



## wwPDB EM Validation Summary Report ⓘ

Mar 20, 2025 – 06:58 PM EDT

PDB ID : 4V7D  
EMDB ID : EMD-5800  
Title : Structure of the Ribosome with Elongation Factor G Trapped in the Pre-Translocation State (pre-translocation 70S\*tRNA\*EF-G structure)  
Authors : Brilot, A.F.; Korostelev, A.A.; Ermolenko, D.N.; Grigorieff, N.  
Deposited on : 2013-11-21  
Resolution : 7.60 Å (reported)  
Based on initial models : 1MMS, 3U4M, 1ZAV, 1DD3, 3R8S

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

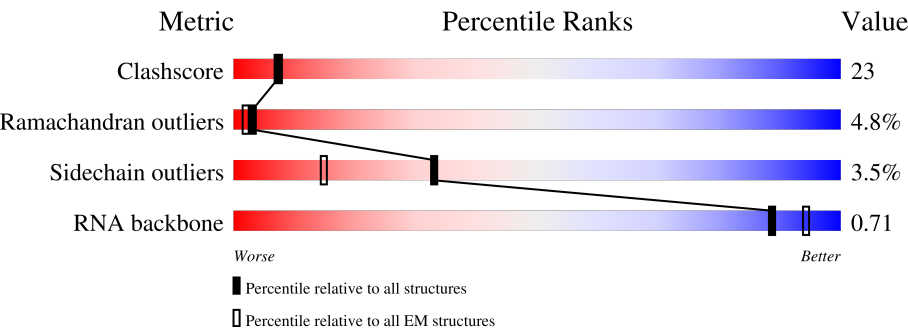
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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 7.60 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	2903	<div><div></div><div>52%</div><div>43%</div><div>6%</div></div>
2	AB	119	<div><div></div><div>56%</div><div>38%</div><div>6%</div></div>
3	AC	233	<div><div>50%</div><div>49%</div><div>47%</div><div>..</div></div>
4	AD	272	<div><div></div><div>43%</div><div>53%</div><div>.</div></div>
5	AE	209	<div><div>7%</div><div>58%</div><div>40%</div><div>.</div></div>
6	AF	201	<div><div>6%</div><div>55%</div><div>43%</div><div>.</div></div>
7	AG	178	<div><div>7%</div><div>36%</div><div>59%</div><div>..</div></div>



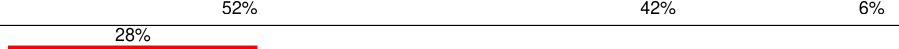
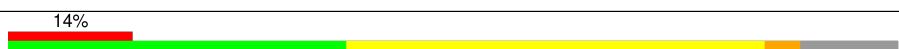
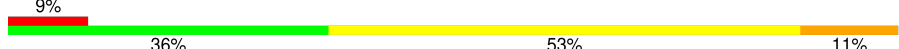

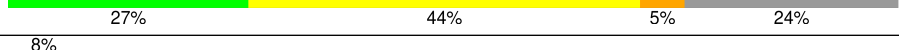
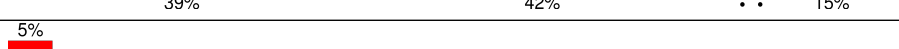
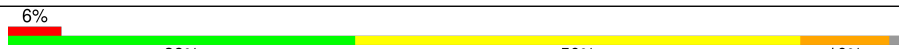

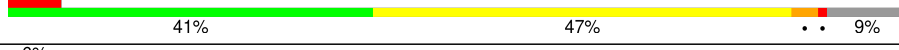
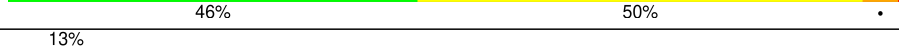
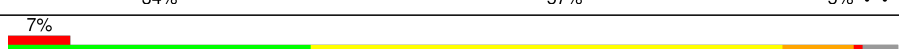
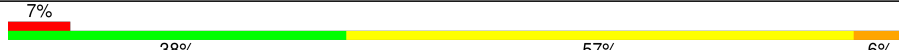


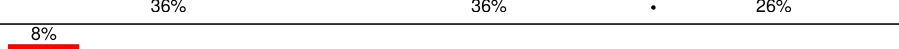
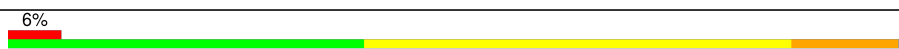
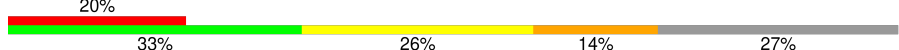






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Mol	Chain	Length	Quality of chain
8	AH	176	
9	AI	149	
10	AJ	165	
11	AK	141	
12	AL	120	
13	AM	142	
14	AN	123	
15	AO	144	
16	AP	136	
17	AQ	127	
18	AR	117	
19	AS	114	
20	AT	117	
21	AU	103	
22	AV	110	
23	AW	100	
24	AX	103	
25	AY	94	
26	AZ	84	
27	A1	77	
28	A2	63	
29	A3	58	
30	A4	56	
31	A5	54	
32	A6	46	

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Mol	Chain	Length	Quality of chain
33	A7	64	
34	A8	38	
35	BA	1542	
36	BB	240	
37	BC	232	
38	BD	205	
39	BE	166	
40	BF	131	
41	BG	178	
42	BH	129	
43	BI	129	
44	BJ	103	
45	BK	128	
46	BL	123	
47	BM	117	
48	BN	100	
49	BO	88	
50	BP	82	
51	BQ	83	
52	BR	74	
53	BS	91	
54	BT	86	
55	BU	70	
56	BV	76	
56	BW	76	

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Mol	Chain	Length	Quality of chain
57	BX	18	
58	BZ	711	
59	BY	6	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	5OH	BY	6	-	-	X	-

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 153817 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	2897	Total	C	N	O	P	0	0
			62192	27744	11444	20107	2897		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	225	Total	C	N	O	S	0	0
			1675	1047	305	317	6		

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	53	Total	C	N	O	S	0	0
			409	261	74	73	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 11 is a protein called 50S ribosomal protein L11.

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

- Molecule 12 is a protein called 50S ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AL	68	Total	C	N	O	0	0
			487	306	82	99		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

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

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.



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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

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

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A4	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	A5	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	1538	Total	C	N	O	P	0	0
			32995	14716	6050	10691	1538		

- Molecule 36 is a protein called 30S ribosomal protein S2.

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

- Molecule 37 is a protein called 30S ribosomal protein S3.

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

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

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

- Molecule 40 is a protein called 30S ribosomal protein S6.

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

- Molecule 41 is a protein called 30S ribosomal protein S7.

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

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

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

- Molecule 45 is a protein called 30S ribosomal protein S11.

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

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

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

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

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

- Molecule 51 is a protein called 30S ribosomal protein S17.

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

- Molecule 52 is a protein called 30S ribosomal protein S18.

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

- Molecule 53 is a protein called 30S ribosomal protein S19.

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

- Molecule 54 is a protein called 30S ribosomal protein S20.

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

- Molecule 55 is a protein called 30S ribosomal protein S21.

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

- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		
56	BW	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BX	18	Total	C	N	O	P	0	0
			386	173	71	124	18		

- Molecule 58 is a protein called Elongation Factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BZ	686	Total	C	N	O	S	0	0
			5301	3341	912	1025	23		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BZ	705	LEU	-	expression tag	UNP P0A6M8
BZ	706	GLU	-	expression tag	UNP P0A6M8
BZ	707	HIS	-	expression tag	UNP P0A6M8
BZ	708	HIS	-	expression tag	UNP P0A6M8
BZ	709	HIS	-	expression tag	UNP P0A6M8
BZ	710	HIS	-	expression tag	UNP P0A6M8
BZ	711	HIS	-	expression tag	UNP P0A6M8
BZ	712	HIS	-	expression tag	UNP P0A6M8

- Molecule 59 is a protein called viomycin.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	BY	6	Total	C	N	O	0	0
			48	25	13	10		

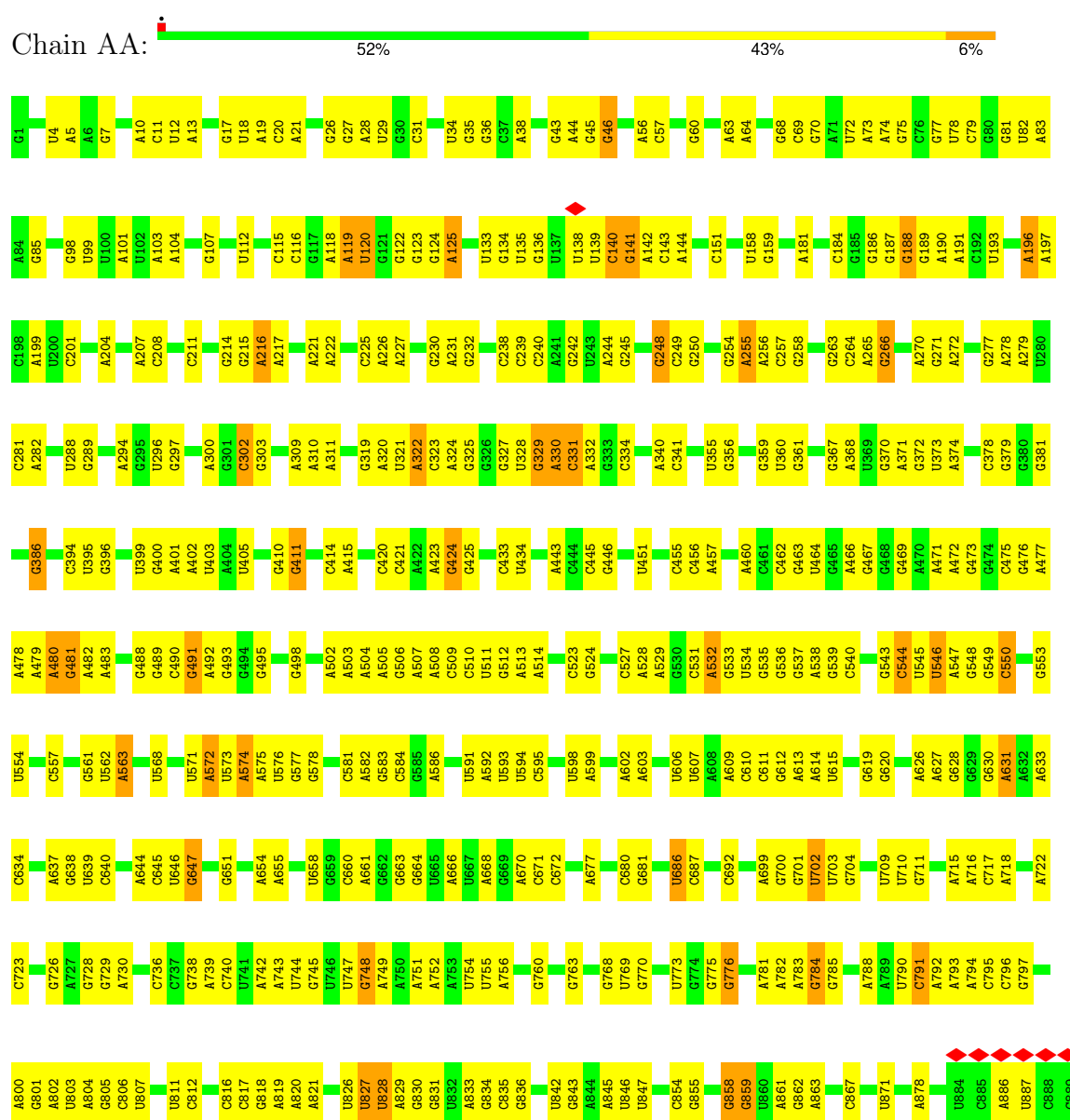
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	A8	1	Total	Zn	0
			1	1	

