



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 05:09 pm GMT

PDB ID : 5JU8  
EMDB ID : EMD-8176  
Title : Cryo-EM structure of an ErmBL-stalled ribosome in complex with P-, and E-tRNA  
Authors : Arenz, S.; Bock, L.V.; Graf, M.; Innis, C.A.; Beckmann, R.; Grubmueller, H.; Vaiana, A.C.; Wilson, D.N.  
Deposited on : 2016-05-10  
Resolution : 3.60 Å (reported)  
Based on initial model : 5AFI

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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

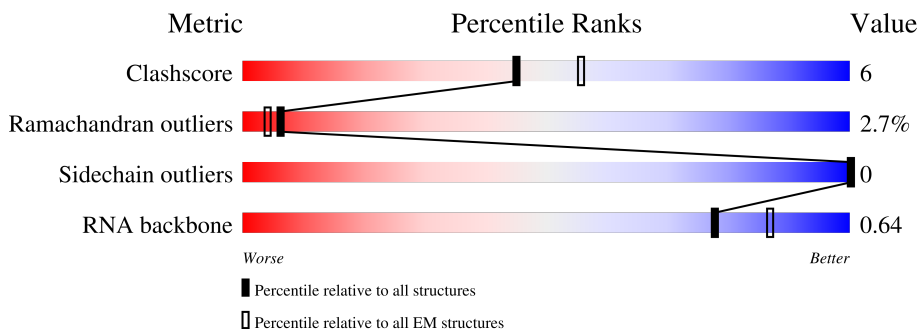
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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	AA	1539	<div> <div>15%</div> <div>54%</div> <div>34%</div> <div>11%</div> <div>.</div> </div>
2	AB	240	<div> <div>90%</div> <div>66%</div> <div>25%</div> <div>9%</div> </div>
3	AC	233	<div> <div>76%</div> <div>64%</div> <div>24%</div> <div>12%</div> </div>
4	AD	206	<div> <div>81%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
5	AE	167	<div> <div>56%</div> <div>67%</div> <div>21%</div> <div>.</div> <div>10%</div> </div>
6	AF	135	<div> <div>53%</div> <div>55%</div> <div>17%</div> <div>.</div> <div>26%</div> </div>
7	AG	179	<div> <div>67%</div> <div>66%</div> <div>18%</div> <div>16%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	10	
23	AX	77	
24	AY	71	
25	BA	2903	
26	BB	120	
27	BC	273	
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	
32	BH	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	BI	142	
34	BJ	142	
35	BK	123	
36	BL	144	
37	BM	136	
38	BN	127	
39	BO	117	
40	BP	115	
41	BQ	118	
42	BR	103	
43	BS	110	
44	BT	100	
45	BU	104	
46	BV	94	
47	BW	85	
48	BX	78	
49	BY	63	
50	BZ	59	
51	B0	57	
52	B1	55	
53	B2	46	
54	B3	65	
55	B4	38	
56	B5	9	

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145158 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	36	ALA	-	insertion	UNP P0AG59

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0
			218	98	44	66	10		

- Molecule 23 is a RNA chain called P-site tRNA Aspartate.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	AX	77	Total	C	N	O	P	S	0	0
			1656	741	290	547	77	1		

- Molecule 24 is a RNA chain called E-site tRNA Valine.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AY	71	Total	C	N	O	P	S	0	0
			1525	682	276	496	70	1		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	120	A	-	expression tag	GB 991970073

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

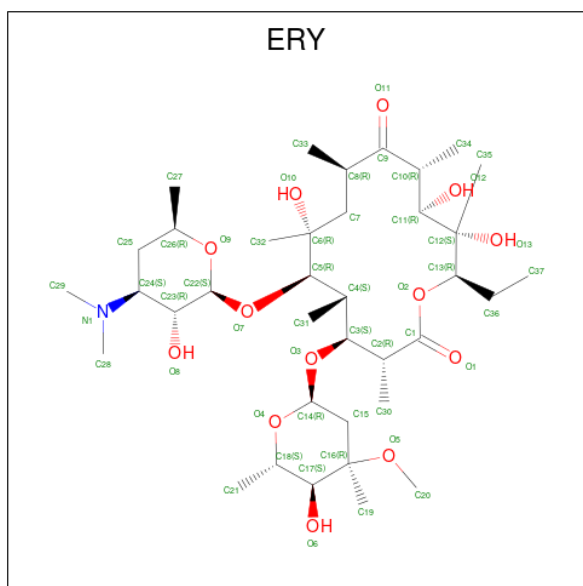
- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is a protein called ErmBL.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	9	Total	C	N	O	S	0	0
			74	46	14	13	1		

- Molecule 57 is ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ).

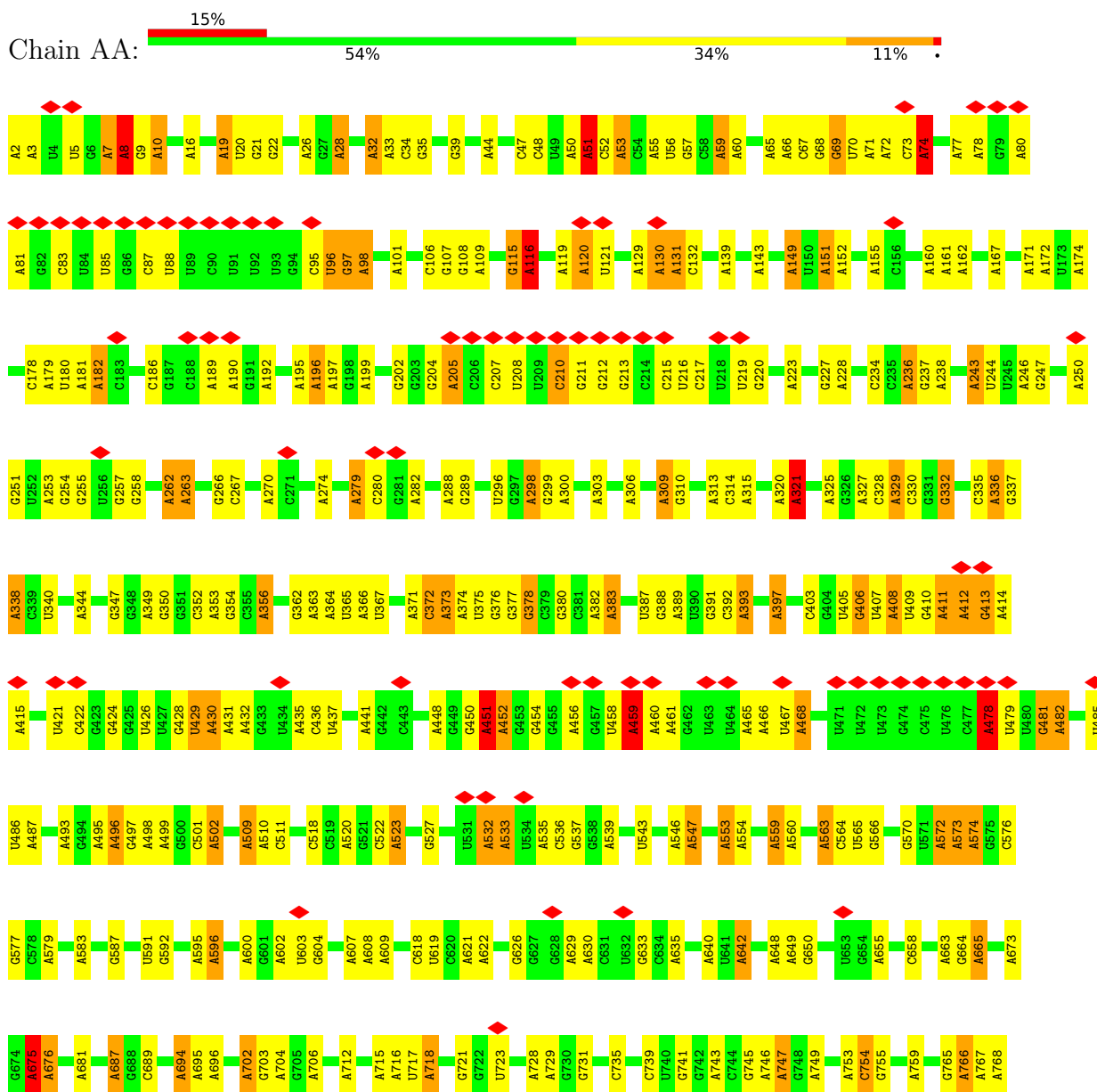


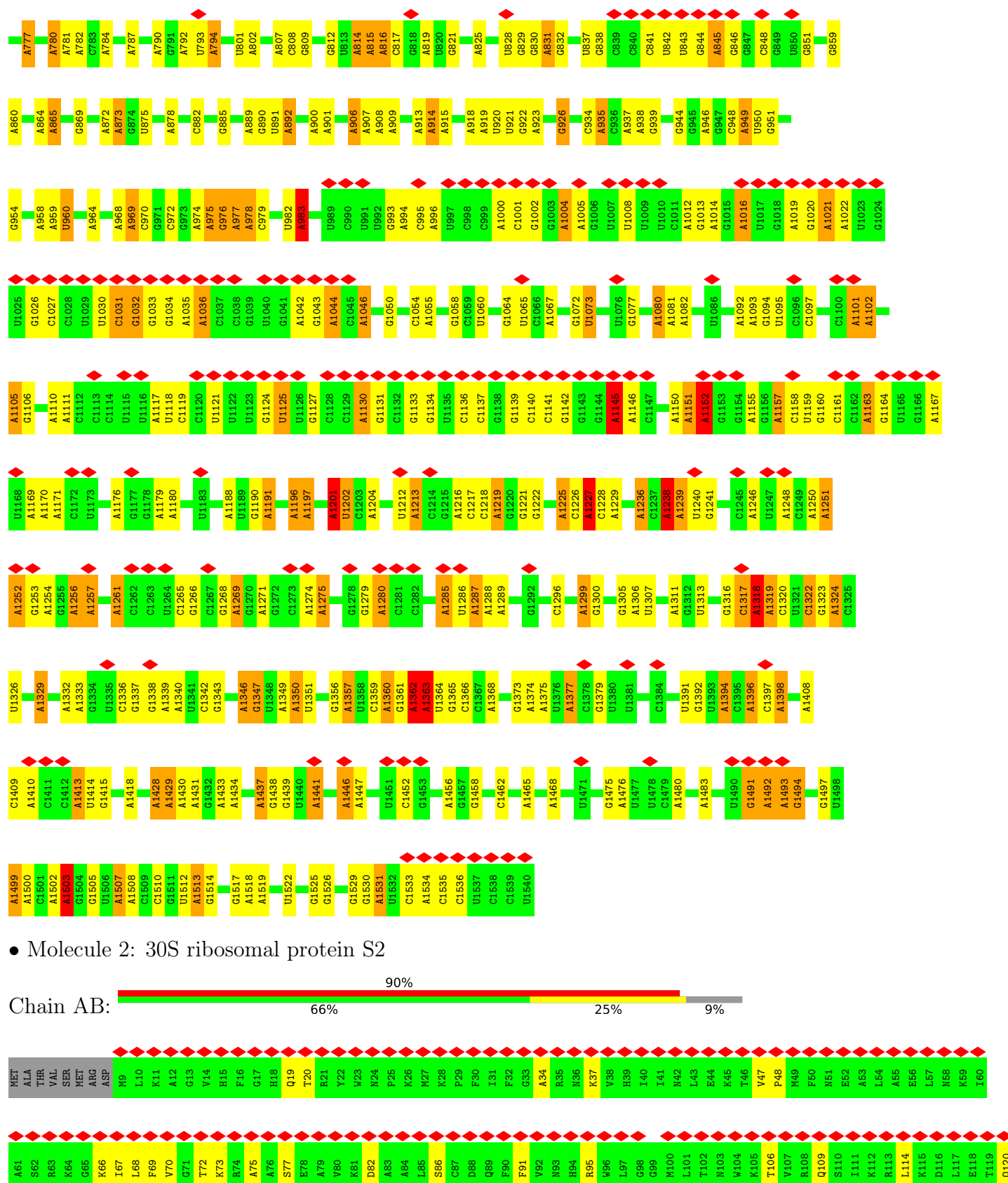
Mol	Chain	Residues	Atoms				AltConf
57	BA	1	Total	C	N	O	0
			51	37	1	13	

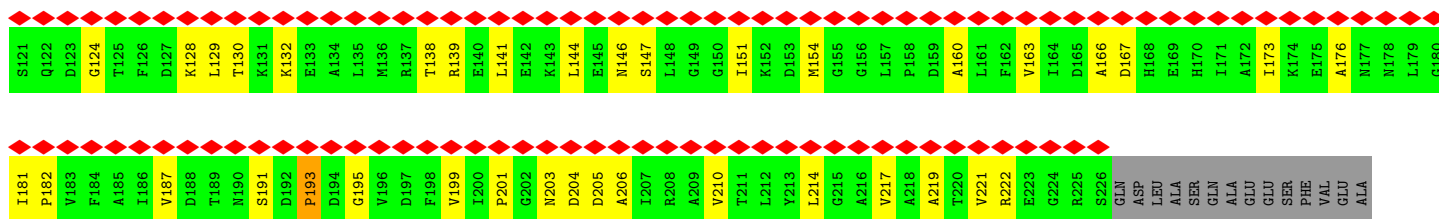
### 3 Residue-property plots

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

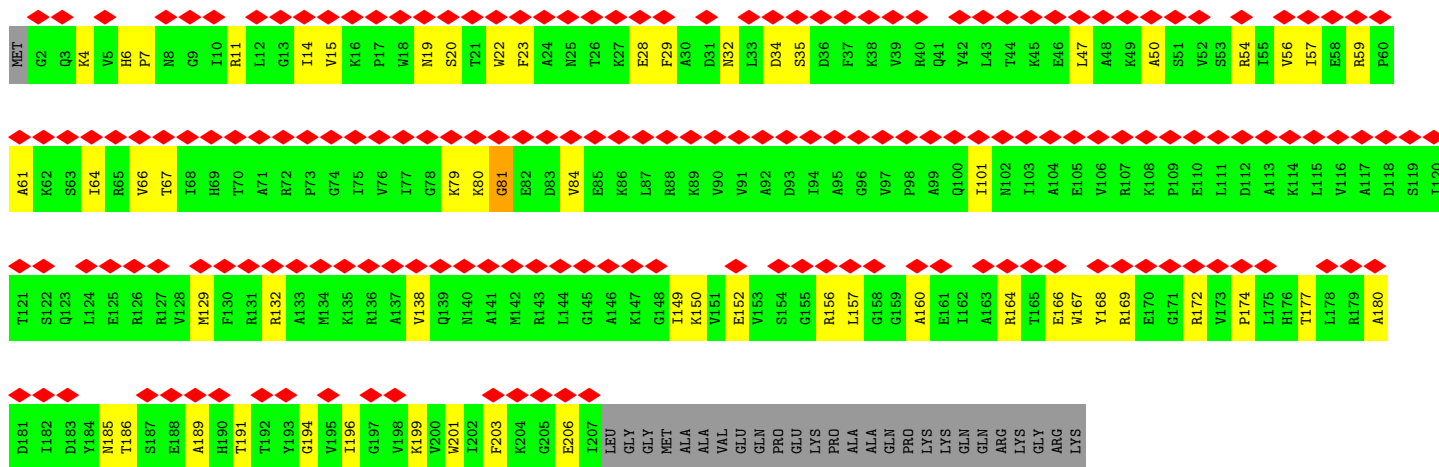
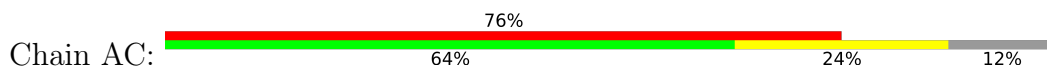
#### • Molecule 1: 16S ribosomal RNA



