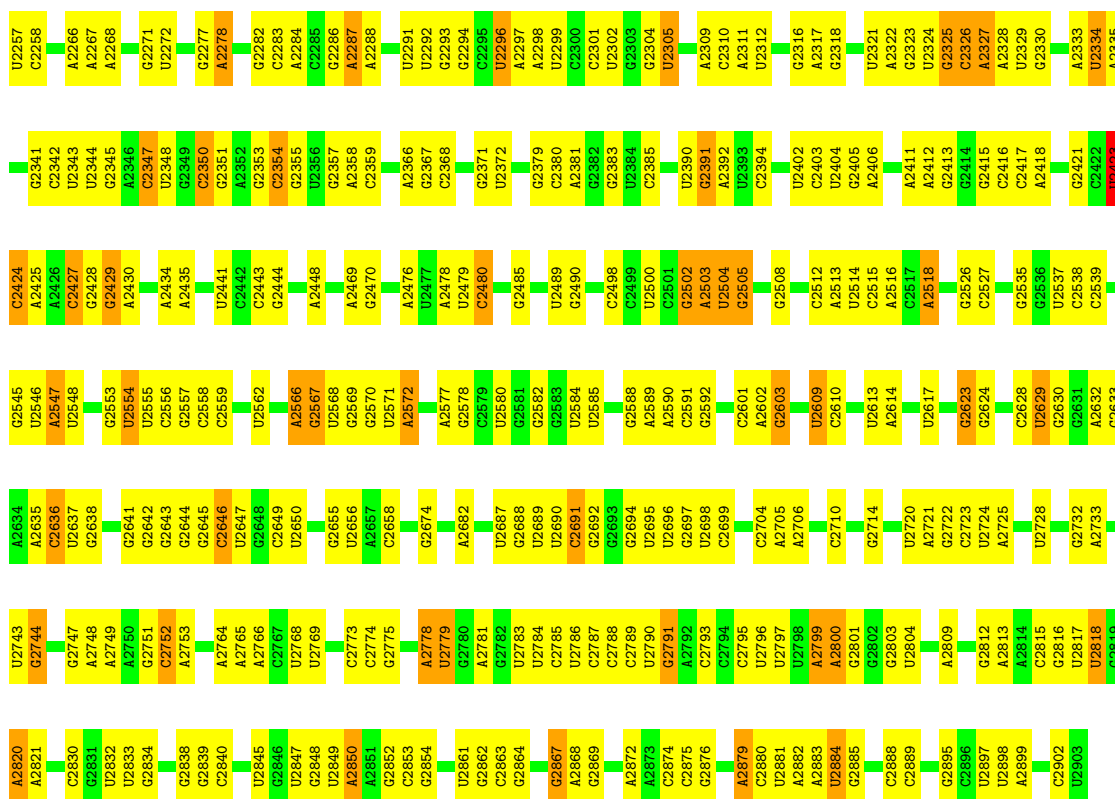


• Molecule 54: 23S ribosomal RNA

Chain 01: 50% 43% 7%

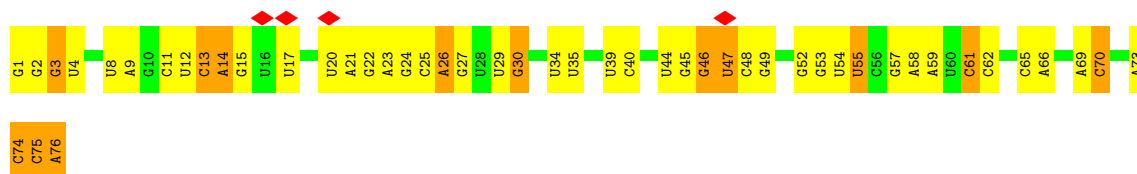


U2166	A2170	A2171	U2172	A2173	U2176	C2177	U2182	A2183	A2184	U2189	G2190	A2191	U2192	U2194	G2195	U2197	A2198	U2203	G2204	G2208	G2209	U2210	A2211	U2213	C2214	G2215	G2216	G2224	A2225	C2226	U2233	G2234	G2235	U2236	G2237	G2238	G2239	U2243	U2244	U2245	G2246	A2247	G2250	G2251	G2252								
C2091	U2092	G2093	C2096	A2097	U2098	U2099	C2103	C2104	C2105	U2106	G2107	A2108	U2109	G2110	U2111	U2112	U2113	A2114	G2115	U2117	A2118	A2119	U2122	G2123	G2124	G2125	G2126	G2127	U2130	U2131	U2132	G2133	A2134	G2141	C2145	C2146	A2147	G2148	U2151	G2152	C2153	U2154	U2155	U2156	U2157	U2158	G2159	C2160	U2161	G2162			
A2020	C2021	U2022	C2023	G2024	A2030	A2031	G2032	A2033	U2034	G2035	C2036	A2037	U2038	U2039	G2040	U2041	A2042	C2043	C2045	G1964	C1965	A1966	C1967	C2055	G2056	G2057	A2060	G2061	A2062	C2063	C2064	G2065	C2066	G2067	U2068	G2069	A2070	A2071	C2072	C2073	U2074	U2075	U2076	U2079	A2080	U2081	C2084	U2085	U2086	G2087	A2088	C2089	A2090
U1841	G1842	C1843	C1844	G1845	A1848	G1849	G1850	C1851	U1852	U1856	G1857	A1858	G1863	G1869	C1870	A1871	G1872	G1873	C1874	G1875	A1876	A1877	G1878	C1879	U1880	C1881	U1882	U1883	G1884	A1885	U1886	C1887	G1888	A1889	G1890	G1891	C1892	C1893	C1894	A1899	A1900	A1901	C1902	G1903	G1906	U1911	U1912	A1913	C1914	A1918			
G1929	G1930	U1931	A1932	G1933	C1934	G1935	A1936	A1937	U1938	U1939	C1940	A1941	G1942	U1943	U1944	U1955	G1959	A1960	G1964	C1965	A1966	C1967	C1970	A1971	A1974	C1975	U1976	G1977	C1800	A1801	A1805	C1806	G1807	A1808	G1809	A1810	U1811	U1812	G1813	C1816	G1817	U1818	U1827	G1828	A1829	C1830	G1831	G1835	C1836	U1837			
A1669	C1670	A1671	A1672	G1673	G1674	U1675	A1676	U1679	U1680	G1681	G1682	A1689	A1690	U1693	C1694	G1695	G1696	A1698	G1699	C1610	A1611	A1616	A1626	G1627	A1634	U1635	U1636	A1637	C1638	A1641	G1642	G1645	C1646	U1647	U1648	G1651	A1652	G1653	A1654	A1655	C1656	U1657	C1658	U1659	G1661	G1663	A1664	A1665	G1666				
C1498	C1499	G1500	A1503	A1504	A1505	U1506	A1508	A1509	G1510	G1511	C1512	U1513	A1515	G1518	U1519	A1522	U1523	A1524	A1525	C1526	A1527	G1528	G1529	A1532	C1533	U1534	C1535	G1537	G1538	G1539	G1540	C1541	U1542	G1543	A1548	A1549	G1555	U1559	A1560	U1563	C1564	C1565	A1566	G1567	A1568	A1569	A1570	A1571					
G1410	U1411	G1416	A1417	G1418	A1419	A1420	G1421	G1422	G1423	A1427	C1428	G1432	A1433	A1434	G1435	G1436	U1438	U1443	G1444	G1445	G1446	A1447	G1448	C1451	U1452	A1453	C1454	C1461	C1462	C1463	U1468	A1469	A1470	G1471	C1472	G1473	U1474	G1475	U1476	A1477	G1478	G1482	G1483	U1484	U1485	A1490	A1491	G1492					
C1319	C1320	G1324	U1325	A1328	U1329	C1330	G1331	G1332	C1335	A1336	G1337	G1338	G1339	U1340	G1341	U1344	C1345	C1346	C1351	U1352	A1353	U1354	G1355	G1356	C1357	C1358	G1364	A1365	A1366	G1367	G1368	G1369	C1370	G1371	U1372	A1373	A1378	U1379	A1383	C1386	A1387	A1394	U1395	G1310	A1213	A1214	G1215	U1222	G1223	U1224			
A1142	A1143	C1146	A1147	U1148	G1149	A1150	A1151	C1152	C1153	G1154	A1155	A1156	G1157	C1161	G1162	C1167	U1168	A1169	C1170	G1171	C1172	U1173	U1174	A1175	U1176	G1177	A1178	U1179	U1180	U1181	G1182	U1183	G1186	G1187	U1188	A1189	G1190	G1191	U1198	U1199	U1203	A1204	A1205	G1206	G1212	A1213	A1214	G1215	U1222	G1223	U1224		
U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	A1070	G1071	C1072	A1073	C1074	A1075	C1076	U1077	U1078	C1079	U1083	A1084	A1085	A1086	G1087	A1088	C1092	G1093	U1094	U1097	U1101	C1102	A1103	C1104	U1105	G1106	A1111	G1112	U1113	C1114	C1123	G1124	A1129	U1130	U1132	A1133	A1134	C1135	G1138	G1139	C1140	U1141				