### 3 Residue-property plots [i](#)

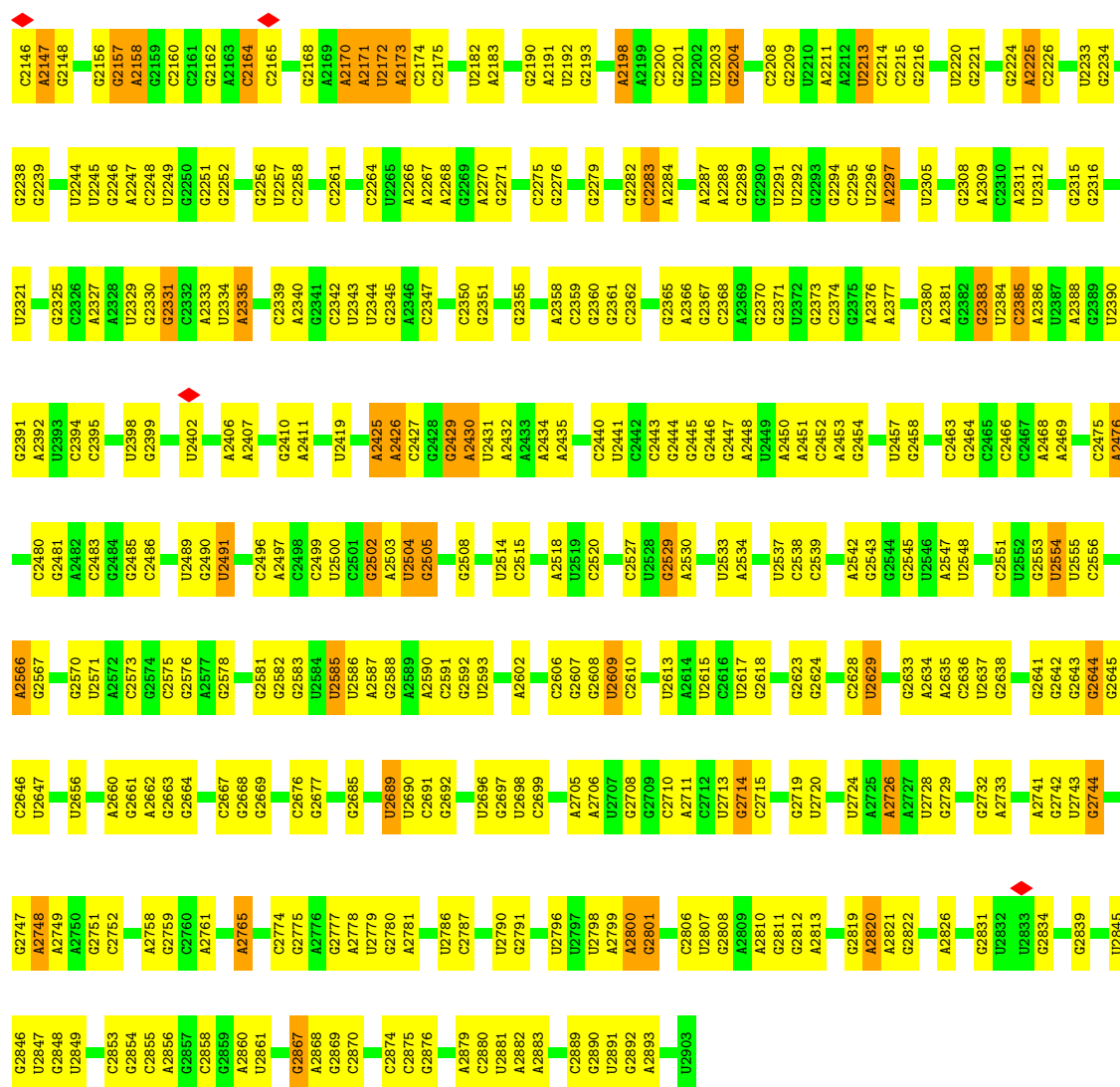
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

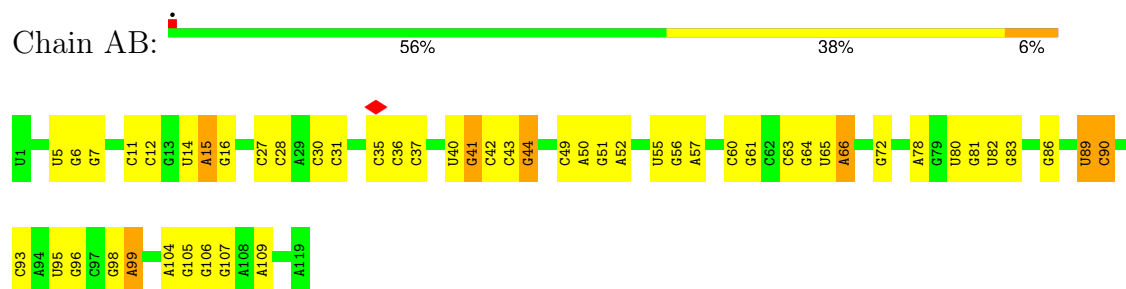






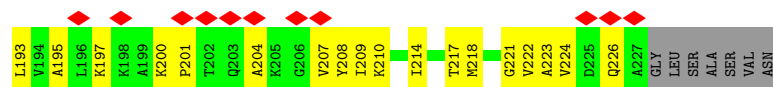
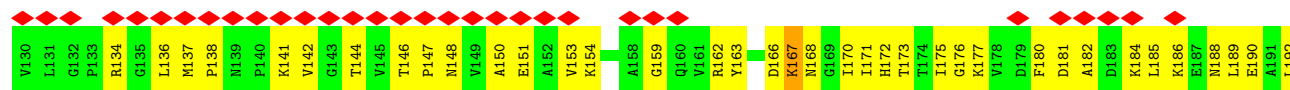


### • Molecule 2: 5S ribosomal RNA

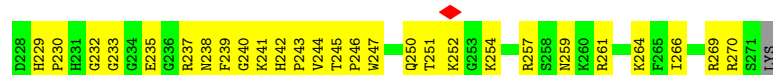
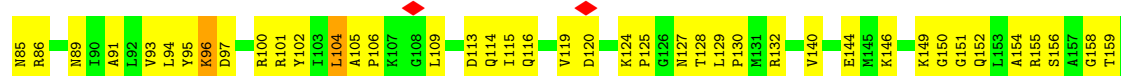


### • Molecule 3: 50S ribosomal protein L1

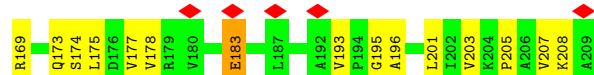
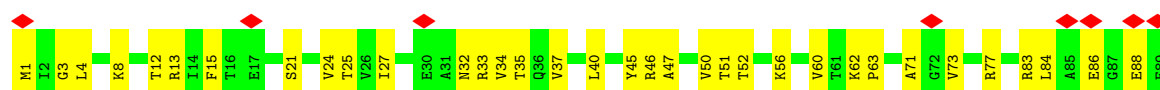