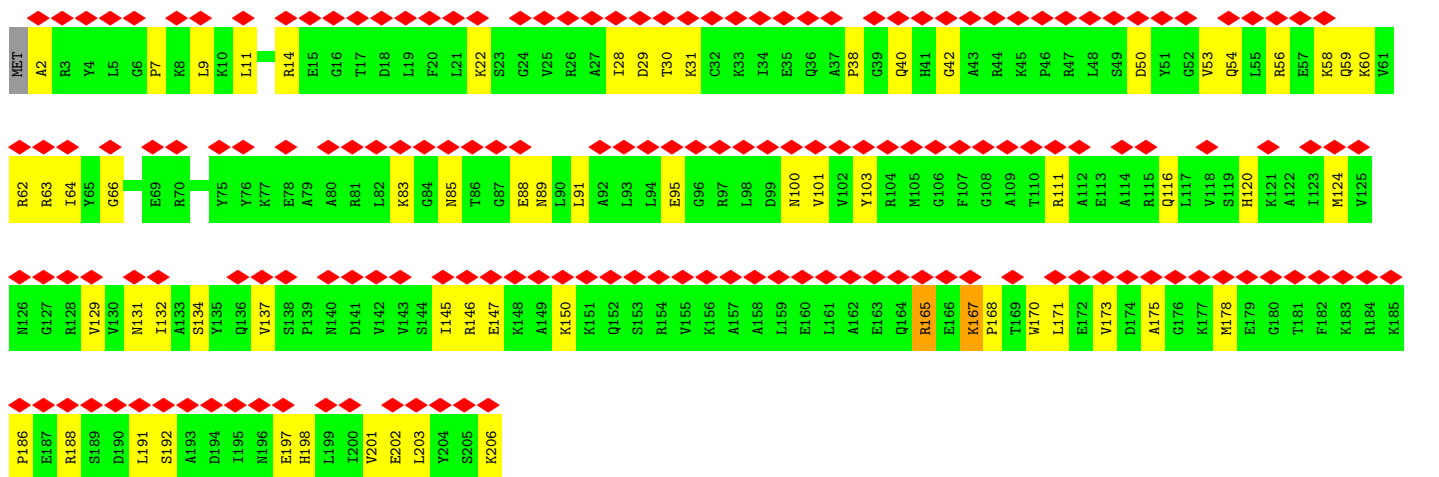
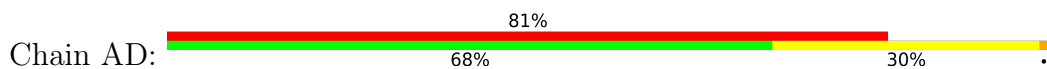




• Molecule 3: 30S ribosomal protein S3

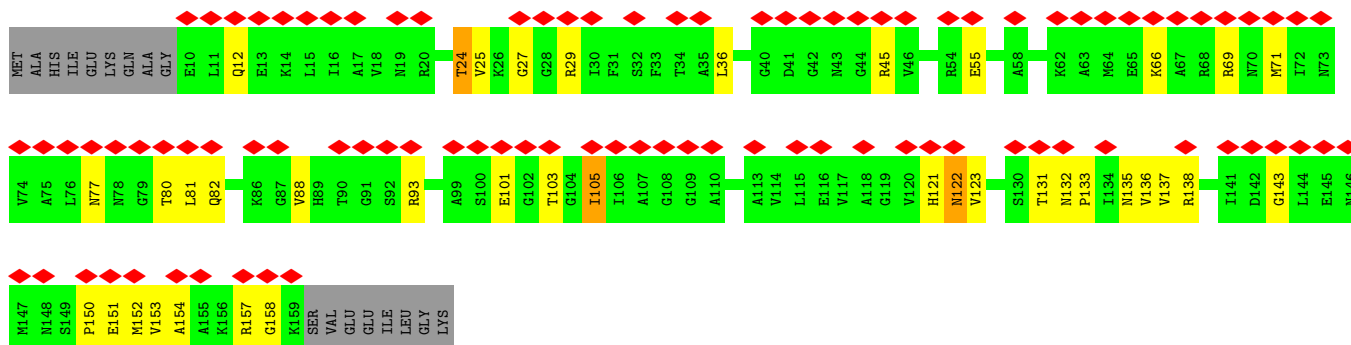


• Molecule 4: 30S ribosomal protein S4

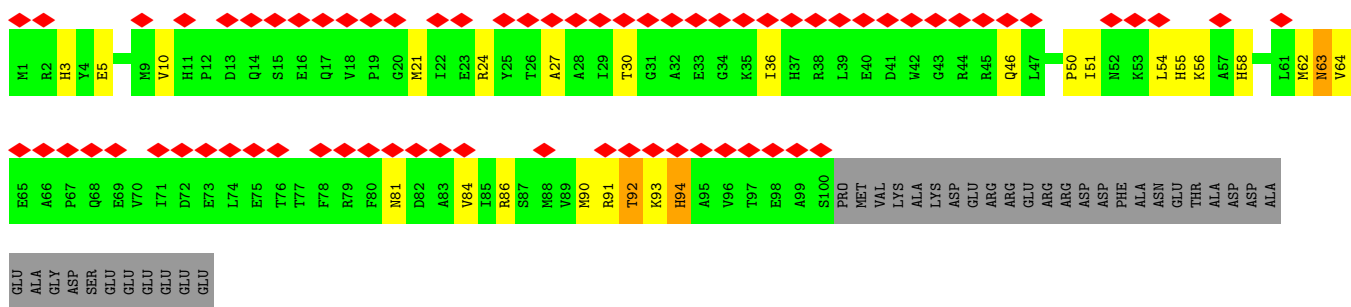


• Molecule 5: 30S ribosomal protein S5

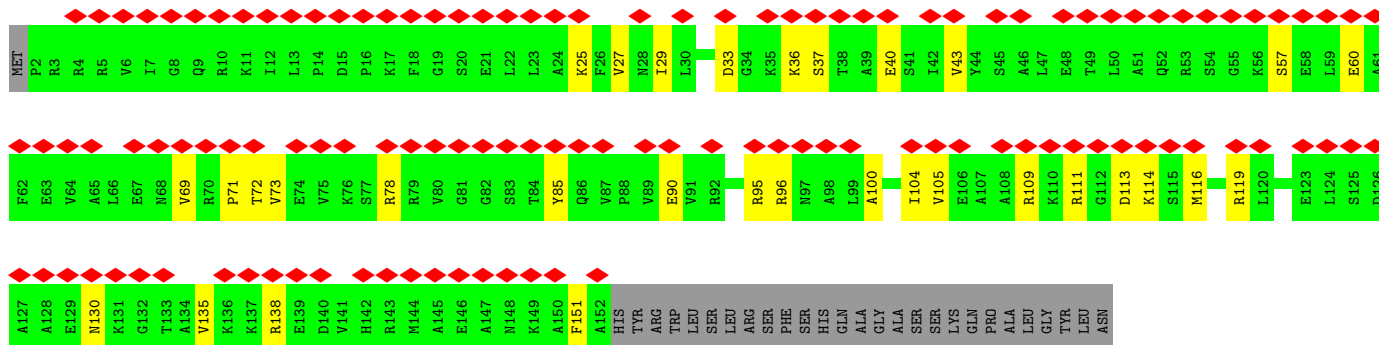




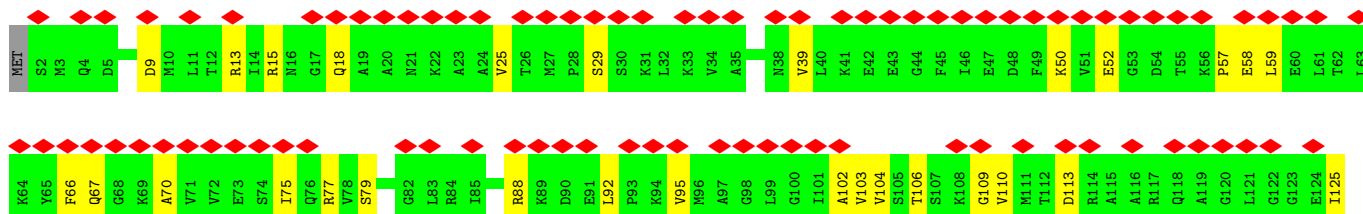
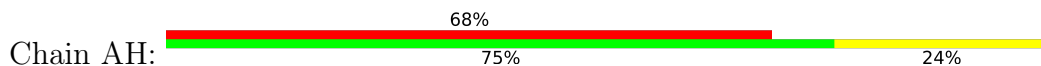
• Molecule 6: 30S ribosomal protein S6

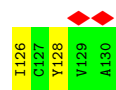


• Molecule 7: 30S ribosomal protein S7

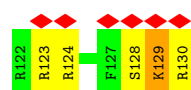
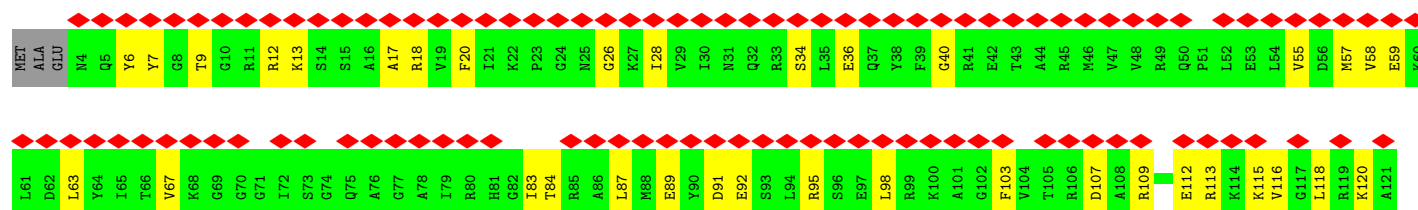
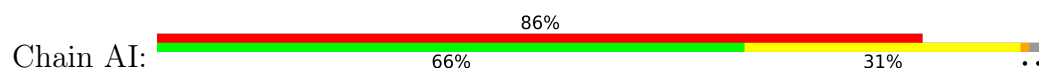


• Molecule 8: 30S ribosomal protein S8

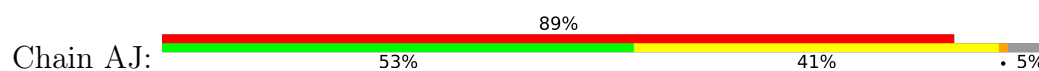




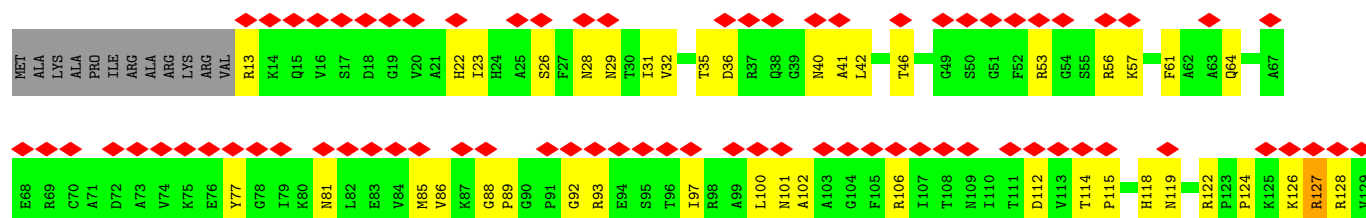
• Molecule 9: 30S ribosomal protein S9



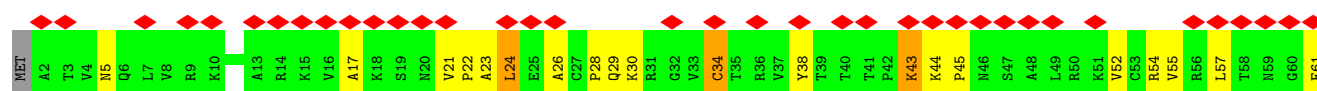
• Molecule 10: 30S ribosomal protein S10

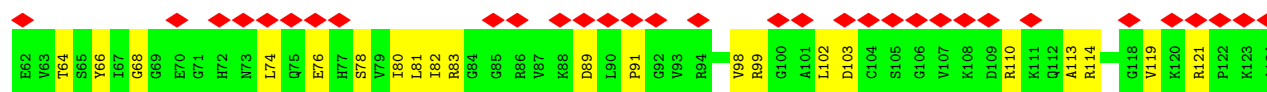


• Molecule 11: 30S ribosomal protein S11

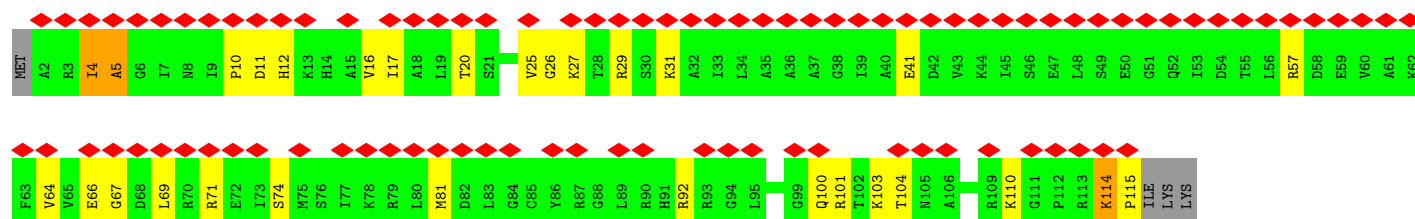
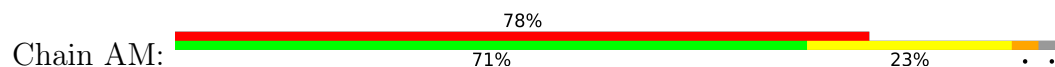


• Molecule 12: 30S ribosomal protein S12

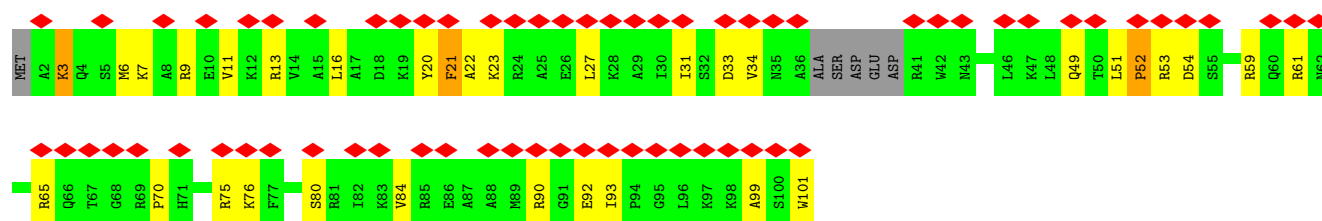




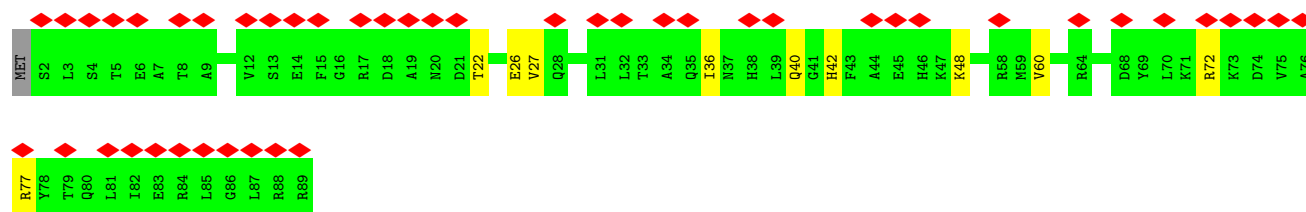
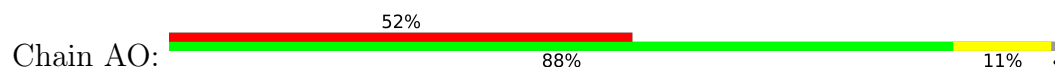
• Molecule 13: 30S ribosomal protein S13



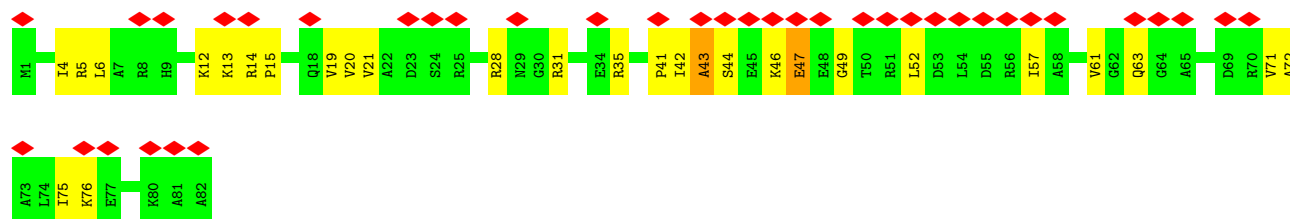
• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15