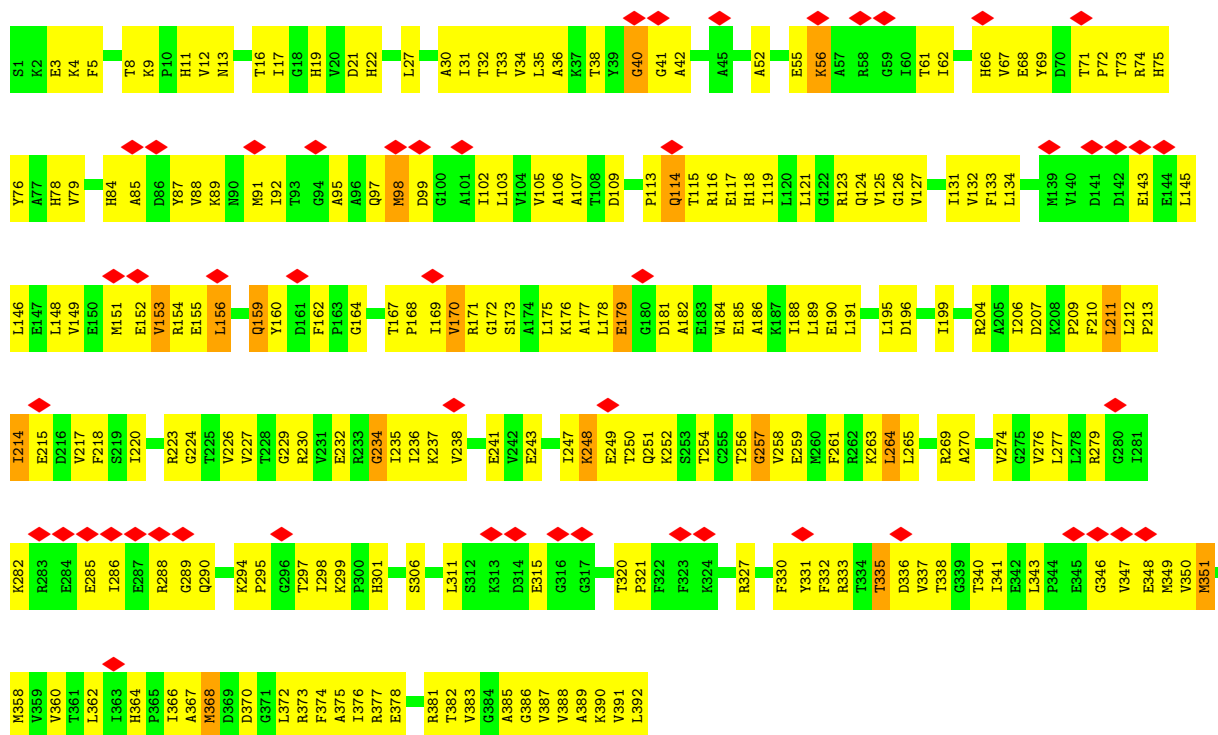




• Molecule 58: tRNA^{Lys}



• Molecule 59: Elongation factor Tu 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND3 was used to determine CTF values. FREALIGN applied CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	60976	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.791	Depositor
Minimum map value	-6.406	Depositor
Average map value	-0.340	Depositor
Map value standard deviation	1.063	Depositor
Recommended contour level	2.85	Depositor
Map size ($\text{\AA}$)	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, FME, MG, U8U

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	04	0.37	0/2122	0.94	10/2852 (0.4%)
2	05	0.39	0/1586	0.90	0/2134
3	06	0.37	0/1571	0.98	8/2113 (0.4%)
4	07	0.39	0/1435	0.84	2/1926 (0.1%)
5	08	0.39	0/1343	0.96	7/1816 (0.4%)
6	09	0.43	0/1122	1.04	9/1515 (0.6%)
7	10	0.48	0/1002	1.16	13/1350 (1.0%)
8	11	0.50	0/1046	1.11	5/1410 (0.4%)
9	12	0.37	0/1152	0.87	2/1551 (0.1%)
10	13	0.39	0/948	0.95	3/1268 (0.2%)
11	14	0.38	0/1054	1.09	8/1403 (0.6%)
12	15	0.39	0/1093	0.91	5/1460 (0.3%)
13	16	0.38	0/974	1.01	5/1301 (0.4%)
14	17	0.35	0/902	0.96	5/1209 (0.4%)
15	18	0.38	0/929	0.88	1/1242 (0.1%)
16	19	0.35	0/960	0.92	4/1278 (0.3%)
17	20	0.44	0/829	0.98	6/1107 (0.5%)
18	21	0.37	0/864	0.85	2/1156 (0.2%)
19	22	0.38	0/745	0.89	1/994 (0.1%)
20	23	0.38	0/788	0.90	3/1051 (0.3%)
21	24	0.39	0/766	0.91	1/1025 (0.1%)
22	25	0.37	0/582	0.89	2/769 (0.3%)
23	26	0.34	0/635	0.86	1/848 (0.1%)
24	27	0.33	0/510	0.94	0/677
25	28	0.38	0/453	0.86	0/605
26	29	0.40	0/532	0.95	2/709 (0.3%)
27	30	0.35	0/450	0.85	1/599 (0.2%)
28	31	0.41	0/417	0.87	1/554 (0.2%)
29	32	0.40	0/380	0.91	0/498
30	33	0.36	0/513	0.93	1/676 (0.1%)
31	34	0.38	0/303	0.90	2/397 (0.5%)
32	B	0.40	0/1736	1.04	18/2338 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	C	0.38	0/1652	0.88	3/2225 (0.1%)
34	D	0.40	0/1665	0.98	7/2227 (0.3%)
35	E	0.40	0/1170	0.95	3/1573 (0.2%)
36	F	0.40	0/836	0.93	4/1128 (0.4%)
37	G	0.38	0/1196	0.99	10/1602 (0.6%)
38	H	0.38	0/989	0.88	0/1326
39	I	0.38	0/1034	1.02	8/1375 (0.6%)
40	J	0.40	0/797	0.92	3/1077 (0.3%)
41	K	0.38	0/886	0.99	3/1195 (0.3%)
42	L	0.39	0/969	0.97	8/1300 (0.6%)
43	M	0.37	0/893	1.04	7/1193 (0.6%)
44	N	0.35	0/817	0.97	6/1088 (0.6%)
45	O	0.37	0/722	0.93	1/964 (0.1%)
46	P	0.37	0/659	1.00	3/884 (0.3%)
47	Q	0.41	0/658	0.99	3/881 (0.3%)
48	R	0.47	0/545	1.07	6/731 (0.8%)
49	S	0.40	0/653	0.86	0/877
50	T	0.35	0/671	1.00	5/888 (0.6%)
51	U	0.42	0/551	1.12	8/728 (1.1%)
52	03	0.53	0/1034	1.10	8/1387 (0.6%)
53	A	0.43	0/36963	0.55	17/57662 (0.0%)
54	01	0.43	0/69796	0.54	13/108888 (0.0%)
55	02	0.44	0/2872	0.54	1/4479 (0.0%)
56	W	0.44	0/1832	0.53	0/2855
56	X	0.48	0/1832	0.61	1/2855 (0.0%)
57	V	0.46	0/446	0.57	0/696
58	Y	0.45	0/1780	0.59	0/2767
59	Z	0.45	0/3085	1.04	23/4173 (0.6%)
All	All	0.42	0/166745	0.69	279/248855 (0.1%)

There are no bond length outliers.