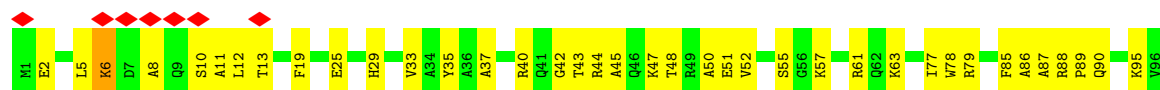
• Molecule 4: 50S ribosomal protein L2

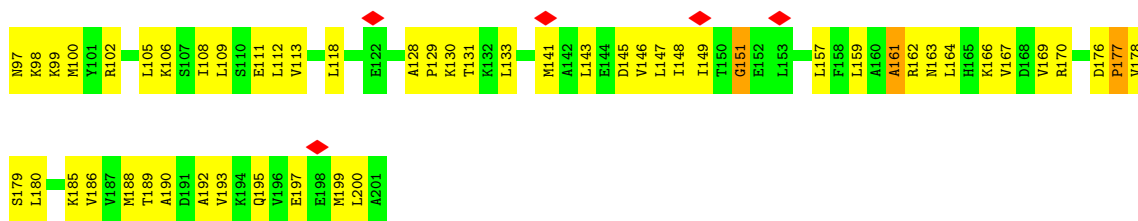


• Molecule 5: 50S ribosomal protein L3

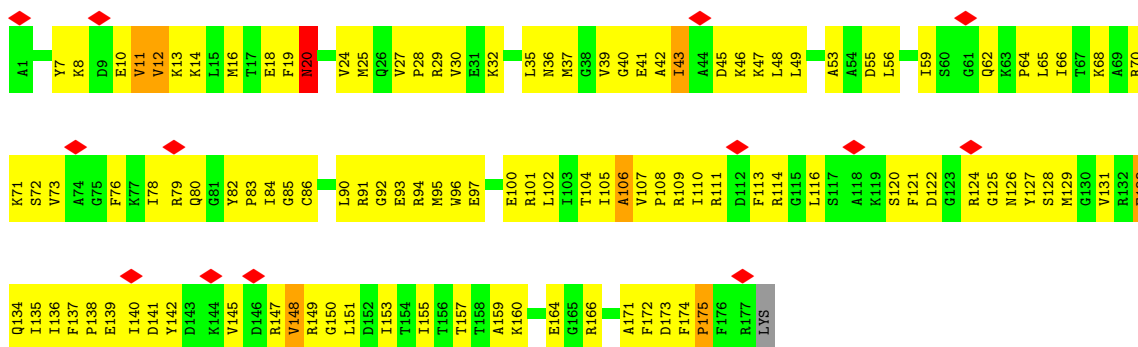


• Molecule 6: 50S ribosomal protein L4

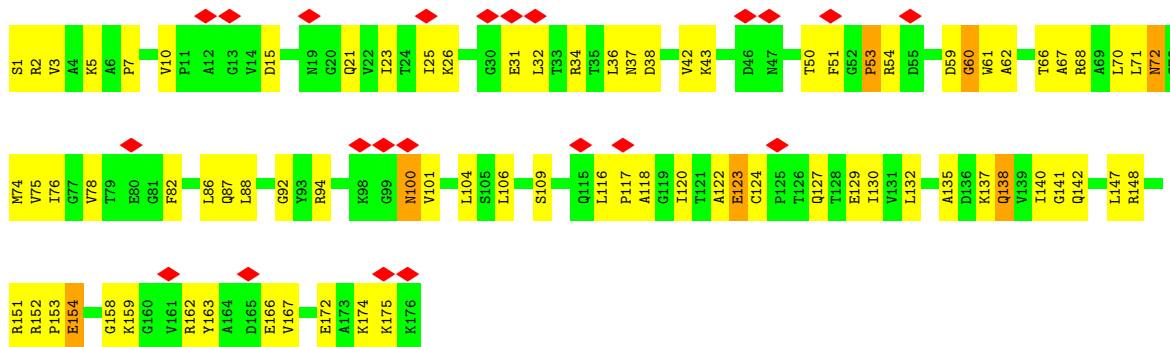




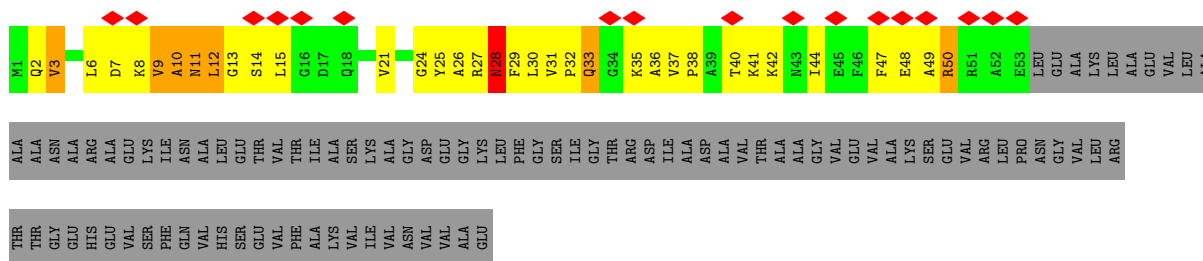
• Molecule 7: 50S ribosomal protein L5



• Molecule 8: 50S ribosomal protein L6

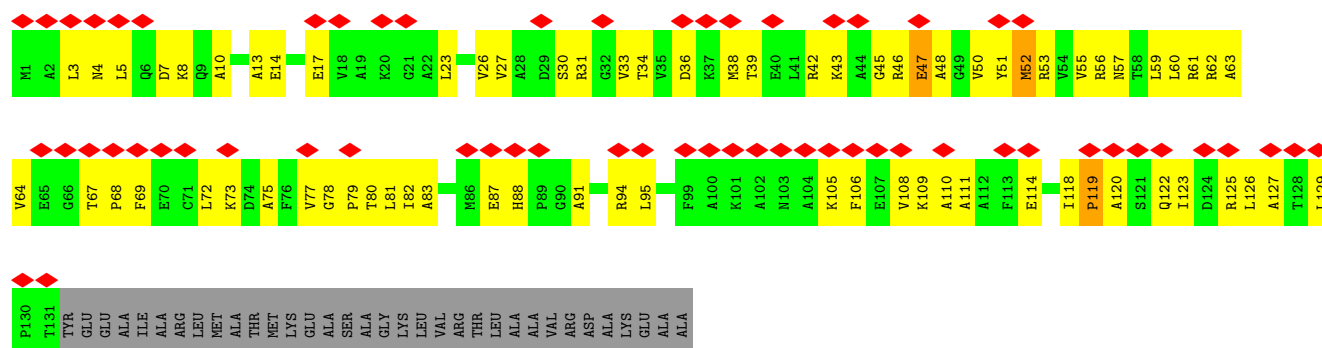


• Molecule 9: 50S ribosomal protein L9



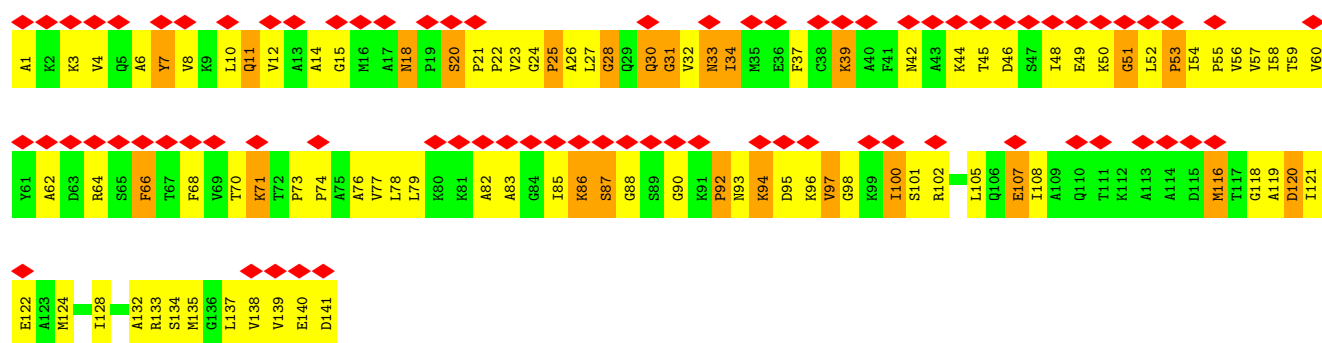
• Molecule 10: 50S ribosomal protein L10

Chain AJ: 




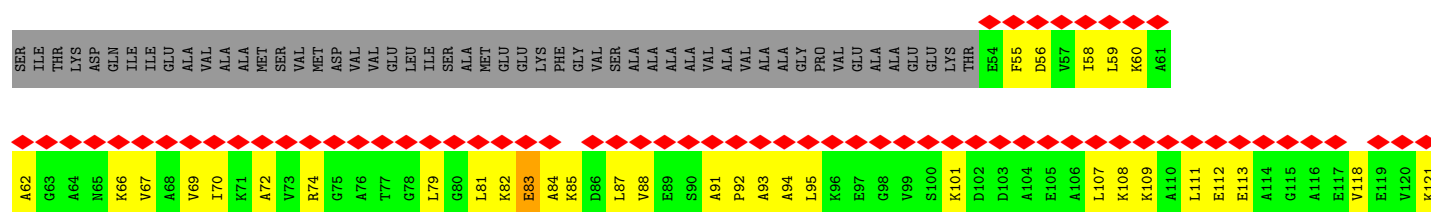
• Molecule 11: 50S ribosomal protein L11

Chain AK: 



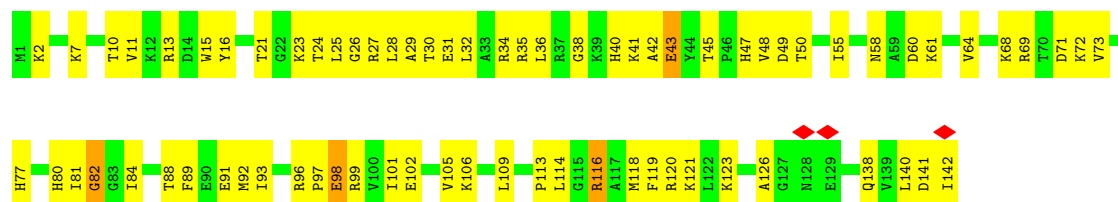
• Molecule 12: 50S ribosomal protein L12

Chain AL: 

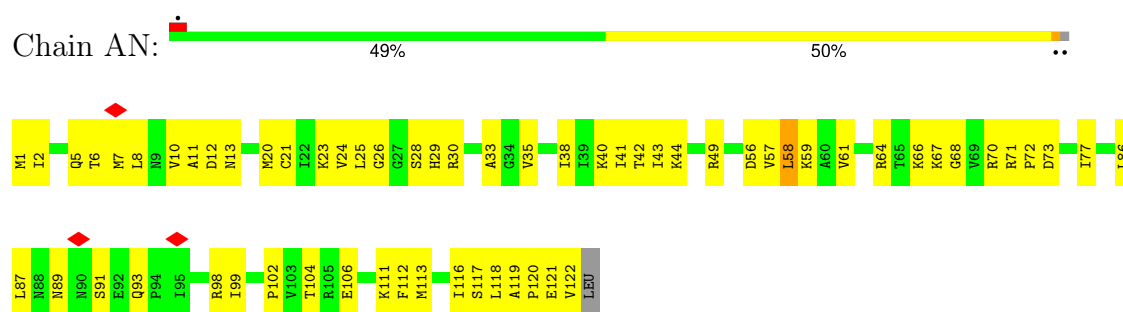


• Molecule 13: 50S ribosomal protein L13

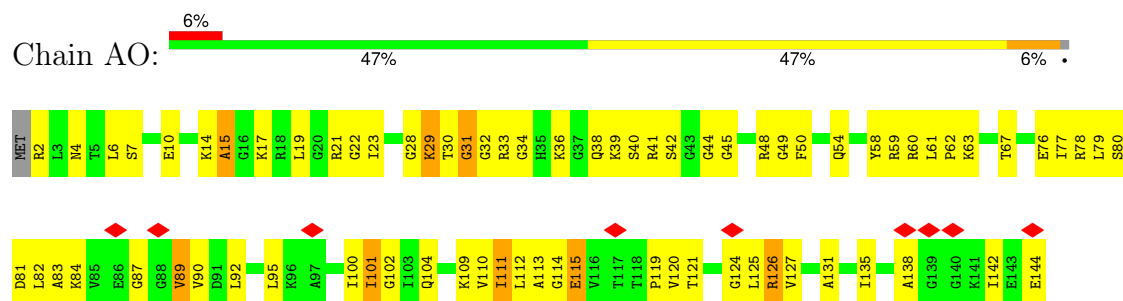
Chain AM: 



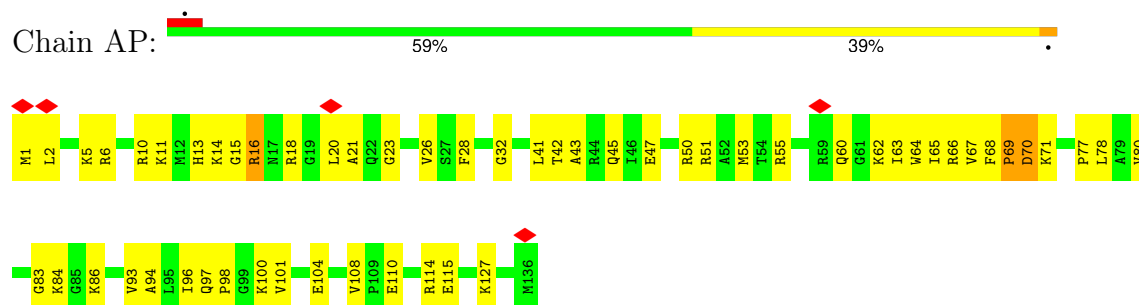
• Molecule 14: 50S ribosomal protein L14



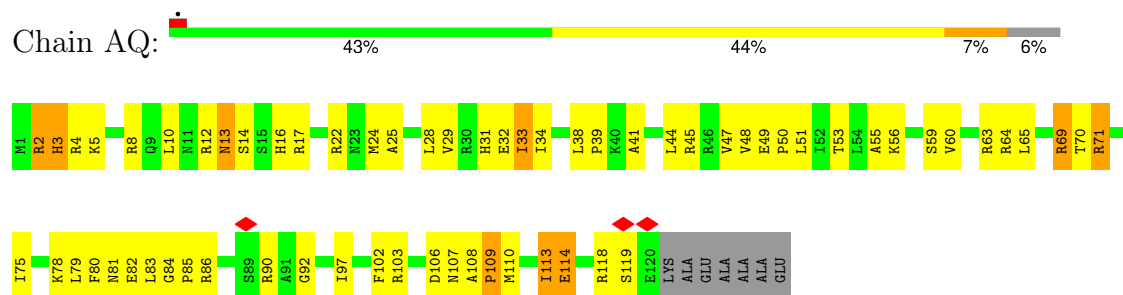
• Molecule 15: 50S ribosomal protein L15



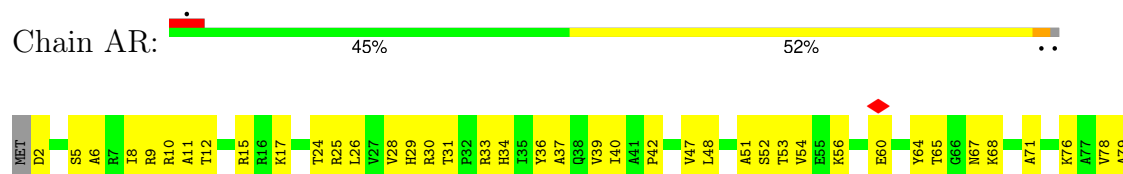
• Molecule 16: 50S ribosomal protein L16

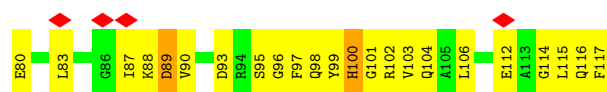


• Molecule 17: 50S ribosomal protein L17

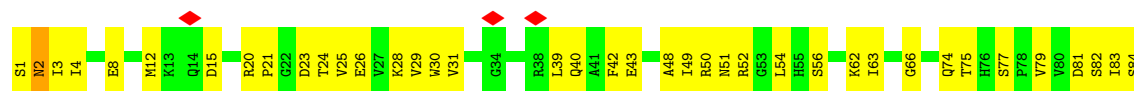


• Molecule 18: 50S ribosomal protein L18





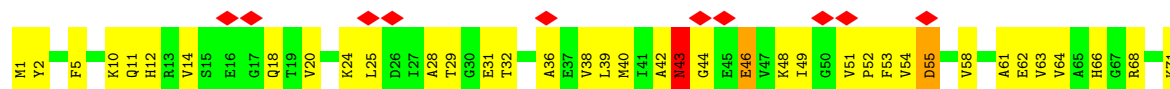
- Molecule 19: 50S ribosomal protein L19



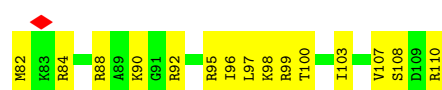
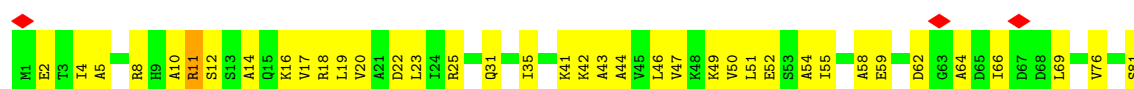
- Molecule 20: 50S ribosomal protein L20



- Molecule 21: 50S ribosomal protein L21

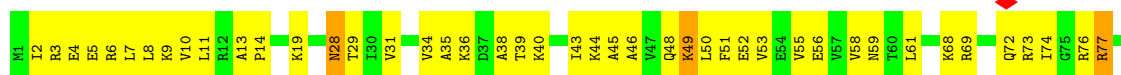


- Molecule 22: 50S ribosomal protein L22



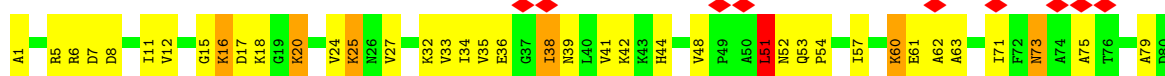
- Molecule 23: 50S ribosomal protein L23

Chain AW: 