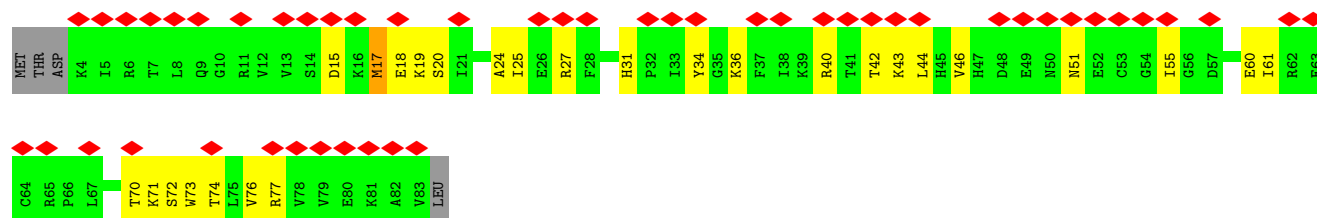


• Molecule 16: 30S ribosomal protein S16




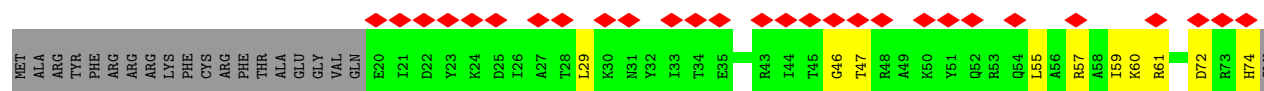
• Molecule 17: 30S ribosomal protein S17

Chain AQ: 



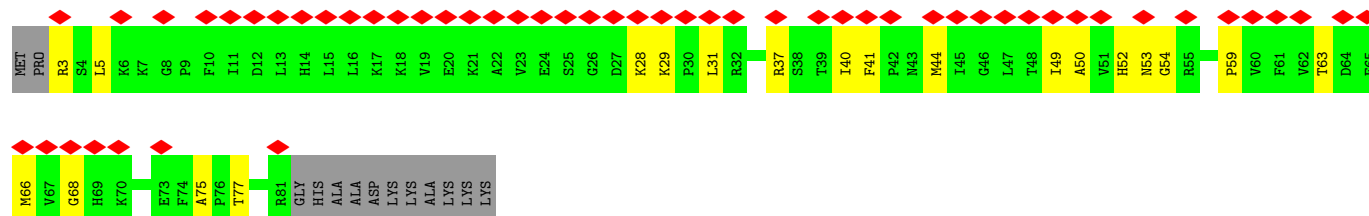
- Molecule 18: 30S ribosomal protein S18

Chain AR: 



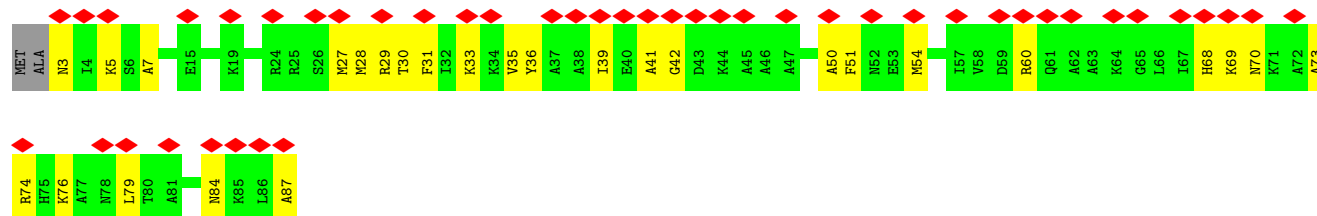
- Molecule 19: 30S ribosomal protein S19

Chain AS: 



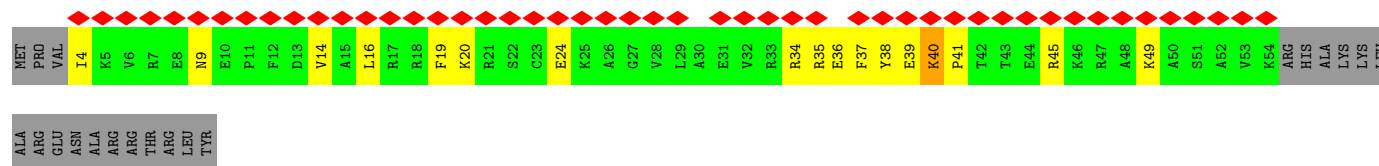
- Molecule 20: 30S ribosomal protein S20

Chain AT: 



- Molecule 21: 30S ribosomal protein S21

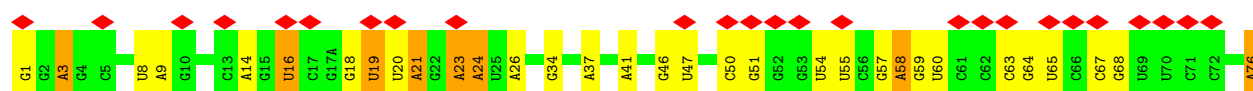
Chain AU: 



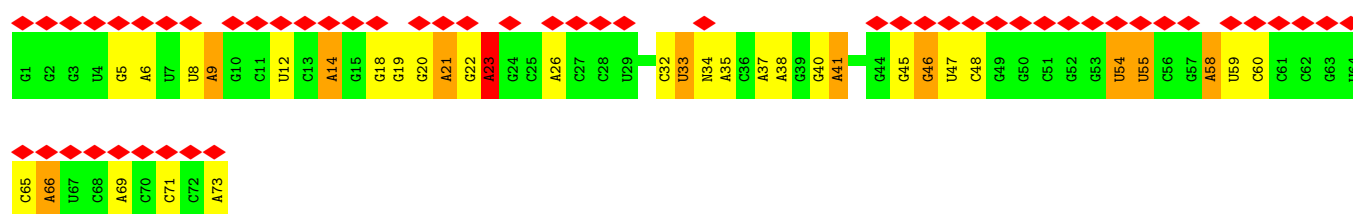
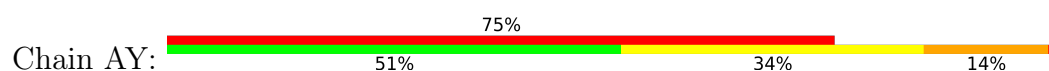
- Molecule 22: mRNA