The worst 5 of 279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	246	A	C2'-C3'-O3'	11.74	127.11	109.50
11	14	95	LEU	N-CA-C	-11.43	98.71	112.89
7	10	77	VAL	N-CA-C	-10.69	102.40	111.91
59	Z	98	MET	N-CA-C	10.38	124.02	110.43
1	04	12	ARG	N-CA-C	-9.96	100.03	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	04	2083	0	2157	87	0
2	05	1565	0	1616	64	0
3	06	1552	0	1619	59	0
4	07	1411	0	1447	75	0
5	08	1323	0	1374	47	0
6	09	1111	0	1148	33	0
7	10	989	0	1025	61	0
8	11	1032	0	1088	70	0
9	12	1129	0	1162	52	0
10	13	939	0	1012	37	0
11	14	1045	0	1117	54	0
12	15	1074	0	1157	35	0
13	16	961	0	1000	46	0
14	17	892	0	923	39	0
15	18	917	0	965	54	0
16	19	947	0	1022	43	0
17	20	816	0	839	37	0
18	21	857	0	922	42	0
19	22	739	0	807	31	0
20	23	780	0	834	33	0
21	24	753	0	780	32	0
22	25	575	0	592	18	0
23	26	625	0	655	24	0
24	27	509	0	543	28	0
25	28	449	0	491	14	0
26	29	523	0	524	18	0
27	30	444	0	461	23	0
28	31	410	0	440	14	0
29	32	377	0	418	14	0
30	33	504	0	574	20	0
31	34	302	0	343	16	0
32	B	1705	0	1732	88	0
33	C	1625	0	1699	68	0
34	D	1643	0	1710	76	0
35	E	1157	0	1199	49	0
36	F	818	0	808	44	0
37	G	1182	0	1240	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	979	0	1034	38	0
39	I	1022	0	1070	65	0
40	J	787	0	828	39	0
41	K	870	0	878	48	0
42	L	955	0	1019	56	0
43	M	884	0	944	50	0
44	N	805	0	847	44	0
45	O	714	0	737	25	0
46	P	649	0	666	36	0
47	Q	649	0	691	37	0
48	R	536	0	552	25	0
49	S	638	0	665	39	0
50	T	665	0	714	34	0
51	U	545	0	579	35	0
52	03	1027	0	1092	53	0
53	A	33012	0	16618	557	0
54	01	62317	0	31346	1039	0
55	02	2568	0	1303	56	0
56	W	1640	0	836	18	0
56	X	1640	0	837	35	0
57	V	395	0	198	5	0
58	Y	1618	0	820	44	0
59	Z	3029	0	3043	177	0
60	W	10	0	10	0	0
61	Y	9	0	12	1	0
62	Z	1	0	0	0	0
63	Z	32	0	14	3	0
All	All	153759	0	104796	3712	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 14.

The worst 5 of 3712 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)
54:01:45:G:H5''	54:01:46:G:H5'	1.41	1.03
58:Y:13:C:H2'	58:Y:14:A:H5''	1.39	1.00
12:15:45:GLN:HE21	54:01:2485:G:H5''	1.30	0.96
59:Z:88:VAL:HG11	59:Z:121:LEU:HD13	1.45	0.96
42:L:33:CYS:H	42:L:54:VAL:HG13	1.32	0.95

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
1	04	269/271 (99%)	236 (88%)	31 (12%)	2 (1%)	18	51
2	05	207/209 (99%)	174 (84%)	28 (14%)	5 (2%)	4	29
3	06	199/201 (99%)	167 (84%)	26 (13%)	6 (3%)	3	25
4	07	175/177 (99%)	156 (89%)	15 (9%)	4 (2%)	5	30
5	08	174/176 (99%)	155 (89%)	15 (9%)	4 (2%)	5	30
6	09	147/149 (99%)	124 (84%)	21 (14%)	2 (1%)	9	37
7	10	129/131 (98%)	90 (70%)	29 (22%)	10 (8%)	1	11
8	11	139/141 (99%)	111 (80%)	20 (14%)	8 (6%)	1	15
9	12	140/142 (99%)	123 (88%)	16 (11%)	1 (1%)	18	51
10	13	120/122 (98%)	94 (78%)	22 (18%)	4 (3%)	3	24
11	14	141/143 (99%)	112 (79%)	23 (16%)	6 (4%)	2	19
12	15	134/136 (98%)	107 (80%)	23 (17%)	4 (3%)	3	25
13	16	118/120 (98%)	100 (85%)	15 (13%)	3 (2%)	4	28
14	17	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	6	33
15	18	112/114 (98%)	92 (82%)	20 (18%)	0	100	100
16	19	115/117 (98%)	101 (88%)	13 (11%)	1 (1%)	14	45
17	20	101/103 (98%)	87 (86%)	10 (10%)	4 (4%)	2	20
18	21	108/110 (98%)	88 (82%)	19 (18%)	1 (1%)	14	45
19	22	91/93 (98%)	78 (86%)	12 (13%)	1 (1%)	11	41
20	23	100/102 (98%)	83 (83%)	10 (10%)	7 (7%)	1	12
21	24	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
22	25	73/75 (97%)	61 (84%)	9 (12%)	3 (4%)	2	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	26	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
24	27	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
25	28	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
26	29	64/66 (97%)	49 (77%)	14 (22%)	1 (2%)	7	35
27	30	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
28	31	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
29	32	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
30	33	62/64 (97%)	52 (84%)	8 (13%)	2 (3%)	3	24
31	34	36/38 (95%)	29 (81%)	7 (19%)	0	100	100
32	B	216/218 (99%)	173 (80%)	35 (16%)	8 (4%)	2	21
33	C	204/206 (99%)	182 (89%)	21 (10%)	1 (0%)	24	57
34	D	203/205 (99%)	163 (80%)	34 (17%)	6 (3%)	3	25
35	E	155/157 (99%)	125 (81%)	21 (14%)	9 (6%)	1	15
36	F	98/100 (98%)	81 (83%)	14 (14%)	3 (3%)	3	25
37	G	149/151 (99%)	124 (83%)	23 (15%)	2 (1%)	9	38
38	H	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	7	35
39	I	125/127 (98%)	93 (74%)	23 (18%)	9 (7%)	1	12
40	J	96/98 (98%)	76 (79%)	13 (14%)	7 (7%)	1	11
41	K	114/116 (98%)	93 (82%)	15 (13%)	6 (5%)	1	16
42	L	121/123 (98%)	92 (76%)	25 (21%)	4 (3%)	3	24
43	M	112/114 (98%)	92 (82%)	17 (15%)	3 (3%)	4	27
44	N	98/100 (98%)	79 (81%)	17 (17%)	2 (2%)	6	32
45	O	86/88 (98%)	71 (83%)	13 (15%)	2 (2%)	5	30
46	P	80/82 (98%)	63 (79%)	15 (19%)	2 (2%)	4	28
47	Q	78/80 (98%)	62 (80%)	13 (17%)	3 (4%)	2	21
48	R	63/65 (97%)	45 (71%)	13 (21%)	5 (8%)	1	10
49	S	77/79 (98%)	63 (82%)	13 (17%)	1 (1%)	9	38
50	T	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
51	U	63/65 (97%)	44 (70%)	16 (25%)	3 (5%)	2	17
52	03	130/223 (58%)	106 (82%)	18 (14%)	6 (5%)	2	18
59	Z	390/392 (100%)	331 (85%)	51 (13%)	8 (2%)	5	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6366/6563 (97%)	5310 (83%)	883 (14%)	173 (3%)	6	27

5 of 173 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	05	134	HIS
3	06	84	THR
3	06	89	PRO
4	07	173	ASP
5	08	174	LYS

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	
1	04	216/216 (100%)	212 (98%)	4 (2%)	50	66
2	05	164/164 (100%)	162 (99%)	2 (1%)	63	72
3	06	165/165 (100%)	164 (99%)	1 (1%)	78	79
4	07	148/148 (100%)	148 (100%)	0	100	100
5	08	137/137 (100%)	136 (99%)	1 (1%)	76	77
6	09	114/114 (100%)	114 (100%)	0	100	100
7	10	100/100 (100%)	98 (98%)	2 (2%)	48	65
8	11	109/109 (100%)	108 (99%)	1 (1%)	70	74
9	12	116/116 (100%)	114 (98%)	2 (2%)	53	67
10	13	103/103 (100%)	103 (100%)	0	100	100
11	14	102/102 (100%)	99 (97%)	3 (3%)	37	58
12	15	109/109 (100%)	109 (100%)	0	100	100
13	16	100/100 (100%)	100 (100%)	0	100	100
14	17	86/86 (100%)	85 (99%)	1 (1%)	63	72
15	18	99/99 (100%)	98 (99%)	1 (1%)	68	74
16	19	89/89 (100%)	88 (99%)	1 (1%)	65	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	20	84/84 (100%)	82 (98%)	2 (2%)	43	62
18	21	93/93 (100%)	91 (98%)	2 (2%)	45	63
19	22	80/80 (100%)	80 (100%)	0	100	100
20	23	83/83 (100%)	80 (96%)	3 (4%)	31	54
21	24	78/78 (100%)	77 (99%)	1 (1%)	61	71
22	25	57/57 (100%)	56 (98%)	1 (2%)	51	67
23	26	67/67 (100%)	67 (100%)	0	100	100
24	27	55/55 (100%)	54 (98%)	1 (2%)	51	67
25	28	48/48 (100%)	48 (100%)	0	100	100
26	29	59/59 (100%)	59 (100%)	0	100	100
27	30	47/47 (100%)	47 (100%)	0	100	100
28	31	45/45 (100%)	44 (98%)	1 (2%)	45	63
29	32	38/38 (100%)	37 (97%)	1 (3%)	40	60
30	33	51/51 (100%)	51 (100%)	0	100	100
31	34	34/34 (100%)	33 (97%)	1 (3%)	37	58
32	B	180/180 (100%)	178 (99%)	2 (1%)	65	73
33	C	170/170 (100%)	169 (99%)	1 (1%)	78	79
34	D	172/172 (100%)	169 (98%)	3 (2%)	53	67
35	E	119/119 (100%)	118 (99%)	1 (1%)	73	76
36	F	87/87 (100%)	85 (98%)	2 (2%)	44	63
37	G	124/124 (100%)	123 (99%)	1 (1%)	73	76
38	H	104/104 (100%)	103 (99%)	1 (1%)	68	74
39	I	105/105 (100%)	104 (99%)	1 (1%)	68	74
40	J	86/86 (100%)	85 (99%)	1 (1%)	63	72
41	K	89/89 (100%)	87 (98%)	2 (2%)	45	63
42	L	103/103 (100%)	100 (97%)	3 (3%)	37	58
43	M	92/92 (100%)	90 (98%)	2 (2%)	45	63
44	N	83/83 (100%)	81 (98%)	2 (2%)	43	62
45	O	76/76 (100%)	75 (99%)	1 (1%)	61	71
46	P	65/65 (100%)	64 (98%)	1 (2%)	57	69
47	Q	74/74 (100%)	72 (97%)	2 (3%)	39	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	R	56/56 (100%)	55 (98%)	1 (2%)	51	67
49	S	70/70 (100%)	70 (100%)	0	100	100
50	T	65/65 (100%)	65 (100%)	0	100	100
51	U	55/55 (100%)	55 (100%)	0	100	100
52	03	110/174 (63%)	107 (97%)	3 (3%)	39	59
59	Z	324/325 (100%)	318 (98%)	6 (2%)	50	66
All	All	5285/5350 (99%)	5217 (99%)	68 (1%)	59	71