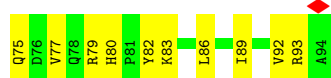
- Molecule 24: 50S ribosomal protein L24

Chain AX: 



- Molecule 25: 50S ribosomal protein L25

Chain AY: 



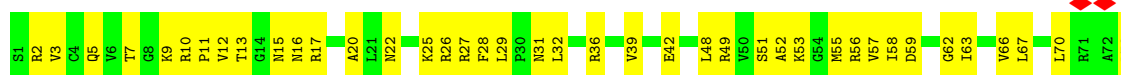
- Molecule 26: 50S ribosomal protein L27

Chain AZ: 

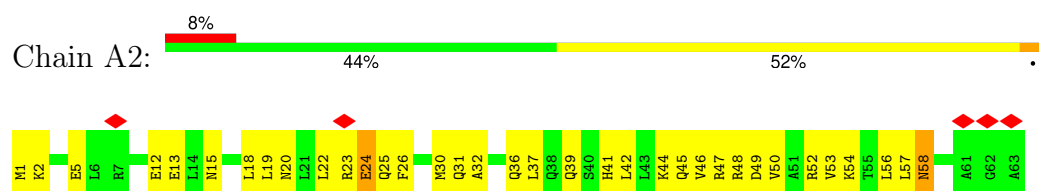


- Molecule 27: 50S ribosomal protein L28

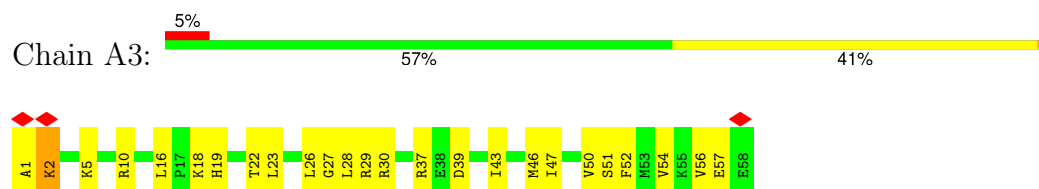
Chain A1: 



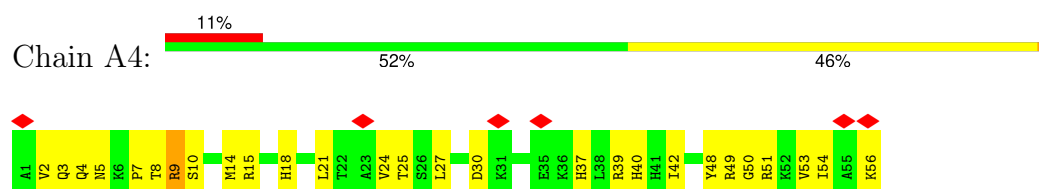
- Molecule 28: 50S ribosomal protein L29



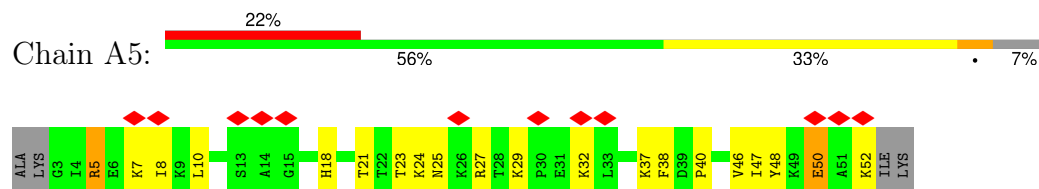
- Molecule 29: 50S ribosomal protein L30



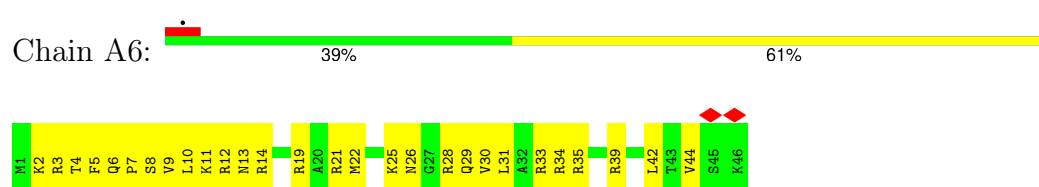
- Molecule 30: 50S ribosomal protein L32



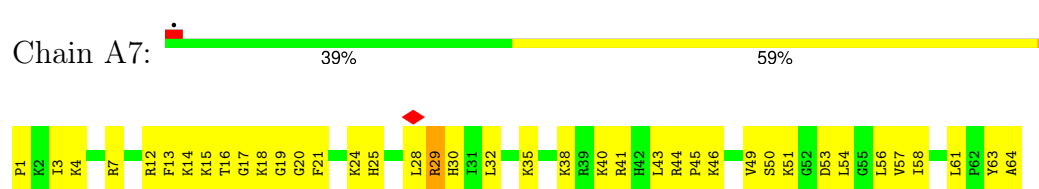
- Molecule 31: 50S ribosomal protein L33



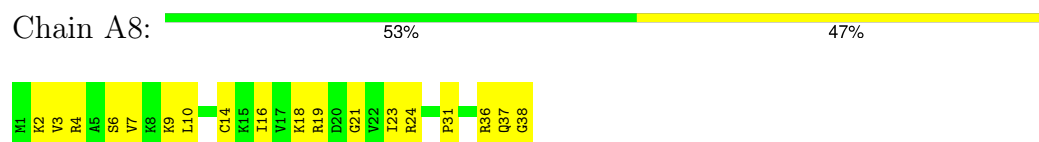
- Molecule 32: 50S ribosomal protein L34



- Molecule 33: 50S ribosomal protein L35

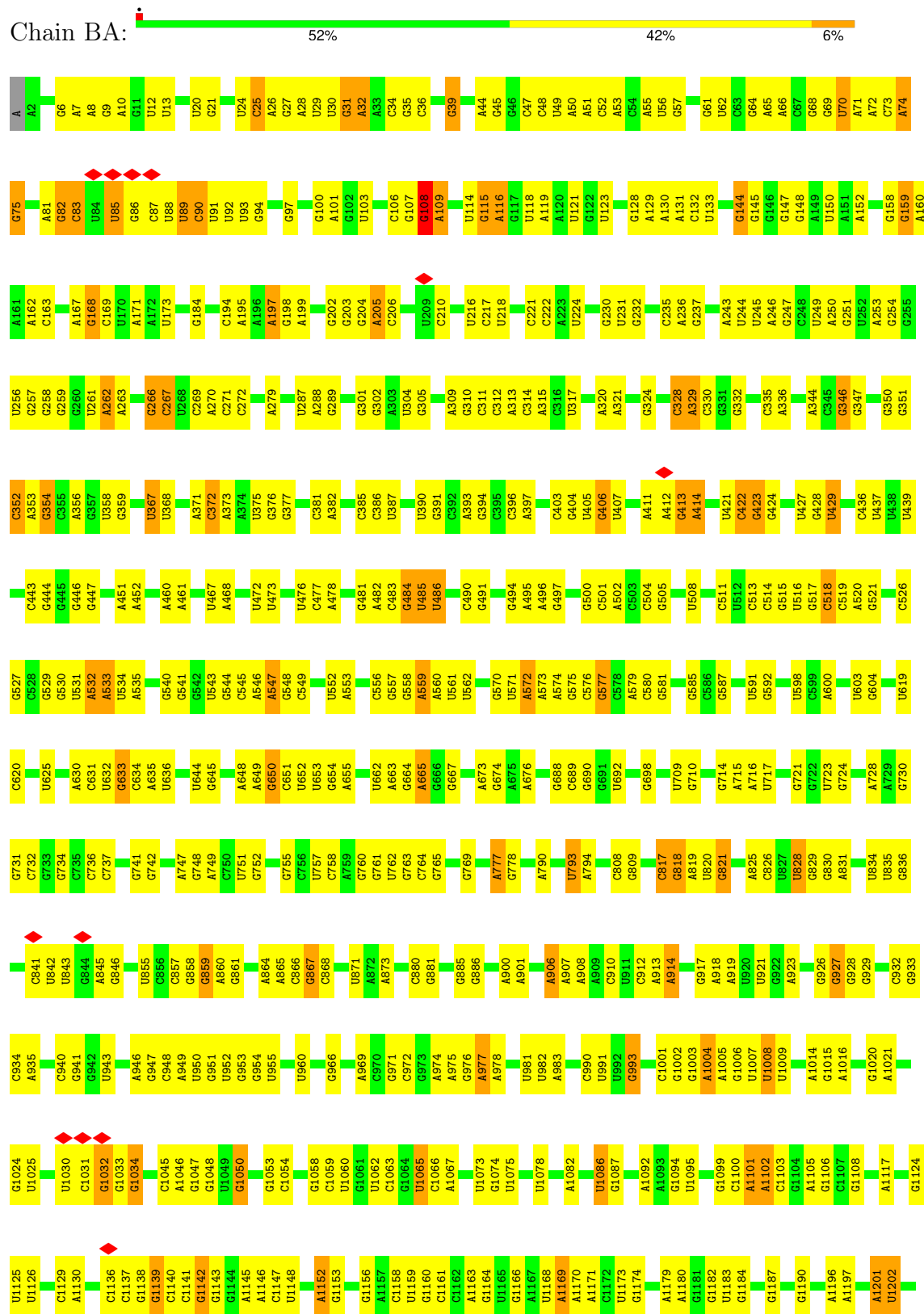


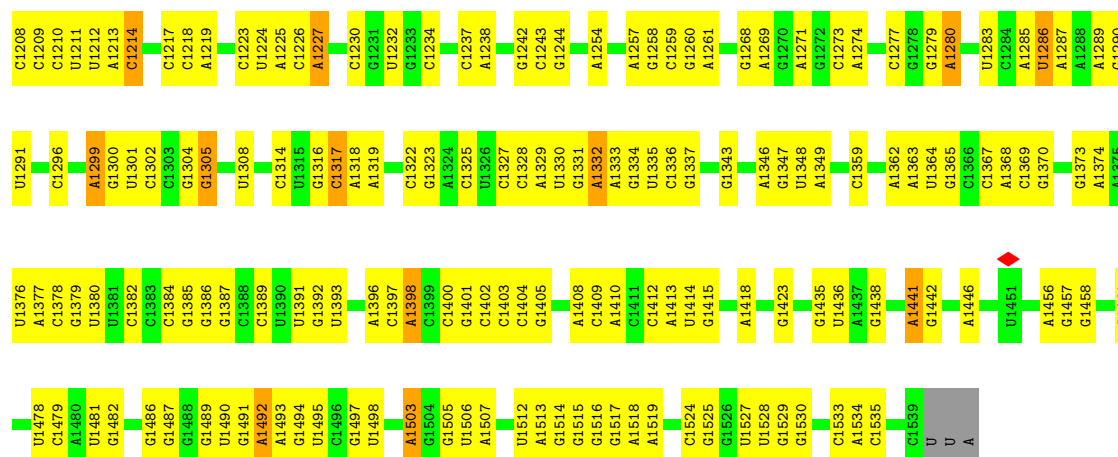
- Molecule 34: 50S ribosomal protein L36



