



## wwPDB EM Validation Summary Report ⓘ

Mar 27, 2025 – 02:45 PM EDT

PDB ID : 9NLB  
EMDB ID : EMD-40929  
Title : E. coli initiation complex with EQ2-EttA in Hydrolytic 2 conformation  
Authors : Singh, S.; Hunt, J.F.  
Deposited on : 2025-03-03  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

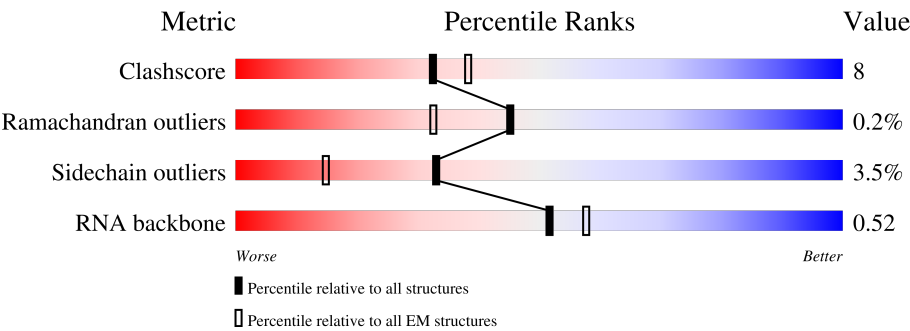
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

# 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 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	220	<div><div>97%</div><div><div></div><div>84%</div><div>15%</div><div>.</div></div></div>
2	13	142	<div><div>11%</div><div><div></div><div>80%</div><div>19%</div><div>.</div></div></div>
3	14	122	<div><div>16%</div><div><div></div><div>70%</div><div>28%</div><div>.</div></div></div>
4	15	143	<div><div>8%</div><div><div></div><div>83%</div><div>17%</div><div>.</div></div></div>
5	16	136	<div><div>15%</div><div><div></div><div>79%</div><div>19%</div><div>.</div></div></div>
6	17	120	<div><div>5%</div><div><div></div><div>84%</div><div>16%</div><div>.</div></div></div>
7	18	116	<div><div>22%</div><div><div></div><div>80%</div><div>19%</div><div>.</div></div></div>


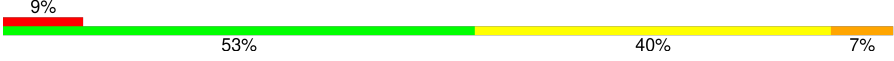

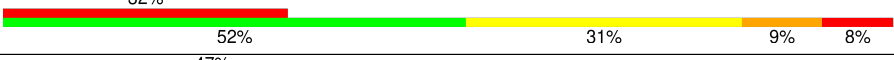
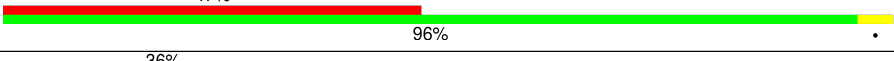
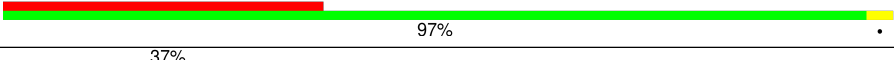
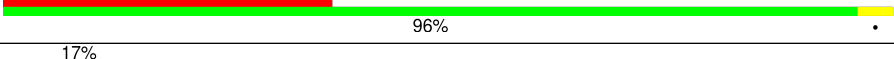
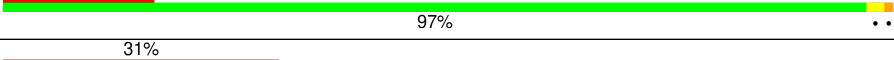
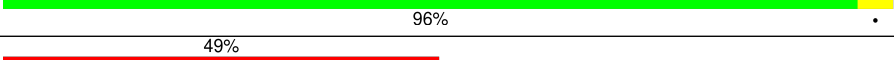
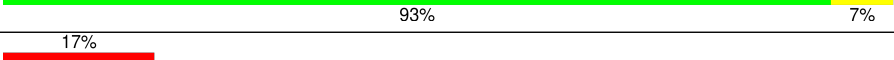
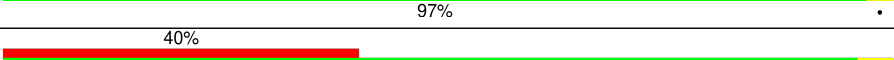
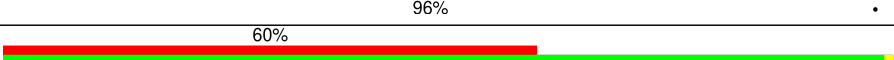
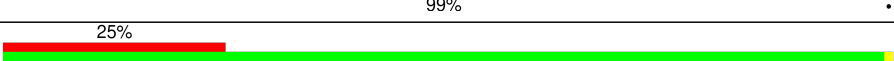
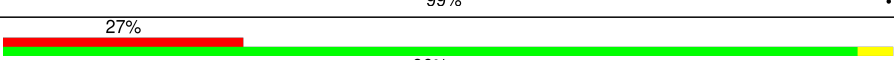
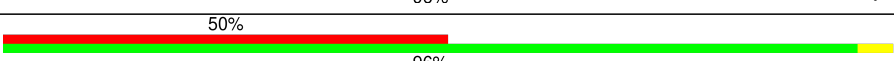
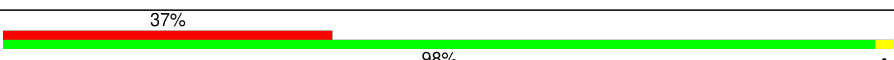
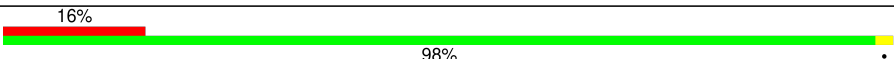
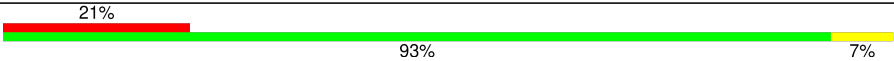
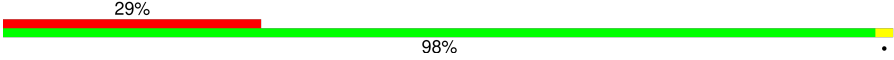
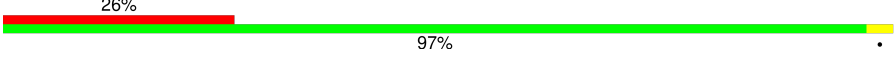
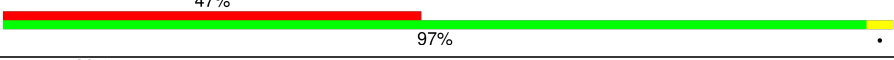
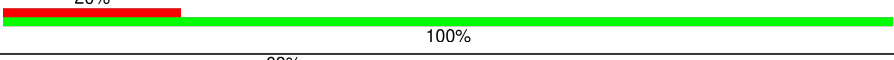
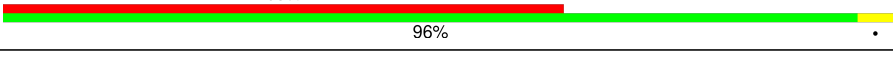

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	19	114	
9	2	271	
10	20	117	
11	21	103	
12	22	110	
13	23	93	
14	24	102	
15	25	94	
16	27	76	
17	28	77	
18	29	63	
19	3	209	
20	30	58	
21	31	66	
22	32	56	
23	33	50	
24	34	46	
25	35	64	
26	36	38	
27	4	201	
28	5	177	
29	6	176	
30	9	149	
31	E	552	
32	M	9	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	R1	2903	
34	R2	119	
35	R3	1531	
36	T	77	
37	sb	218	
38	sc	206	
39	sd	205	
40	se	157	
41	sf	100	
42	sg	151	
43	sh	129	
44	si	127	
45	sj	98	
46	sk	116	
47	sl	123	
48	sm	114	
49	sn	100	
50	so	88	
51	sp	82	
52	sq	80	
53	sr	65	
54	ss	79	
55	st	85	
56	su	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	H2U	T	20	X	-	-	-
36	4OC	T	32	X	-	-	-
36	MUM	T	54	X	-	-	-
36	PSU	T	55	X	-	-	-
36	4SU	T	8	X	-	-	-

## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 150087 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 Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	220	Total	C	N	O	S	0	0
			1353	804	270	277	2		

- Molecule 2 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	13	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 3 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	14	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 4 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	15	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 5 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	16	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	17	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	18	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 8 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	19	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 10 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	20	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 11 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	21	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 12 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	22	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	23	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	24	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	25	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	27	76	Total	C	N	O	S		
			582	360	117	104	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	28	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	29	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	209	Total	C	N	O	S		
			1565	979	288	294	4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	30	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL31.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	33	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 25 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 31 is a protein called Energy-dependent translational throttle protein EttA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	552	Total	C	N	O	S	0	0
			4360	2745	774	829	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	188	GLN	GLU	conflict	UNP P0A9W3
E	341	SER	ASP	conflict	UNP P0A9W3
E	470	GLN	GLU	conflict	UNP P0A9W3

- Molecule 32 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	9	Total	C	N	O	P	0	0
			195	88	40	58	9		

- Molecule 33 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R1	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R1	1847	G	A	conflict	GB 2019144442

- Molecule 34 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R2	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	R3	1531	Total	C	N	O	P	0	0
			32850	14652	6028	10640	1530		

- Molecule 36 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	T	77	Total	C	N	O	P	S	0	0
			1639	734	294	534	76	1		

- Molecule 37 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	sb	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 38 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	se	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 41 is a protein called 30S ribosomal protein S6, non-modified isoform.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

- Molecule 44 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 47 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 50 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 51 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 52 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	sr	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	ss	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

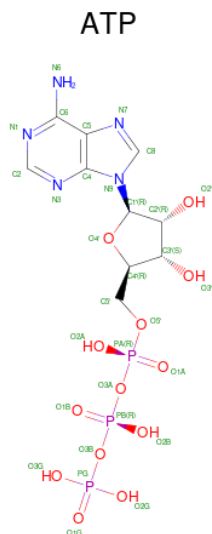
- Molecule 56 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	su	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	15	1	Total	Mg	0
			1	1	
57	2	1	Total	Mg	0
			1	1	
57	32	1	Total	Mg	0
			1	1	
57	R1	199	Total	Mg	0
			199	199	
57	R3	77	Total	Mg	0
			77	77	

- Molecule 58 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

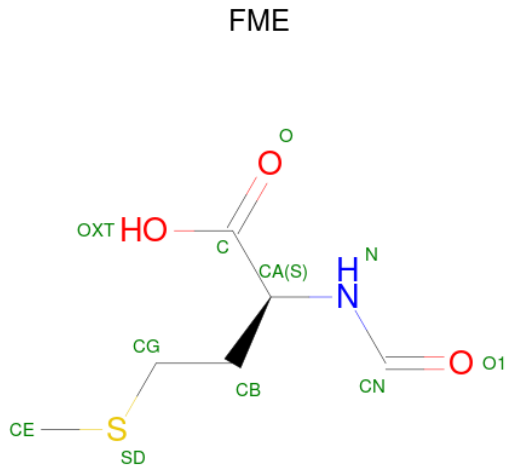


Mol	Chain	Residues	Atoms					AltConf
58	E	1	Total 31	C 10	N 5	O 13	P 3	0
58	E	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 59 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
59	E	2	Total 2	Na 2	0

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $\text{C}_6\text{H}_{11}\text{NO}_3\text{S}$ ).



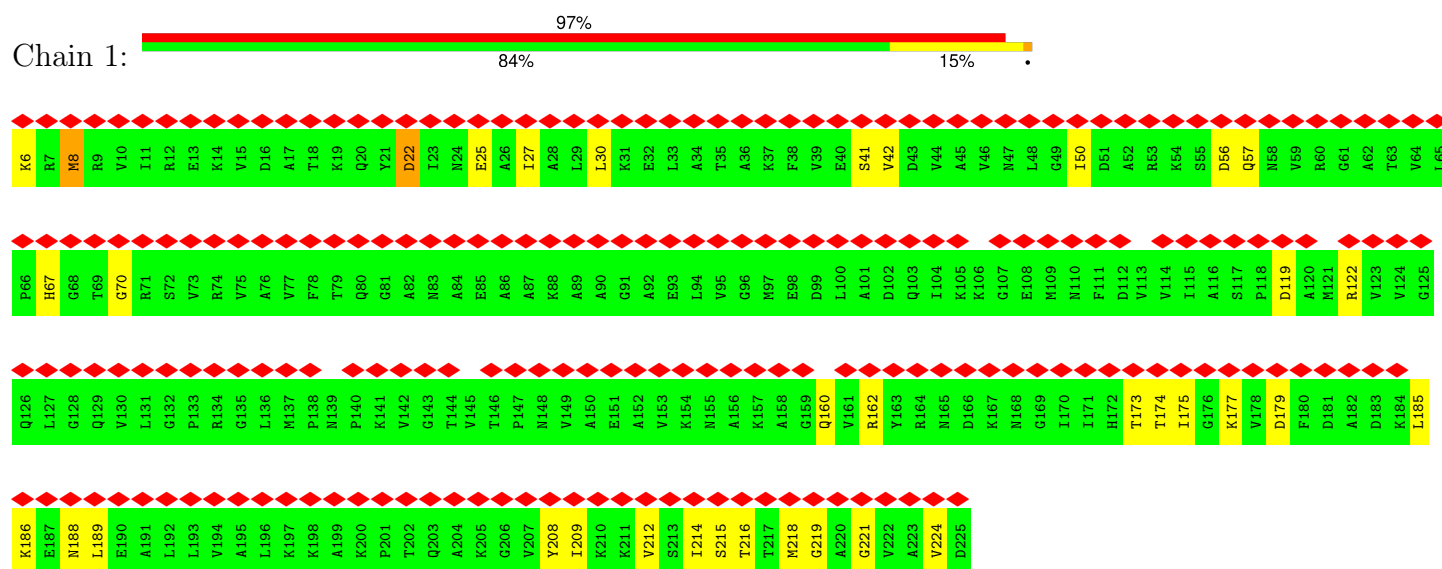
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	T	1	10	6	1	2	1	0



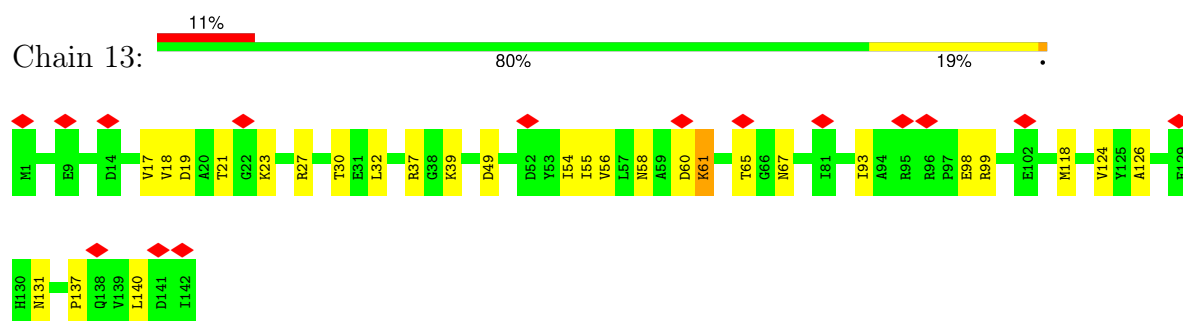
### 3 Residue-property plots

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.