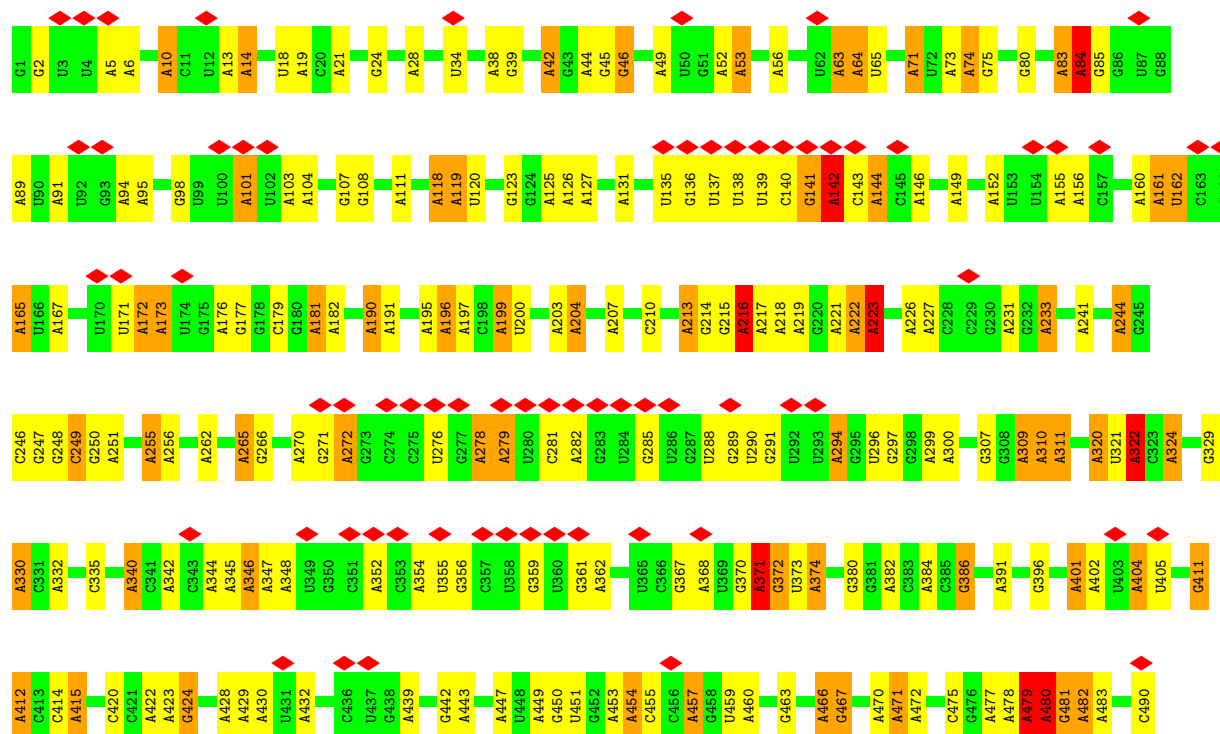
- Molecule 23: P-site tRNA Aspartate

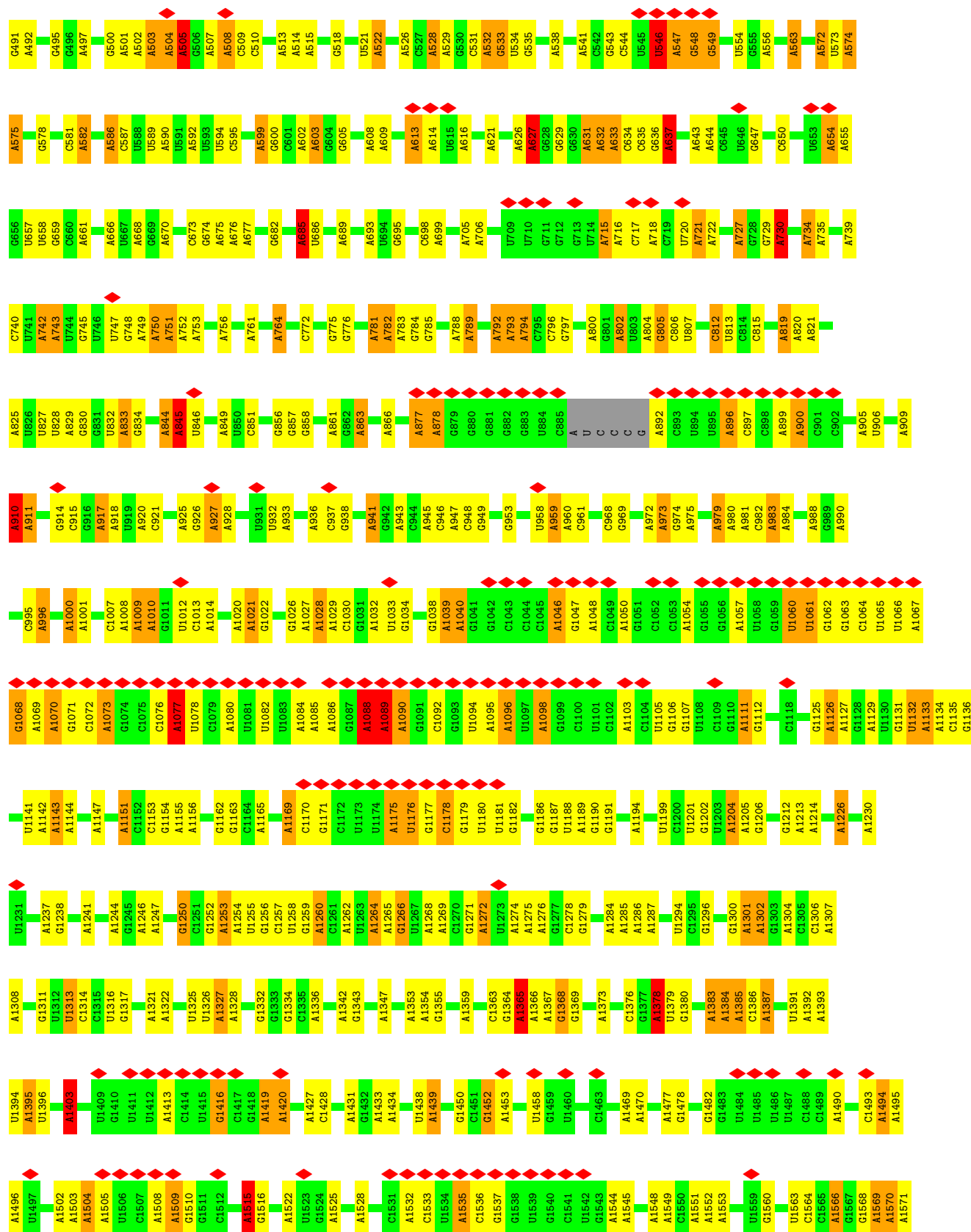


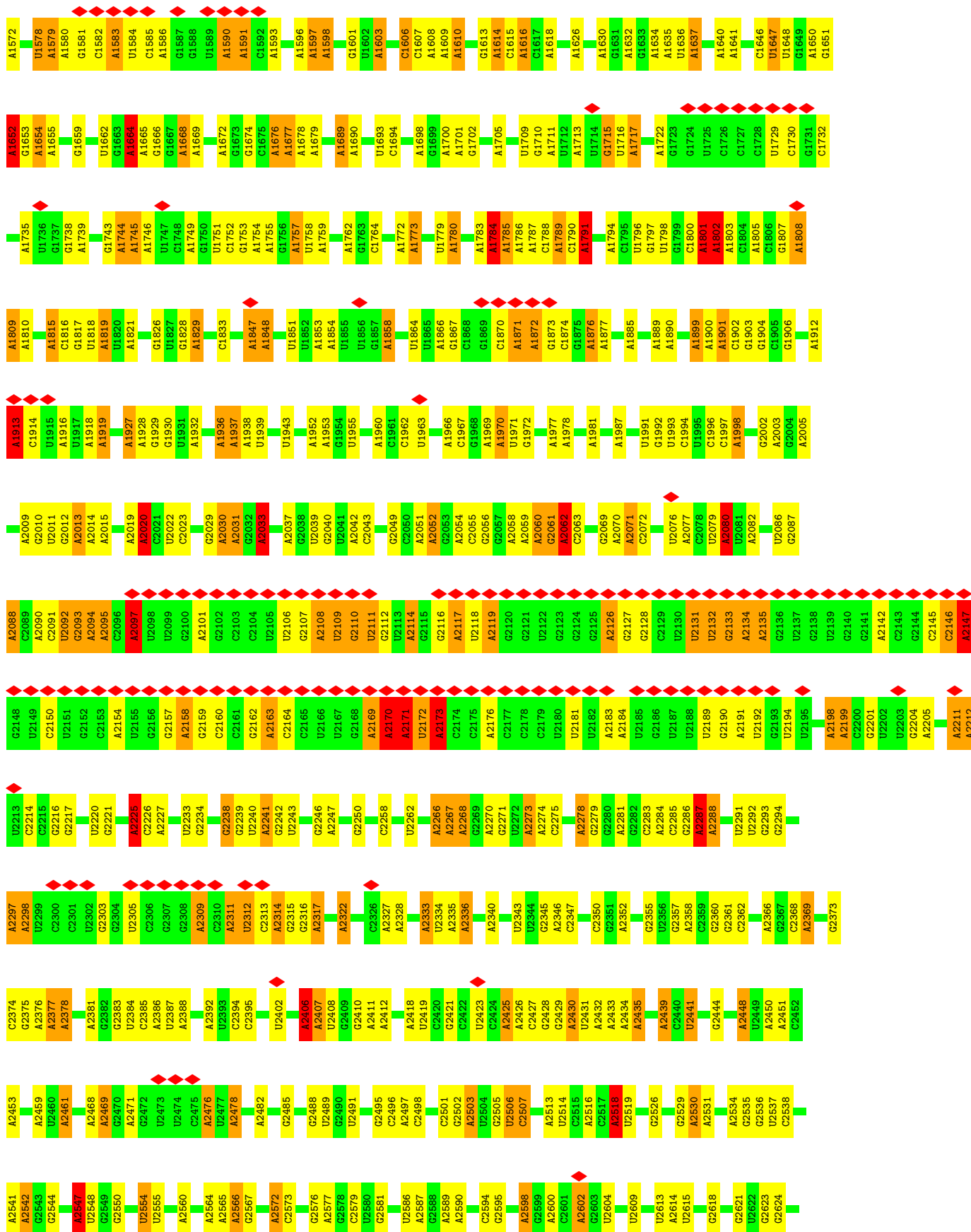
- Molecule 24: E-site tRNA Valine

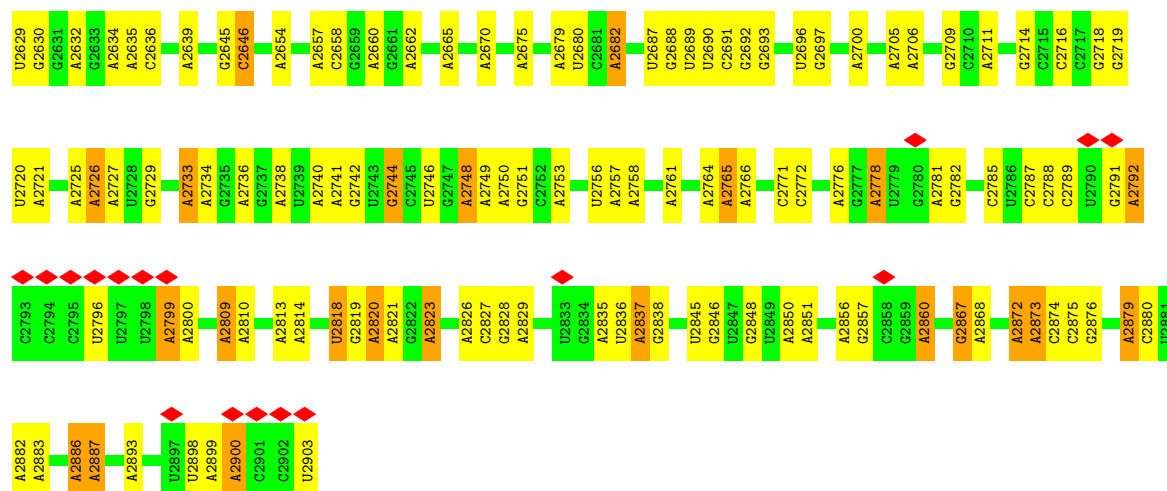


- Molecule 25: 23S ribosomal RNA

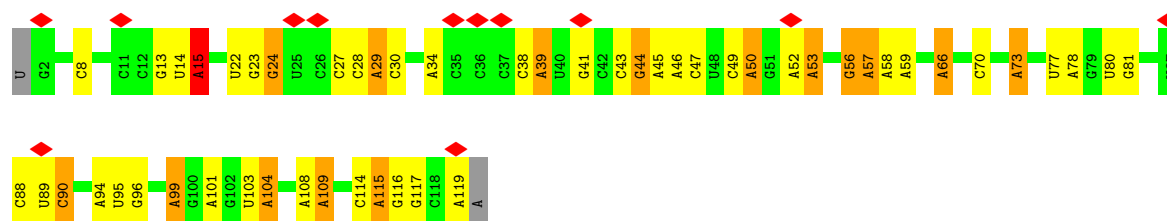




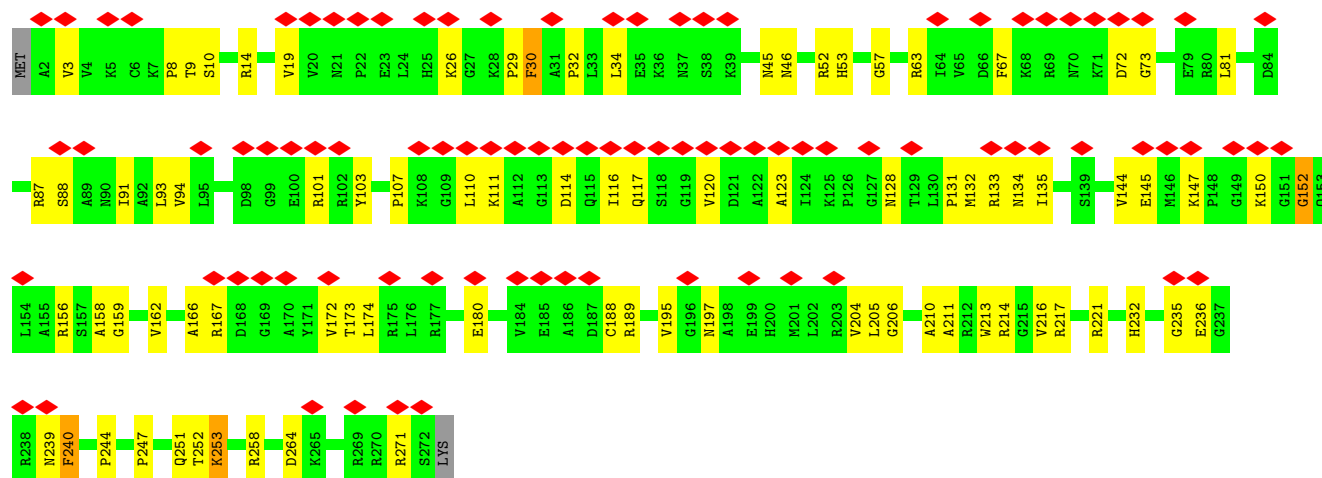




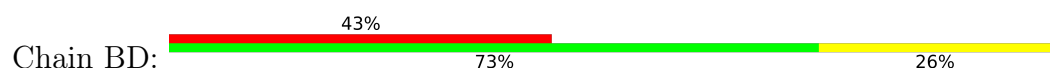
• Molecule 26: 5S ribosomal RNA

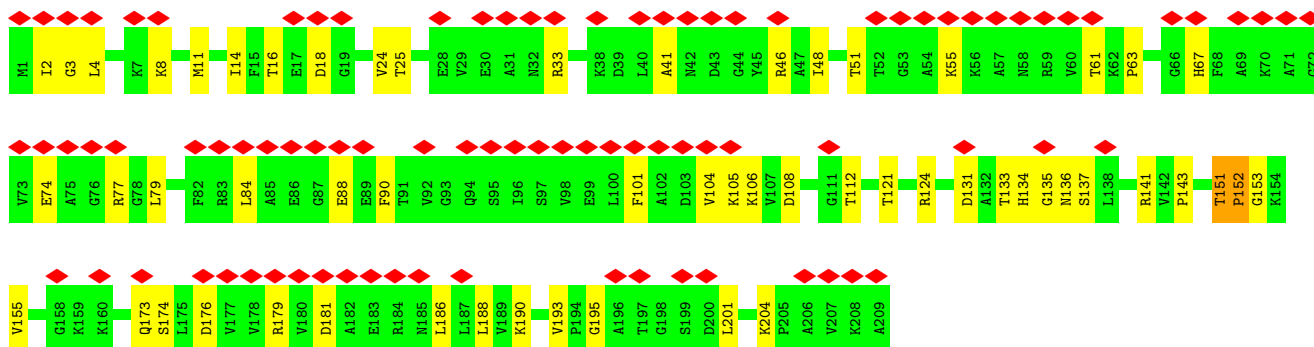


• Molecule 27: 50S ribosomal protein L2

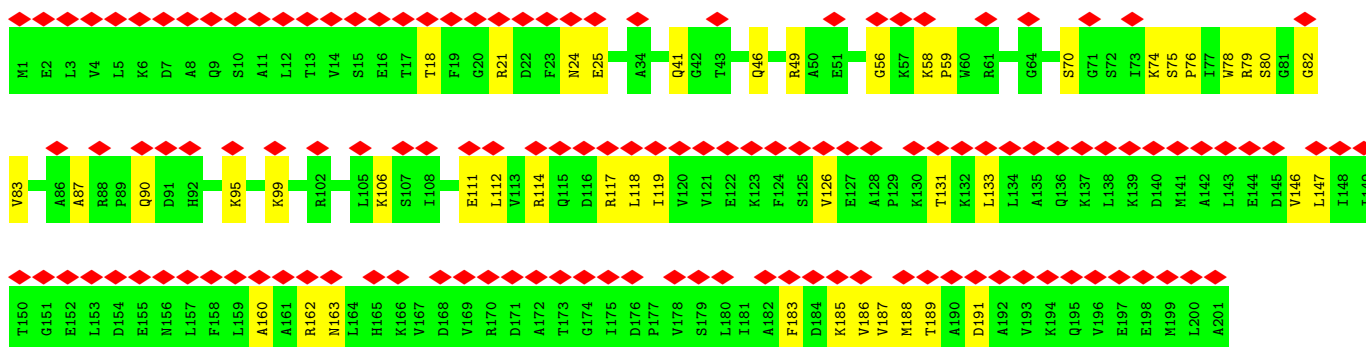
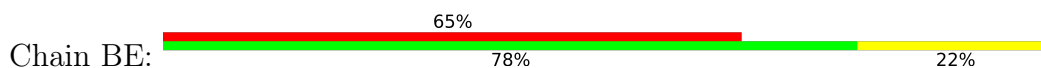


• Molecule 28: 50S ribosomal protein L3

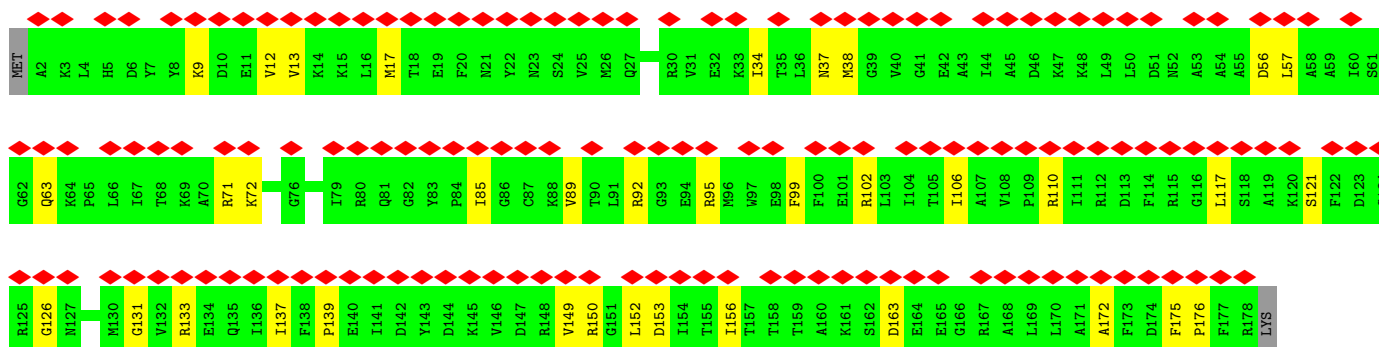
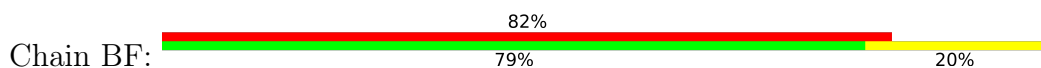




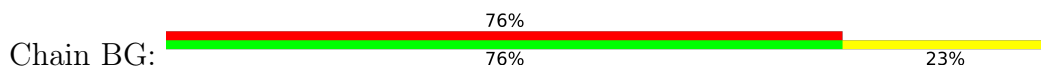
• Molecule 29: 50S ribosomal protein L4



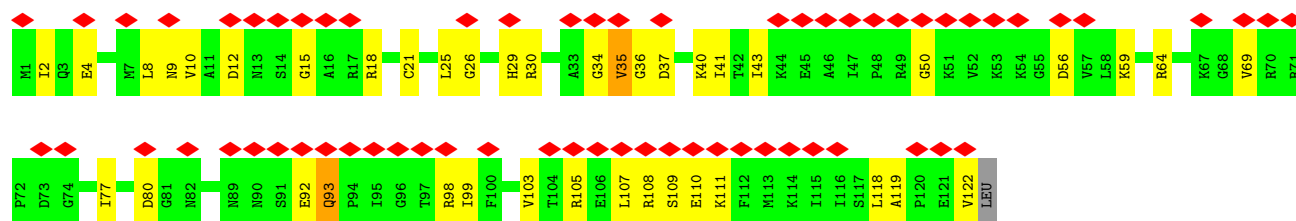
• Molecule 30: 50S ribosomal protein L5



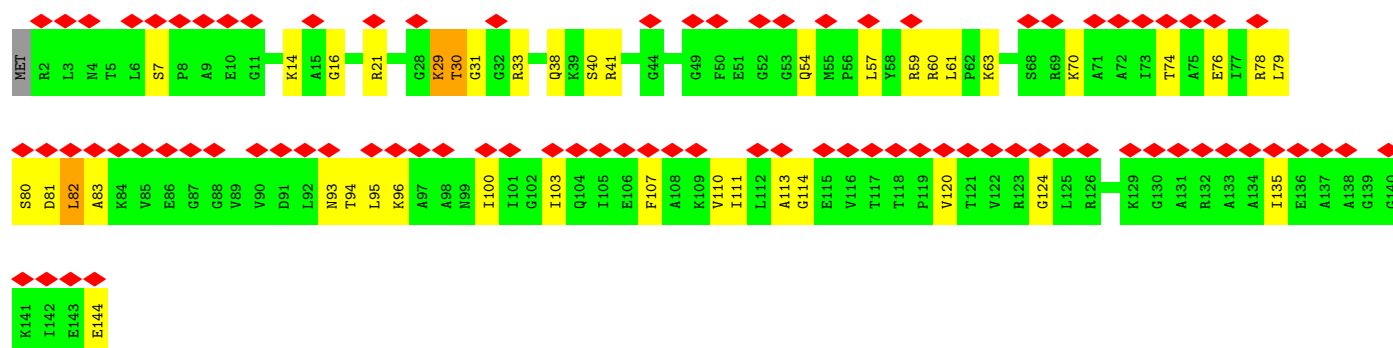
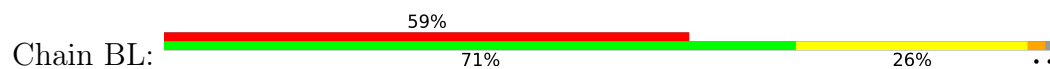
• Molecule 31: 50S ribosomal protein L6



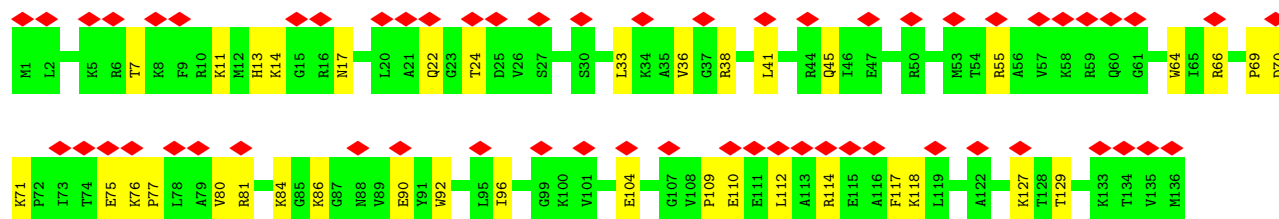
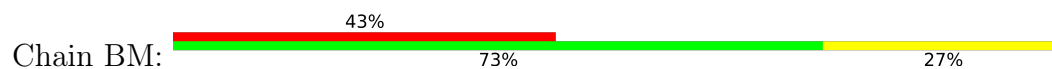




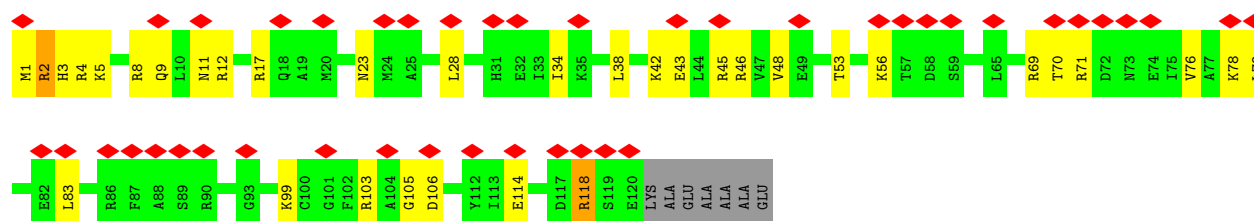
• Molecule 36: 50S ribosomal protein L15



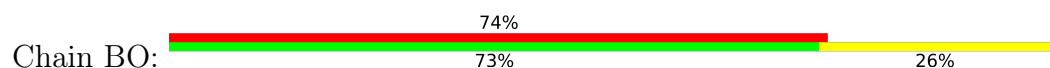
• Molecule 37: 50S ribosomal protein L16