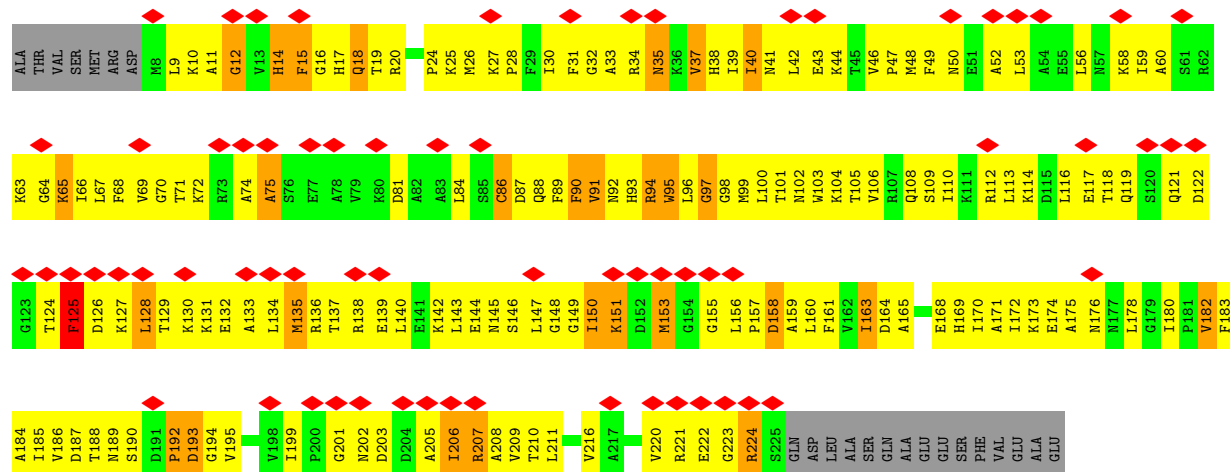


## ● Molecule 35: 16S ribosomal RNA

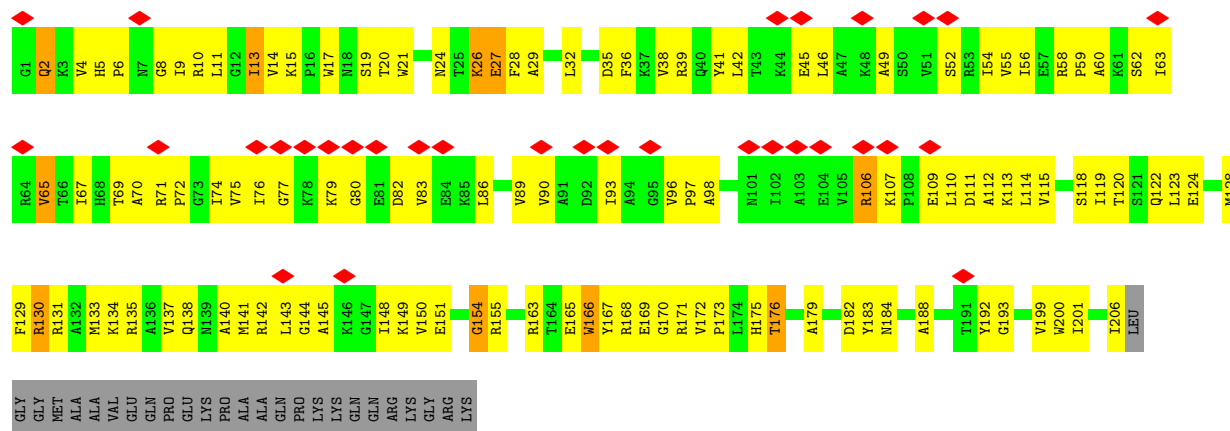




• Molecule 36: 30S ribosomal protein S2

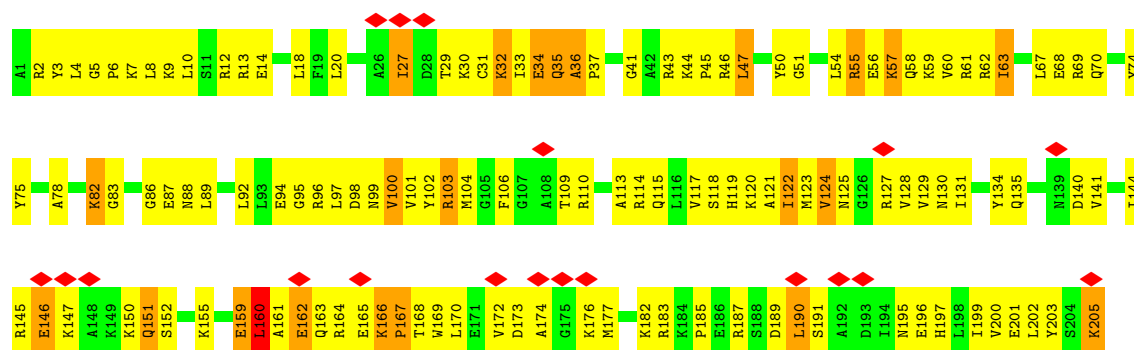


• Molecule 37: 30S ribosomal protein S3



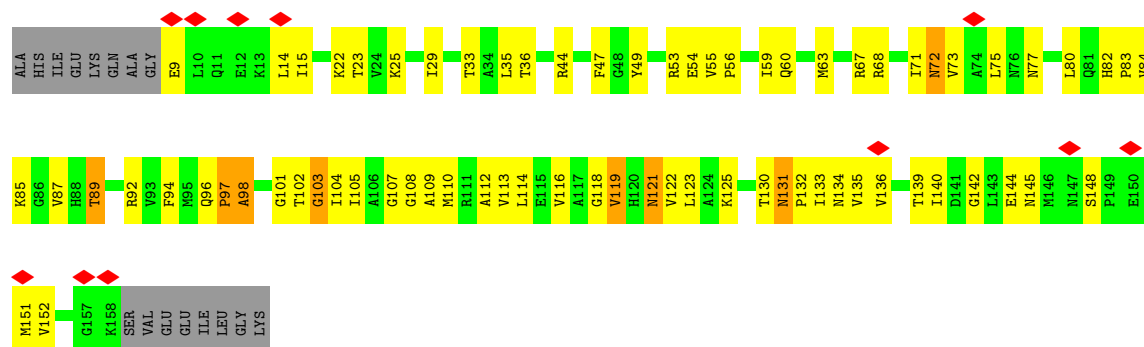
- Molecule 38: 30S ribosomal protein S4

Chain BD: 



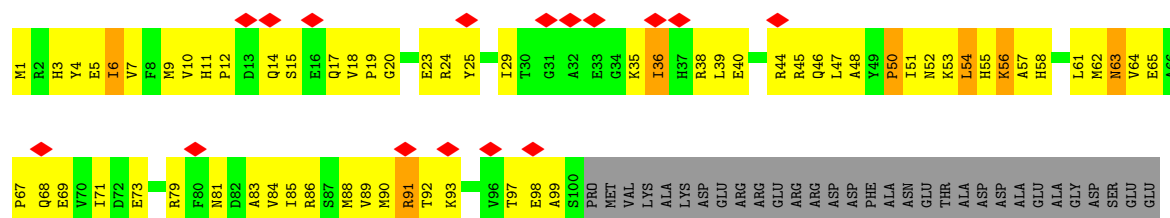
- Molecule 39: 30S ribosomal protein S5

Chain BE: 




- Molecule 40: 30S ribosomal protein S6

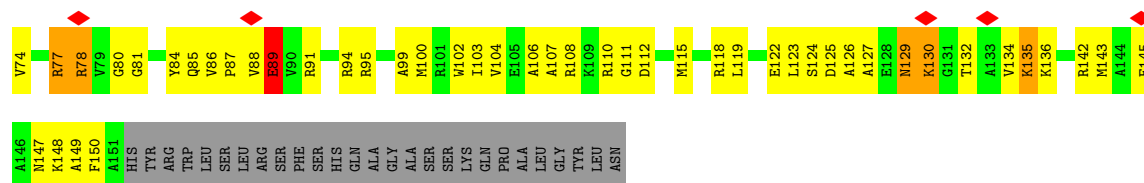
Chain BF: 



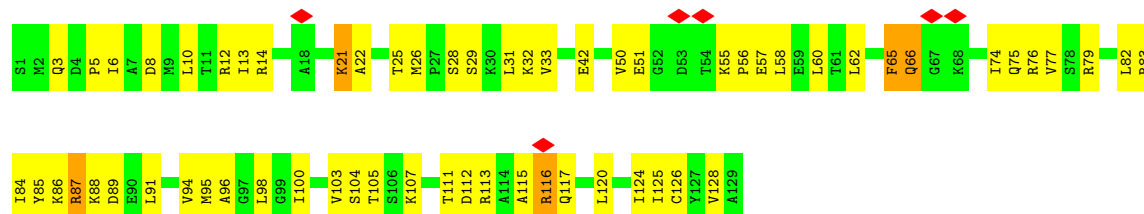
- Molecule 41: 30S ribosomal protein S7

Chain BG: 

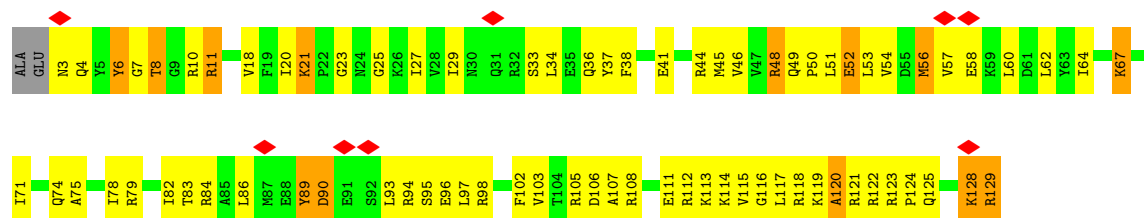




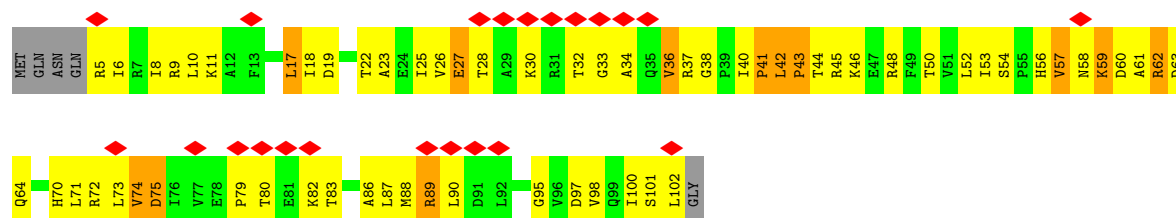
• Molecule 42: 30S ribosomal protein S8



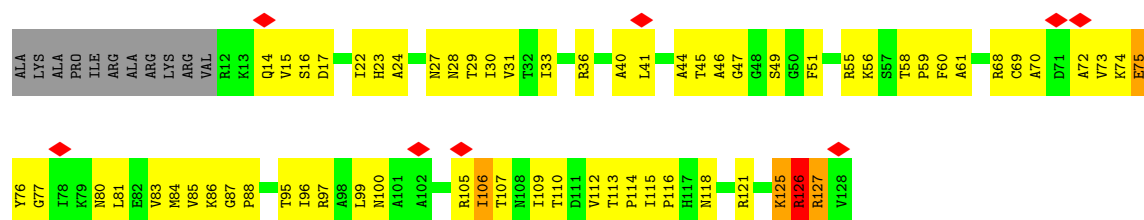
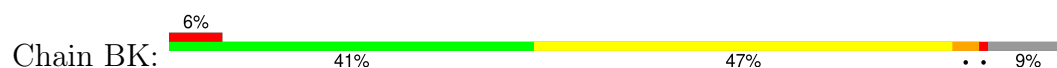
• Molecule 43: 30S ribosomal protein S9



• Molecule 44: 30S ribosomal protein S10

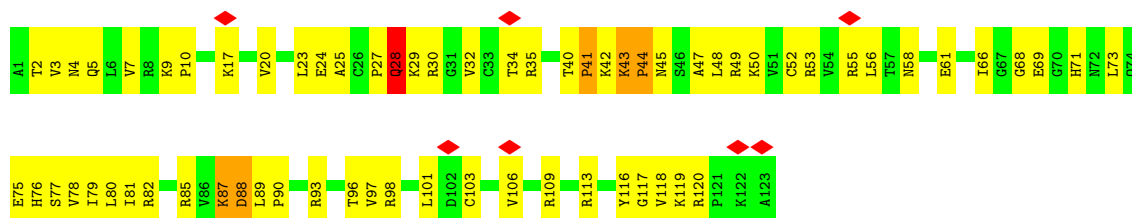


• Molecule 45: 30S ribosomal protein S11



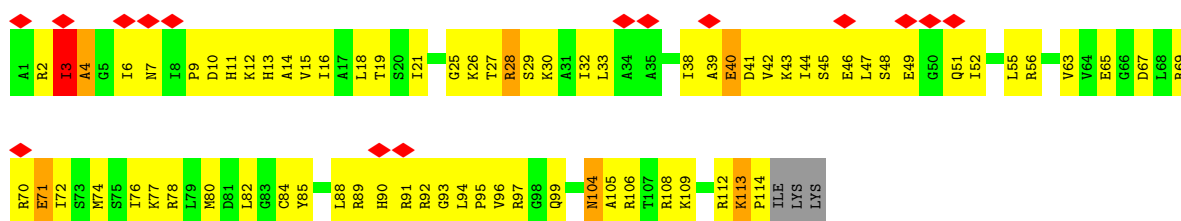
- Molecule 46: 30S ribosomal protein S12

Chain BL: 