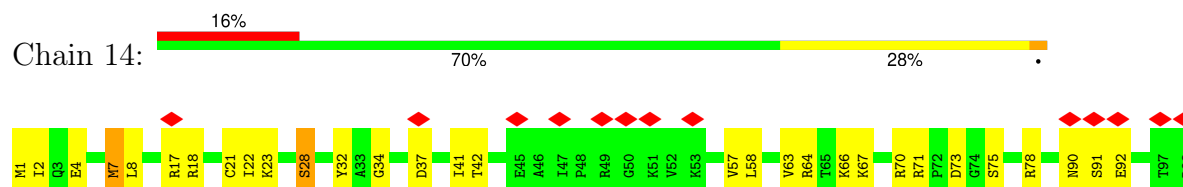
#### • Molecule 1: Large ribosomal subunit protein uL1



#### • Molecule 2: Large ribosomal subunit protein uL13

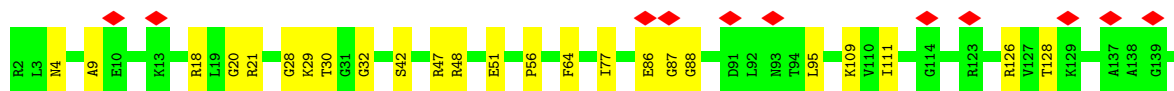
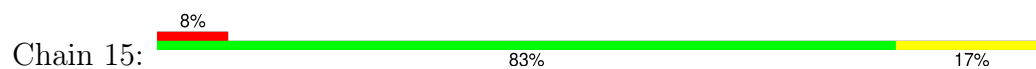


#### • Molecule 3: 50S ribosomal protein L14

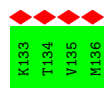
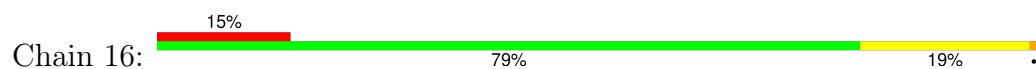




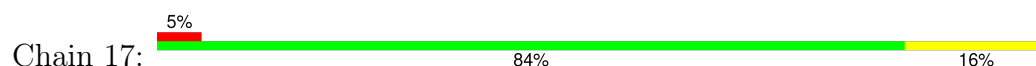
- Molecule 4: 50S ribosomal protein L15



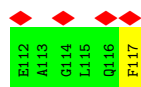
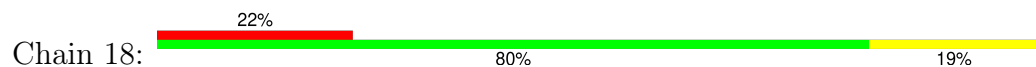
- Molecule 5: 50S ribosomal protein L16



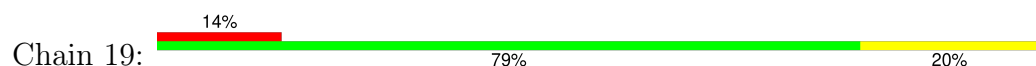
- Molecule 6: Large ribosomal subunit protein bL17

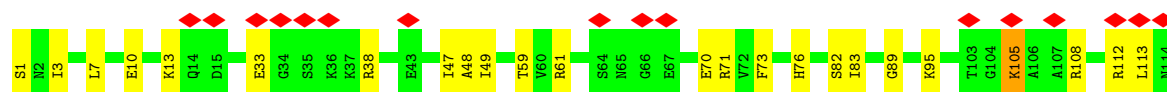


- Molecule 7: Large ribosomal subunit protein uL18

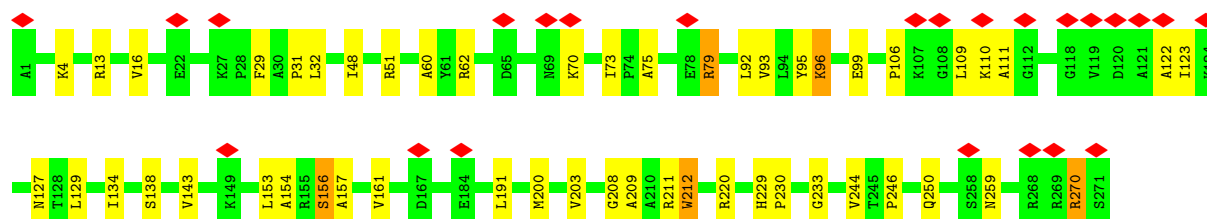
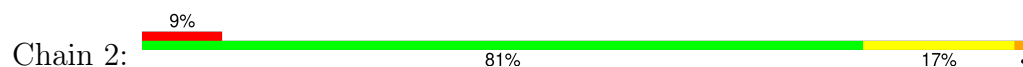


- Molecule 8: 50S ribosomal protein L19





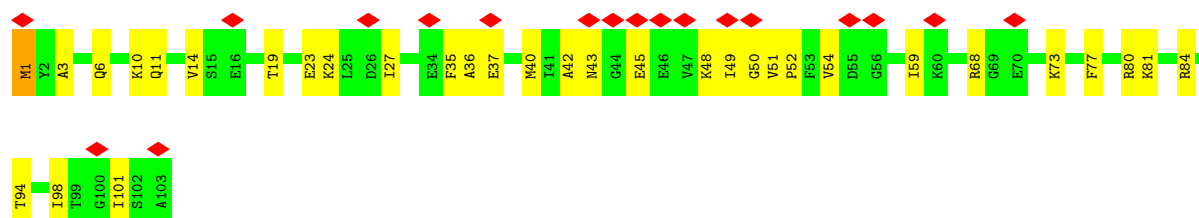
- Molecule 9: 50S ribosomal protein L2



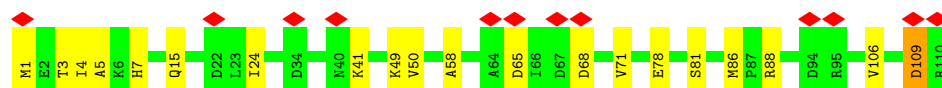
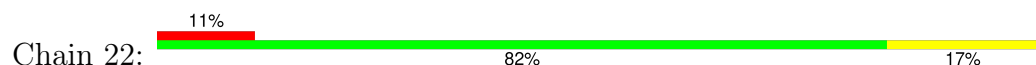
- Molecule 10: Large ribosomal subunit protein bL20



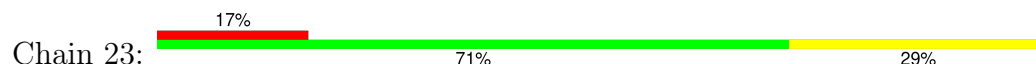
- Molecule 11: Large ribosomal subunit protein bL21



- Molecule 12: Large ribosomal subunit protein uL22

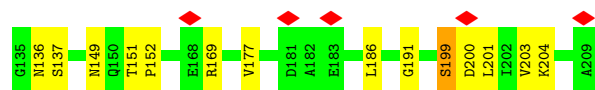


- Molecule 13: Large ribosomal subunit protein uL23

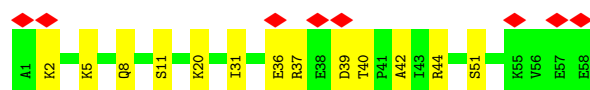
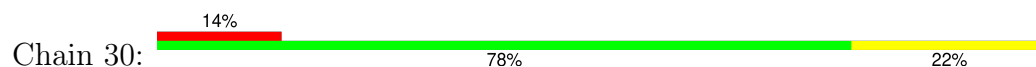


- Molecule 14: Large ribosomal subunit protein uL24

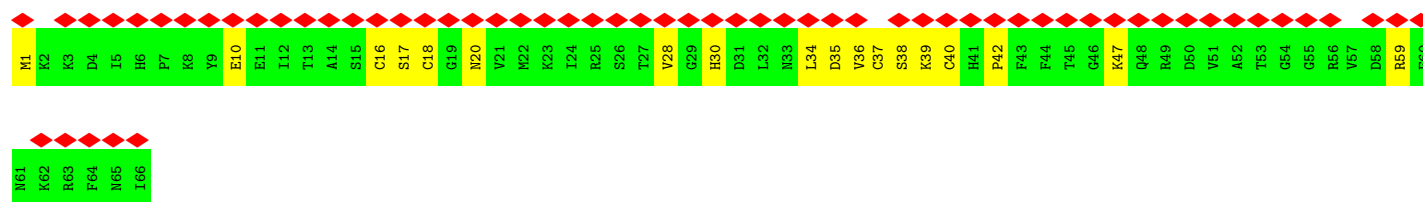




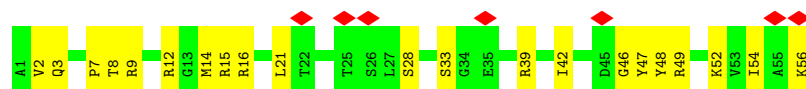
- Molecule 20: 50S ribosomal protein L30



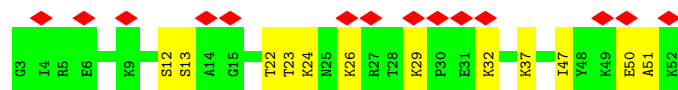
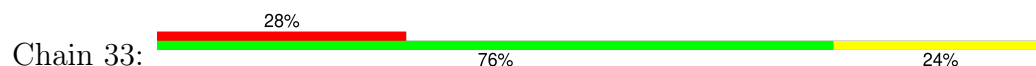
- Molecule 21: Large ribosomal subunit protein bL31



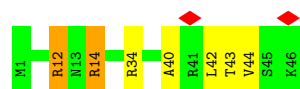
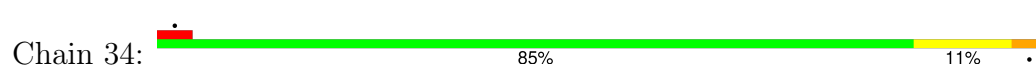
- Molecule 22: 50S ribosomal protein L32



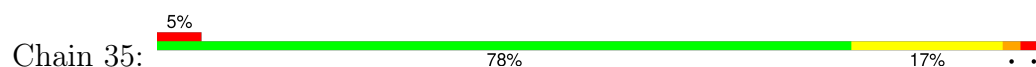
- Molecule 23: Large ribosomal subunit protein bL33

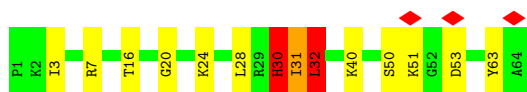


- Molecule 24: 50S ribosomal protein L34

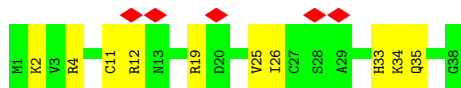
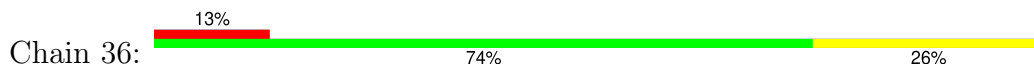


- Molecule 25: Large ribosomal subunit protein bL35

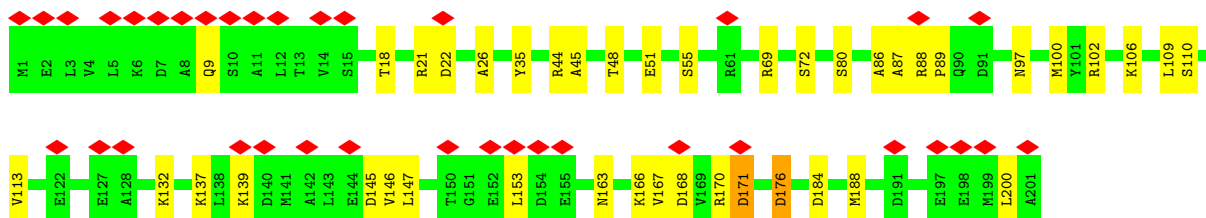




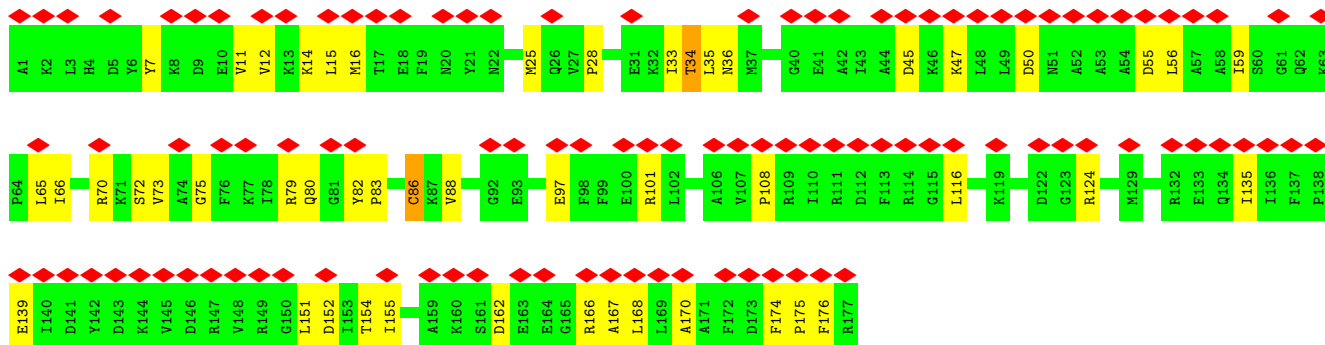
- Molecule 26: 50S ribosomal protein L36



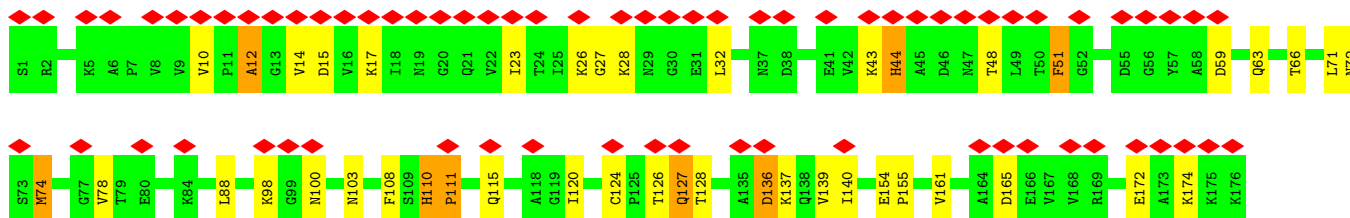
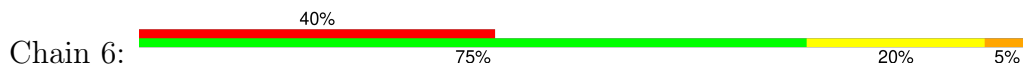
- Molecule 27: Large ribosomal subunit protein uL4