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	Q	69	THR
52	03	5	THR
59	Z	211	LEU
20	23	82	VAL
20	23	65	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
44	N	34	ASN
46	P	9	HIS
59	Z	19	HIS
14	17	38	GLN
14	17	29	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	170 (11%)	11 (0%)
54	01	2902/2903 (99%)	398 (13%)	17 (0%)
55	02	119/120 (99%)	12 (10%)	1 (0%)
56	W	76/77 (98%)	7 (9%)	0
56	X	76/77 (98%)	13 (17%)	0
57	V	17/18 (94%)	1 (5%)	0
58	Y	75/76 (98%)	19 (25%)	0
All	All	4803/4810 (99%)	620 (12%)	29 (0%)

5 of 620 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	7	A
53	A	9	G
53	A	22	G
53	A	32	A
53	A	39	G

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	01	421	C
54	01	2655	G
54	01	859	G
54	01	1940	U
54	01	774	G

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
58	U8U	Y	34	58,57	20,24,25	1.21	2 (10%)	22,34,37	0.93	2 (9%)

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
58	U8U	Y	34	58,57	-	1/10/28/29	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Y	34	U8U	C6-N1	3.88	1.44	1.38
58	Y	34	U8U	C4-C5	2.06	1.50	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Y	34	U8U	C2'-C1'-N1	2.29	119.64	113.25
58	Y	34	U8U	C5-C6-N1	2.00	125.64	122.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	Y	34	U8U	C5-C-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
63	GCP	Z	402	62	32,34,34	1.86	5 (15%)	49,54,54	2.59	14 (28%)
61	LYS	Y	101	58	7,8,9	0.66	0	3,8,10	0.27	0
60	FME	W	101	-	8,9,10	0.67	0	8,9,11	1.23	1 (12%)

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
63	GCP	Z	402	62	-	9/19/38/38	0/3/3/3
61	LYS	Y	101	58	-	0/6/7/9	-
60	FME	W	101	-	-	3/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	Z	402	GCP	PA-O3A	-5.83	1.53	1.59
63	Z	402	GCP	PB-O3A	-5.14	1.52	1.58
63	Z	402	GCP	PB-O2B	-2.38	1.50	1.56
63	Z	402	GCP	O4'-C1'	2.38	1.47	1.42
63	Z	402	GCP	C1'-N9	2.24	1.53	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	Z	402	GCP	C1'-N9-C4	8.58	151.82	126.49
63	Z	402	GCP	C1'-N9-C8	-8.51	102.55	126.73
63	Z	402	GCP	O1G-PG-C3B	-6.97	96.17	111.37
63	Z	402	GCP	O5'-PA-O1A	-3.95	93.27	108.94
63	Z	402	GCP	O2B-PB-O1B	3.65	121.84	109.95

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

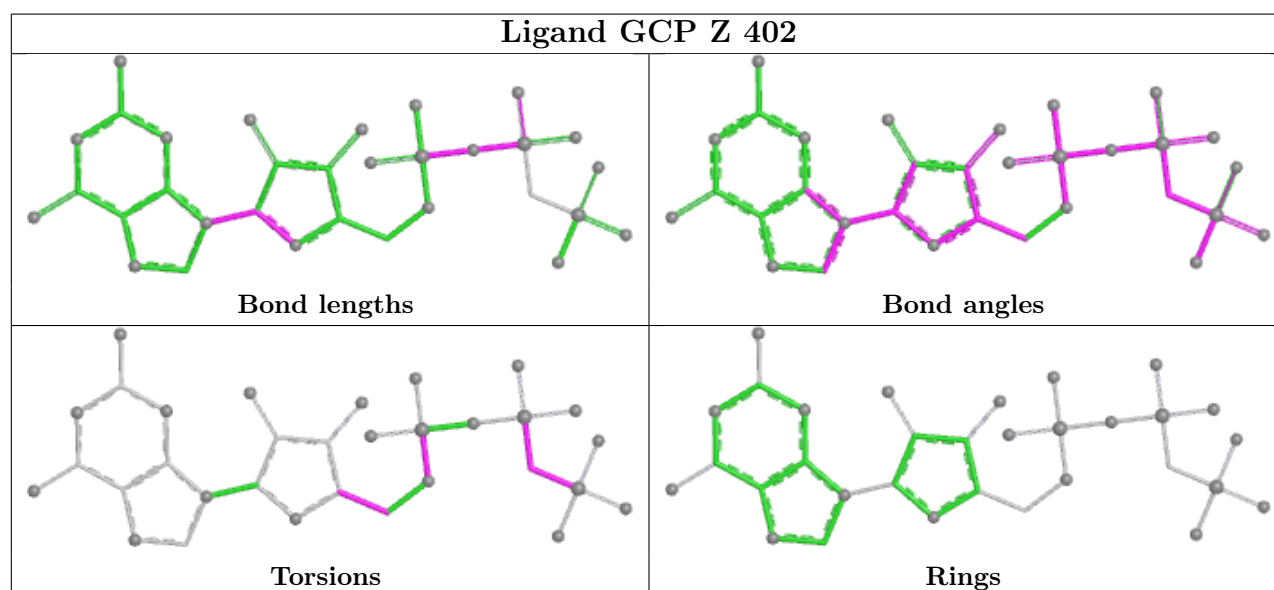
Mol	Chain	Res	Type	Atoms
60	W	101	FME	O1-CN-N-CA
60	W	101	FME	O-C-CA-CB
63	Z	402	GCP	PB-C3B-PG-O1G
63	Z	402	GCP	PB-C3B-PG-O2G
63	Z	402	GCP	PG-C3B-PB-O1B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	Z	402	GCP	3	0
61	Y	101	LYS	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

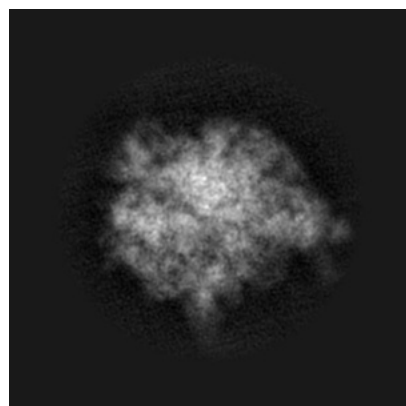
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8620. These allow visual inspection of the internal detail of the map and identification of artifacts.