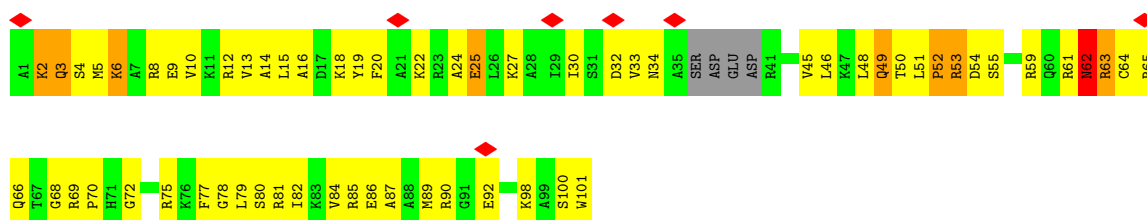
- Molecule 47: 30S ribosomal protein S13

Chain BM: 



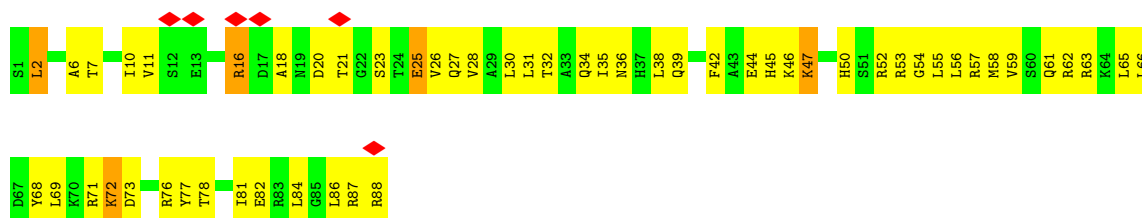
- Molecule 48: 30S ribosomal protein S14

Chain BN: 



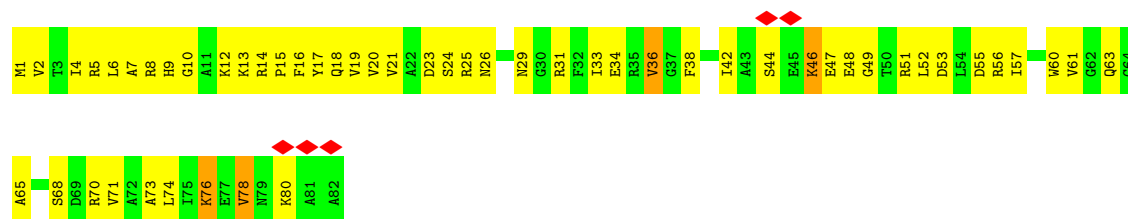
- Molecule 49: 30S ribosomal protein S15

Chain BO: 



- Molecule 50: 30S ribosomal protein S16

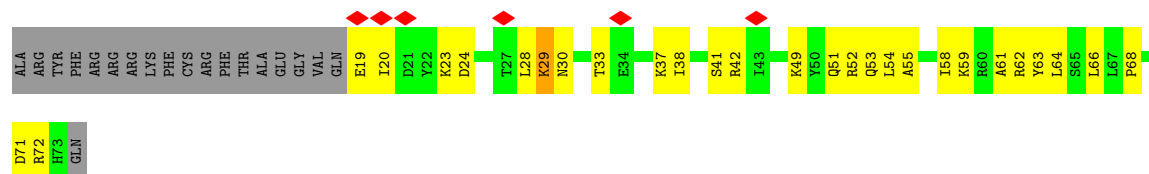
Chain BP: 



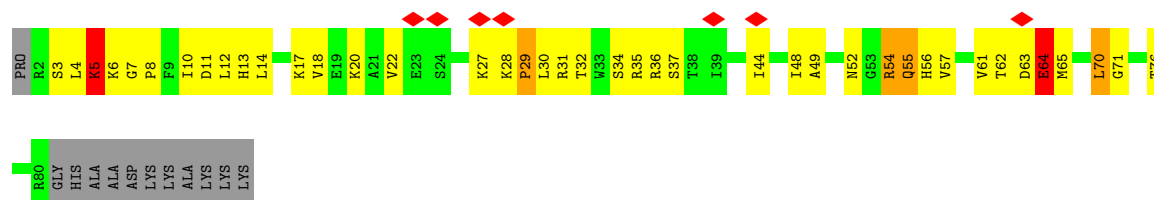
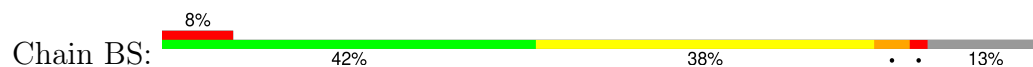
• Molecule 51: 30S ribosomal protein S17



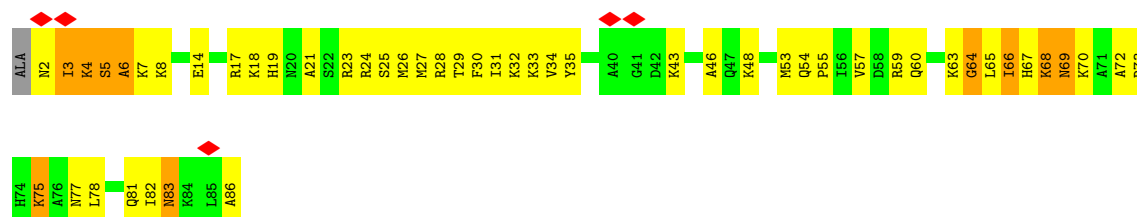
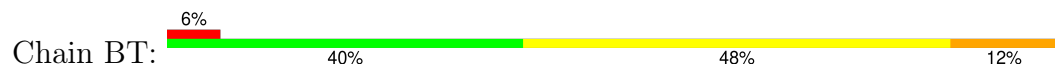
• Molecule 52: 30S ribosomal protein S18



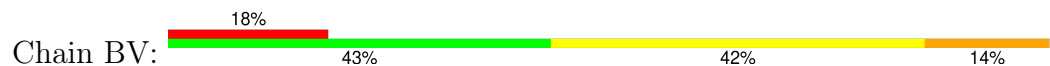
• Molecule 53: 30S ribosomal protein S19

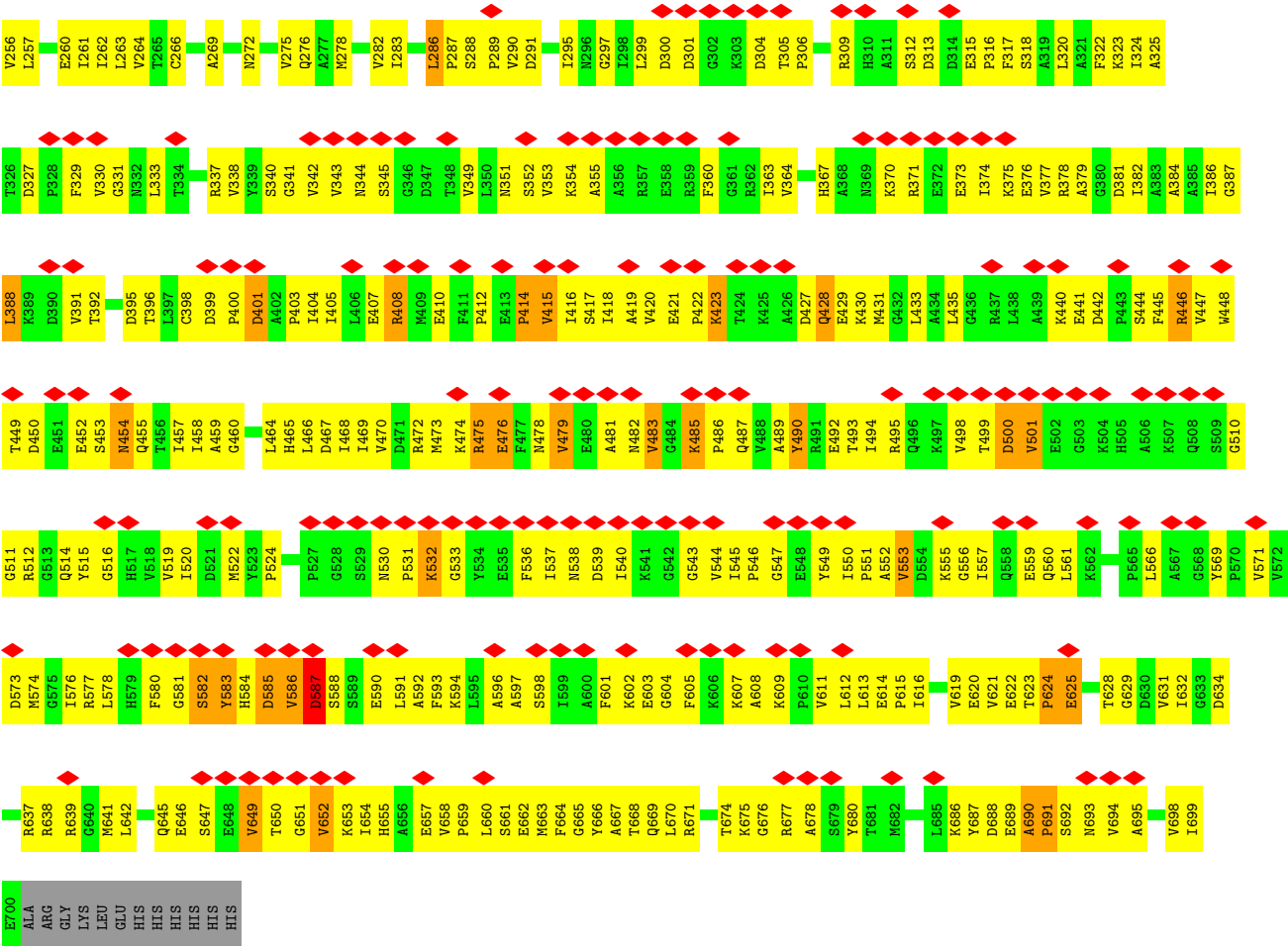


• Molecule 54: 30S ribosomal protein S20



- Chain BU: 





● Molecule 59: viomycin



KBE1
A2
S3
S4
UAL5
50H6



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85115	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND3, FREALIGN per micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1150	Depositor
Maximum defocus (nm)	6950	Depositor
Magnification	134615	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	1.446	Depositor
Minimum map value	-0.459	Depositor
Average map value	-0.029	Depositor
Map value standard deviation	0.177	Depositor
Recommended contour level	0.32	Depositor
Map size ( $\text{\AA}$ )	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.04, 1.04, 1.04	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KBE, DPP, ZN, UAL, 5OH

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	0.33	11/69653 (0.0%)	0.64	18/108657 (0.0%)
2	AB	0.23	0/2847	0.62	0/4440
3	AC	0.22	0/1690	0.41	0/2278
4	AD	0.22	0/2121	0.41	0/2852
5	AE	0.24	0/1586	0.41	0/2134
6	AF	0.23	0/1571	0.40	0/2113
7	AG	0.26	0/1434	0.40	0/1926
8	AH	0.23	0/1343	0.41	0/1816
9	AI	0.27	0/414	0.43	0/556
10	AJ	0.25	0/1001	0.42	0/1350
11	AK	0.24	0/1046	0.44	0/1410
12	AL	0.23	0/488	0.40	0/652
13	AM	0.23	0/1152	0.40	0/1551
14	AN	0.23	0/947	0.42	0/1268
15	AO	0.24	0/1054	0.42	0/1403
16	AP	0.25	0/1093	0.41	0/1460
17	AQ	0.25	0/973	0.39	0/1301
18	AR	0.23	0/902	0.38	0/1209
19	AS	0.24	0/929	0.41	0/1242
20	AT	0.25	0/960	0.37	0/1278
21	AU	0.25	0/829	0.43	0/1107
22	AV	0.21	0/864	0.41	0/1156
23	AW	0.22	0/744	0.41	0/994
24	AX	0.25	0/787	0.41	0/1051
25	AY	0.25	0/766	0.39	0/1025
26	AZ	0.26	0/582	0.37	0/769
27	A1	0.25	0/635	0.39	0/848
28	A2	0.24	0/510	0.42	0/677
29	A3	0.23	0/453	0.42	0/605
30	A4	0.23	0/450	0.40	0/599
31	A5	0.27	0/416	0.41	0/554
32	A6	0.25	0/380	0.39	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	A7	0.25	0/513	0.40	0/676
34	A8	0.24	0/303	0.40	0/397
35	BA	0.28	4/36944 (0.0%)	0.65	4/57632 (0.0%)
36	BB	0.25	0/1735	0.43	0/2338
37	BC	0.24	0/1651	0.41	0/2225
38	BD	0.23	0/1665	0.40	0/2227
39	BE	0.24	0/1118	0.43	0/1504
40	BF	0.24	0/835	0.43	0/1128
41	BG	0.23	0/1195	0.42	0/1602
42	BH	0.24	0/989	0.41	0/1326
43	BI	0.24	0/1034	0.42	0/1375
44	BJ	0.22	0/796	0.45	0/1077
45	BK	0.24	0/893	0.41	0/1205
46	BL	0.22	0/969	0.42	0/1300
47	BM	0.21	0/892	0.42	0/1193
48	BN	0.24	0/785	0.39	0/1043
49	BO	0.23	0/722	0.41	0/964
50	BP	0.25	0/659	0.39	0/884
51	BQ	0.24	0/657	0.43	0/881
52	BR	0.23	0/462	0.40	0/621
53	BS	0.25	0/652	0.43	0/877
54	BT	0.24	0/671	0.41	0/888
55	BU	0.26	0/430	0.43	0/570
56	BV	0.33	2/1809 (0.1%)	0.73	6/2819 (0.2%)
56	BW	0.33	1/1812 (0.1%)	0.65	0/2823
57	BX	0.37	0/432	0.67	0/671
58	BZ	0.29	0/5398	0.59	1/7304 (0.0%)
59	BY	2.44	2/11 (18.2%)	0.76	0/13
All	All	0.29	20/166652 (0.0%)	0.59	29/248342 (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
1	AA	0	2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1911	U	O3'-P	-49.96	1.01	1.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	867	G	O3'-P	15.84	1.80	1.61
1	AA	867	C	O3'-P	12.49	1.76	1.61
35	BA	906	A	O3'-P	10.44	1.73	1.61
1	AA	1425	G	O3'-P	7.22	1.69	1.61