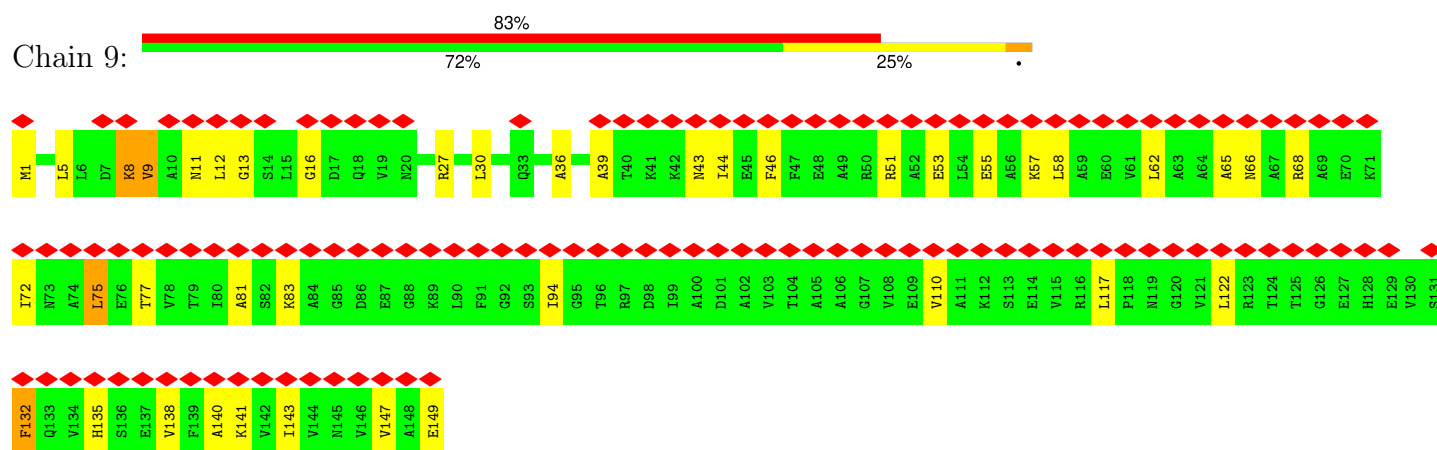
- Molecule 28: 50S ribosomal protein L5



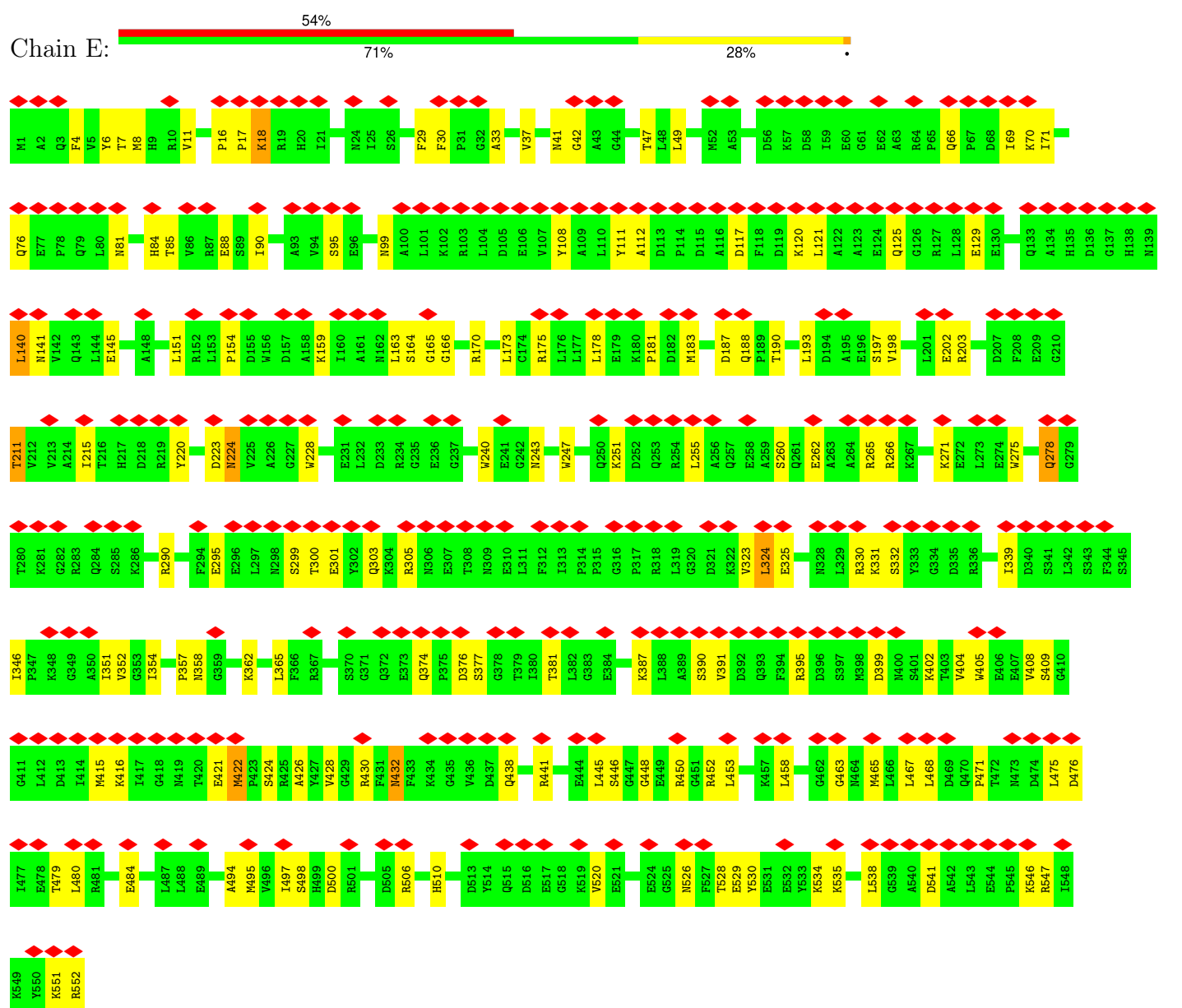
- Molecule 29: Large ribosomal subunit protein uL6



- Molecule 30: Large ribosomal subunit protein bL9

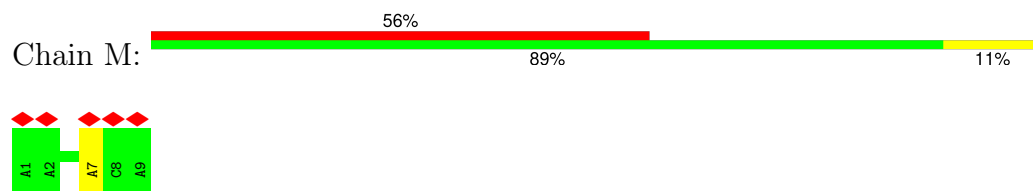


• Molecule 31: Energy-dependent translational throttle protein EttA



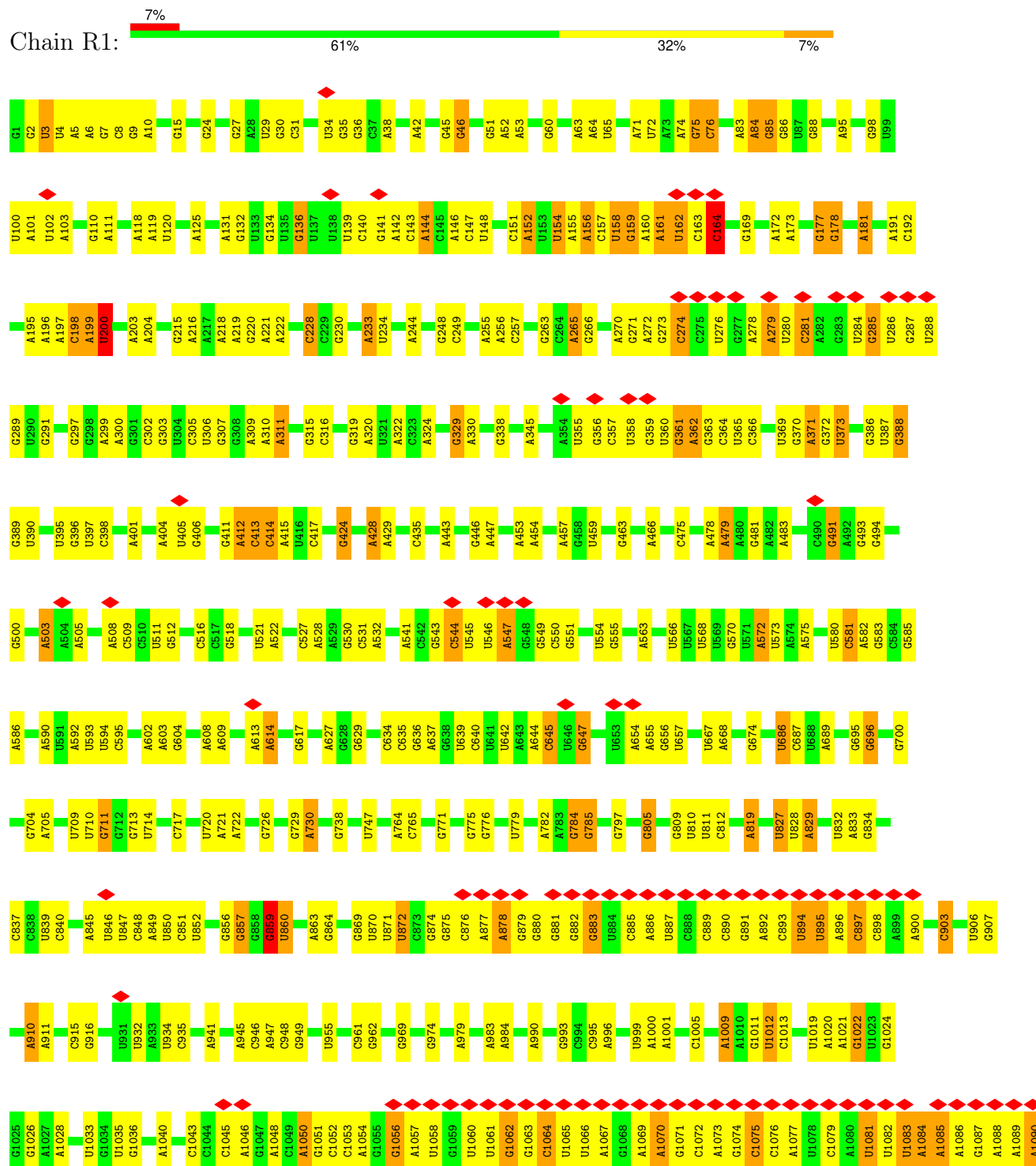
- Molecule 32: mRNA

Chain M:



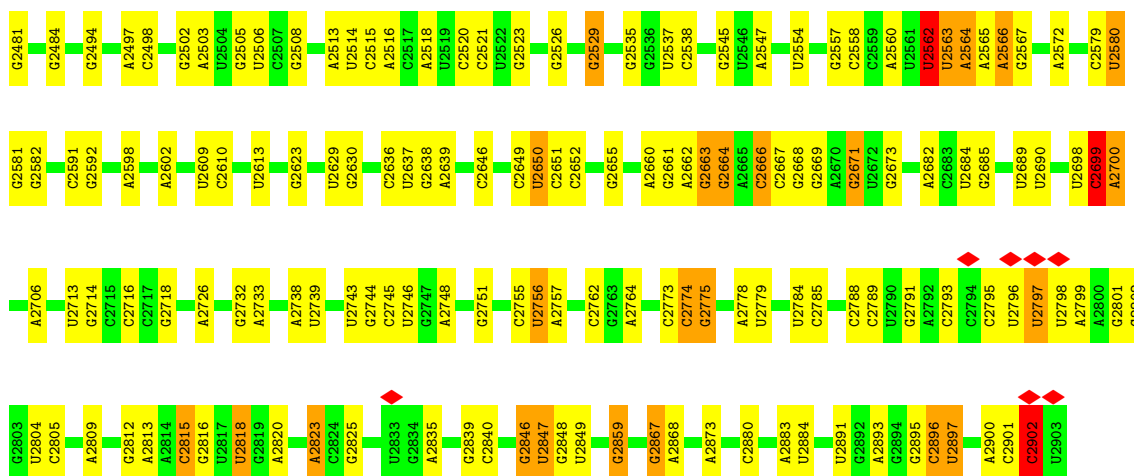
- Molecule 33: 23S ribosomal RNA

Chain R1:

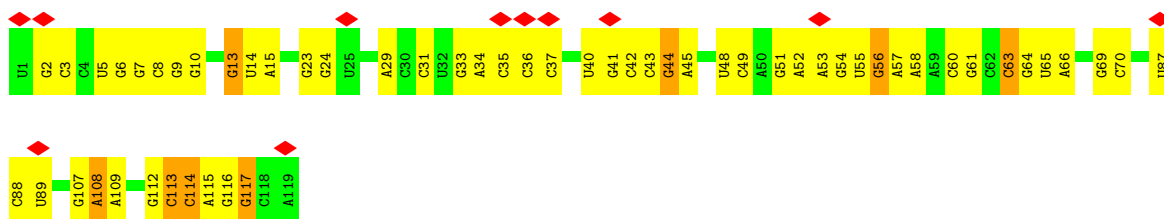




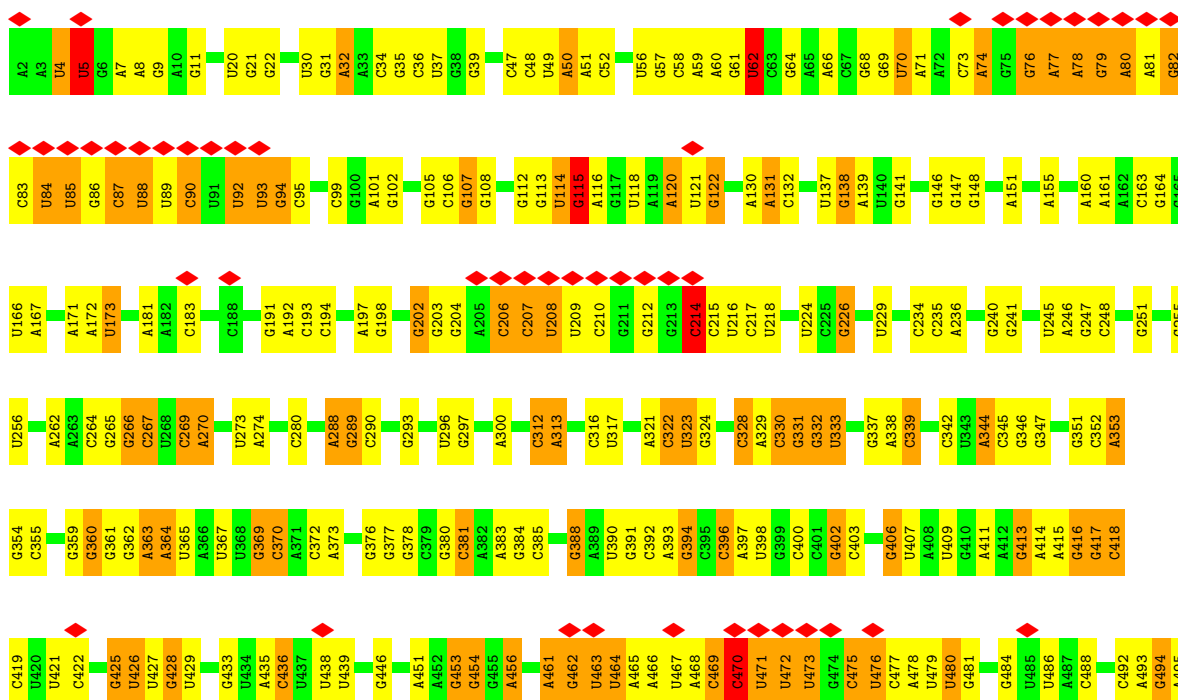


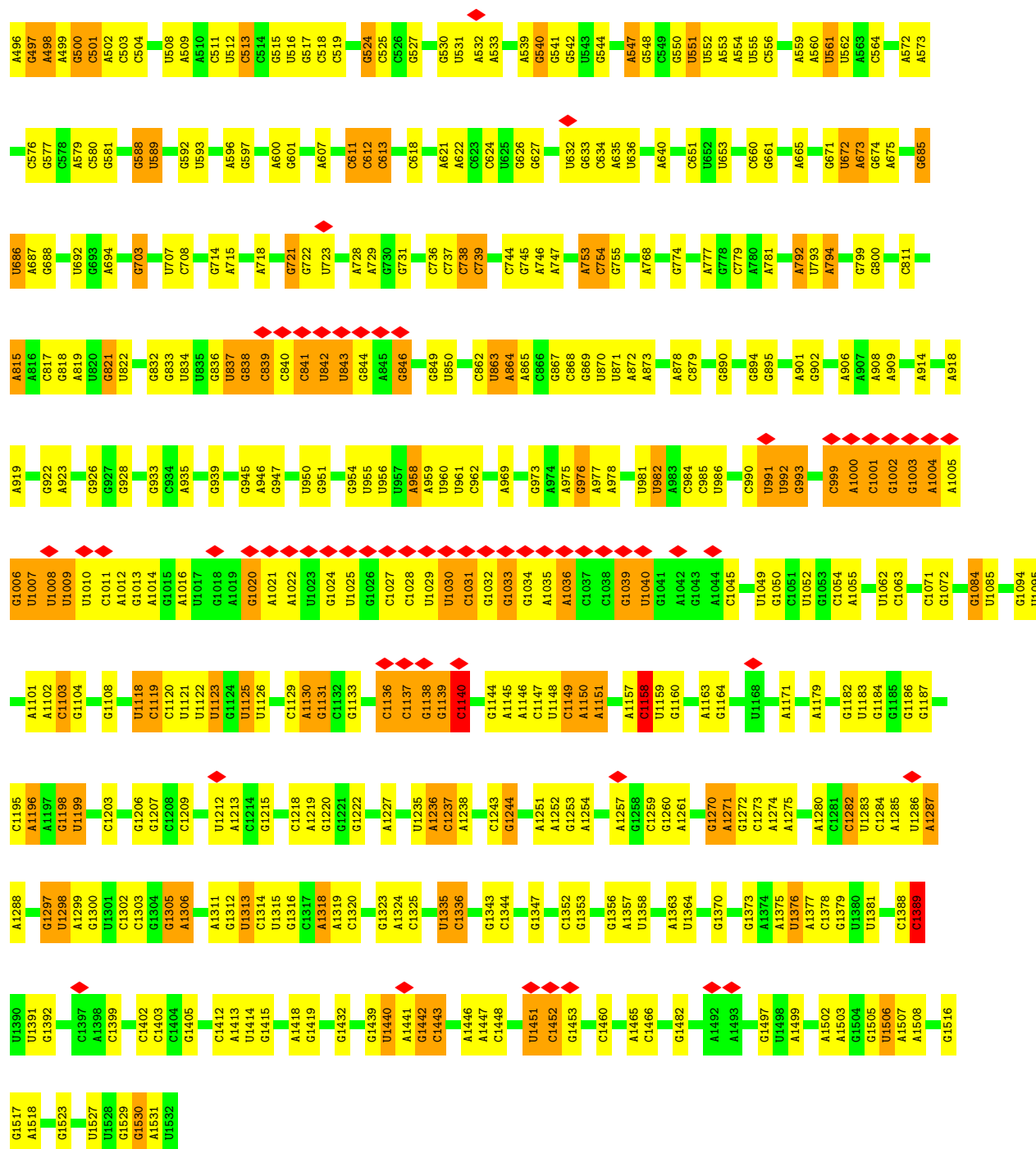


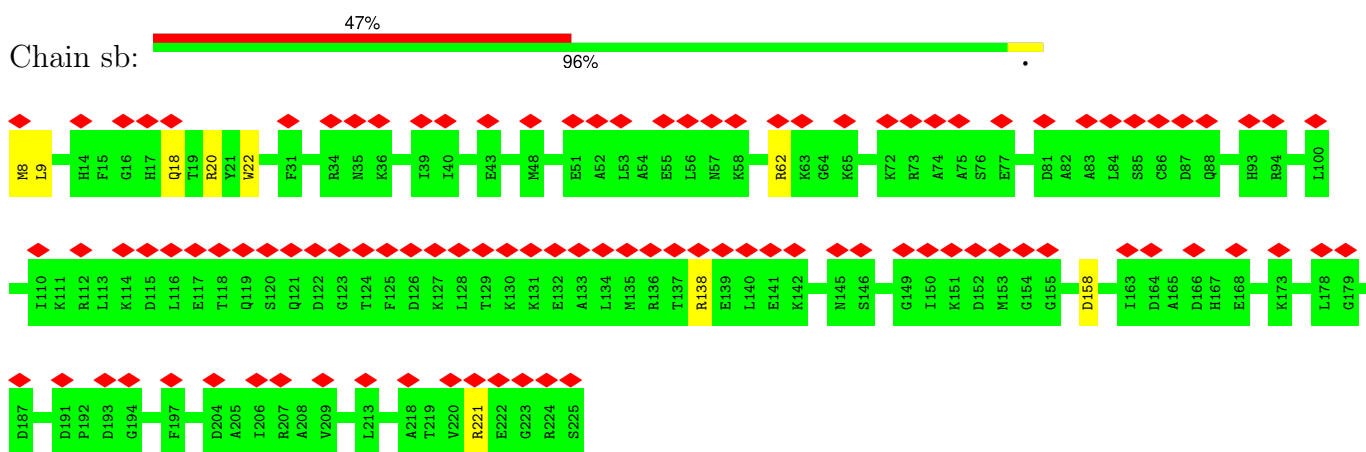
• Molecule 34: 5S ribosomal RNA



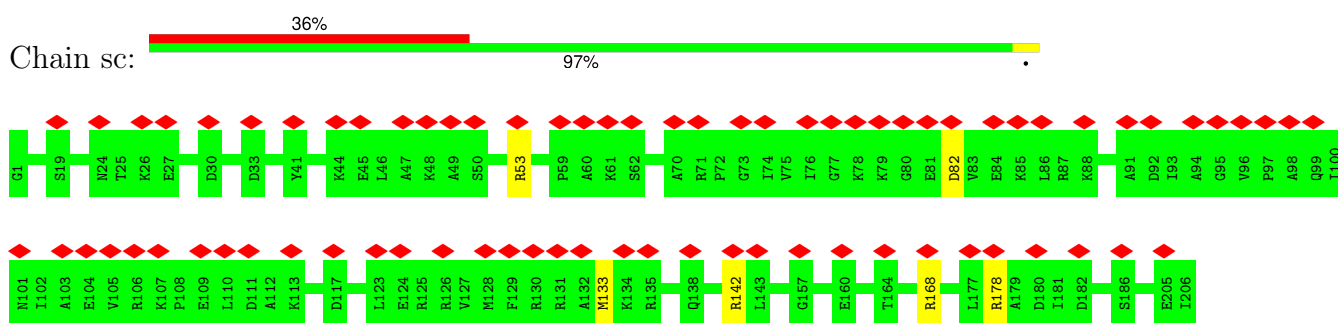
• Molecule 35: 16S ribosomal RNA



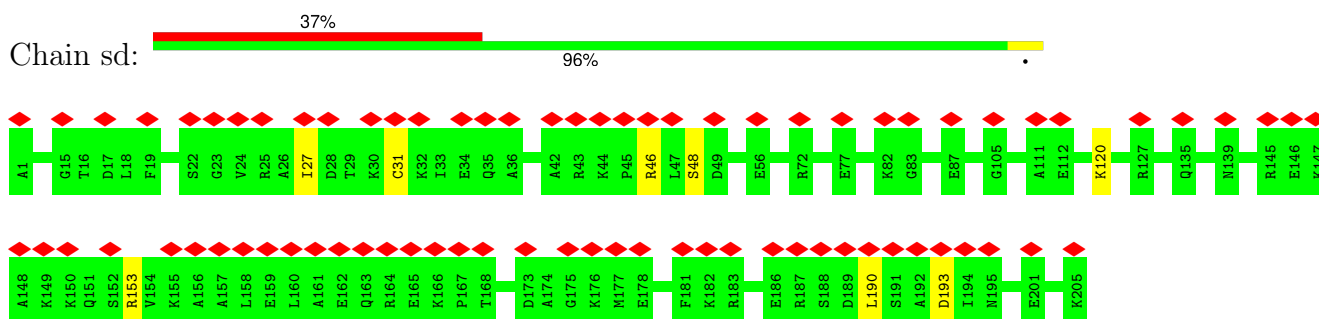




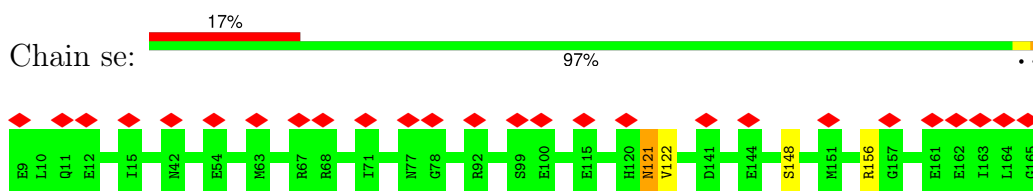
• Molecule 38: Small ribosomal subunit protein uS3



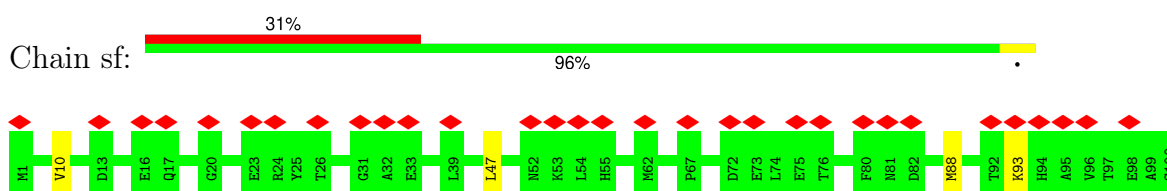
• Molecule 39: 30S ribosomal protein S4



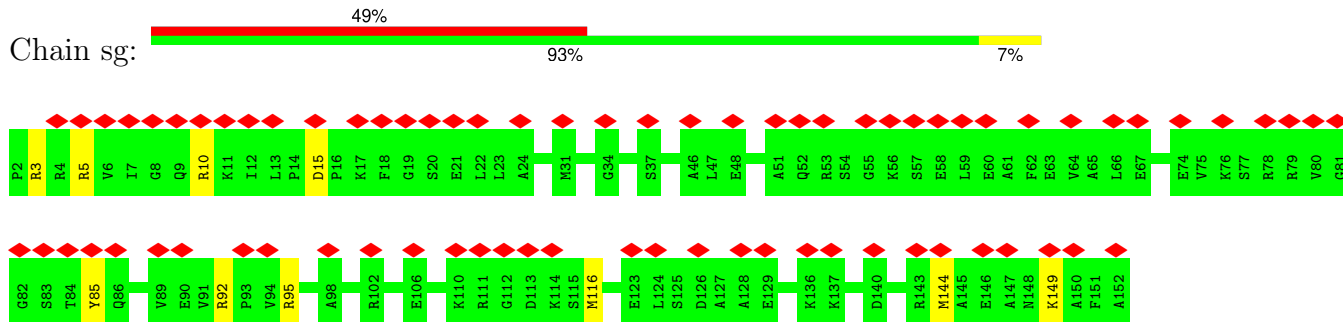
• Molecule 40: Small ribosomal subunit protein uS5



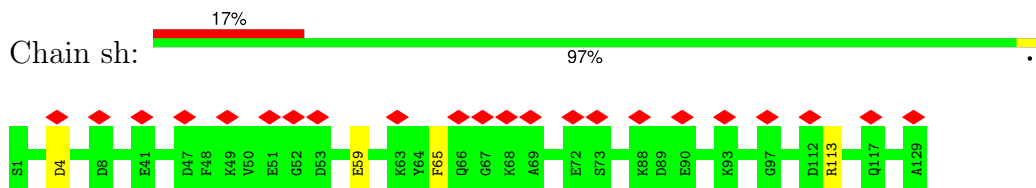
• Molecule 41: 30S ribosomal protein S6, non-modified isoform



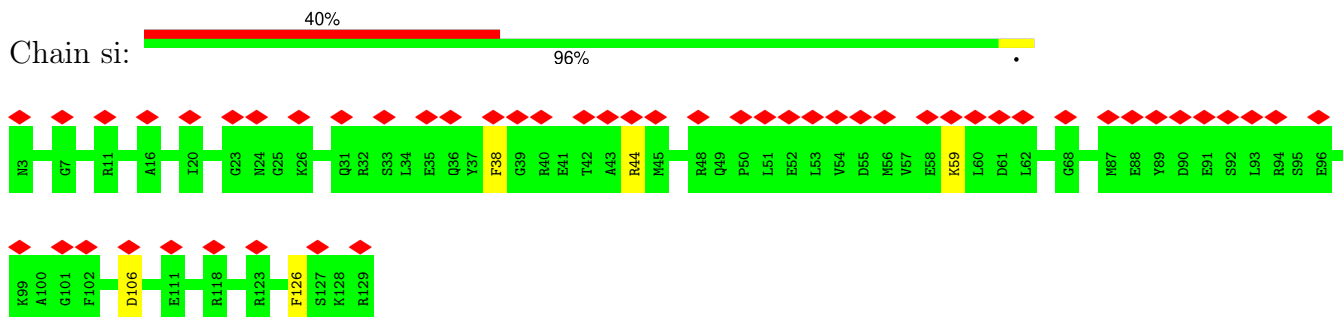
- Molecule 42: 30S ribosomal protein S7



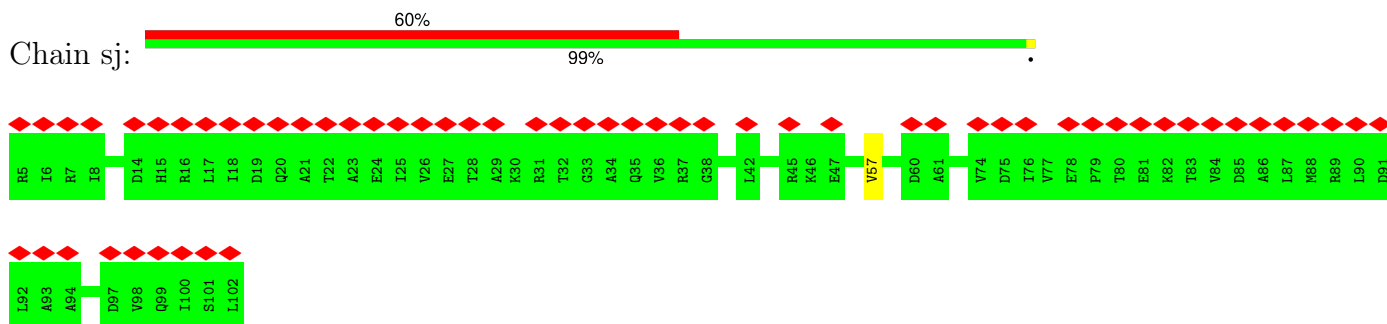
- Molecule 43: 30S ribosomal protein S8



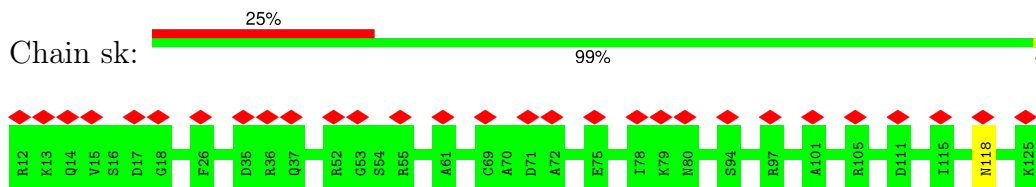
- Molecule 44: Small ribosomal subunit protein uS9



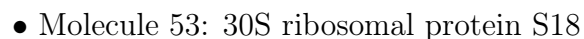
- Molecule 45: 30S ribosomal protein S10

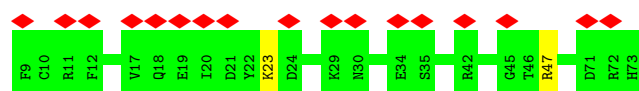


- Molecule 46: Small ribosomal subunit protein uS11

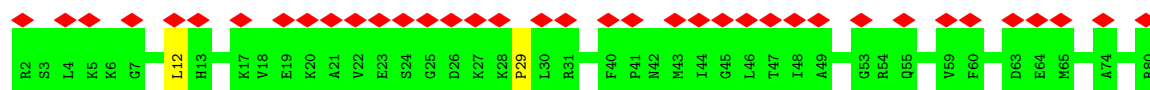


- Molecule 47: Small ribosomal subunit protein uS12

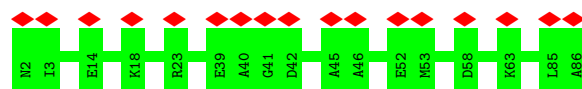




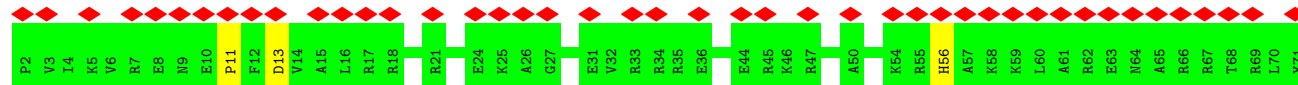
- Molecule 54: 30S ribosomal protein S19



- Molecule 55: 30S ribosomal protein S20



- Molecule 56: Small ribosomal subunit protein bS21



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.378	Depositor
Minimum map value	-1.183	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, PSU, FME, MG, 4OC, MUM, 4SU, ATP, NA

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	1	0.24	0/1361	0.52	0/1796
2	13	0.32	0/1152	0.56	1/1551 (0.1%)
3	14	0.32	0/947	0.60	0/1268
4	15	0.32	0/1054	0.59	0/1403
5	16	0.31	0/1093	0.59	0/1460
6	17	0.31	0/973	0.60	0/1301
7	18	0.28	0/902	0.54	0/1209
8	19	0.31	0/929	0.56	0/1242
9	2	0.34	0/2121	0.58	0/2852
10	20	0.36	0/960	0.53	0/1278
11	21	0.32	0/829	0.57	0/1107
12	22	0.29	0/864	0.53	0/1156
13	23	0.31	0/744	0.54	0/994
14	24	0.30	0/787	0.55	0/1051
15	25	0.29	0/766	0.53	0/1025
16	27	0.32	0/589	0.54	0/779
17	28	0.29	0/635	0.56	0/848
18	29	0.25	0/510	0.54	0/677
19	3	0.33	0/1586	0.56	0/2134
20	30	0.27	0/453	0.55	0/605
21	31	0.28	0/531	0.54	0/709
22	32	0.32	0/450	0.61	0/599
23	33	0.32	0/416	0.53	0/554
24	34	0.31	0/380	0.66	0/498
25	35	0.32	0/513	0.67	1/676 (0.1%)
26	36	0.31	0/303	0.59	0/397
27	4	0.30	0/1571	0.51	0/2113
28	5	0.28	0/1434	0.53	0/1926
29	6	0.78	3/1343 (0.2%)	1.02	6/1816 (0.3%)
30	9	0.27	0/1122	0.58	0/1515
31	E	0.29	0/4441	0.55	1/5993 (0.0%)
32	M	0.32	0/219	0.72	0/339

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	R1	0.54	0/69797	0.82	27/108890 (0.0%)
34	R2	0.42	0/2847	0.85	1/4440 (0.0%)
35	R3	0.47	0/36782	0.85	25/57377 (0.0%)
36	T	0.39	0/1716	0.85	3/2672 (0.1%)
37	sb	0.28	0/1735	0.52	0/2338
38	sc	0.28	0/1651	0.55	0/2225
39	sd	0.28	0/1665	0.56	0/2227
40	se	0.30	0/1169	0.59	0/1573
41	sf	0.31	0/835	0.64	1/1128 (0.1%)
42	sg	0.27	0/1195	0.54	0/1602
43	sh	0.30	0/989	0.55	0/1326
44	si	0.30	0/1034	0.65	0/1375
45	sj	0.29	0/796	0.62	0/1077
46	sk	0.29	0/885	0.56	0/1195
47	sl	0.30	0/969	0.61	0/1300
48	sm	0.27	0/892	0.59	0/1193
49	sn	0.27	0/817	0.60	0/1088
50	so	0.27	0/722	0.57	0/964
51	sp	0.31	0/659	0.59	0/884
52	sq	0.30	0/657	0.58	0/881
53	sr	0.30	0/544	0.57	0/731
54	ss	0.54	2/652 (0.3%)	1.13	4/877 (0.5%)
55	st	0.26	0/671	0.48	0/888
56	su	0.30	0/598	0.64	1/792 (0.1%)
All	All	0.46	5/162255 (0.0%)	0.77	71/241914 (0.0%)