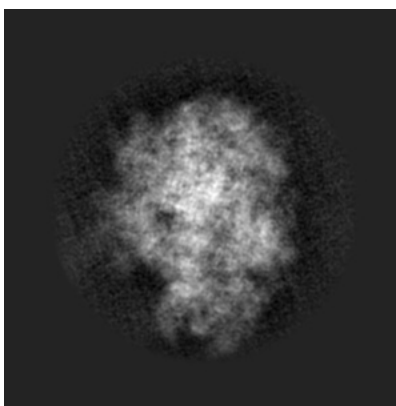
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

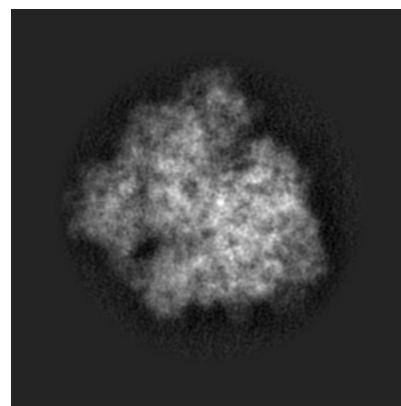
6.1.1 Primary map



X

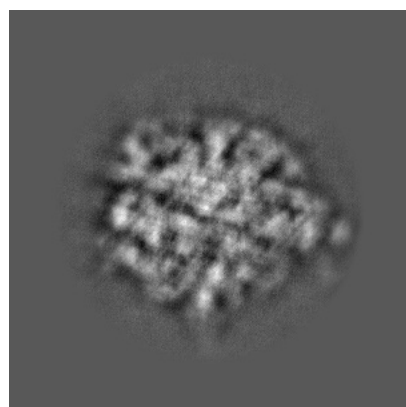


Y

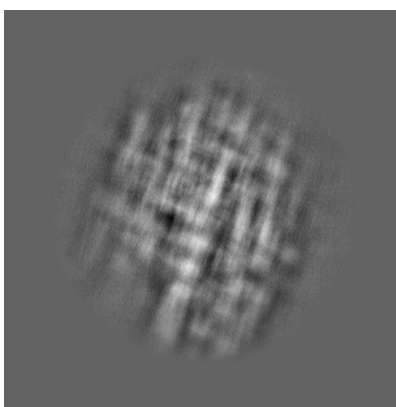


Z

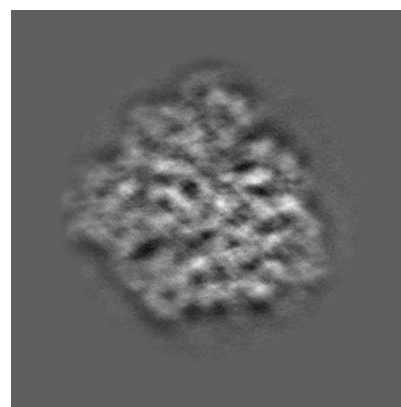
6.1.2 Raw map



X



Y

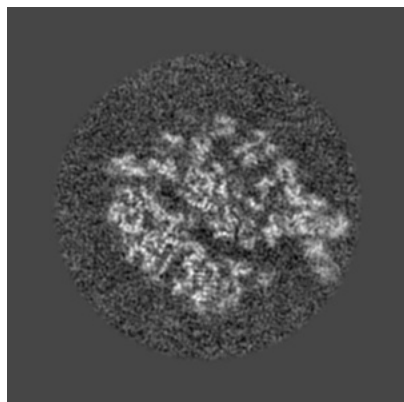


Z

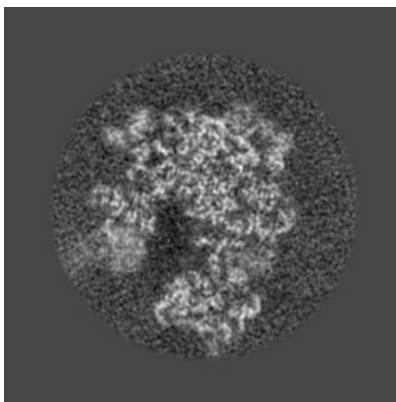
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

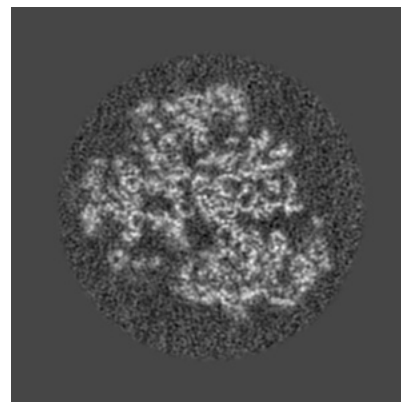
6.2.1 Primary map



X Index: 240

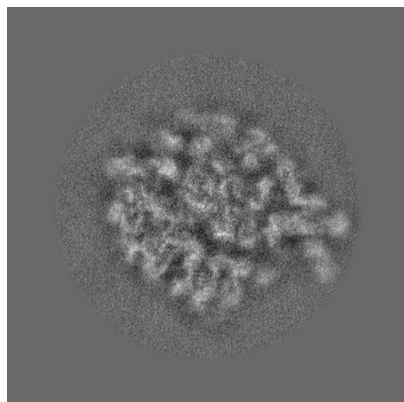


Y Index: 240

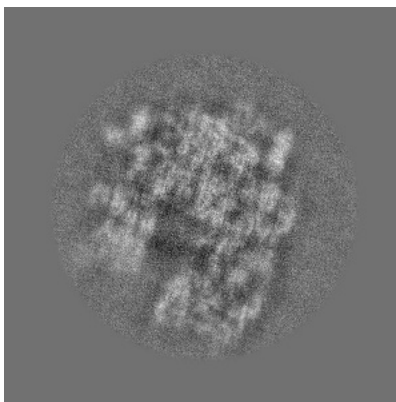


Z Index: 240

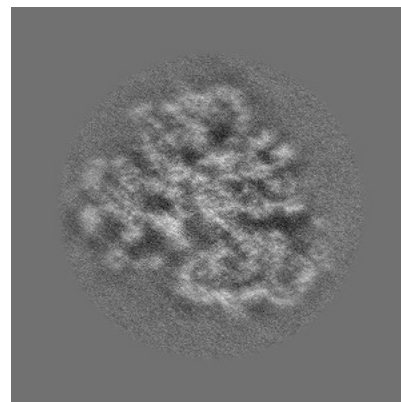
6.2.2 Raw map



X Index: 240



Y Index: 240

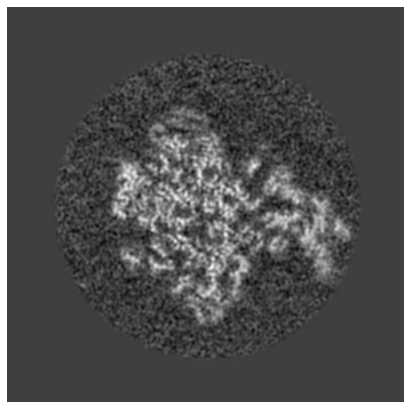


Z Index: 240

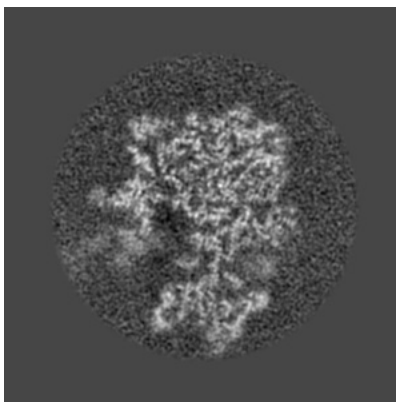
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