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	906	A	P-O3'-C3'	-25.65	88.92	119.70
35	BA	906	A	O3'-P-O5'	18.08	138.35	104.00
1	AA	1911	U	P-O3'-C3'	-15.29	101.35	119.70
35	BA	906	A	OP1-P-O3'	-12.39	77.94	105.20
1	AA	1911	U	OP2-P-O3'	10.59	128.49	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1913	A	Sidechain
1	AA	1915	U	Sidechain

## 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	62192	0	31283	1405	0
2	AB	2548	0	1292	51	0
3	AC	1675	0	1763	103	0
4	AD	2082	0	2157	180	0
5	AE	1565	0	1616	93	0
6	AF	1552	0	1619	117	0
7	AG	1410	0	1447	129	0
8	AH	1323	0	1374	82	0
9	AI	409	0	429	37	0
10	AJ	988	0	1025	87	0
11	AK	1032	0	1088	123	0
12	AL	487	0	515	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AM	1129	0	1162	72	0
14	AN	938	0	1012	64	0
15	AO	1045	0	1117	115	0
16	AP	1074	0	1157	65	0
17	AQ	960	0	1000	69	0
18	AR	892	0	923	59	0
19	AS	917	0	965	62	0
20	AT	947	0	1022	76	0
21	AU	816	0	839	67	0
22	AV	857	0	922	56	0
23	AW	738	0	807	73	0
24	AX	779	0	834	54	0
25	AY	753	0	780	42	0
26	AZ	575	0	589	39	0
27	A1	625	0	655	43	0
28	A2	509	0	543	42	0
29	A3	449	0	491	30	0
30	A4	444	0	461	42	0
31	A5	409	0	440	19	0
32	A6	377	0	418	41	0
33	A7	504	0	574	59	0
34	A8	302	0	343	32	0
35	BA	32995	0	16607	686	0
36	BB	1704	0	1732	194	0
37	BC	1624	0	1699	120	0
38	BD	1643	0	1710	171	0
39	BE	1105	0	1148	79	0
40	BF	817	0	808	70	0
41	BG	1181	0	1240	98	0
42	BH	979	0	1034	85	0
43	BI	1022	0	1070	118	0
44	BJ	786	0	828	81	0
45	BK	877	0	887	76	0
46	BL	955	0	1019	99	0
47	BM	883	0	944	82	0
48	BN	774	0	827	92	0
49	BO	714	0	737	56	0
50	BP	649	0	666	63	0
51	BQ	648	0	691	59	0
52	BR	455	0	478	37	0
53	BS	637	0	665	38	0
54	BT	665	0	714	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BU	425	0	449	33	0
56	BV	1619	0	822	56	0
56	BW	1622	0	821	47	0
57	BX	386	0	194	11	0
58	BZ	5301	0	5269	667	0
59	BY	48	0	40	13	0
60	A8	1	0	0	0	0
All	All	153817	0	105761	5995	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 23.

The worst 5 of 5995 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:1912:A:C2	1:AA:1919:A:C5	2.13	1.37
1:AA:1052:C:OP1	1:AA:2752:C:H5'	1.10	1.21
1:AA:2876:G:H5''	19:AS:2:ASN:HB2	1.19	1.19
1:AA:1916:A:H2	35:BA:1409:C:OP1	1.21	1.19
1:AA:250:G:H4'	15:AO:59:ARG:HD3	1.18	1.17

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	
3	AC	223/233 (96%)	203 (91%)	18 (8%)	2 (1%)	14	52
4	AD	269/272 (99%)	222 (82%)	39 (14%)	8 (3%)	3	23
5	AE	207/209 (99%)	179 (86%)	22 (11%)	6 (3%)	3	23
6	AF	199/201 (99%)	170 (85%)	24 (12%)	5 (2%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	175/178 (98%)	145 (83%)	21 (12%)	9 (5%)	1	15
8	AH	174/176 (99%)	144 (83%)	24 (14%)	6 (3%)	3	21
9	AI	51/149 (34%)	28 (55%)	15 (29%)	8 (16%)	0	3
10	AJ	129/165 (78%)	108 (84%)	16 (12%)	5 (4%)	2	19
11	AK	139/141 (99%)	77 (55%)	39 (28%)	23 (16%)	0	2
12	AL	66/120 (55%)	55 (83%)	10 (15%)	1 (2%)	8	40
13	AM	140/142 (99%)	118 (84%)	21 (15%)	1 (1%)	19	57
14	AN	120/123 (98%)	102 (85%)	13 (11%)	5 (4%)	2	17
15	AO	141/144 (98%)	110 (78%)	21 (15%)	10 (7%)	1	11
16	AP	134/136 (98%)	115 (86%)	15 (11%)	4 (3%)	3	23
17	AQ	118/127 (93%)	98 (83%)	14 (12%)	6 (5%)	1	15
18	AR	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	3	20
19	AS	112/114 (98%)	94 (84%)	14 (12%)	4 (4%)	3	20
20	AT	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	14	52
21	AU	101/103 (98%)	81 (80%)	16 (16%)	4 (4%)	2	18
22	AV	108/110 (98%)	88 (82%)	18 (17%)	2 (2%)	6	32
23	AW	91/100 (91%)	79 (87%)	11 (12%)	1 (1%)	12	47
24	AX	100/103 (97%)	76 (76%)	17 (17%)	7 (7%)	1	11
25	AY	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
26	AZ	74/84 (88%)	63 (85%)	10 (14%)	1 (1%)	9	41
27	A1	75/77 (97%)	65 (87%)	10 (13%)	0	100	100
28	A2	61/63 (97%)	51 (84%)	8 (13%)	2 (3%)	3	21
29	A3	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
30	A4	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
31	A5	48/54 (89%)	38 (79%)	8 (17%)	2 (4%)	2	17
32	A6	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
33	A7	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	8	38
34	A8	36/38 (95%)	28 (78%)	7 (19%)	1 (3%)	4	24
36	BB	216/240 (90%)	140 (65%)	51 (24%)	25 (12%)	0	5
37	BC	204/232 (88%)	169 (83%)	28 (14%)	7 (3%)	3	21
38	BD	203/205 (99%)	161 (79%)	26 (13%)	16 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BE	148/166 (89%)	111 (75%)	27 (18%)	10 (7%)	1	12
40	BF	98/131 (75%)	71 (72%)	20 (20%)	7 (7%)	1	11
41	BG	149/178 (84%)	123 (83%)	21 (14%)	5 (3%)	3	21
42	BH	127/129 (98%)	112 (88%)	11 (9%)	4 (3%)	3	22
43	BI	125/129 (97%)	95 (76%)	25 (20%)	5 (4%)	2	18
44	BJ	96/103 (93%)	65 (68%)	19 (20%)	12 (12%)	0	4
45	BK	115/128 (90%)	88 (76%)	22 (19%)	5 (4%)	2	17
46	BL	121/123 (98%)	95 (78%)	18 (15%)	8 (7%)	1	12
47	BM	112/117 (96%)	94 (84%)	12 (11%)	6 (5%)	1	15
48	BN	92/100 (92%)	67 (73%)	19 (21%)	6 (6%)	1	12
49	BO	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	5	28
50	BP	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	1	13
51	BQ	78/83 (94%)	56 (72%)	14 (18%)	8 (10%)	0	6
52	BR	53/74 (72%)	49 (92%)	4 (8%)	0	100	100
53	BS	77/91 (85%)	56 (73%)	14 (18%)	7 (9%)	0	8
54	BT	83/86 (96%)	69 (83%)	7 (8%)	7 (8%)	0	9
55	BU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	4
58	BZ	680/711 (96%)	565 (83%)	76 (11%)	39 (6%)	1	14
59	BY	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	6622/7186 (92%)	5360 (81%)	943 (14%)	319 (5%)	3	16

5 of 319 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	104	VAL
8	AH	37	ASN
8	AH	118	ALA
9	AI	3	VAL
9	AI	9	VAL

### 5.3.2 Protein sidechains ⓘ

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



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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	175/180 (97%)	173 (99%)	2 (1%)	70	80
4	AD	216/217 (100%)	213 (99%)	3 (1%)	62	75
5	AE	164/164 (100%)	162 (99%)	2 (1%)	67	78
6	AF	165/165 (100%)	165 (100%)	0	100	100
7	AG	148/149 (99%)	145 (98%)	3 (2%)	50	68
8	AH	137/137 (100%)	132 (96%)	5 (4%)	30	50
9	AI	42/114 (37%)	39 (93%)	3 (7%)	12	32
10	AJ	100/123 (81%)	99 (99%)	1 (1%)	73	82
11	AK	109/109 (100%)	98 (90%)	11 (10%)	6	20
12	AL	47/84 (56%)	46 (98%)	1 (2%)	48	66
13	AM	116/116 (100%)	113 (97%)	3 (3%)	41	59
14	AN	103/104 (99%)	102 (99%)	1 (1%)	73	82
15	AO	102/103 (99%)	100 (98%)	2 (2%)	50	68
16	AP	109/109 (100%)	106 (97%)	3 (3%)	38	57
17	AQ	100/103 (97%)	96 (96%)	4 (4%)	27	47
18	AR	86/87 (99%)	85 (99%)	1 (1%)	67	78
19	AS	99/99 (100%)	97 (98%)	2 (2%)	50	68
20	AT	89/89 (100%)	89 (100%)	0	100	100
21	AU	84/84 (100%)	82 (98%)	2 (2%)	44	62
22	AV	93/93 (100%)	93 (100%)	0	100	100
23	AW	80/84 (95%)	77 (96%)	3 (4%)	28	49
24	AX	83/84 (99%)	78 (94%)	5 (6%)	16	37
25	AY	78/78 (100%)	76 (97%)	2 (3%)	41	59
26	AZ	56/62 (90%)	55 (98%)	1 (2%)	54	71
27	A1	67/67 (100%)	66 (98%)	1 (2%)	60	75
28	A2	55/55 (100%)	54 (98%)	1 (2%)	54	71
29	A3	48/48 (100%)	47 (98%)	1 (2%)	48	66
30	A4	47/47 (100%)	45 (96%)	2 (4%)	25	46
31	A5	45/48 (94%)	45 (100%)	0	100	100
32	A6	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	A7	51/51 (100%)	50 (98%)	1 (2%)	50	68
34	A8	34/34 (100%)	34 (100%)	0	100	100
36	BB	180/198 (91%)	168 (93%)	12 (7%)	13	34
37	BC	170/189 (90%)	162 (95%)	8 (5%)	22	44
38	BD	172/172 (100%)	159 (92%)	13 (8%)	11	30
39	BE	113/125 (90%)	109 (96%)	4 (4%)	31	51
40	BF	87/112 (78%)	84 (97%)	3 (3%)	32	51
41	BG	124/146 (85%)	119 (96%)	5 (4%)	27	47
42	BH	104/104 (100%)	101 (97%)	3 (3%)	37	56
43	BI	105/106 (99%)	96 (91%)	9 (9%)	8	26
44	BJ	86/90 (96%)	83 (96%)	3 (4%)	31	51
45	BK	90/98 (92%)	84 (93%)	6 (7%)	13	34
46	BL	103/103 (100%)	101 (98%)	2 (2%)	52	69
47	BM	92/95 (97%)	89 (97%)	3 (3%)	33	52
48	BN	79/83 (95%)	73 (92%)	6 (8%)	11	30
49	BO	76/76 (100%)	73 (96%)	3 (4%)	27	48
50	BP	65/65 (100%)	62 (95%)	3 (5%)	23	44
51	BQ	74/77 (96%)	69 (93%)	5 (7%)	13	34
52	BR	48/64 (75%)	47 (98%)	1 (2%)	48	66
53	BS	70/78 (90%)	66 (94%)	4 (6%)	17	38
54	BT	65/65 (100%)	62 (95%)	3 (5%)	23	44
55	BU	44/60 (73%)	40 (91%)	4 (9%)	7	24
58	BZ	563/585 (96%)	539 (96%)	24 (4%)	25	46
59	BY	2/2 (100%)	2 (100%)	0	100	100
All	All	5478/5818 (94%)	5288 (96%)	190 (4%)	33	51