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
25	35	0	1
29	6	0	1
30	9	0	1
36	T	8	0
39	sd	0	1
40	se	0	1
41	sf	0	1
49	sn	0	1
All	All	8	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	6	111	PRO	CG-CD	-20.93	0.81	1.50
29	6	111	PRO	CB-CG	15.30	2.26	1.50
54	ss	29	PRO	CG-CD	-8.88	1.21	1.50
54	ss	29	PRO	CB-CG	-7.31	1.13	1.50
29	6	111	PRO	N-CD	5.28	1.55	1.47

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	6	111	PRO	N-CD-CG	-20.10	73.05	103.20
54	ss	29	PRO	N-CD-CG	-18.37	75.64	103.20
29	6	111	PRO	CA-CB-CG	-17.57	70.61	104.00
29	6	111	PRO	N-CA-CB	-15.99	84.11	103.30
29	6	111	PRO	CB-CG-CD	-14.69	49.22	106.50

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	T	8	4SU	C1',C2'
36	T	20	H2U	C2'
36	T	32	4OC	C2'
36	T	54	MUM	C5,C4',C3'
36	T	55	PSU	C4'

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	35	30	HIS	Peptide
29	6	12	ALA	Peptide
30	9	8	LYS	Peptide
39	sd	27	ILE	Peptide
40	se	121	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1353	0	1159	23	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	13	1129	0	1162	15	0
3	14	938	0	1012	23	0
4	15	1045	0	1117	23	0
5	16	1074	0	1157	15	0
6	17	960	0	1000	11	0
7	18	892	0	923	15	0
8	19	917	0	965	17	0
9	2	2082	0	2157	34	0
10	20	947	0	1022	10	0
11	21	816	0	839	24	0
12	22	857	0	922	15	0
13	23	738	0	807	16	0
14	24	779	0	834	21	0
15	25	753	0	780	13	0
16	27	582	0	599	7	0
17	28	625	0	655	10	0
18	29	509	0	543	8	0
19	3	1565	0	1616	27	0
20	30	449	0	491	7	0
21	31	522	0	524	12	0
22	32	444	0	461	17	0
23	33	409	0	440	9	0
24	34	377	0	418	5	0
25	35	504	0	574	15	0
26	36	302	0	343	9	0
27	4	1552	0	1619	27	0
28	5	1410	0	1447	38	0
29	6	1323	0	1374	28	0
30	9	1111	0	1148	28	0
31	E	4360	0	4336	101	0
32	M	195	0	99	0	0
33	R1	62318	0	31344	639	0
34	R2	2546	0	1292	38	0
35	R3	32850	0	16534	371	0
36	T	1639	0	831	29	0
37	sb	1704	0	1732	0	0
38	sc	1624	0	1699	0	0
39	sd	1643	0	1710	0	0
40	se	1156	0	1199	0	0
41	sf	817	0	808	0	0
42	sg	1181	0	1238	0	0
43	sh	979	0	1034	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	si	1022	0	1070	0	0
45	sj	786	0	828	0	0
46	sk	869	0	878	0	0
47	sl	955	0	1019	0	0
48	sm	883	0	944	0	0
49	sn	805	0	847	0	0
50	so	714	0	737	0	0
51	sp	649	0	666	0	0
52	sq	648	0	691	0	0
53	sr	535	0	552	0	0
54	ss	637	0	665	0	0
55	st	665	0	714	0	0
56	su	590	0	629	0	0
57	15	1	0	0	0	0
57	2	1	0	0	0	0
57	32	1	0	0	0	0
57	R1	199	0	0	0	0
57	R3	77	0	0	0	0
58	E	62	0	24	4	0
59	E	2	0	0	0	0
60	T	10	0	10	1	0
All	All	150087	0	102238	1576	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 8.

The worst 5 of 1576 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)
33:R1:136:G:N1	33:R1:142:A:C2	2.28	1.02
33:R1:134:G:H1	33:R1:144:A:N6	1.62	0.98
33:R1:136:G:N1	33:R1:142:A:H2	1.59	0.96
35:R3:359:G:HO2'	35:R3:360:G:H8	0.96	0.91
33:R1:2138:G:N1	33:R1:2153:C:N3	2.20	0.89

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	1	218/220 (99%)	189 (87%)	29 (13%)	0	100	100
2	13	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
3	14	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
4	15	141/143 (99%)	123 (87%)	18 (13%)	0	100	100
5	16	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
6	17	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
7	18	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
8	19	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
9	2	269/271 (99%)	244 (91%)	25 (9%)	0	100	100
10	20	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
11	21	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
12	22	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
13	23	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
14	24	100/102 (98%)	90 (90%)	10 (10%)	0	100	100
15	25	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
16	27	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
17	28	75/77 (97%)	75 (100%)	0	0	100	100
18	29	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
19	3	207/209 (99%)	186 (90%)	21 (10%)	0	100	100
20	30	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
21	31	64/66 (97%)	54 (84%)	10 (16%)	0	100	100
22	32	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
23	33	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
24	34	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
25	35	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	8	37

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	36	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
27	4	199/201 (99%)	184 (92%)	15 (8%)	0	100	100
28	5	175/177 (99%)	160 (91%)	15 (9%)	0	100	100
29	6	174/176 (99%)	157 (90%)	17 (10%)	0	100	100
30	9	147/149 (99%)	126 (86%)	19 (13%)	2 (1%)	9	40
31	E	550/552 (100%)	496 (90%)	51 (9%)	3 (0%)	25	60
37	sb	216/218 (99%)	190 (88%)	25 (12%)	1 (0%)	25	60
38	sc	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
39	sd	203/205 (99%)	180 (89%)	23 (11%)	0	100	100
40	se	155/157 (99%)	135 (87%)	18 (12%)	2 (1%)	10	41
41	sf	98/100 (98%)	80 (82%)	18 (18%)	0	100	100
42	sg	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
43	sh	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
44	si	125/127 (98%)	106 (85%)	19 (15%)	0	100	100
45	sj	96/98 (98%)	85 (88%)	10 (10%)	1 (1%)	13	47
46	sk	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
47	sl	121/123 (98%)	91 (75%)	30 (25%)	0	100	100
48	sm	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
49	sn	98/100 (98%)	75 (76%)	23 (24%)	0	100	100
50	so	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
51	sp	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
52	sq	78/80 (98%)	66 (85%)	12 (15%)	0	100	100
53	sr	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
54	ss	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
55	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
56	su	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
All	All	6352/6454 (98%)	5731 (90%)	611 (10%)	10 (0%)	45	75

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	35	31	ILE
31	E	18	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
37	sb	18	GLN
40	se	122	VAL
31	E	211	THR

### 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	1	106/171 (62%)	104 (98%)	2 (2%)	52	76
2	13	116/116 (100%)	112 (97%)	4 (3%)	32	63
3	14	103/103 (100%)	98 (95%)	5 (5%)	21	54
4	15	102/102 (100%)	101 (99%)	1 (1%)	73	87
5	16	109/109 (100%)	105 (96%)	4 (4%)	29	62
6	17	100/100 (100%)	99 (99%)	1 (1%)	73	87
7	18	86/86 (100%)	84 (98%)	2 (2%)	45	72
8	19	99/99 (100%)	97 (98%)	2 (2%)	50	75
9	2	216/216 (100%)	207 (96%)	9 (4%)	25	58
10	20	89/89 (100%)	89 (100%)	0	100	100
11	21	84/84 (100%)	82 (98%)	2 (2%)	44	71
12	22	93/93 (100%)	91 (98%)	2 (2%)	47	73
13	23	80/80 (100%)	77 (96%)	3 (4%)	28	60
14	24	83/83 (100%)	80 (96%)	3 (4%)	30	62
15	25	78/78 (100%)	72 (92%)	6 (8%)	10	39
16	27	58/58 (100%)	57 (98%)	1 (2%)	56	78
17	28	67/67 (100%)	65 (97%)	2 (3%)	36	66
18	29	55/55 (100%)	53 (96%)	2 (4%)	30	62
19	3	164/164 (100%)	160 (98%)	4 (2%)	44	71
20	30	48/48 (100%)	46 (96%)	2 (4%)	25	58
21	31	59/59 (100%)	57 (97%)	2 (3%)	32	63

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	32	47/47 (100%)	46 (98%)	1 (2%)	48	74
23	33	45/45 (100%)	44 (98%)	1 (2%)	47	73
24	34	38/38 (100%)	36 (95%)	2 (5%)	19	52
25	35	51/51 (100%)	49 (96%)	2 (4%)	27	60
26	36	34/34 (100%)	34 (100%)	0	100	100
27	4	165/165 (100%)	155 (94%)	10 (6%)	15	47
28	5	148/148 (100%)	143 (97%)	5 (3%)	32	63
29	6	137/137 (100%)	129 (94%)	8 (6%)	17	49
30	9	114/114 (100%)	110 (96%)	4 (4%)	31	63
31	E	461/464 (99%)	444 (96%)	17 (4%)	29	62
37	sb	180/180 (100%)	172 (96%)	8 (4%)	24	57
38	sc	170/170 (100%)	164 (96%)	6 (4%)	31	63
39	sd	172/172 (100%)	165 (96%)	7 (4%)	26	59
40	se	119/119 (100%)	117 (98%)	2 (2%)	56	78
41	sf	87/87 (100%)	85 (98%)	2 (2%)	45	72
42	sg	124/124 (100%)	114 (92%)	10 (8%)	9	36
43	sh	104/104 (100%)	100 (96%)	4 (4%)	28	60
44	si	105/105 (100%)	100 (95%)	5 (5%)	21	55
45	sj	86/86 (100%)	86 (100%)	0	100	100
46	sk	89/89 (100%)	88 (99%)	1 (1%)	70	86
47	sl	103/103 (100%)	98 (95%)	5 (5%)	21	54
48	sm	92/92 (100%)	87 (95%)	5 (5%)	18	51
49	sn	83/83 (100%)	82 (99%)	1 (1%)	67	85
50	so	76/76 (100%)	74 (97%)	2 (3%)	41	70
51	sp	65/65 (100%)	59 (91%)	6 (9%)	7	29
52	sq	74/74 (100%)	72 (97%)	2 (3%)	40	69
53	sr	56/56 (100%)	54 (96%)	2 (4%)	30	62
54	ss	70/70 (100%)	69 (99%)	1 (1%)	62	82
55	st	65/65 (100%)	65 (100%)	0	100	100
56	su	60/60 (100%)	58 (97%)	2 (3%)	33	64
All	All	5215/5283 (99%)	5035 (96%)	180 (4%)	33	63

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	sb	158	ASP
42	sg	149	LYS
38	sc	133	MET
40	se	148	SER
44	si	59	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
31	E	99	ASN
41	sf	94	HIS
31	E	188	GLN
45	sj	58	ASN
41	sf	3	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	M	8/9 (88%)	1 (12%)	0
33	R1	2902/2903 (99%)	571 (19%)	21 (0%)
34	R2	118/119 (99%)	17 (14%)	0
35	R3	1529/1531 (99%)	390 (25%)	23 (1%)
36	T	74/77 (96%)	19 (25%)	3 (4%)
All	All	4631/4639 (99%)	998 (21%)	47 (1%)

5 of 998 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	M	7	A
33	R1	2	G
33	R1	3	U
33	R1	10	A
33	R1	15	G

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	R3	472	U
35	R3	685	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	R3	497	G
35	R3	588	G
35	R3	837	U

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

5 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$
36	4OC	T	32	36	20,23,24	2.70	5 (25%)	25,32,35	1.09	2 (8%)
36	MUM	T	54	36	18,22,22	3.39	6 (33%)	19,32,32	2.17	5 (26%)
36	4SU	T	8	36	18,21,22	3.64	8 (44%)	25,30,33	2.27	5 (20%)
36	H2U	T	20	36	18,21,22	4.56	5 (27%)	19,30,33	3.83	6 (31%)
36	PSU	T	55	36	18,21,22	2.23	7 (38%)	21,30,33	2.16	5 (23%)

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
36	4OC	T	32	36	1/1/5/6	1/9/29/30	0/2/2/2
36	MUM	T	54	36	3/3/9/10	3/7/41/41	0/2/2/2
36	4SU	T	8	36	2/2/5/5	0/7/25/26	0/2/2/2
36	H2U	T	20	36	1/1/8/9	5/7/38/39	0/2/2/2
36	PSU	T	55	36	1/1/5/5	5/7/25/26	0/2/2/2

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	T	54	MUM	C6-N1	-12.32	1.31	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	T	20	H2U	O4-C4	11.19	1.45	1.23
36	T	8	4SU	O2-C2	10.65	1.41	1.23
36	T	20	H2U	C2-N1	9.58	1.48	1.35
36	T	32	4OC	O2-C2	9.31	1.41	1.23

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	T	20	H2U	O2-C2-N1	-10.22	110.81	123.10
36	T	20	H2U	O4-C4-N3	-7.61	108.57	120.30
36	T	8	4SU	C4-N3-C2	-6.81	120.78	127.31
36	T	55	PSU	N1-C2-N3	6.59	122.12	115.17
36	T	20	H2U	O4-C4-C5	-6.48	108.93	122.20

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	T	20	H2U	C2'
36	T	32	4OC	C2'
36	T	54	MUM	C5
36	T	54	MUM	C4'
36	T	54	MUM	C3'

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	T	20	H2U	O4'-C1'-N1-C2
36	T	20	H2U	O4'-C1'-N1-C6
36	T	54	MUM	O4'-C4'-C5'-O5'
36	T	54	MUM	C3'-C4'-C5'-O5'
36	T	54	MUM	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	T	54	MUM	1	0
36	T	20	H2U	2	0
36	T	55	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 284 ligands modelled in this entry, 281 are 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	$\# Z  > 2$
58	ATP	E	601	59	28,33,33	0.84	1 (3%)	34,52,52	0.60	1 (2%)
60	FME	T	101	36	8,9,10	0.96	0	8,9,11	1.00	0
58	ATP	E	602	59	28,33,33	0.72	0	34,52,52	0.62	1 (2%)

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	ATP	E	601	59	-	5/18/38/38	0/3/3/3
60	FME	T	101	36	-	5/7/9/11	-
58	ATP	E	602	59	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	E	601	ATP	PA-O3A	-2.21	1.57	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	E	602	ATP	C5-C6-N6	2.34	123.87	120.31
58	E	601	ATP	C5-C6-N6	2.33	123.86	120.31