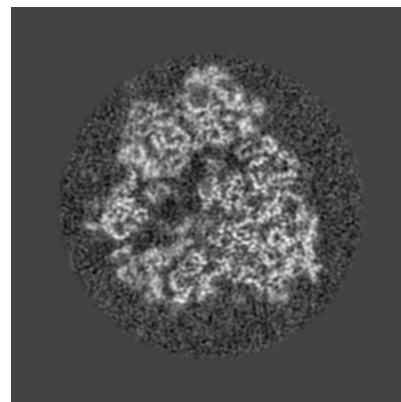
6.3.1 Primary map



X Index: 251

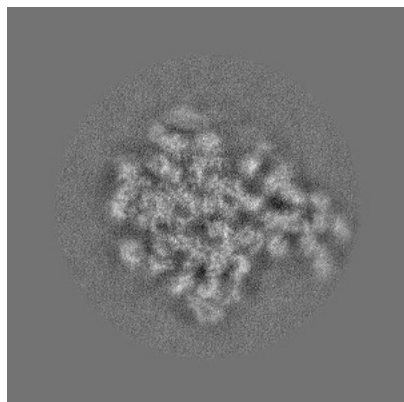


Y Index: 249

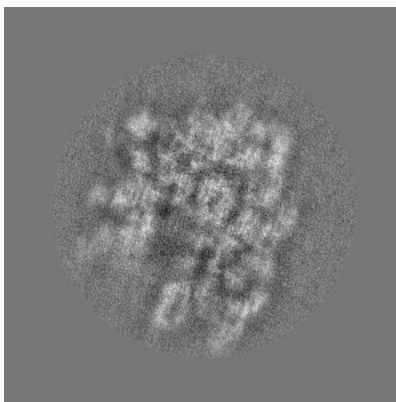


Z Index: 220

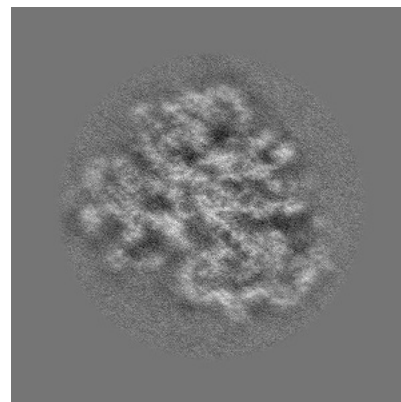
6.3.2 Raw map



X Index: 251



Y Index: 245

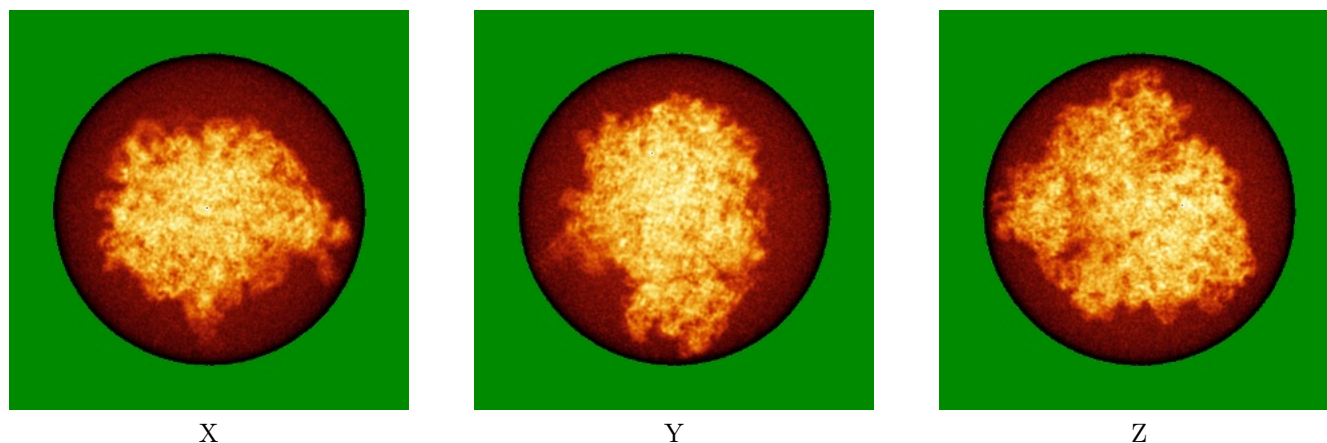


Z Index: 241

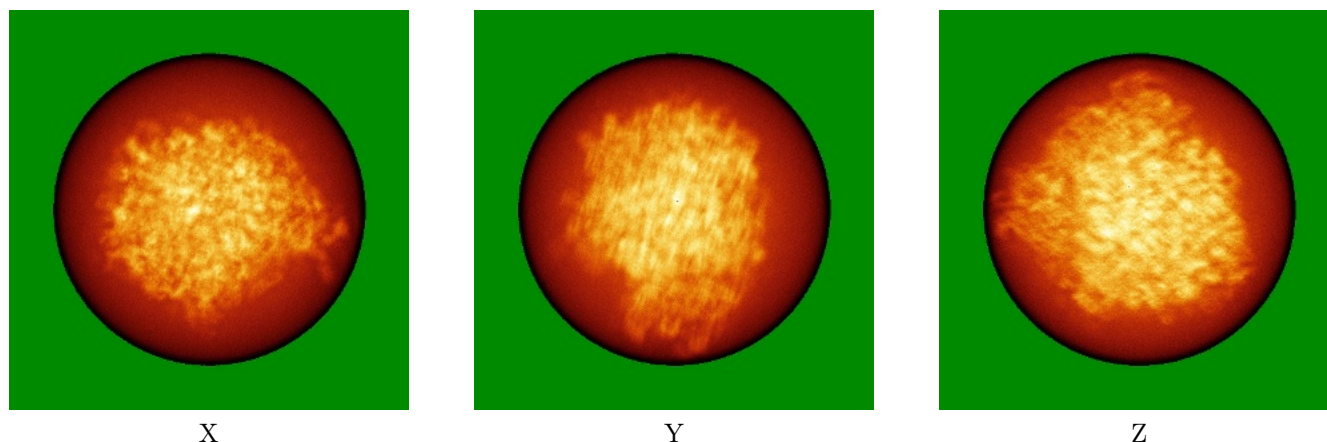
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

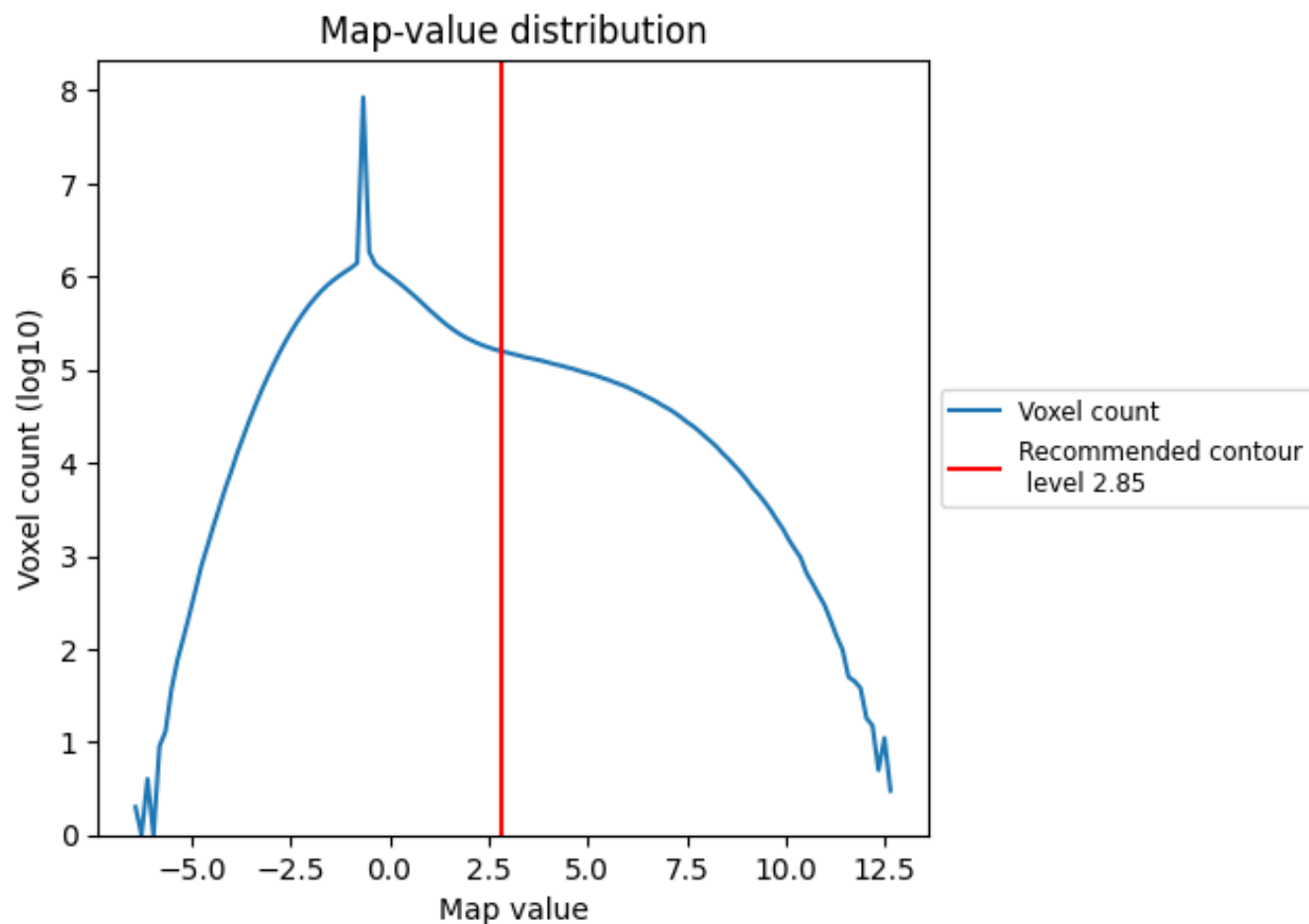
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