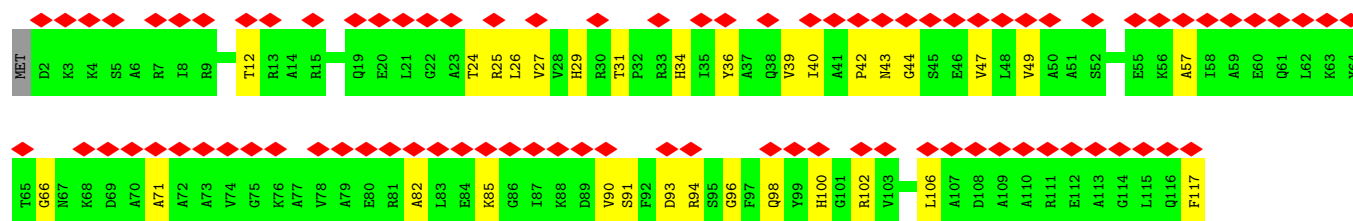


• Molecule 38: 50S ribosomal protein L17

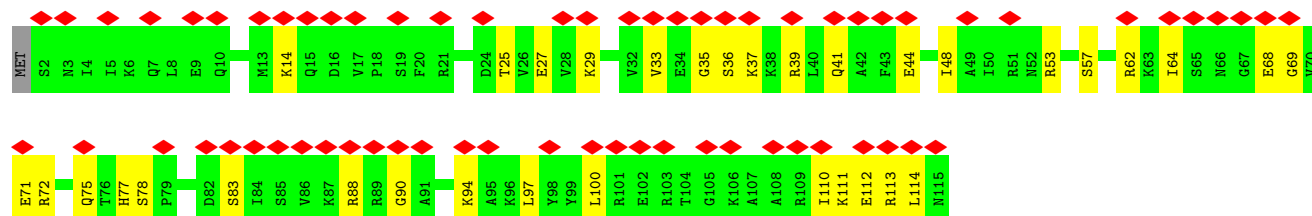


• Molecule 39: 50S ribosomal protein L18

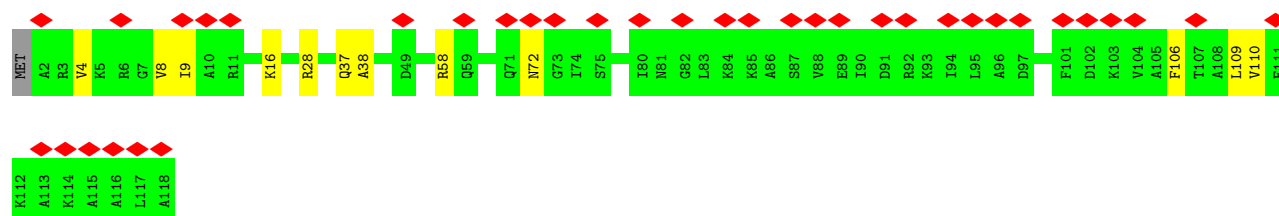
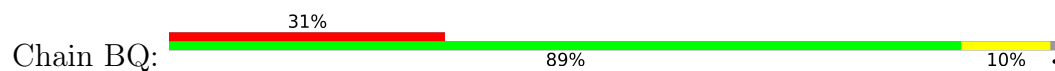


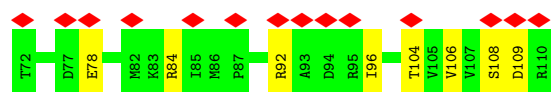


• Molecule 40: 50S ribosomal protein L19

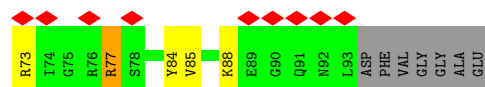
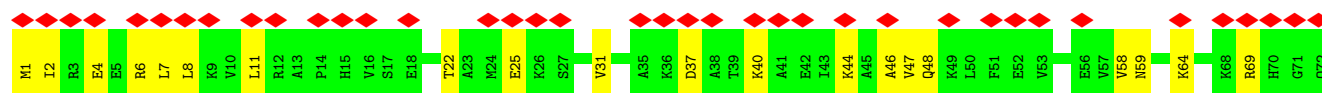


• Molecule 41: 50S ribosomal protein L20

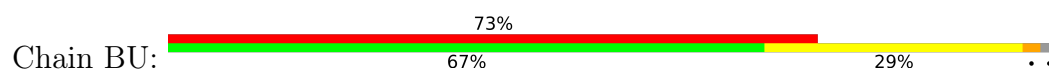




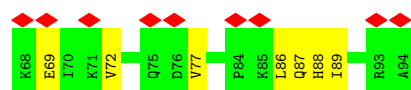
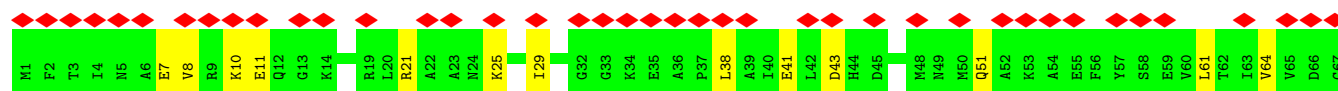
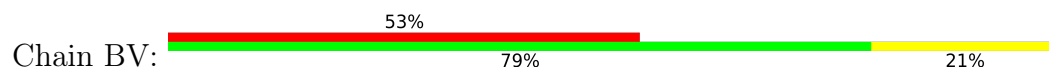
- Molecule 44: 50S ribosomal protein L23



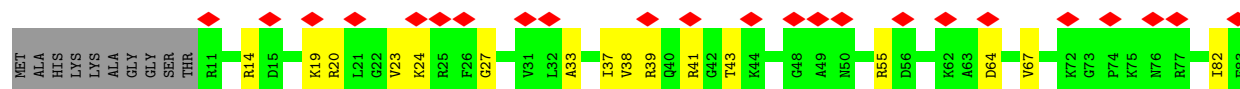
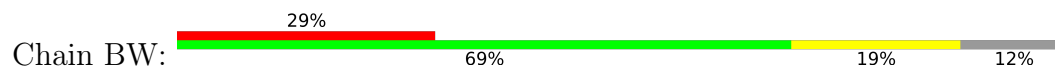
- Molecule 45: 50S ribosomal protein L24



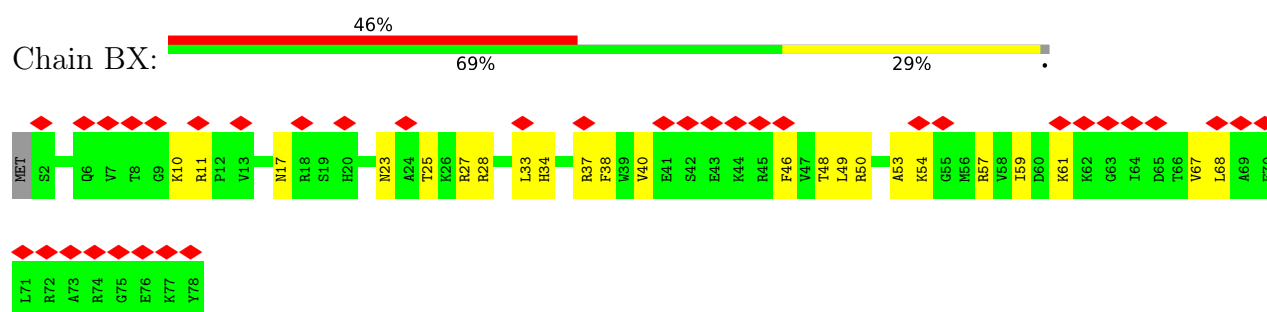
- Molecule 46: 50S ribosomal protein L25



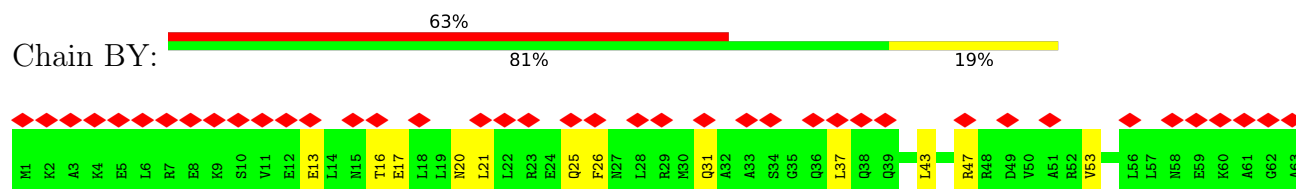
- Molecule 47: 50S ribosomal protein L27



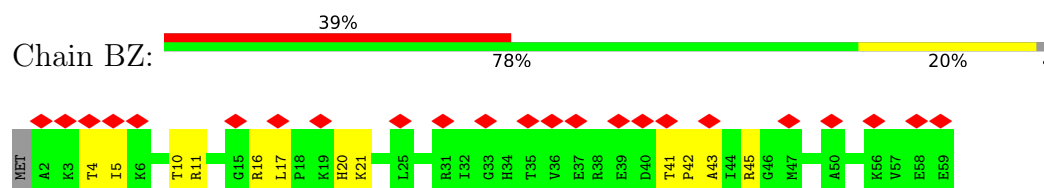
- Molecule 48: 50S ribosomal protein L28



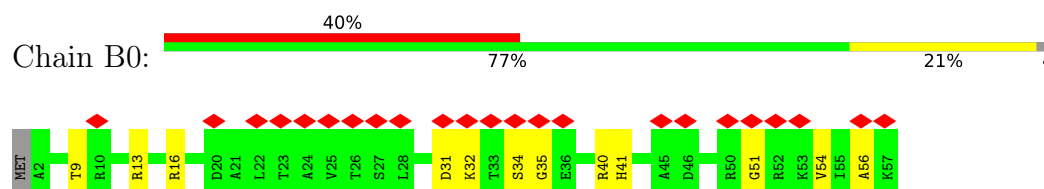
- Molecule 49: 50S ribosomal protein L29



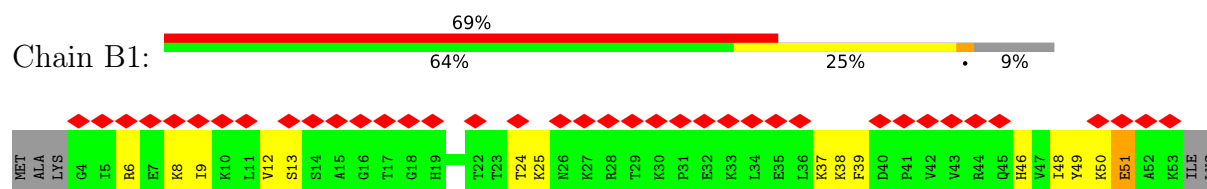
- Molecule 50: 50S ribosomal protein L30



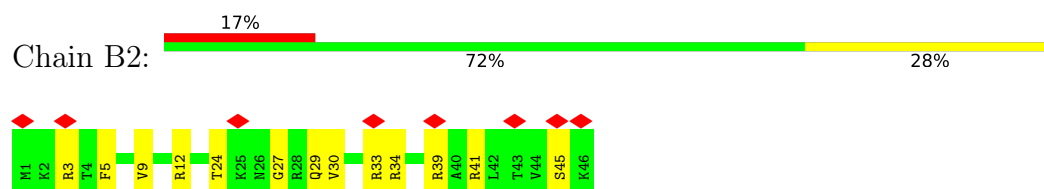
- Molecule 51: 50S ribosomal protein L32



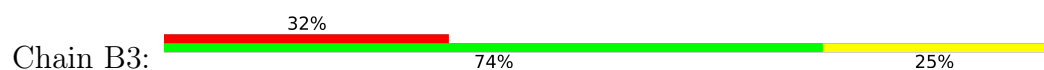
- Molecule 52: 50S ribosomal protein L33

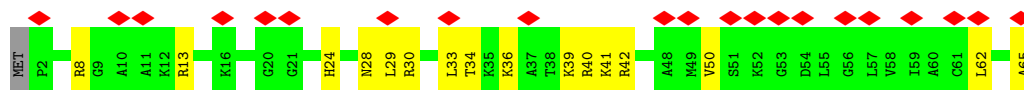


- Molecule 53: 50S ribosomal protein L34

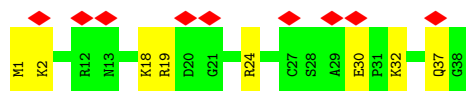
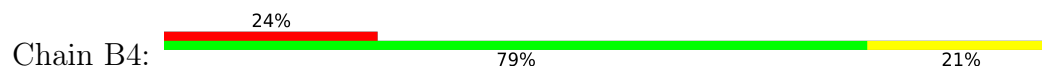


- Molecule 54: 50S ribosomal protein L35





- Molecule 55: 50S ribosomal protein L36



- Molecule 56: ErmBL



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	4	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.007	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00118	Depositor
Map size (Å)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ERY, 2MA, 4SU, H2U, 6MZ, QUO, CM0, PSU, 7MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	2.20	1359/36965 (3.7%)	3.38	4641/57662 (8.0%)
2	AB	0.31	0/1735	0.49	0/2338
3	AC	0.25	0/1651	0.44	0/2225
4	AD	0.27	0/1665	0.45	0/2227
5	AE	0.24	0/1118	0.47	0/1504
6	AF	0.26	0/835	0.46	0/1128
7	AG	0.25	0/1195	0.43	0/1602
8	AH	0.27	0/989	0.45	0/1326
9	AI	0.28	0/1034	0.49	0/1375
10	AJ	0.31	0/796	0.53	0/1077
11	AK	0.25	0/893	0.45	0/1205
12	AL	0.25	0/969	0.45	0/1300
13	AM	0.27	0/892	0.48	0/1193
14	AN	0.24	0/785	0.42	0/1043
15	AO	0.28	0/718	0.45	0/959
16	AP	0.26	0/659	0.44	0/884
17	AQ	0.27	0/657	0.49	0/881
18	AR	0.26	0/462	0.44	0/621
19	AS	0.26	0/652	0.43	0/877
20	AT	0.25	0/671	0.43	0/888
21	AU	0.25	0/430	0.50	0/570
22	AV	3.36	19/245 (7.8%)	5.14	72/380 (18.9%)
23	AX	1.72	36/1602 (2.2%)	2.65	120/2491 (4.8%)
24	AY	1.97	45/1554 (2.9%)	3.05	157/2416 (6.5%)
25	BA	2.25	2658/69659 (3.8%)	3.46	9149/108672 (8.4%)
26	BB	1.94	81/2828 (2.9%)	3.01	277/4410 (6.3%)
27	BC	0.26	0/2121	0.45	0/2852
28	BD	0.27	0/1586	0.46	0/2134
29	BE	0.28	0/1571	0.46	0/2113
30	BF	0.30	0/1434	0.47	0/1926
31	BG	0.27	0/1343	0.44	0/1816
32	BH	0.29	0/364	0.51	0/490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BI	0.28	0/1046	0.49	0/1410
34	BJ	0.27	0/1152	0.45	0/1551
35	BK	0.26	0/947	0.47	0/1268
36	BL	0.23	0/1054	0.44	0/1403
37	BM	0.26	0/1093	0.44	0/1460
38	BN	0.26	0/973	0.44	0/1301
39	BO	0.25	0/902	0.41	0/1209
40	BP	0.24	0/929	0.44	0/1242
41	BQ	0.25	0/960	0.39	0/1278
42	BR	0.25	0/829	0.43	0/1107
43	BS	0.30	0/864	0.48	0/1156
44	BT	0.24	0/744	0.44	0/994
45	BU	0.28	0/787	0.46	0/1051
46	BV	0.27	0/766	0.44	0/1025
47	BW	0.25	0/576	0.39	0/762
48	BX	0.23	0/635	0.40	0/848
49	BY	0.22	0/510	0.39	0/677
50	BZ	0.23	0/453	0.44	0/605
51	B0	0.27	0/450	0.44	0/599
52	B1	0.24	0/416	0.43	0/554
53	B2	0.20	0/380	0.36	0/498
54	B3	0.22	0/513	0.40	0/676
55	B4	0.23	0/303	0.39	0/397
56	B5	0.36	0/74	0.59	0/98
All	All	1.88	4198/157434 (2.7%)	2.96	14416/235754 (6.1%)