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

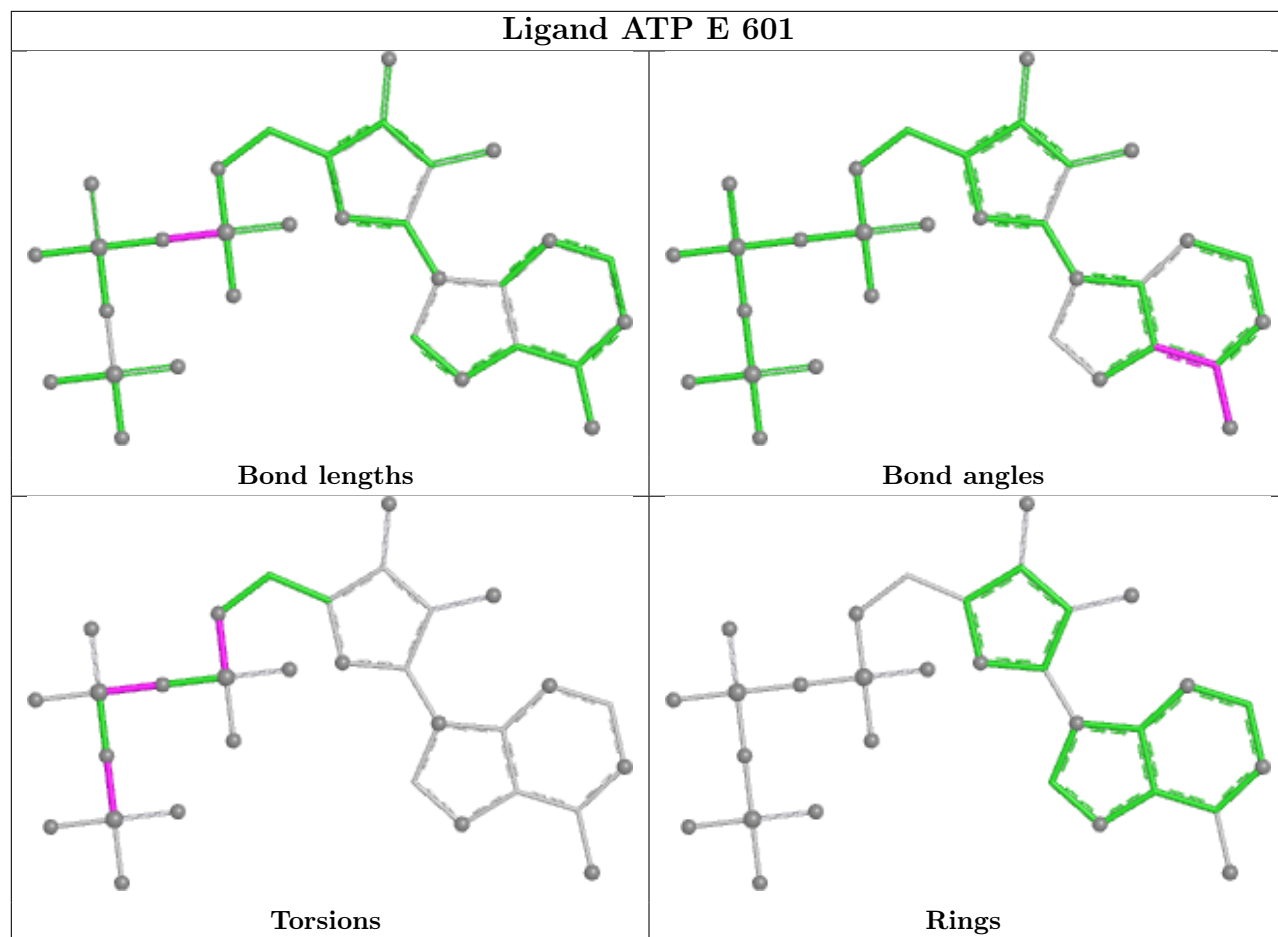
Mol	Chain	Res	Type	Atoms
58	E	601	ATP	PB-O3B-PG-O3G
58	E	601	ATP	C5'-O5'-PA-O2A
58	E	601	ATP	C5'-O5'-PA-O3A
58	E	602	ATP	PB-O3B-PG-O2G
60	T	101	FME	N-CA-CB-CG

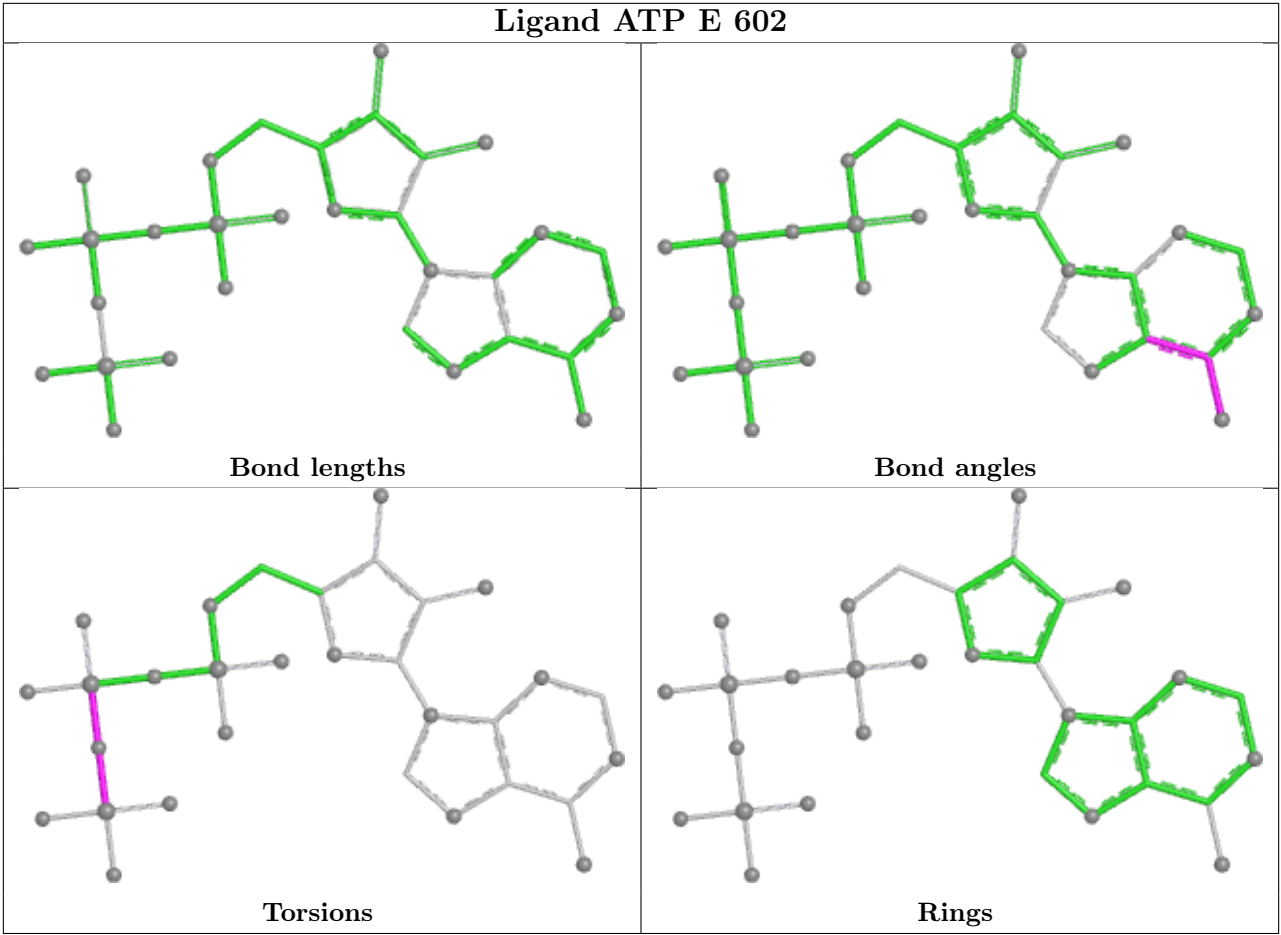
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	E	601	ATP	3	0
60	T	101	FME	1	0
58	E	602	ATP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	R3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	460:A	O3'	461:A	P	5.06
1	R3	210:C	O3'	211:G	P	3.72



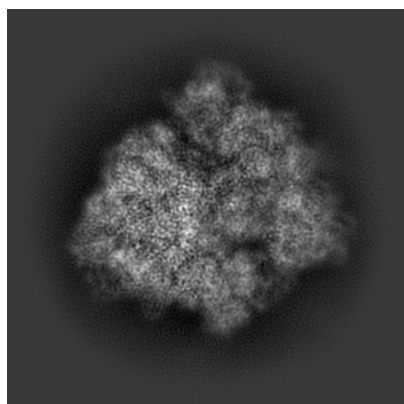
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40929. These allow visual inspection of the internal detail of the map and identification of artifacts.

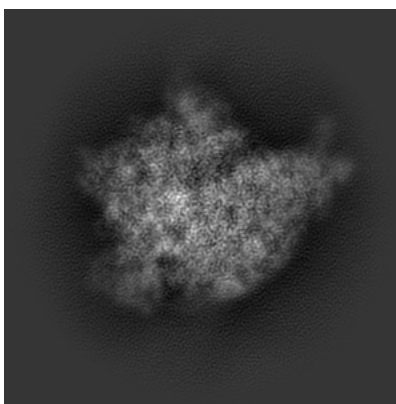
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

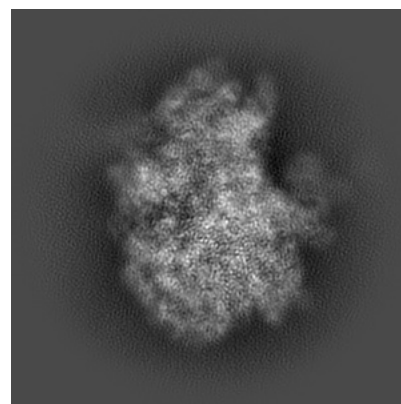
#### 6.1.1 Primary map



X

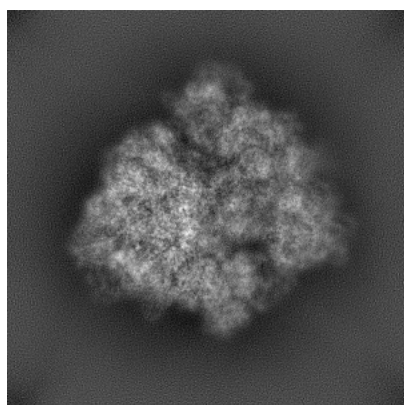


Y

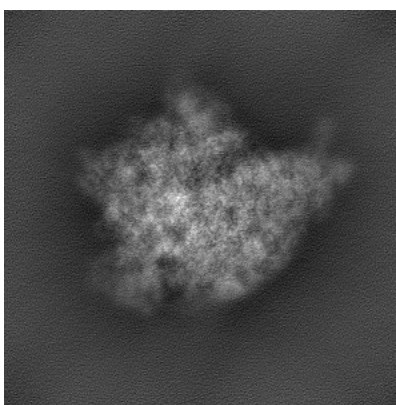


Z

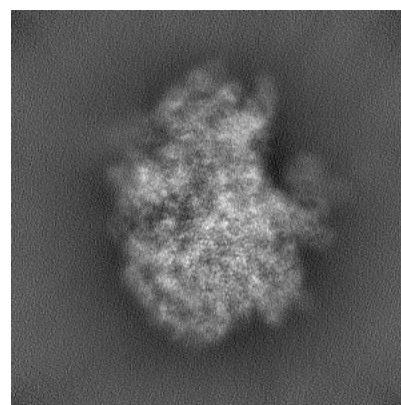
#### 6.1.2 Raw map



X



Y

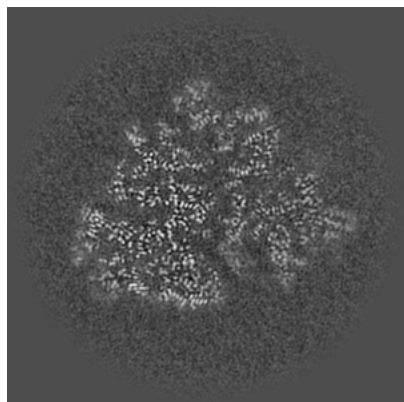


Z

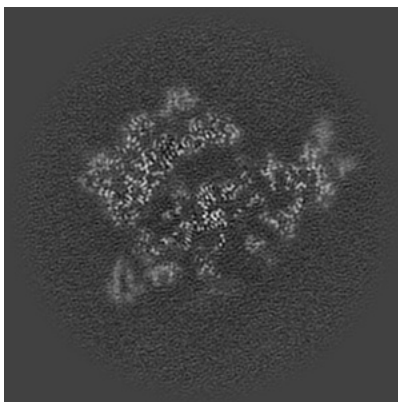
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

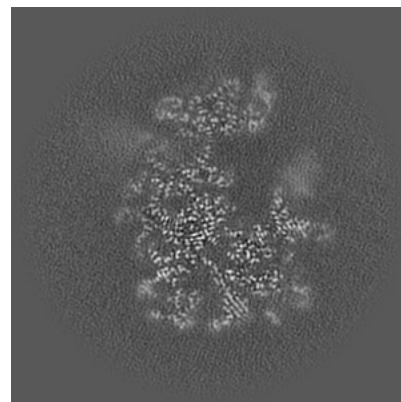
### 6.2.1 Primary map



X Index: 200

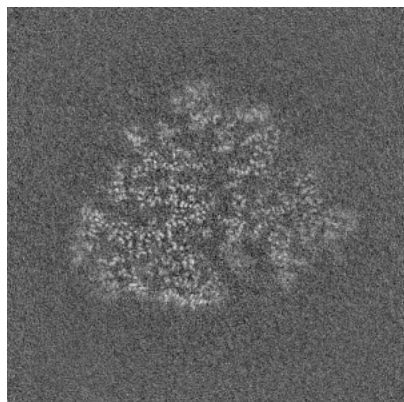


Y Index: 200

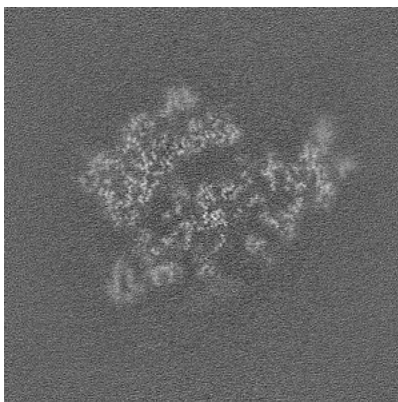


Z Index: 200

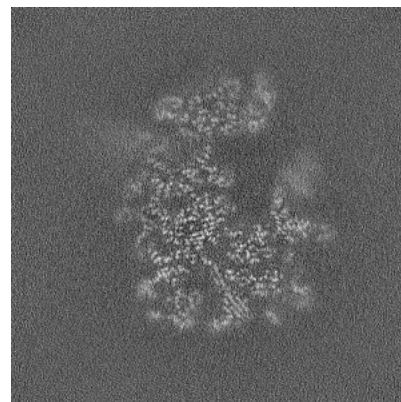
### 6.2.2 Raw map



X Index: 200



Y Index: 200

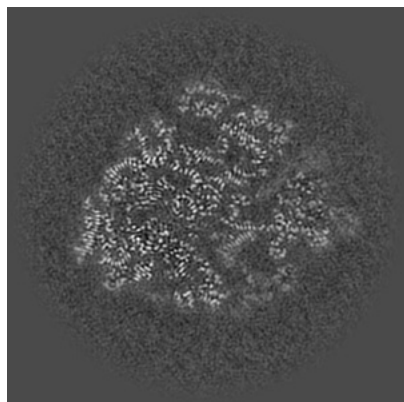


Z Index: 200

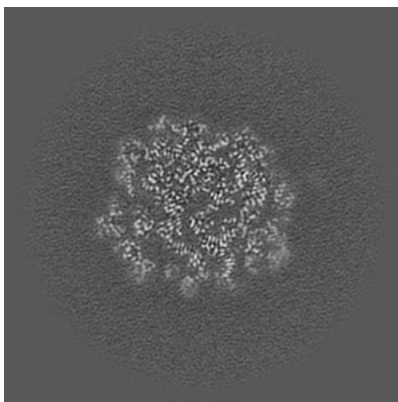
The images above show central slices of the map in three orthogonal directions.