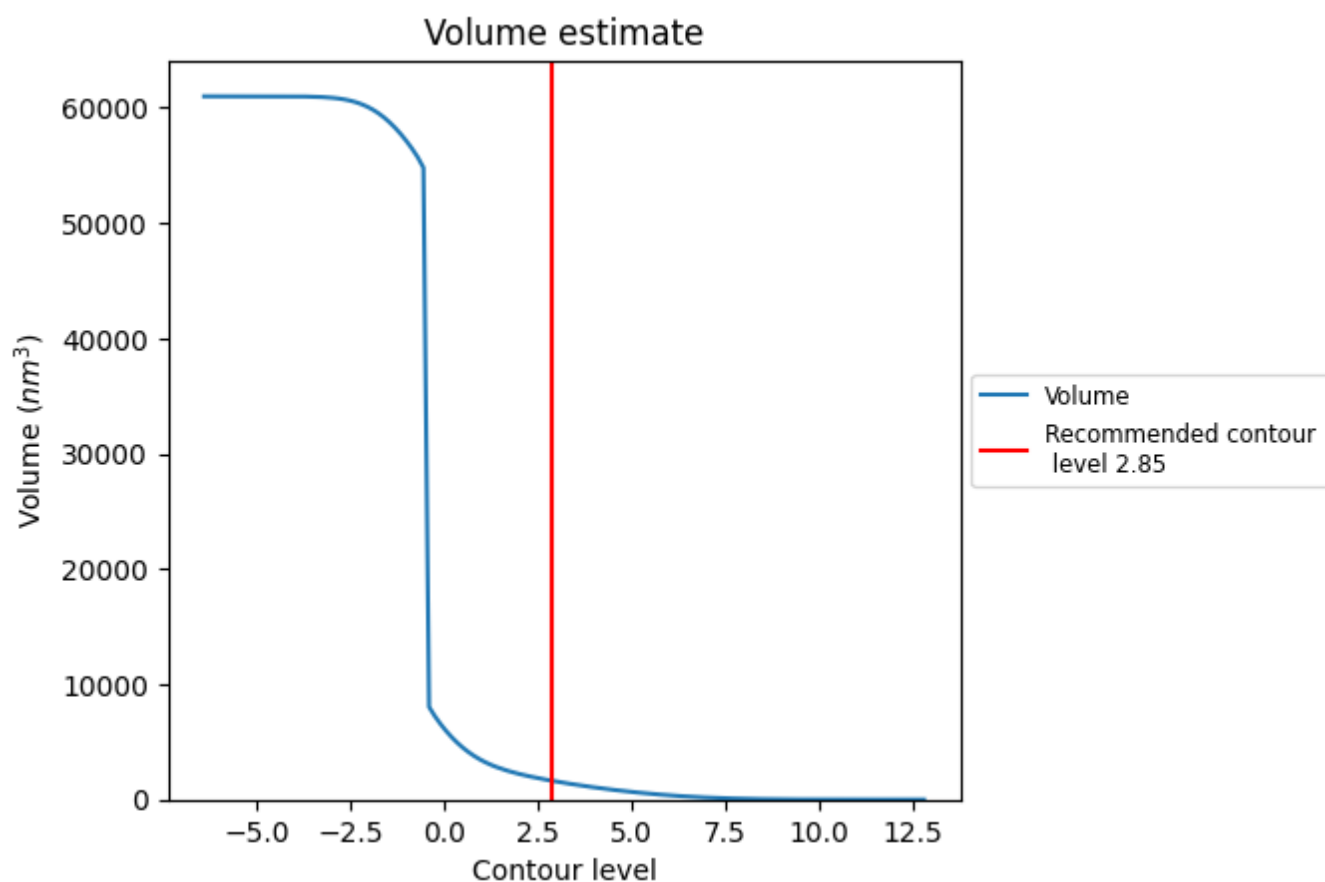
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

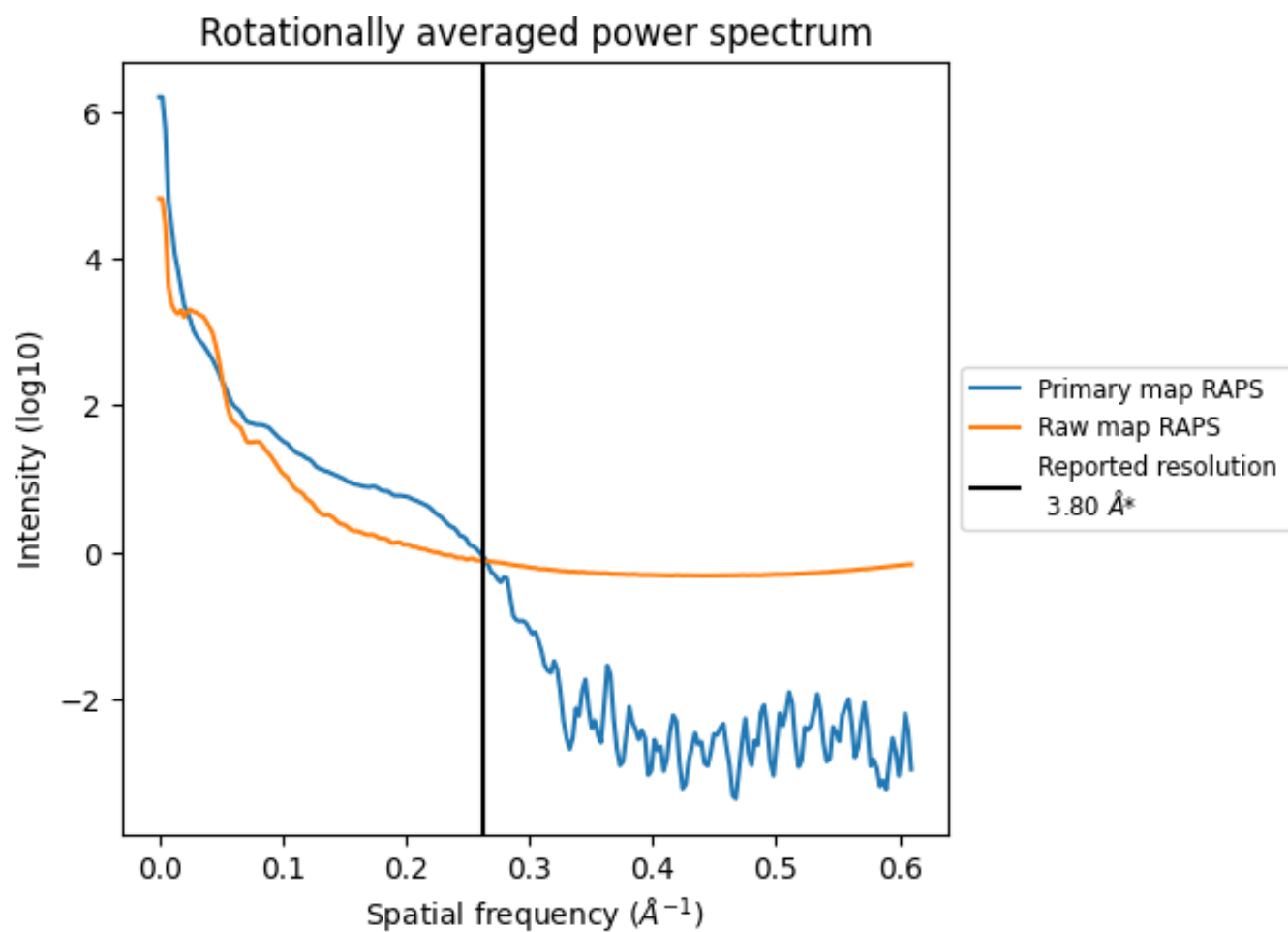
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1643 nm³; this corresponds to an approximate mass of 1484 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 ⓘ

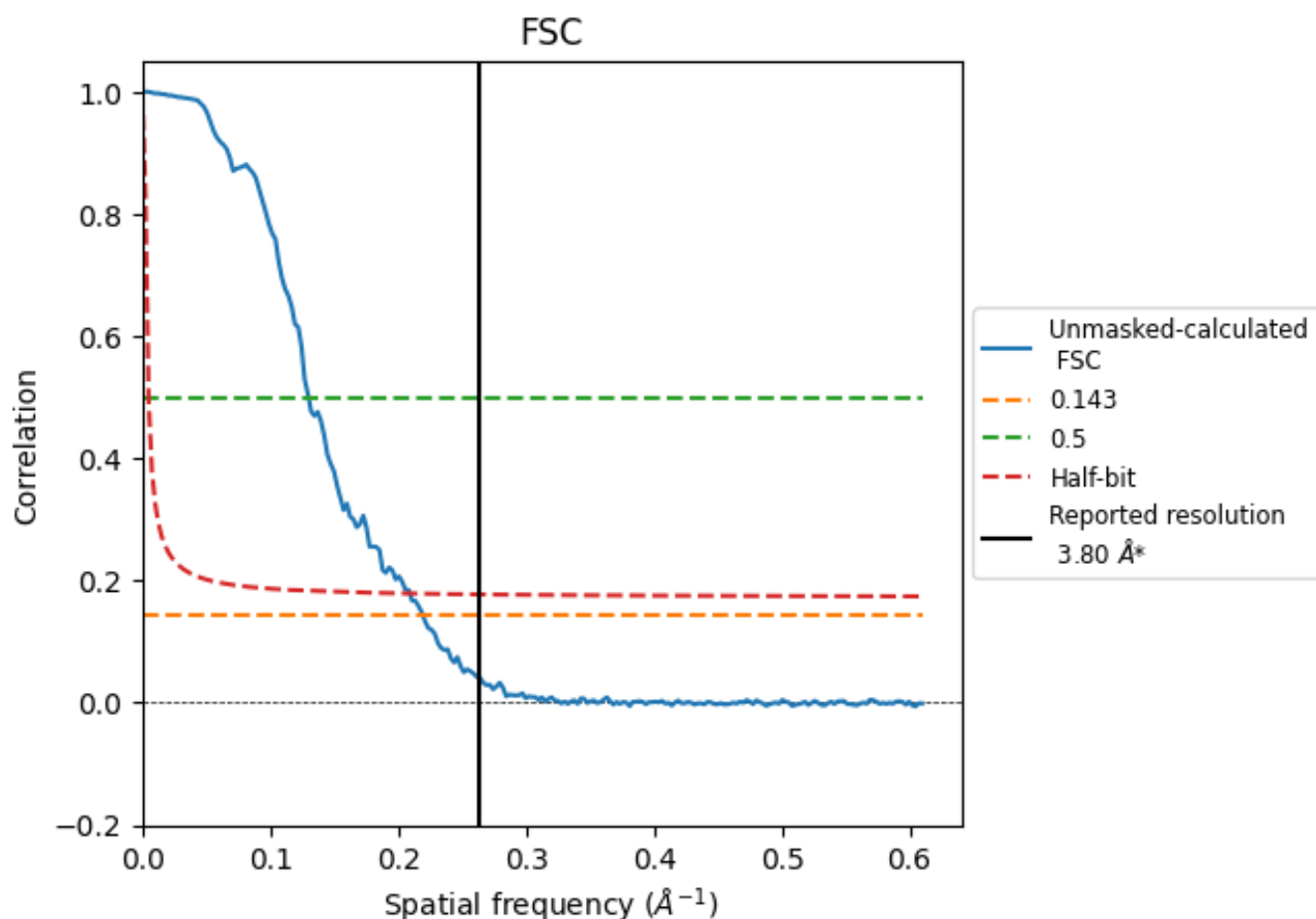


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.56	7.69	4.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.56 differs from the reported value 3.8 by more than 10 %