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
28	BD	0	1

The worst 5 of 4198 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	454	A	C6-N6	17.19	1.47	1.33
1	AA	860	A	C6-N6	17.14	1.47	1.33
1	AA	1227	A	C6-N6	17.12	1.47	1.33
1	AA	1155	A	C6-N6	17.08	1.47	1.33
25	BA	633	A	C6-N6	17.08	1.47	1.33

The worst 5 of 14416 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	983	A	C2-N3-C4	20.28	120.74	110.60
25	BA	278	A	C2-N3-C4	20.21	120.71	110.60
25	BA	2114	A	C2-N3-C4	20.09	120.64	110.60
25	BA	514	A	C2-N3-C4	19.98	120.59	110.60
25	BA	1669	A	C2-N3-C4	19.82	120.51	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BD	151	THR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33015	0	16618	245	0
2	AB	1704	0	1732	31	0
3	AC	1624	0	1696	36	0
4	AD	1643	0	1707	45	0
5	AE	1105	0	1148	24	0
6	AF	817	0	808	14	0
7	AG	1181	0	1238	22	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	23	0
10	AJ	786	0	828	32	0
11	AK	877	0	887	30	0
12	AL	955	0	1016	26	0
13	AM	883	0	941	20	0
14	AN	774	0	824	26	0
15	AO	710	0	728	8	0
16	AP	649	0	666	20	0
17	AQ	648	0	691	19	0
18	AR	455	0	478	8	0
19	AS	637	0	665	12	0
20	AT	665	0	714	21	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	AU	425	0	449	9	0
22	AV	218	0	109	2	0
23	AX	1656	0	855	6	0
24	AY	1525	0	780	7	0
25	BA	62195	0	31280	416	0
26	BB	2529	0	1281	24	0
27	BC	2082	0	2154	55	0
28	BD	1565	0	1616	42	0
29	BE	1552	0	1619	30	0
30	BF	1410	0	1444	21	0
31	BG	1323	0	1371	24	0
32	BH	359	0	381	11	0
33	BI	1032	0	1085	22	0
34	BJ	1129	0	1162	19	0
35	BK	938	0	1012	24	0
36	BL	1045	0	1117	28	0
37	BM	1074	0	1157	24	0
38	BN	960	0	1000	24	0
39	BO	892	0	923	19	0
40	BP	917	0	962	23	0
41	BQ	947	0	1019	10	0
42	BR	816	0	839	12	0
43	BS	857	0	922	17	0
44	BT	738	0	807	17	0
45	BU	779	0	831	23	0
46	BV	753	0	780	13	0
47	BW	569	0	581	14	0
48	BX	625	0	652	18	0
49	BY	509	0	543	8	0
50	BZ	449	0	488	7	0
51	B0	444	0	458	9	0
52	B1	409	0	440	11	0
53	B2	377	0	418	11	0
54	B3	504	0	572	14	0
55	B4	302	0	343	9	0
56	B5	74	0	74	8	0
57	BA	51	0	67	4	0
All	All	145158	0	97077	1425	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 6.

The worst 5 of 1425 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1493:A:H3'	25:BA:1913:A:N1	1.74	1.02
1:AA:1493:A:C3'	25:BA:1913:A:N1	2.26	0.98
1:AA:1409:C:O2	1:AA:1492:A:N6	2.00	0.95
1:AA:1493:A:O3'	25:BA:1913:A:N1	2.02	0.92
1:AA:1493:A:O2'	1:AA:1494:G:OP1	1.91	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/240 (90%)	190 (88%)	19 (9%)	7 (3%)	3	25
3	AC	204/233 (88%)	180 (88%)	18 (9%)	6 (3%)	3	27
4	AD	203/206 (98%)	187 (92%)	10 (5%)	6 (3%)	3	26
5	AE	148/167 (89%)	125 (84%)	16 (11%)	7 (5%)	2	18
6	AF	98/135 (73%)	85 (87%)	8 (8%)	5 (5%)	1	16
7	AG	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	19	53
8	AH	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	16	51
9	AI	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	2	17
10	AJ	96/103 (93%)	82 (85%)	8 (8%)	6 (6%)	1	13
11	AK	115/129 (89%)	98 (85%)	14 (12%)	3 (3%)	4	28
12	AL	121/124 (98%)	107 (88%)	7 (6%)	7 (6%)	1	14
13	AM	112/118 (95%)	104 (93%)	5 (4%)	3 (3%)	4	28
14	AN	92/102 (90%)	78 (85%)	9 (10%)	5 (5%)	1	15
15	AO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	AP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	4	29
17	AQ	78/84 (93%)	65 (83%)	10 (13%)	3 (4%)	2	22

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	AS	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	10	41
20	AT	83/87 (95%)	77 (93%)	3 (4%)	3 (4%)	3	23
21	AU	49/71 (69%)	37 (76%)	7 (14%)	5 (10%)	0	6
27	BC	269/273 (98%)	246 (91%)	17 (6%)	6 (2%)	5	32
28	BD	207/209 (99%)	190 (92%)	15 (7%)	2 (1%)	13	46
29	BE	199/201 (99%)	187 (94%)	10 (5%)	2 (1%)	13	46
30	BF	175/179 (98%)	156 (89%)	14 (8%)	5 (3%)	3	27
31	BG	174/177 (98%)	161 (92%)	10 (6%)	3 (2%)	7	37
32	BH	45/149 (30%)	34 (76%)	8 (18%)	3 (7%)	1	12
33	BI	139/142 (98%)	117 (84%)	14 (10%)	8 (6%)	1	14
34	BJ	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	19	53
35	BK	120/123 (98%)	105 (88%)	10 (8%)	5 (4%)	2	20
36	BL	141/144 (98%)	117 (83%)	17 (12%)	7 (5%)	1	17
37	BM	134/136 (98%)	125 (93%)	6 (4%)	3 (2%)	5	32
38	BN	118/127 (93%)	105 (89%)	8 (7%)	5 (4%)	2	20
39	BO	114/117 (97%)	104 (91%)	7 (6%)	3 (3%)	4	28
40	BP	112/115 (97%)	104 (93%)	6 (5%)	2 (2%)	7	35
41	BQ	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
42	BR	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	3	26
43	BS	108/110 (98%)	98 (91%)	8 (7%)	2 (2%)	6	35
44	BT	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5	32
45	BU	100/104 (96%)	83 (83%)	12 (12%)	5 (5%)	1	17
46	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
47	BW	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
48	BX	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
49	BY	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
50	BZ	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	7	35
51	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
52	B1	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	5	33
53	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	B4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
56	B5	7/9 (78%)	2 (29%)	4 (57%)	1 (14%)	0	3
All	All	5522/5994 (92%)	4969 (90%)	405 (7%)	148 (3%)	6	28

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	105	ILE
9	AI	55	VAL
11	AK	127	ARG
17	AQ	17	MET
17	AQ	51	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/198 (91%)	180 (100%)	0	100	100
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	113/126 (90%)	113 (100%)	0	100	100
6	AF	87/116 (75%)	87 (100%)	0	100	100
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	105 (100%)	0	100	100
10	AJ	86/90 (96%)	86 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	103/104 (99%)	103 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	75/77 (97%)	75 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	70/79 (89%)	70 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	44/61 (72%)	44 (100%)	0	100	100
27	BC	216/218 (99%)	216 (100%)	0	100	100
28	BD	164/164 (100%)	164 (100%)	0	100	100
29	BE	165/165 (100%)	165 (100%)	0	100	100
30	BF	148/150 (99%)	148 (100%)	0	100	100
31	BG	137/138 (99%)	137 (100%)	0	100	100
32	BH	38/114 (33%)	38 (100%)	0	100	100
33	BI	109/110 (99%)	109 (100%)	0	100	100
34	BJ	116/116 (100%)	116 (100%)	0	100	100
35	BK	103/104 (99%)	103 (100%)	0	100	100
36	BL	102/103 (99%)	102 (100%)	0	100	100
37	BM	109/109 (100%)	109 (100%)	0	100	100
38	BN	100/103 (97%)	100 (100%)	0	100	100
39	BO	86/87 (99%)	86 (100%)	0	100	100
40	BP	99/100 (99%)	99 (100%)	0	100	100
41	BQ	89/90 (99%)	89 (100%)	0	100	100
42	BR	84/84 (100%)	84 (100%)	0	100	100
43	BS	93/93 (100%)	93 (100%)	0	100	100
44	BT	80/84 (95%)	80 (100%)	0	100	100
45	BU	83/85 (98%)	83 (100%)	0	100	100
46	BV	78/78 (100%)	78 (100%)	0	100	100
47	BW	56/63 (89%)	56 (100%)	0	100	100
48	BX	67/68 (98%)	67 (100%)	0	100	100
49	BY	55/55 (100%)	55 (100%)	0	100	100
50	BZ	48/49 (98%)	48 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	B0	47/48 (98%)	47 (100%)	0	100	100
52	B1	45/49 (92%)	45 (100%)	0	100	100
53	B2	38/38 (100%)	38 (100%)	0	100	100
54	B3	51/52 (98%)	51 (100%)	0	100	100
55	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	8/8 (100%)	8 (100%)	0	100	100
All	All	4594/4885 (94%)	4594 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
29	BE	163	ASN
36	BL	54	GLN
49	BY	27	ASN
30	BF	63	GLN
33	BI	12	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	220 (14%)	6 (0%)
22	AV	9/10 (90%)	0	0
23	AX	74/77 (96%)	7 (9%)	0
24	AY	67/71 (94%)	13 (19%)	1 (1%)
25	BA	2895/2903 (99%)	428 (14%)	8 (0%)
26	BB	117/120 (97%)	13 (11%)	0
All	All	4699/4720 (99%)	681 (14%)	15 (0%)

5 of 681 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	32	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	271	G
25	BA	2225	A
25	BA	404	A
25	BA	2506	U
25	BA	2109	U

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

16 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
23	4SU	AX	8	23	18,21,22	1.08	2 (11%)	26,30,33	0.83	2 (7%)
23	H2U	AX	16	23	18,21,22	1.02	2 (11%)	21,30,33	1.00	2 (9%)
24	CM0	AY	34	24	22,26,27	0.98	1 (4%)	28,37,40	1.24	3 (10%)
24	PSU	AY	55	24	18,21,22	1.29	3 (16%)	22,30,33	1.60	3 (13%)
23	5MU	AX	54	23	19,22,23	0.92	2 (10%)	28,32,35	1.14	2 (7%)
23	H2U	AX	19	23	18,21,22	1.00	2 (11%)	21,30,33	1.00	2 (9%)
23	PSU	AX	55	23	18,21,22	1.30	3 (16%)	22,30,33	1.63	4 (18%)
23	2MA	AX	37	23	17,25,26	0.94	1 (5%)	17,37,40	0.92	1 (5%)
23	PSU	AX	65	23	18,21,22	1.26	3 (16%)	22,30,33	1.53	5 (22%)
24	6MZ	AY	37	24	18,25,26	1.27	3 (16%)	16,36,39	0.86	0
23	H2U	AX	20	23	18,21,22	1.04	2 (11%)	21,30,33	0.99	2 (9%)
23	QUO	AX	34	23,22	29,35,36	1.33	3 (10%)	31,52,55	1.45	7 (22%)
24	5MU	AY	54	24	19,22,23	0.95	2 (10%)	28,32,35	1.14	2 (7%)
23	7MG	AX	46	23	22,26,27	2.03	3 (13%)	29,39,42	1.21	4 (13%)
24	7MG	AY	46	24	22,26,27	2.04	3 (13%)	29,39,42	1.23	4 (13%)
24	4SU	AY	8	24	18,21,22	1.08	2 (11%)	26,30,33	0.83	2 (7%)

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
23	4SU	AX	8	23	-	0/7/25/26	0/2/2/2
23	H2U	AX	16	23	-	3/7/38/39	0/2/2/2
24	CM0	AY	34	24	-	3/12/30/31	0/2/2/2
24	PSU	AY	55	24	-	0/7/25/26	0/2/2/2
23	5MU	AX	54	23	-	0/7/25/26	0/2/2/2
23	H2U	AX	19	23	-	6/7/38/39	0/2/2/2
23	PSU	AX	55	23	-	0/7/25/26	0/2/2/2
23	2MA	AX	37	23	-	0/3/25/26	0/3/3/3
23	PSU	AX	65	23	-	4/7/25/26	0/2/2/2
24	6MZ	AY	37	24	-	1/5/27/28	0/3/3/3
23	H2U	AX	20	23	-	0/7/38/39	0/2/2/2
23	QUO	AX	34	23,22	-	2/6/43/44	0/4/4/4
24	5MU	AY	54	24	-	2/7/25/26	0/2/2/2
23	7MG	AX	46	23	-	0/7/37/38	0/3/3/3
24	7MG	AY	46	24	-	3/7/37/38	0/3/3/3
24	4SU	AY	8	24	-	0/7/25/26	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	6.22	1.49	1.46
23	AX	46	7MG	C8-N9	6.20	1.49	1.46
24	AY	46	7MG	C5-N7	5.72	1.42	1.35
23	AX	46	7MG	C5-N7	5.69	1.42	1.35
23	AX	34	QUO	C6-N1	3.99	1.43	1.37

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AX	55	PSU	C6-C5-C4	5.07	121.74	118.20
24	AY	55	PSU	C6-C5-C4	4.92	121.64	118.20
23	AX	65	PSU	C6-C5-C4	3.99	120.98	118.20
24	AY	34	CM0	C7-O5-C5	-3.88	112.49	117.58
23	AX	34	QUO	O6-C6-N1	-3.44	116.58	120.65

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AX	19	H2U	O4'-C4'-C5'-O5'
23	AX	19	H2U	O4'-C1'-N1-C6
23	AX	19	H2U	C2'-C1'-N1-C6
23	AX	34	QUO	C16-C12-N11-C10
23	AX	65	PSU	C2'-C1'-C5-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AX	16	H2U	1	0
24	AY	55	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand 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
57	ERY	BA	9000	-	53,53,53	1.14	4 (7%)	82,82,82	1.67	22 (26%)

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
57	ERY	BA	9000	-	-	15/72/107/107	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	9000	ERY	O13-C12	-2.82	1.39	1.44
57	BA	9000	ERY	O10-C6	-2.64	1.40	1.44
57	BA	9000	ERY	O9-C26	-2.52	1.39	1.44
57	BA	9000	ERY	O2-C13	-2.52	1.42	1.46

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	9000	ERY	C36-C13-C12	-3.88	107.85	115.20
57	BA	9000	ERY	C34-C10-C11	-3.87	109.56	114.38
57	BA	9000	ERY	C12-C11-C10	-3.41	112.15	116.43
57	BA	9000	ERY	O13-C12-C13	3.32	112.62	107.28
57	BA	9000	ERY	O2-C1-C2	3.28	118.76	111.56