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

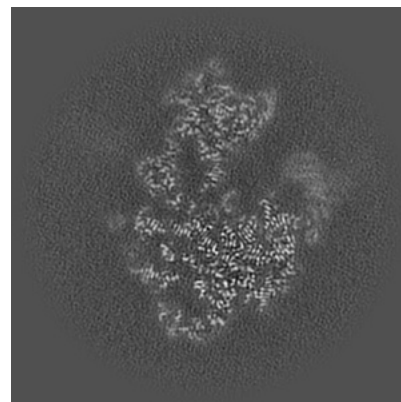
### 6.3.1 Primary map



X Index: 207

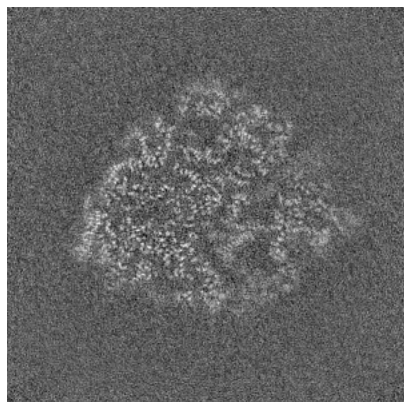


Y Index: 152

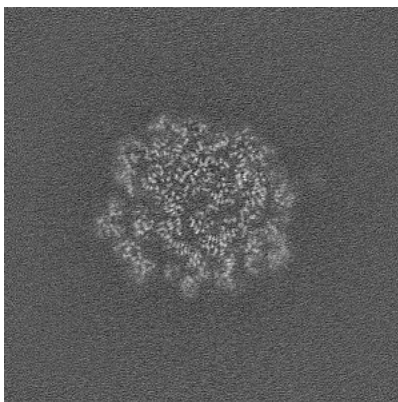


Z Index: 177

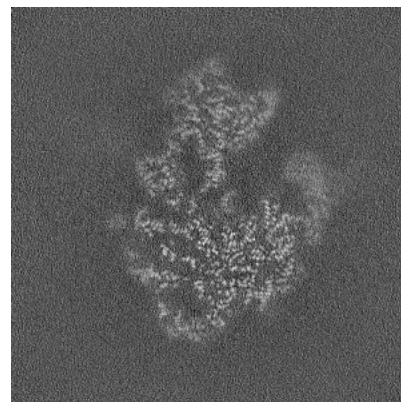
### 6.3.2 Raw map



X Index: 208



Y Index: 152



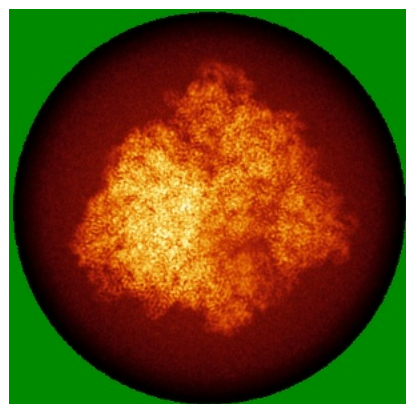
Z Index: 178

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

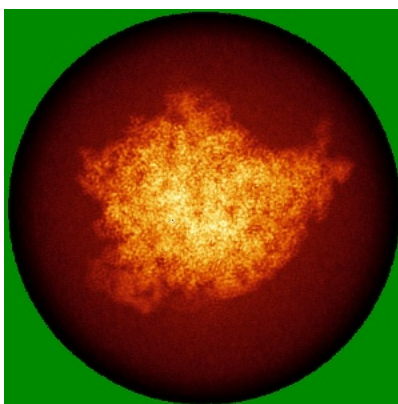


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

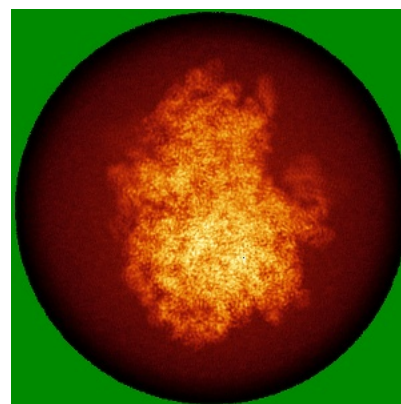
### 6.4.1 Primary map



X

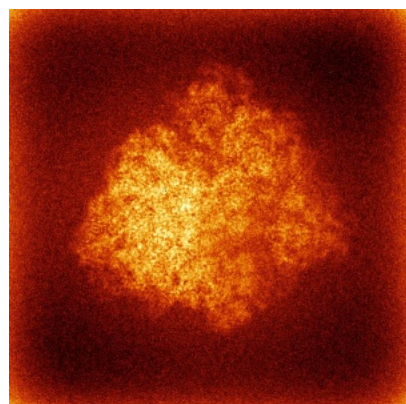


Y

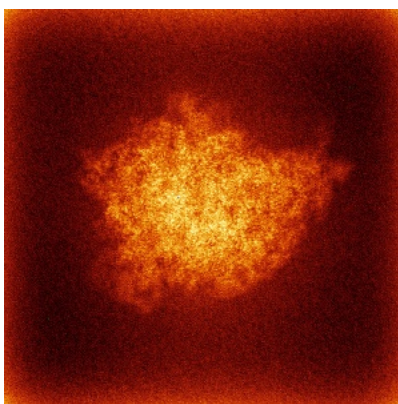


Z

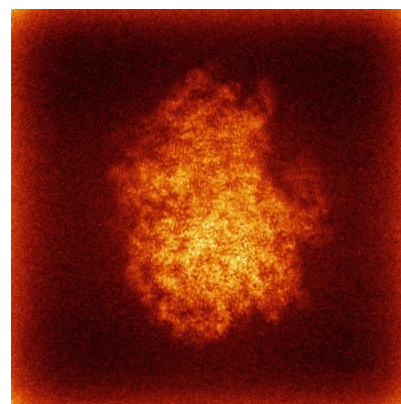
### 6.4.2 Raw map



X



Y

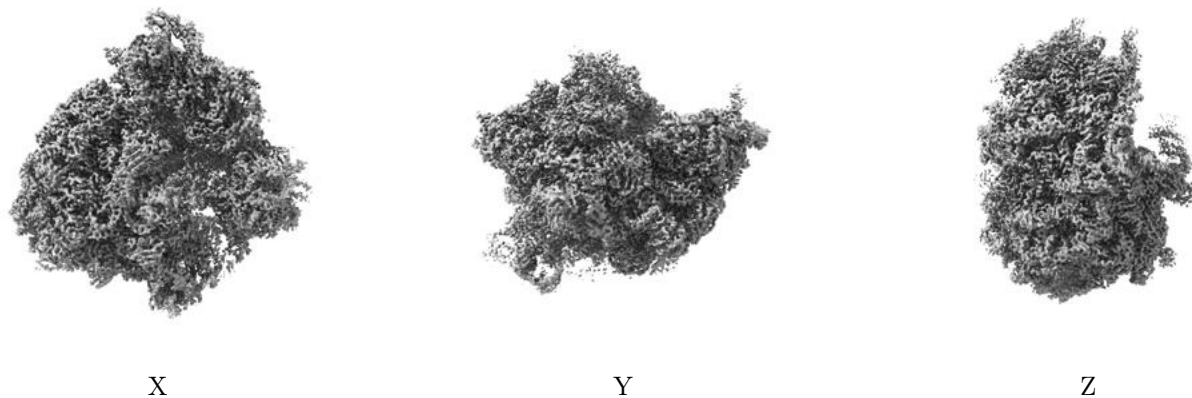


Z

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

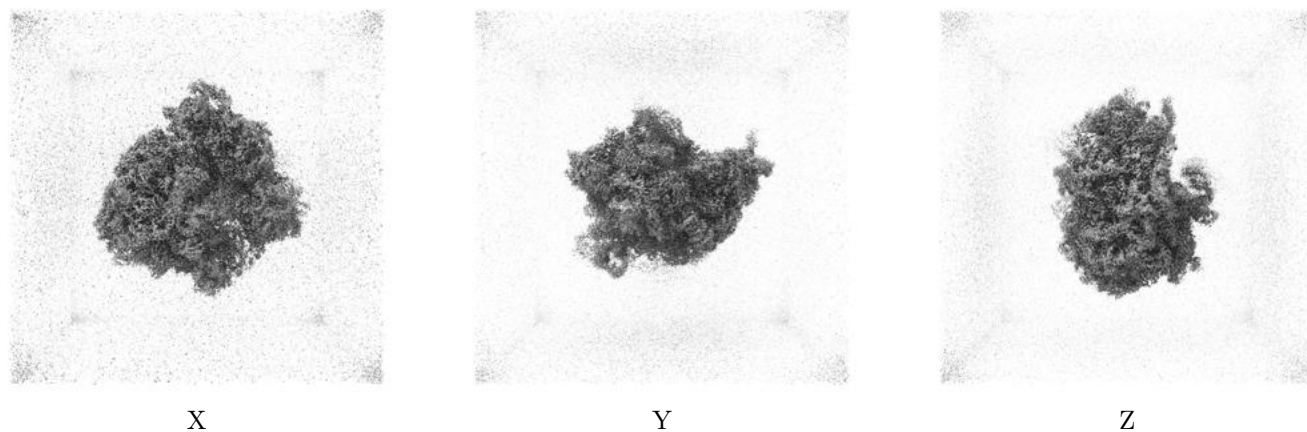
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

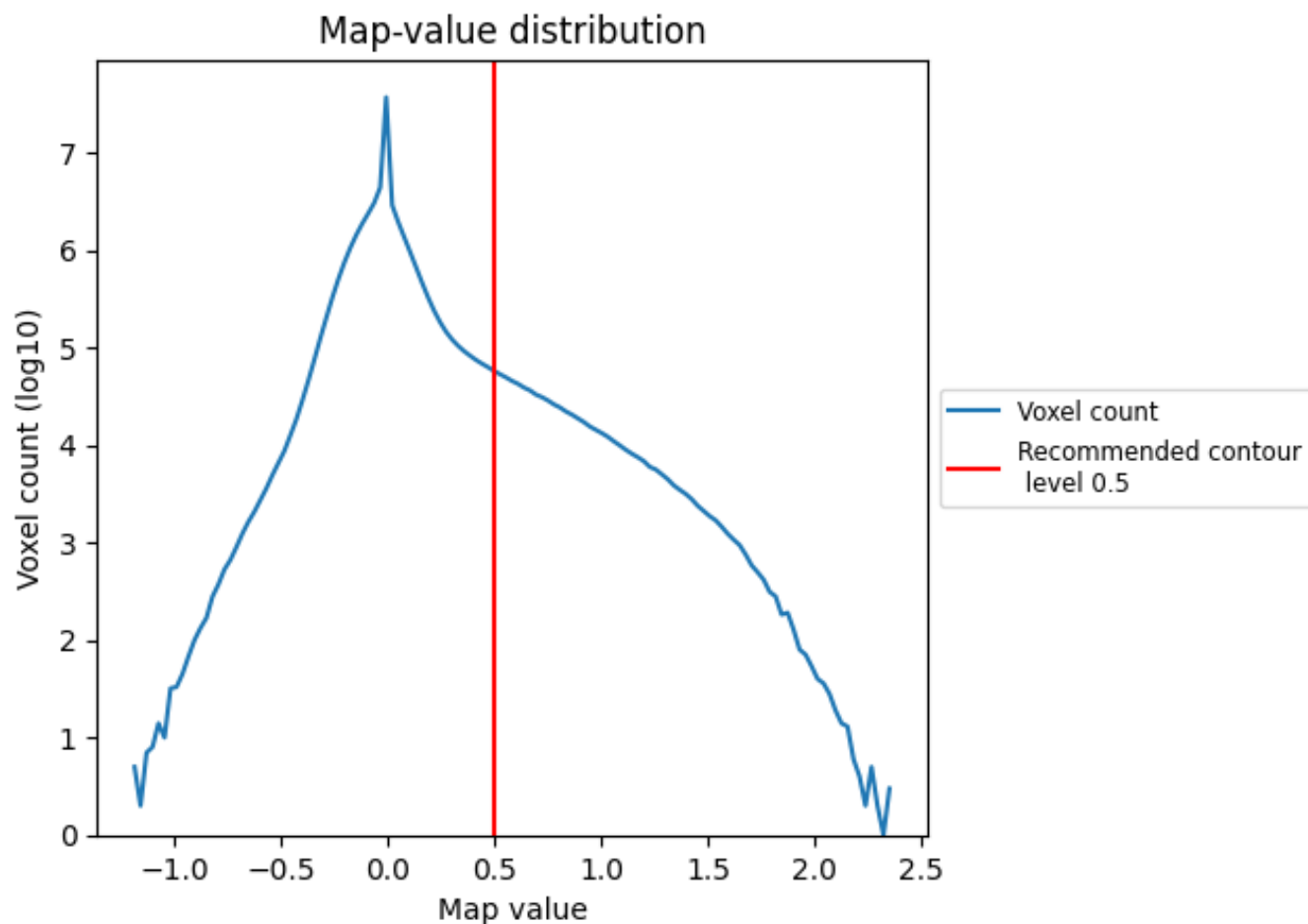
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

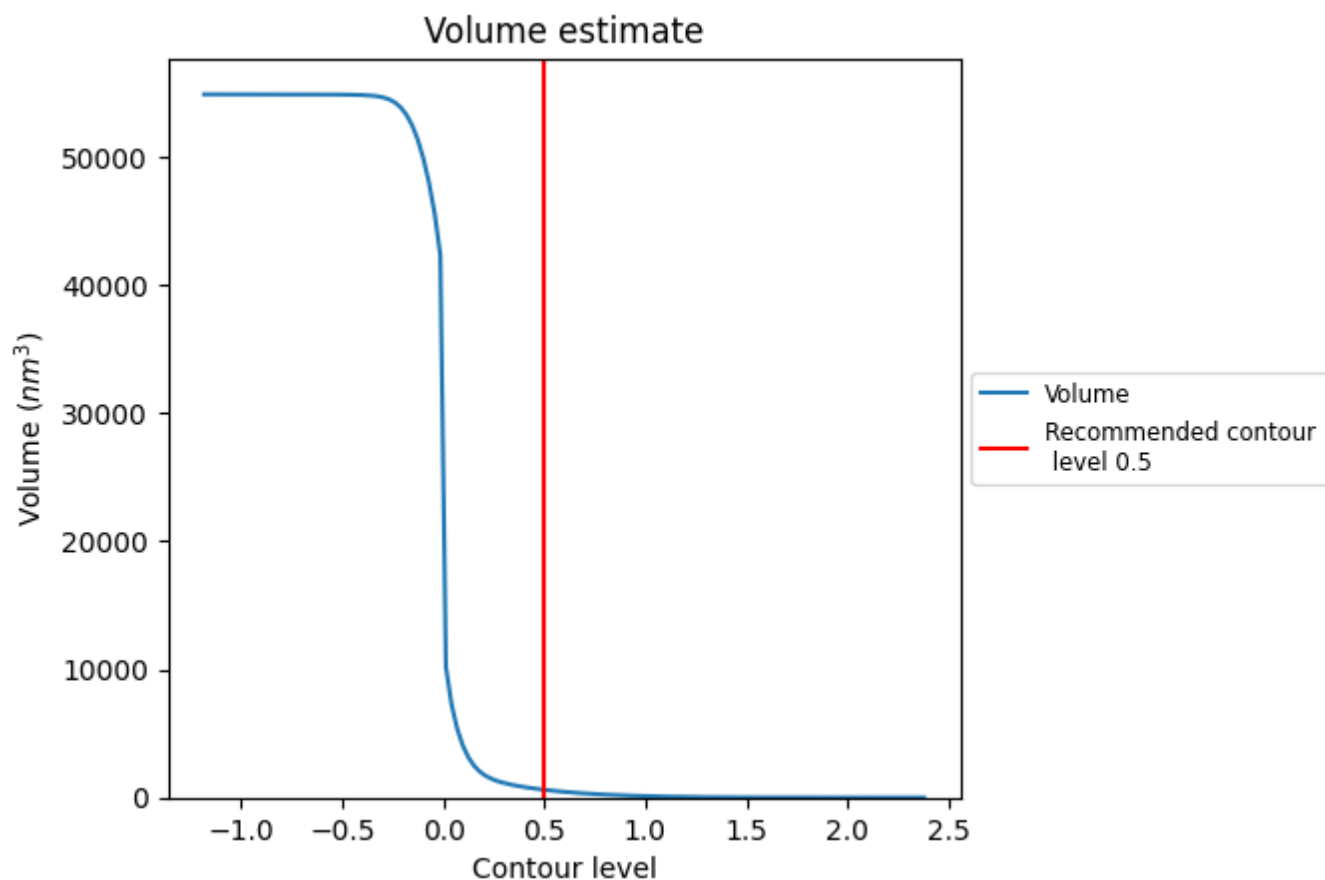
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

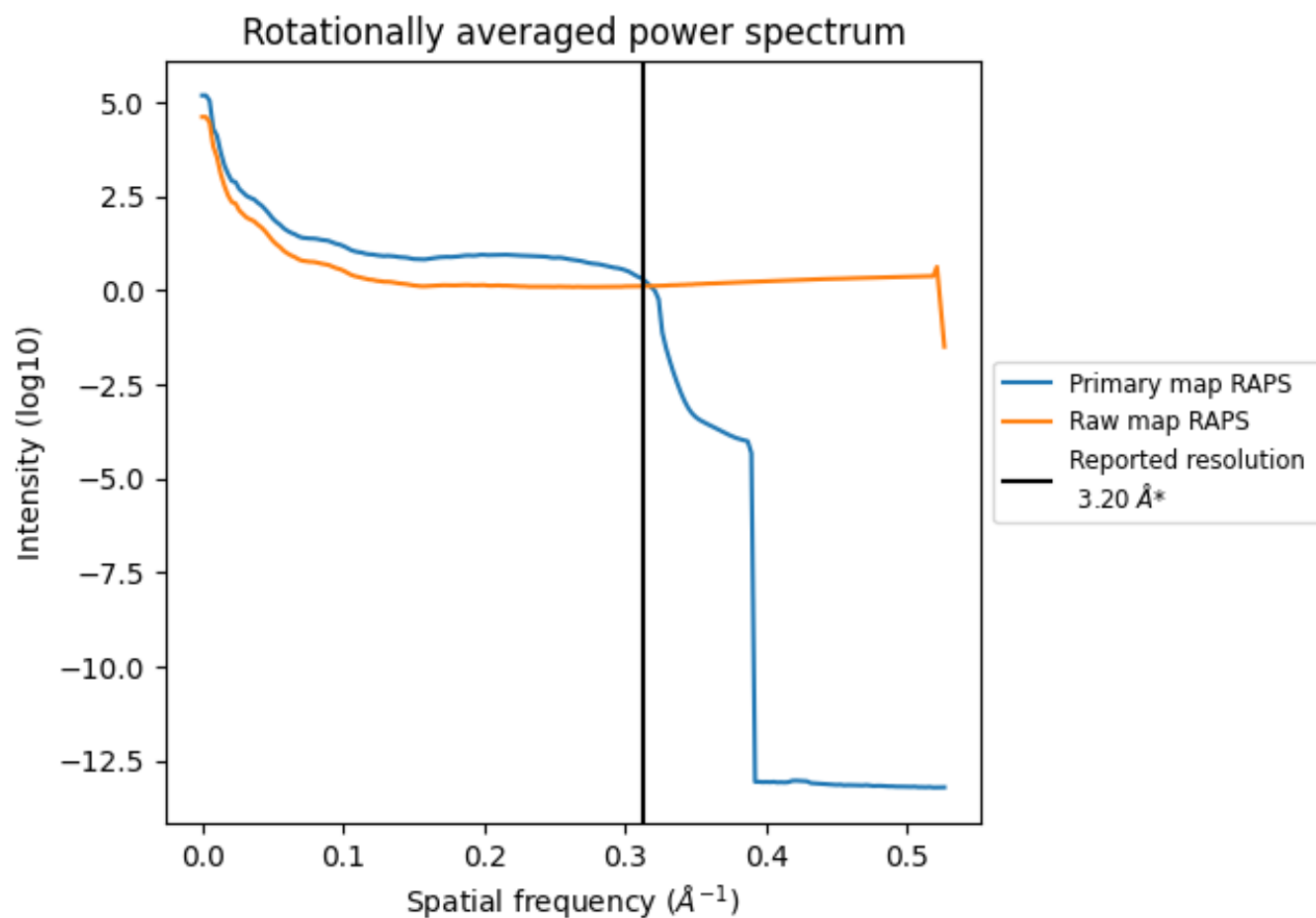
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 605 nm<sup>3</sup>; this corresponds to an approximate mass of 546 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 ⓘ