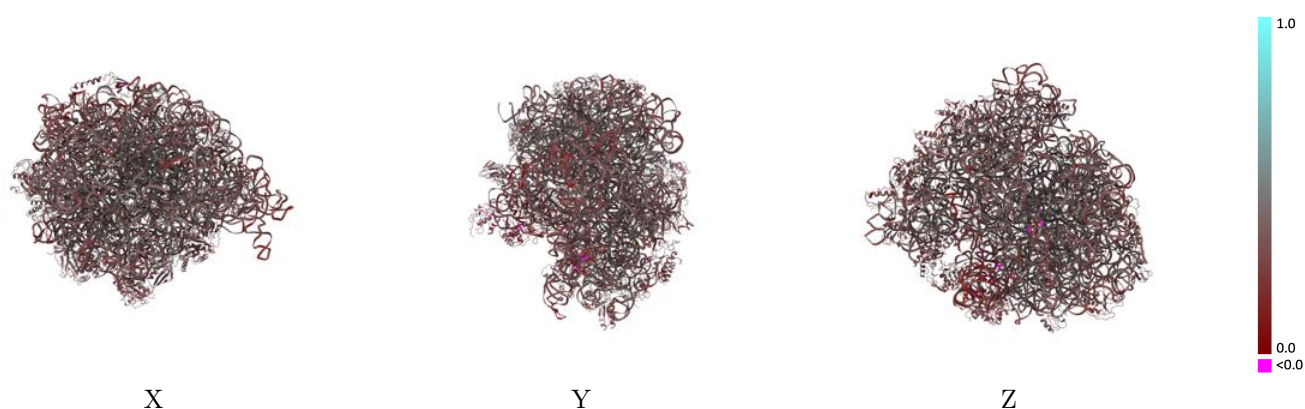
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8620 and PDB model 5UYQ. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)

This section was not generated.

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

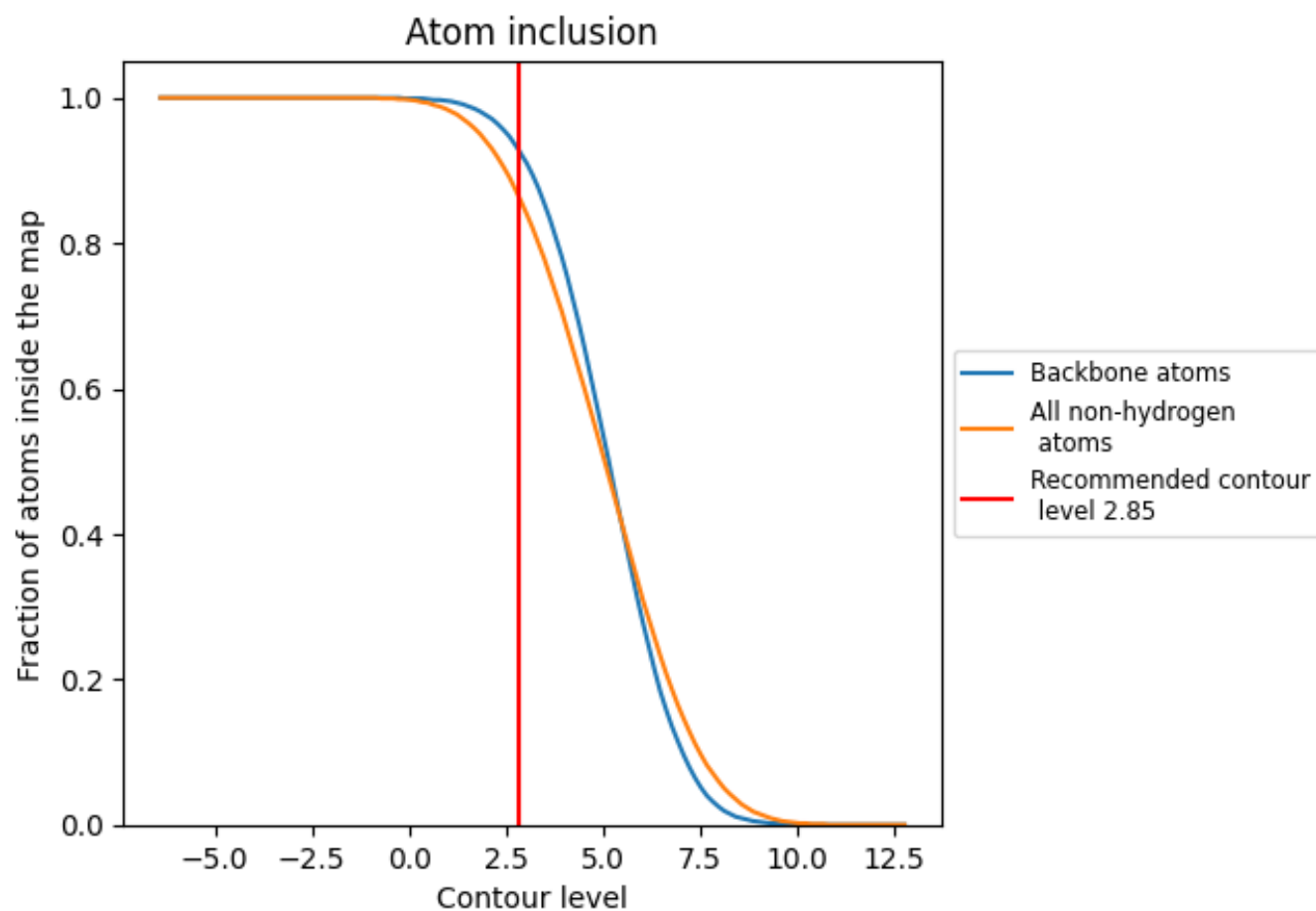


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (2.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.3510
01	 0.9390	 0.3650
02	 0.9390	 0.3420
03	 0.5720	 0.2270
04	 0.7880	 0.3960
05	 0.7480	 0.3970
06	 0.7510	 0.3560
07	 0.7620	 0.3230
08	 0.7760	 0.3490
09	 0.3810	 0.2820
10	 0.3960	 0.2190
11	 0.4750	 0.2300
12	 0.7540	 0.3650
13	 0.6560	 0.3860
14	 0.7830	 0.3670
15	 0.6830	 0.3780
16	 0.8080	 0.3710
17	 0.7990	 0.3370
18	 0.7170	 0.3750
19	 0.8050	 0.3640
20	 0.7750	 0.3860
21	 0.7460	 0.3710
22	 0.7790	 0.3610
23	 0.7920	 0.3470
24	 0.7670	 0.3550
25	 0.7570	 0.4010
26	 0.7540	 0.3720
27	 0.8010	 0.3120
28	 0.7600	 0.3810
29	 0.7790	 0.3040
30	 0.7970	 0.3740
31	 0.7210	 0.3340
32	 0.7970	 0.3730
33	 0.8250	 0.4000
34	 0.7940	 0.3930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
A	 0.9340	 0.3520
B	 0.6920	 0.3210
C	 0.7320	 0.3580
D	 0.6910	 0.2980
E	 0.7510	 0.3560
F	 0.7630	 0.3650
G	 0.7080	 0.3150
H	 0.7720	 0.3720
I	 0.7840	 0.3360
J	 0.6710	 0.3120
K	 0.7810	 0.3530
L	 0.6920	 0.3640
M	 0.7690	 0.3270
N	 0.7760	 0.3410
O	 0.7780	 0.3530
P	 0.7930	 0.3310
Q	 0.7430	 0.3420
R	 0.8020	 0.3570
S	 0.8170	 0.3490
T	 0.7720	 0.3090
U	 0.6060	 0.3210
V	 0.7390	 0.3100
W	 0.8730	 0.3330
X	 0.6650	 0.2080
Y	 0.7930	 0.2760
Z	 0.6840	 0.2940