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

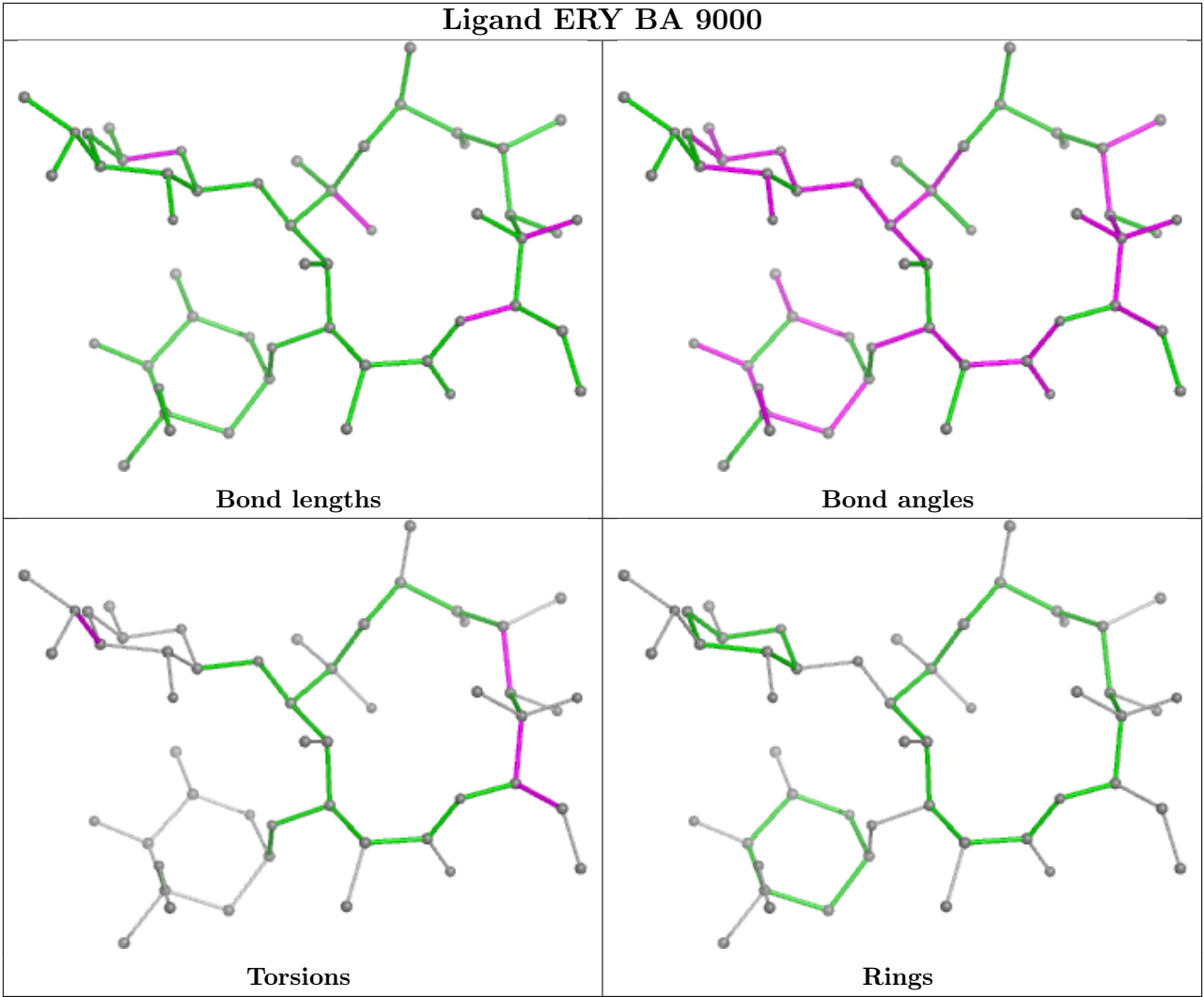
Mol	Chain	Res	Type	Atoms
57	BA	9000	ERY	C9-C10-C11-C12
57	BA	9000	ERY	C34-C10-C11-C12
57	BA	9000	ERY	C34-C10-C11-O12
57	BA	9000	ERY	C35-C12-C13-O2
57	BA	9000	ERY	O13-C12-C13-O2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	9000	ERY	4	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	AY	1
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AY	15:G	O3'	18:G	P	6.79

Continued on next page...

*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	99:C	O3'	100:G	P	3.18

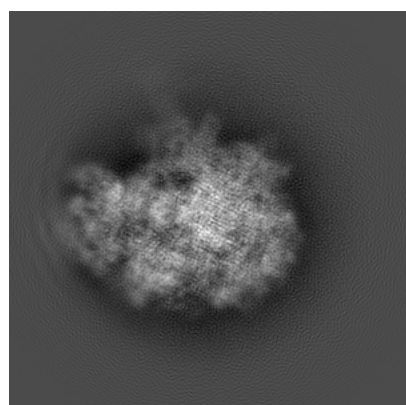
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8176. These allow visual inspection of the internal detail of the map and identification of artifacts.

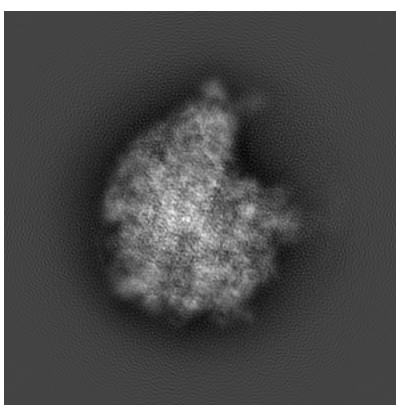
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

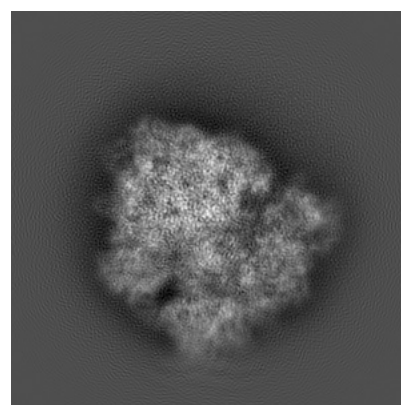
#### 6.1.1 Primary map



X



Y

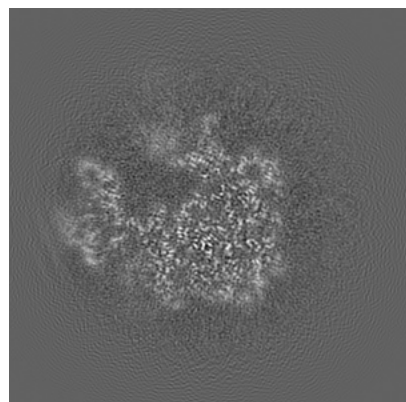


Z

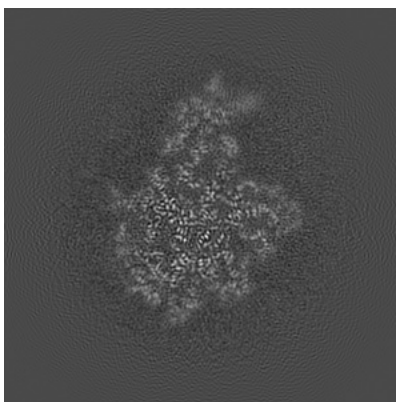
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

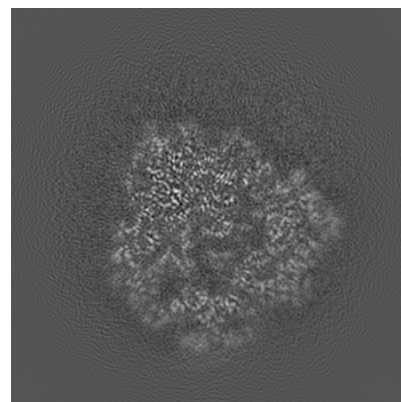
#### 6.2.1 Primary map



X Index: 184



Y Index: 184

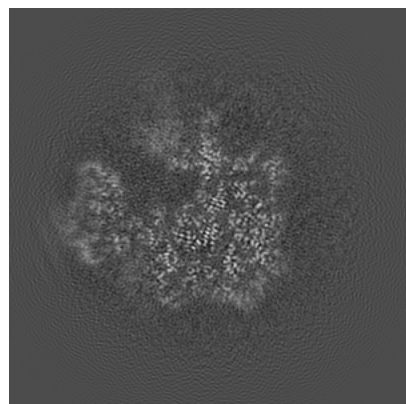


Z Index: 184

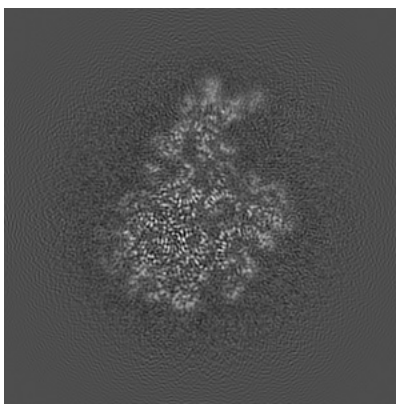
The images above show central slices of the map in three orthogonal directions.

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

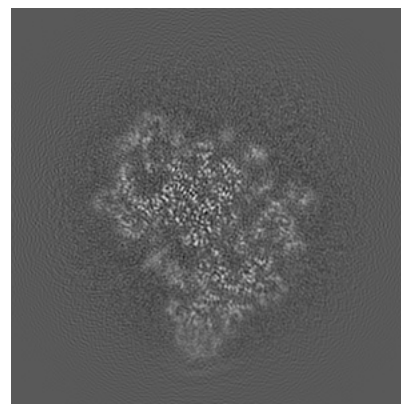
### 6.3.1 Primary map



X Index: 181



Y Index: 176

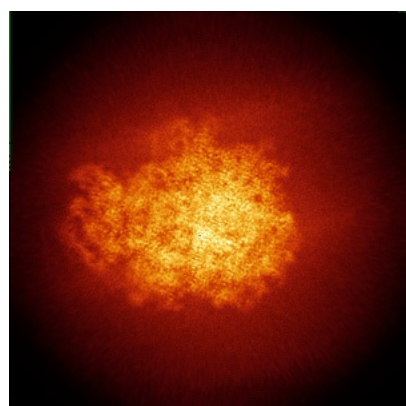


Z Index: 156

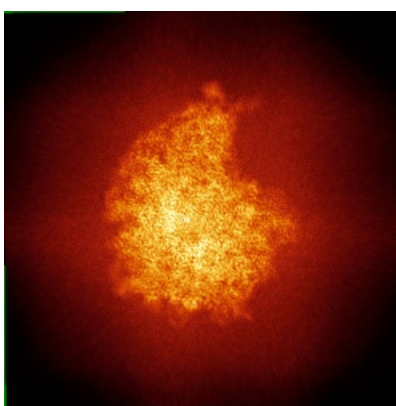
The images above show the largest variance slices of the map in three orthogonal directions.

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

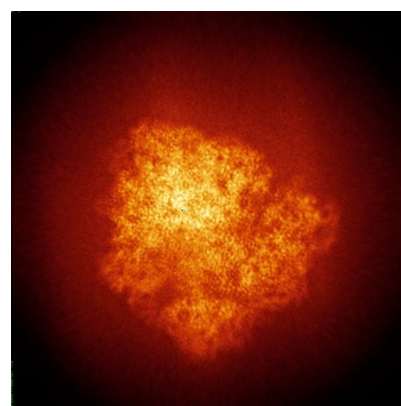
### 6.4.1 Primary map



X



Y



Z

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

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

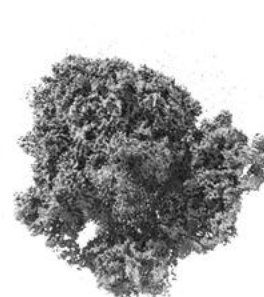
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

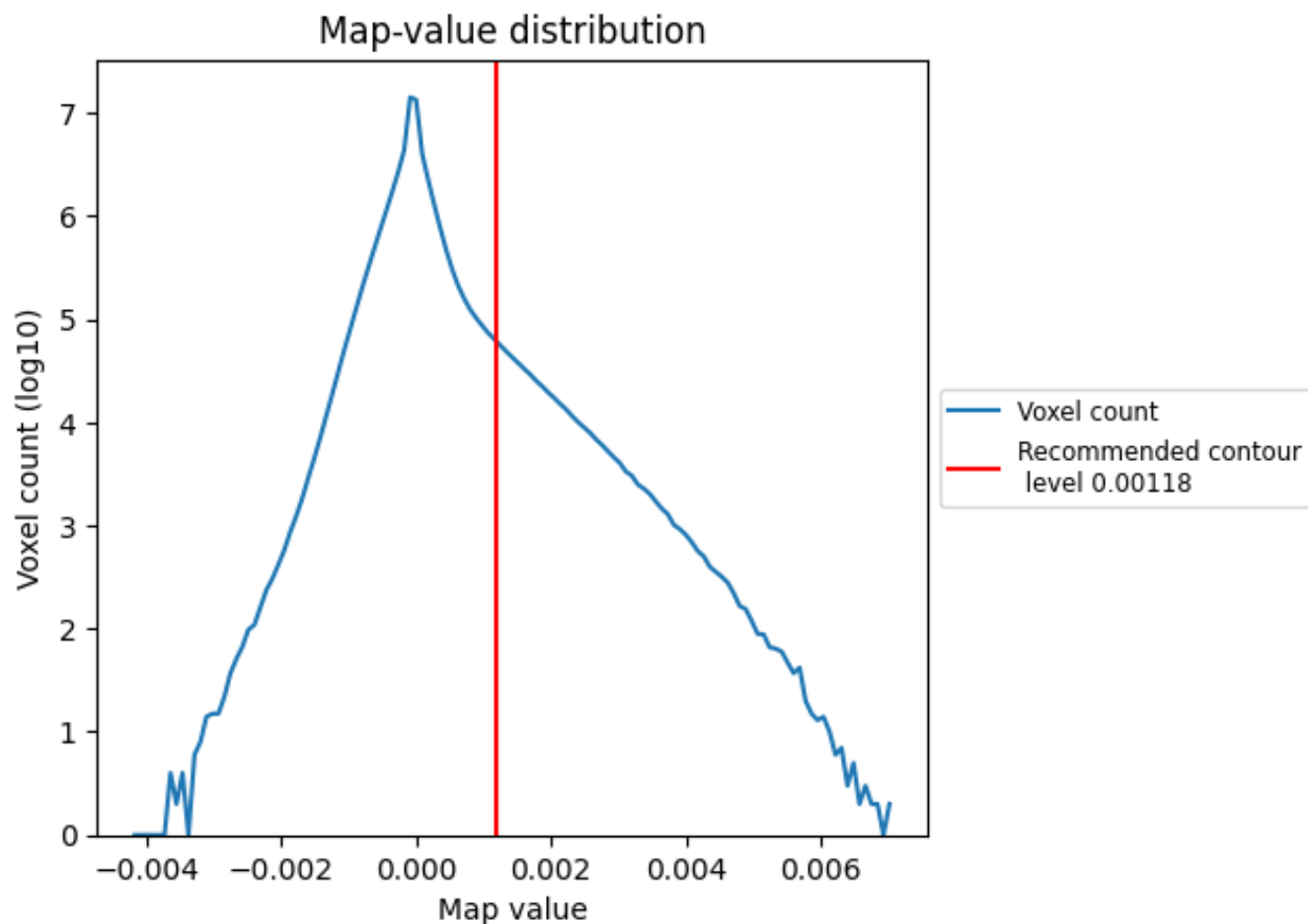
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

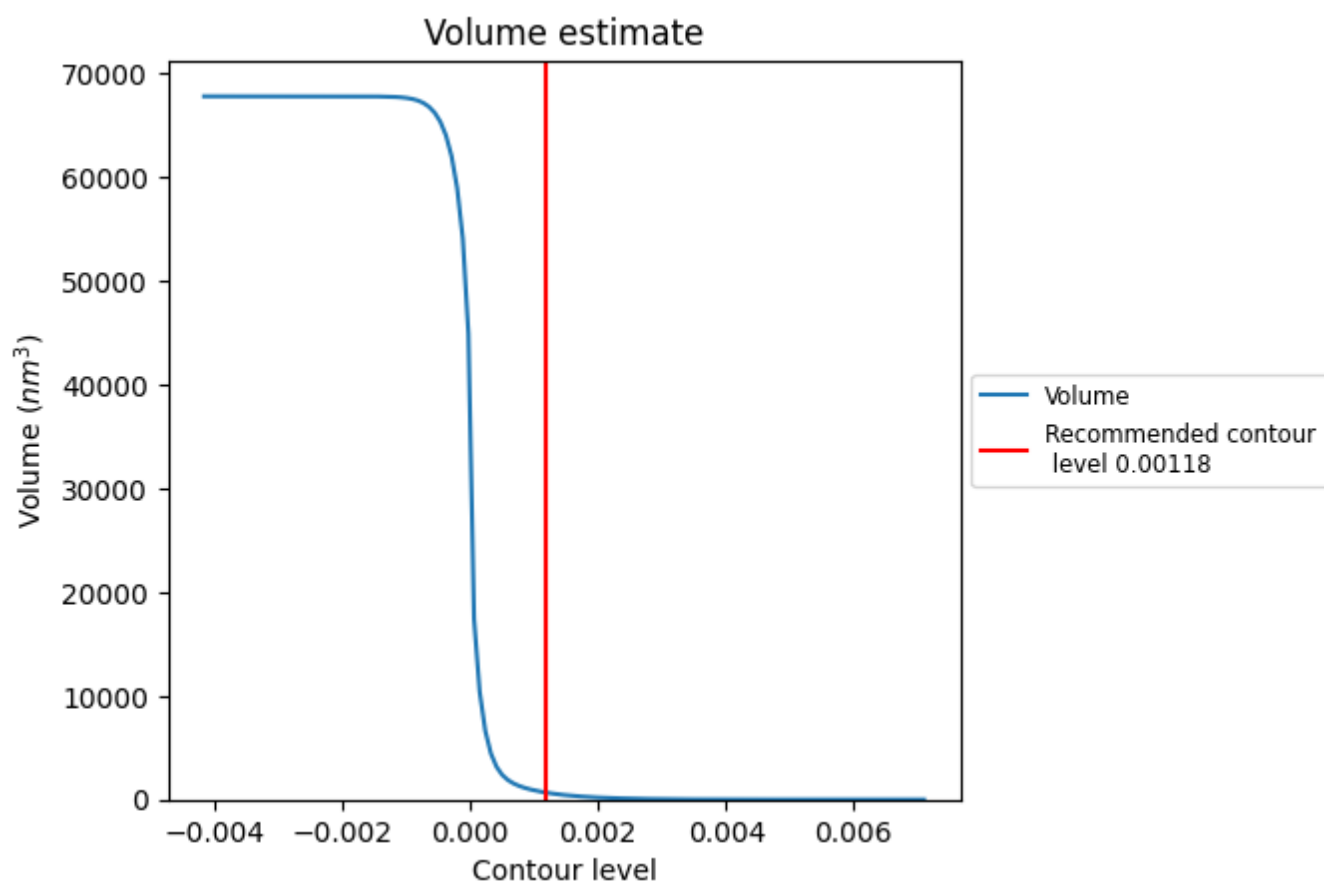
This section contains the results of statistical analysis of the map.