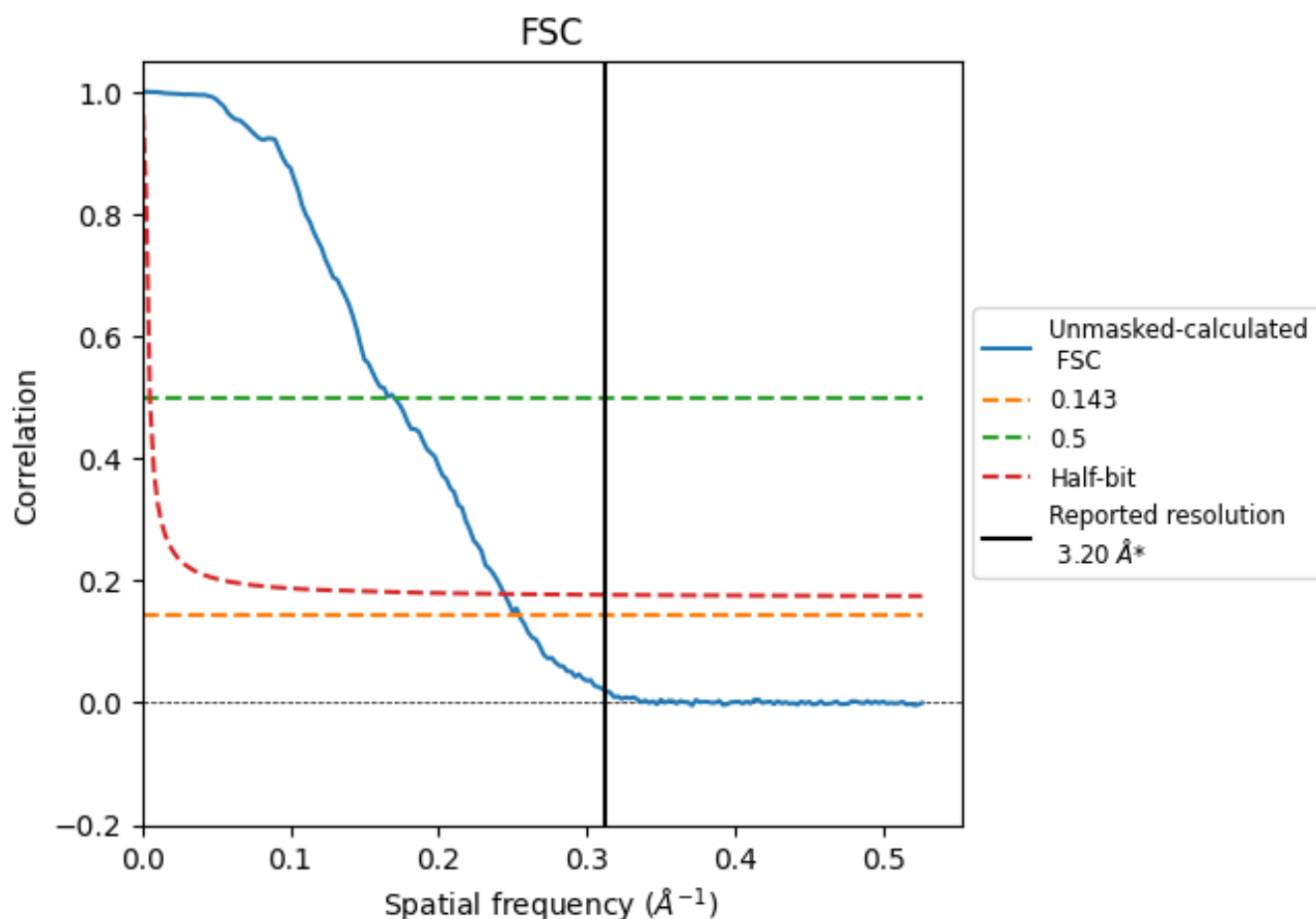
\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

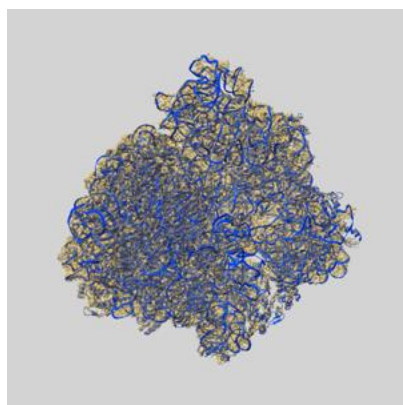
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.93	5.89	4.09

\*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 3.93 differs from the reported value 3.2 by more than 10 %

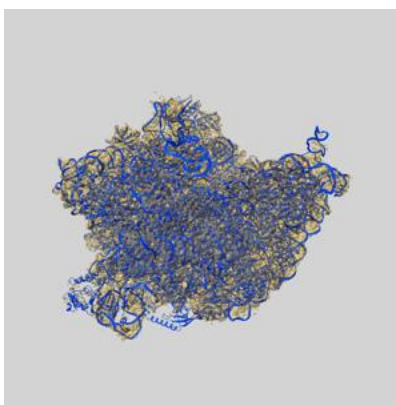
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40929 and PDB model 9NLB. Per-residue inclusion information can be found in section 3 on page 17.

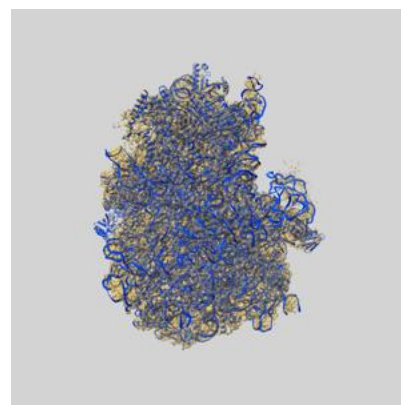
### 9.1 Map-model overlay [i](#)



X



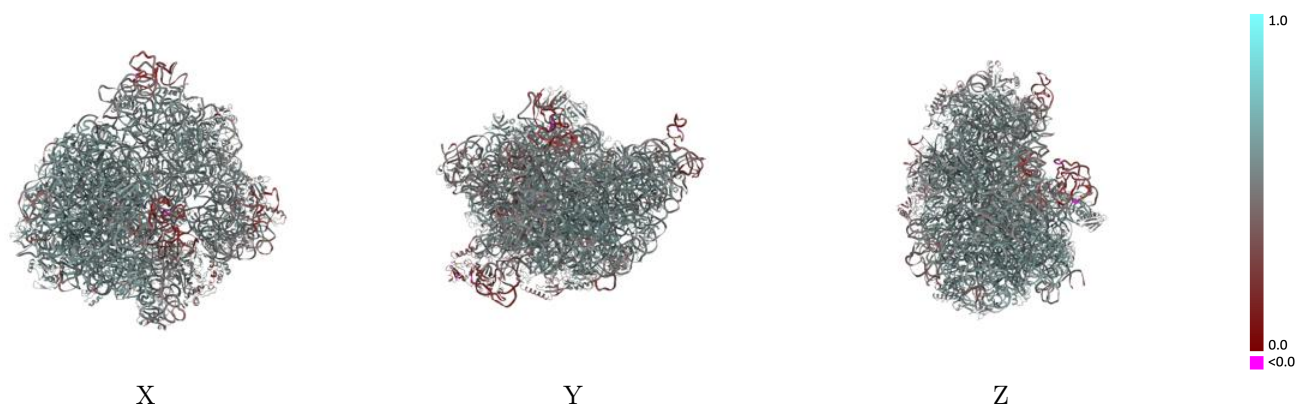
Y



Z

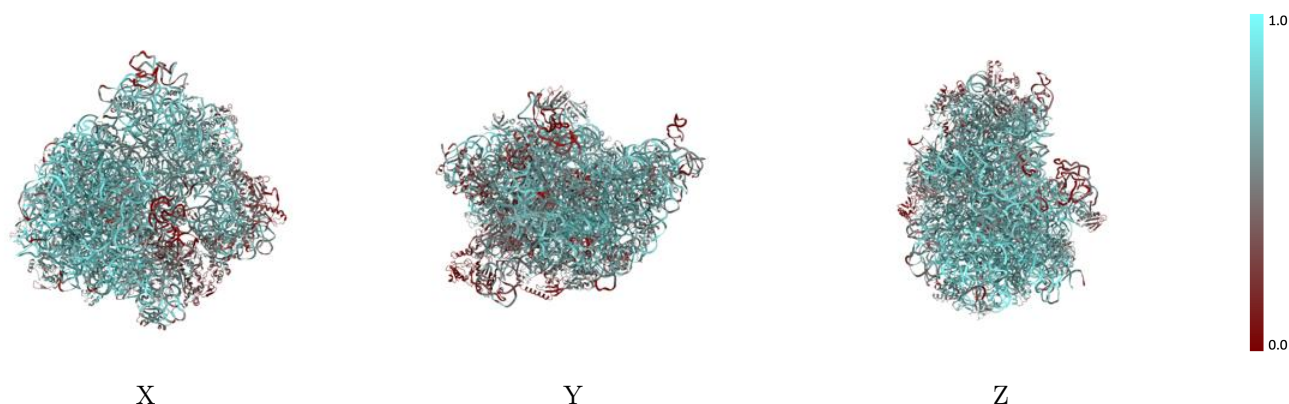
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



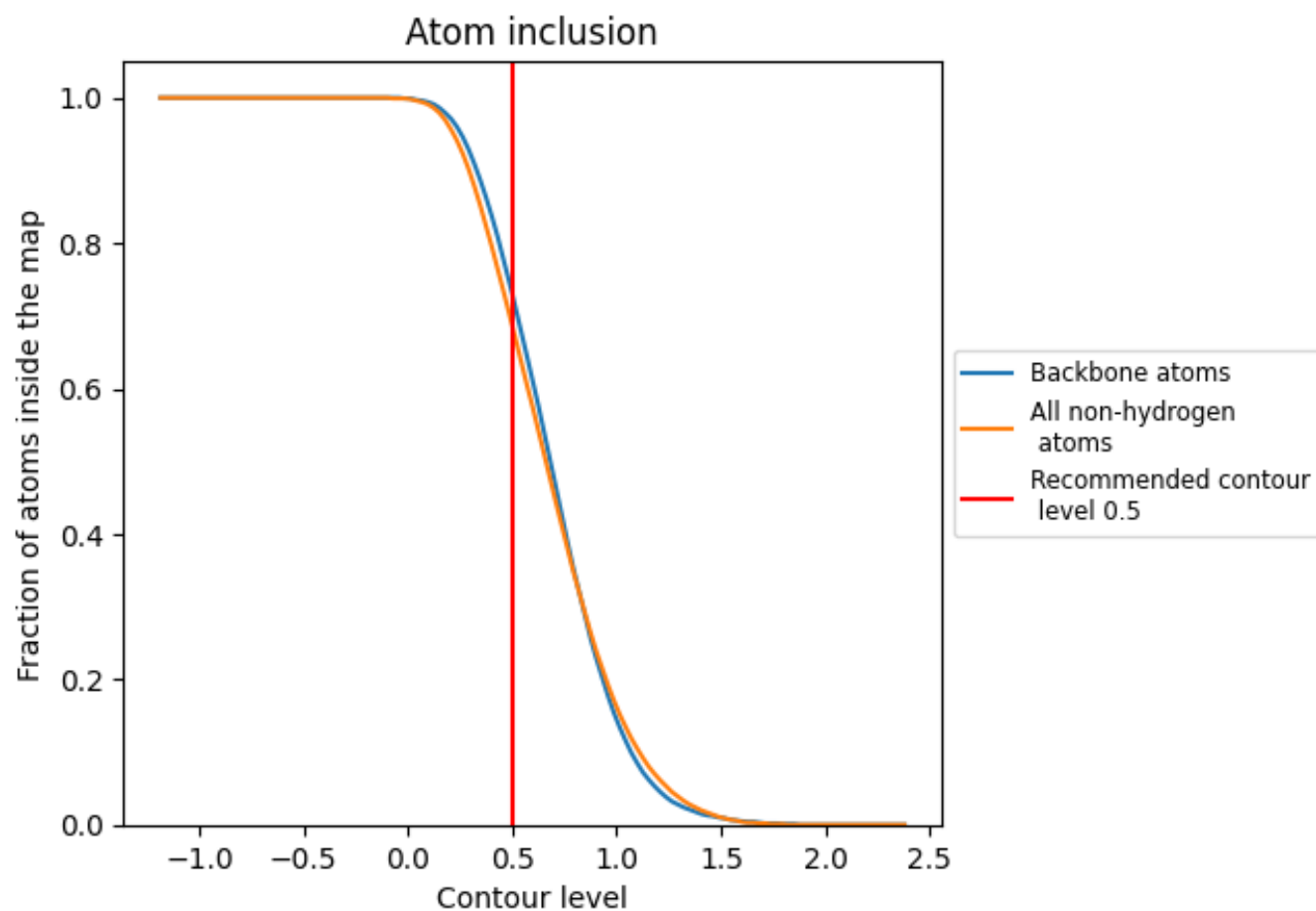
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ













































The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.5230
1	 0.0970	 0.3300
13	 0.6700	 0.5680
14	 0.5980	 0.5620
15	 0.6640	 0.5600
16	 0.6180	 0.5660
17	 0.7220	 0.5740
18	 0.5430	 0.5200
19	 0.6310	 0.5640
2	 0.6780	 0.5790
20	 0.7190	 0.5810
21	 0.6410	 0.5450
22	 0.6600	 0.5620
23	 0.5910	 0.5410
24	 0.5370	 0.5150
25	 0.5850	 0.5430
27	 0.6910	 0.5770
28	 0.6440	 0.5760
29	 0.5760	 0.5160
3	 0.6640	 0.5640
30	 0.6340	 0.5480
31	 0.0920	 0.3690
32	 0.6690	 0.5620
33	 0.5590	 0.5530
34	 0.7210	 0.5910
35	 0.7190	 0.5870
36	 0.6470	 0.5680
4	 0.6110	 0.5490
5	 0.3430	 0.4720
6	 0.4430	 0.4950
9	 0.1590	 0.3960
E	 0.3970	 0.4980
M	 0.3690	 0.4910
R1	 0.7940	 0.5360
R2	 0.7270	 0.4920



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
R3	 0.7420	 0.5110
T	 0.5170	 0.4310
sb	 0.4240	 0.4720
sc	 0.4660	 0.5220
sd	 0.4960	 0.5130
se	 0.5950	 0.5350
sf	 0.5150	 0.5010
sg	 0.4180	 0.5020
sh	 0.5850	 0.5490
si	 0.4640	 0.4950
sj	 0.3720	 0.4720
sk	 0.5480	 0.5390
sl	 0.5340	 0.5350
sm	 0.4170	 0.4940
sn	 0.4920	 0.4970
so	 0.5910	 0.5490
sp	 0.5740	 0.5280
sq	 0.5320	 0.5330
sr	 0.5520	 0.5290
ss	 0.4330	 0.4930
st	 0.5510	 0.5260
su	 0.3660	 0.5190