### 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.

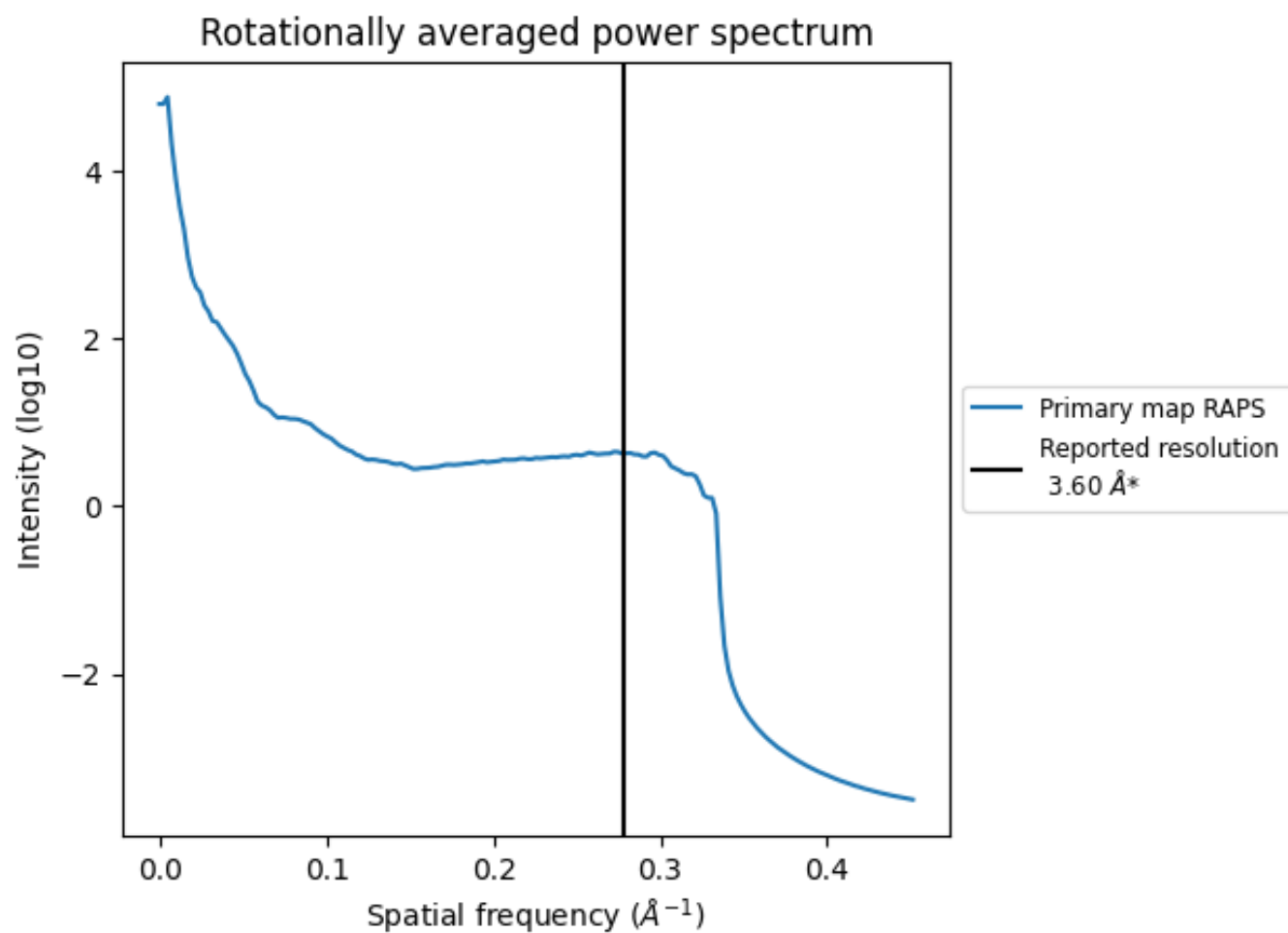
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 675 nm<sup>3</sup>; this corresponds to an approximate mass of 610 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 0.278 Å<sup>-1</sup>

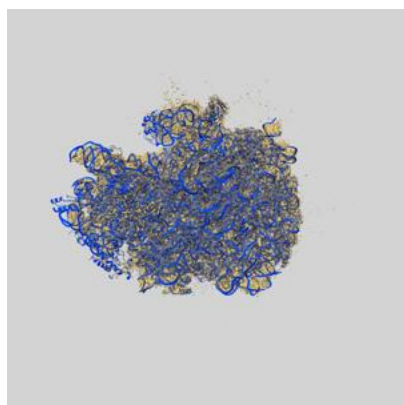
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

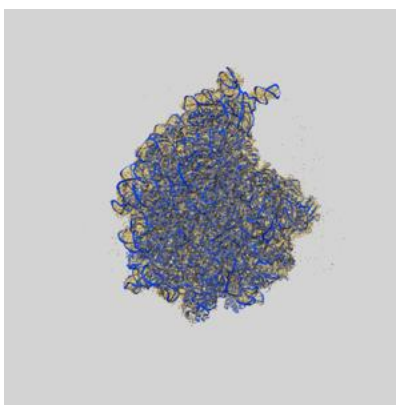
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8176 and PDB model 5JU8. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

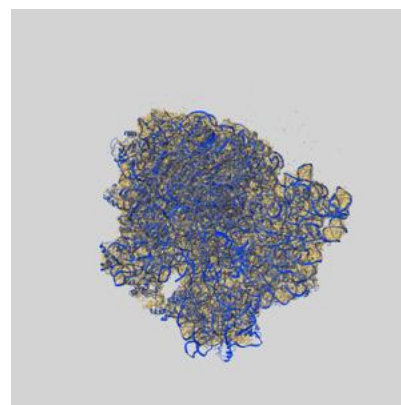
### 9.1 Map-model overlay [i](#)



X



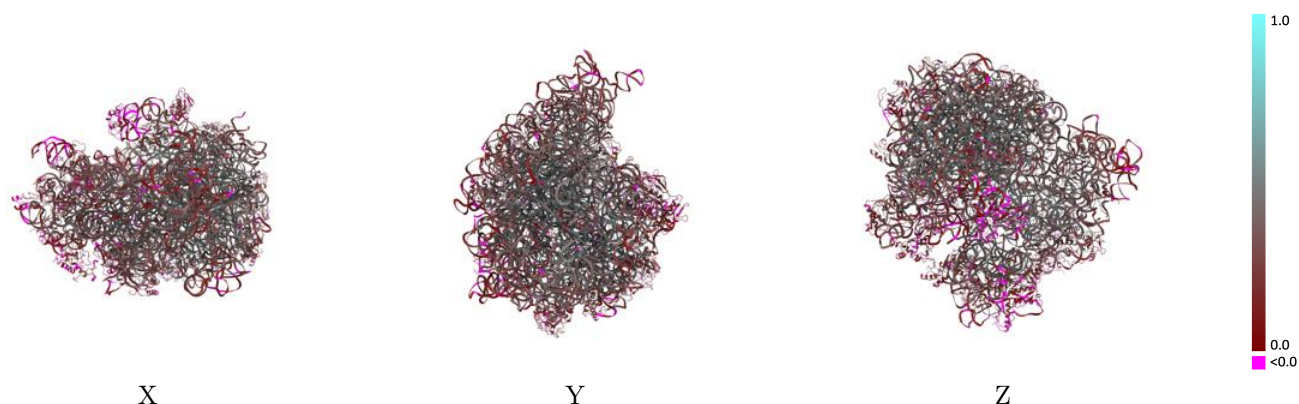
Y



Z

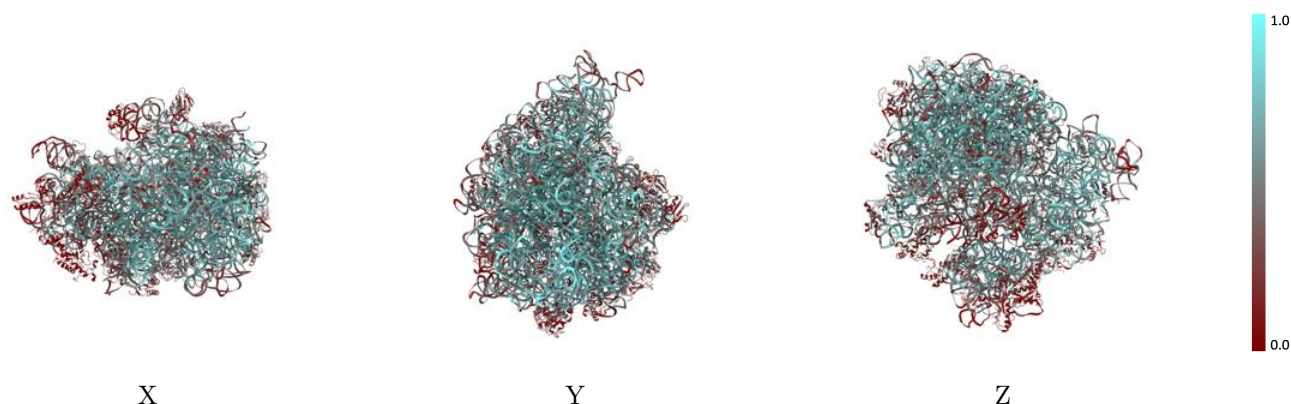
The images above show the 3D surface view of the map at the recommended contour level 0.00118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



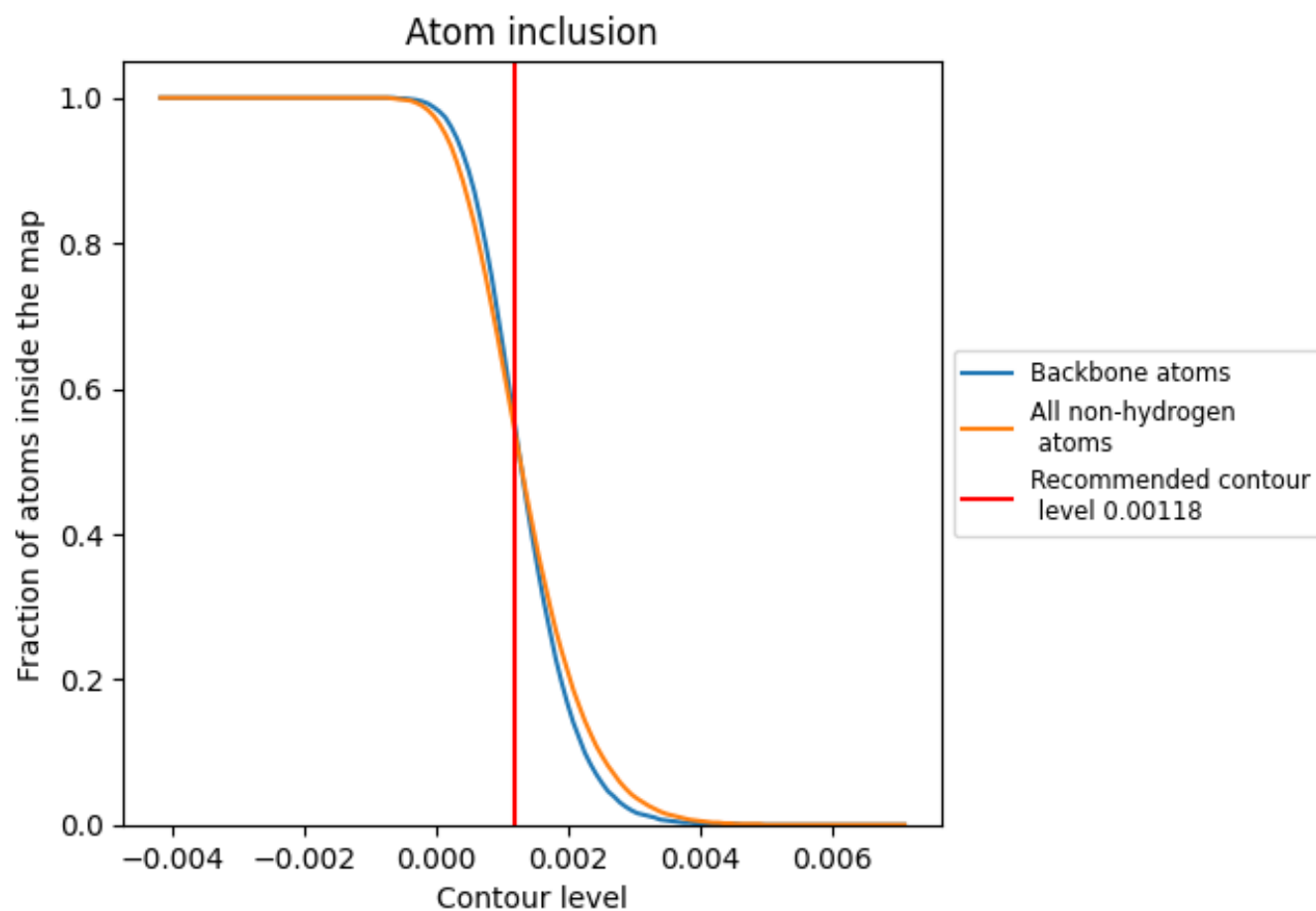
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00118).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 55% 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 (0.00118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5500	 0.3330
AA	 0.6140	 0.3450
AB	 0.0390	 0.1250
AC	 0.2100	 0.2590
AD	 0.2280	 0.2240
AE	 0.3350	 0.2930
AF	 0.2860	 0.2120
AG	 0.2390	 0.2060
AH	 0.3320	 0.2940
AI	 0.1730	 0.2140
AJ	 0.1280	 0.1560
AK	 0.3540	 0.2410
AL	 0.3530	 0.3030
AM	 0.2490	 0.2090
AN	 0.2870	 0.2540
AO	 0.4180	 0.2800
AP	 0.4040	 0.2630
AQ	 0.3320	 0.2440
AR	 0.3920	 0.2730
AS	 0.3290	 0.2330
AT	 0.3990	 0.2580
AU	 0.1060	 0.1150
AV	 0.6100	 0.4270
AX	 0.4840	 0.3130
AY	 0.3270	 0.1900
B0	 0.4670	 0.3370
B1	 0.2520	 0.2500
B2	 0.5630	 0.3770
B3	 0.4970	 0.3730
B4	 0.5340	 0.3630
B5	 0.2920	 0.2820
BA	 0.6710	 0.3830
BB	 0.6110	 0.3090
BC	 0.5130	 0.3560
BD	 0.4430	 0.3510



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
BE	 0.3200	 0.2700
BF	 0.2190	 0.1680
BG	 0.2710	 0.1930
BH	 0.0670	 0.1200
BI	 0.0080	 0.0070
BJ	 0.4720	 0.3350
BK	 0.3880	 0.3420
BL	 0.3900	 0.2860
BM	 0.4590	 0.3170
BN	 0.5030	 0.3620
BO	 0.2750	 0.2450
BP	 0.3890	 0.3140
BQ	 0.5400	 0.3480
BR	 0.3880	 0.2820
BS	 0.4580	 0.3300
BT	 0.3890	 0.2690
BU	 0.2840	 0.1930
BV	 0.4000	 0.2710
BW	 0.4880	 0.3560
BX	 0.4340	 0.2830
BY	 0.3440	 0.2020
BZ	 0.4260	 0.3180