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BI	11	ARG
49	BO	16	ARG
43	BI	67	LYS
45	BK	126	ARG
51	BQ	16	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
41	BG	85	GLN
52	BR	53	GLN
43	BI	49	GLN
46	BL	111	GLN
58	BZ	122	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2894/2903 (99%)	291 (10%)	4 (0%)
2	AB	118/119 (99%)	11 (9%)	0
35	BA	1537/1542 (99%)	164 (10%)	4 (0%)
56	BV	75/76 (98%)	15 (20%)	1 (1%)
56	BW	75/76 (98%)	11 (14%)	0
57	BX	17/18 (94%)	3 (17%)	0
All	All	4716/4734 (99%)	495 (10%)	9 (0%)

5 of 495 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	A
1	AA	34	U
1	AA	35	G
1	AA	46	G
1	AA	74	A

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	1201	A
56	BV	15	G
1	AA	2425	A
35	BA	74	A
35	BA	115	G

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

4 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
59	UAL	BY	5	59	6,8,9	2.28	2 (33%)	4,9,11	1.57	1 (25%)
59	KBE	BY	1	59	8,8,9	0.55	0	6,8,10	0.88	0
59	DPP	BY	2	59	4,5,6	0.48	0	1,5,7	0.31	0
59	5OH	BY	6	59	7,12,13	0.62	0	4,16,18	1.76	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	UAL	BY	5	59	-	0/3/7/9	-
59	KBE	BY	1	59	-	1/7/7/8	-
59	DPP	BY	2	59	-	0/2/4/6	-
59	5OH	BY	6	59	-	0/2/18/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	BY	5	UAL	C1-N1	-4.10	1.34	1.40
59	BY	5	UAL	C-CA	-3.63	1.39	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BY	6	5OH	CR-CB-CA	-3.20	109.22	112.61
59	BY	5	UAL	O-C-CA	-2.79	121.90	125.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	BY	1	KBE	C-CA-CB-N

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	BY	5	UAL	3	0
59	BY	1	KBE	2	0
59	BY	6	5OH	7	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	3
35	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1916:A	O3'	1917:U	P	2.39

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	867:G	O3'	868:C	P	1.80
1	AA	867:C	O3'	868:U	P	1.76
1	AA	1911:U	O3'	1912:A	P	1.01

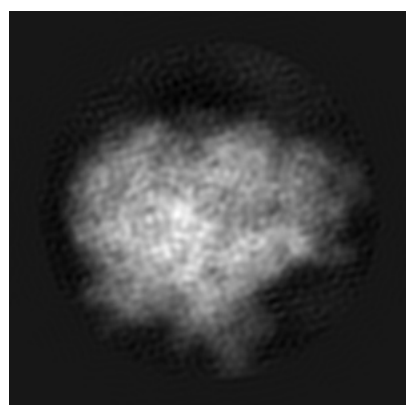
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5800. These allow visual inspection of the internal detail of the map and identification of artifacts.

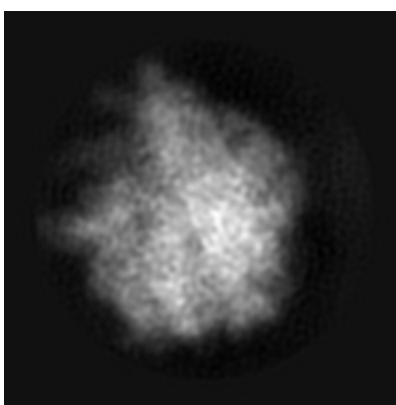
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

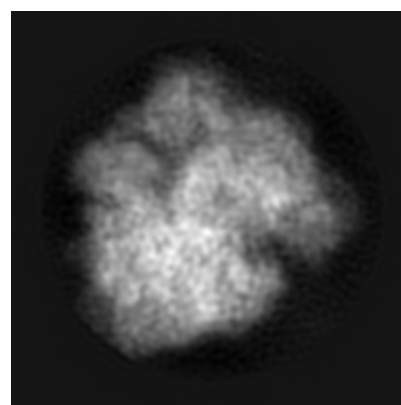
#### 6.1.1 Primary map



X



Y

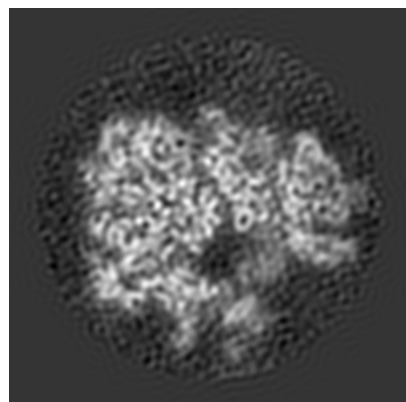


Z

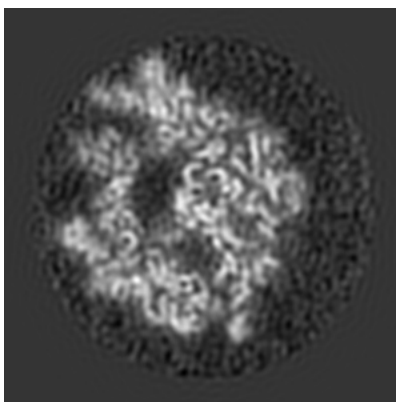
The images above show the map projected in three orthogonal directions.

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

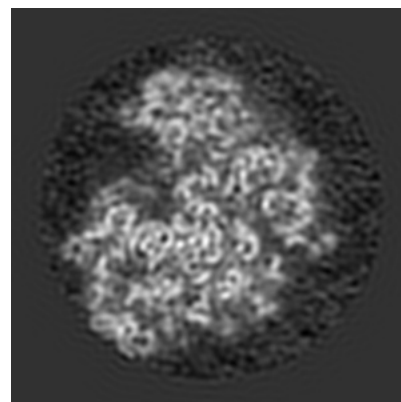
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

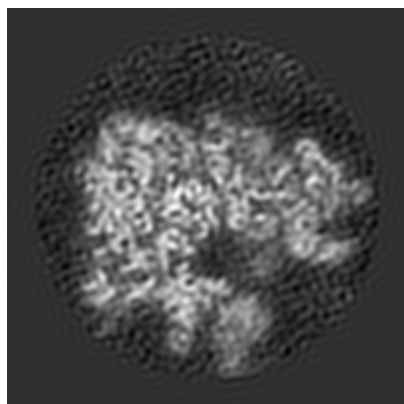


Z Index: 160

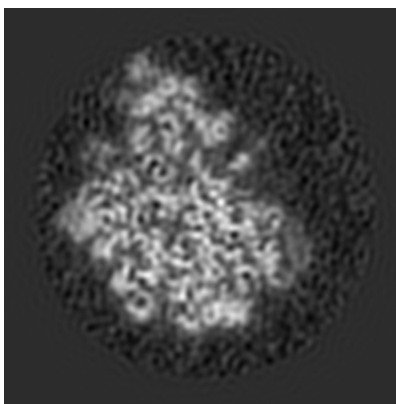
The images above show central slices of the map in three orthogonal directions.

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

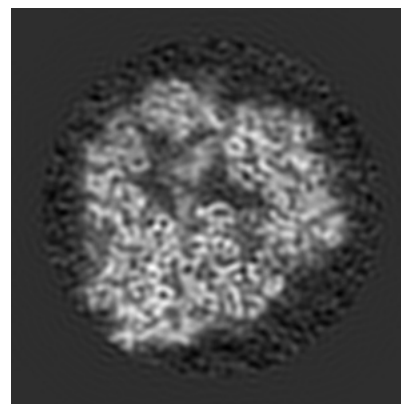
### 6.3.1 Primary map



X Index: 155



Y Index: 144

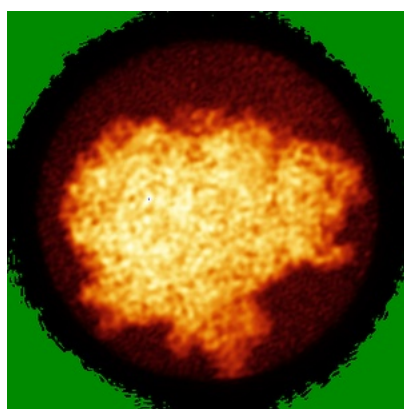


Z Index: 138

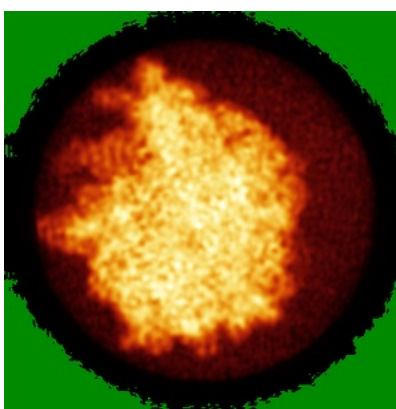
The images above show the largest variance slices of the map in three orthogonal directions.

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

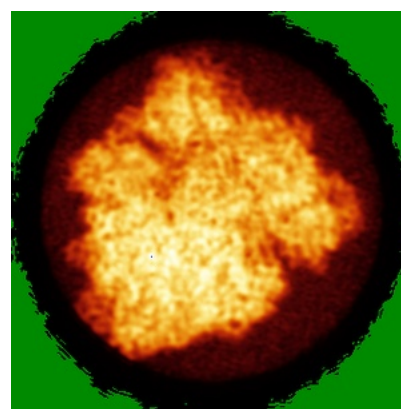
### 6.4.1 Primary map



X



Y



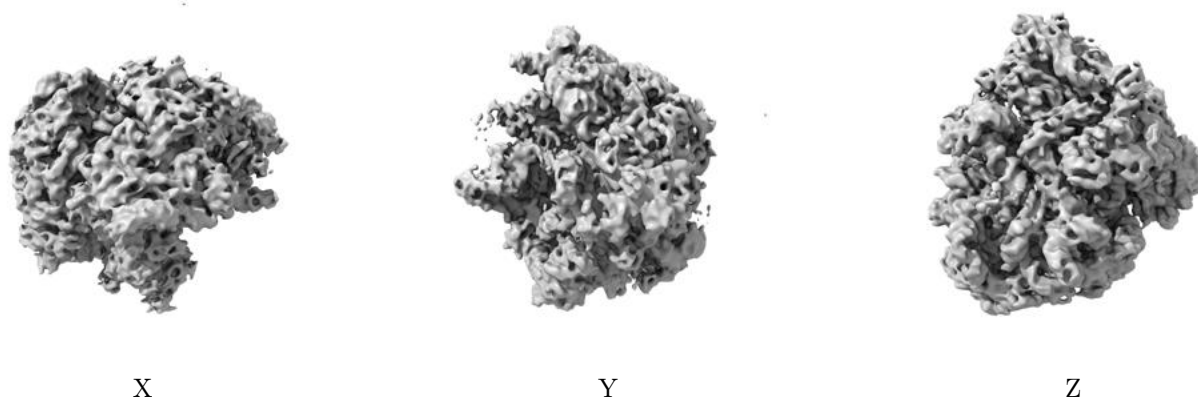
Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

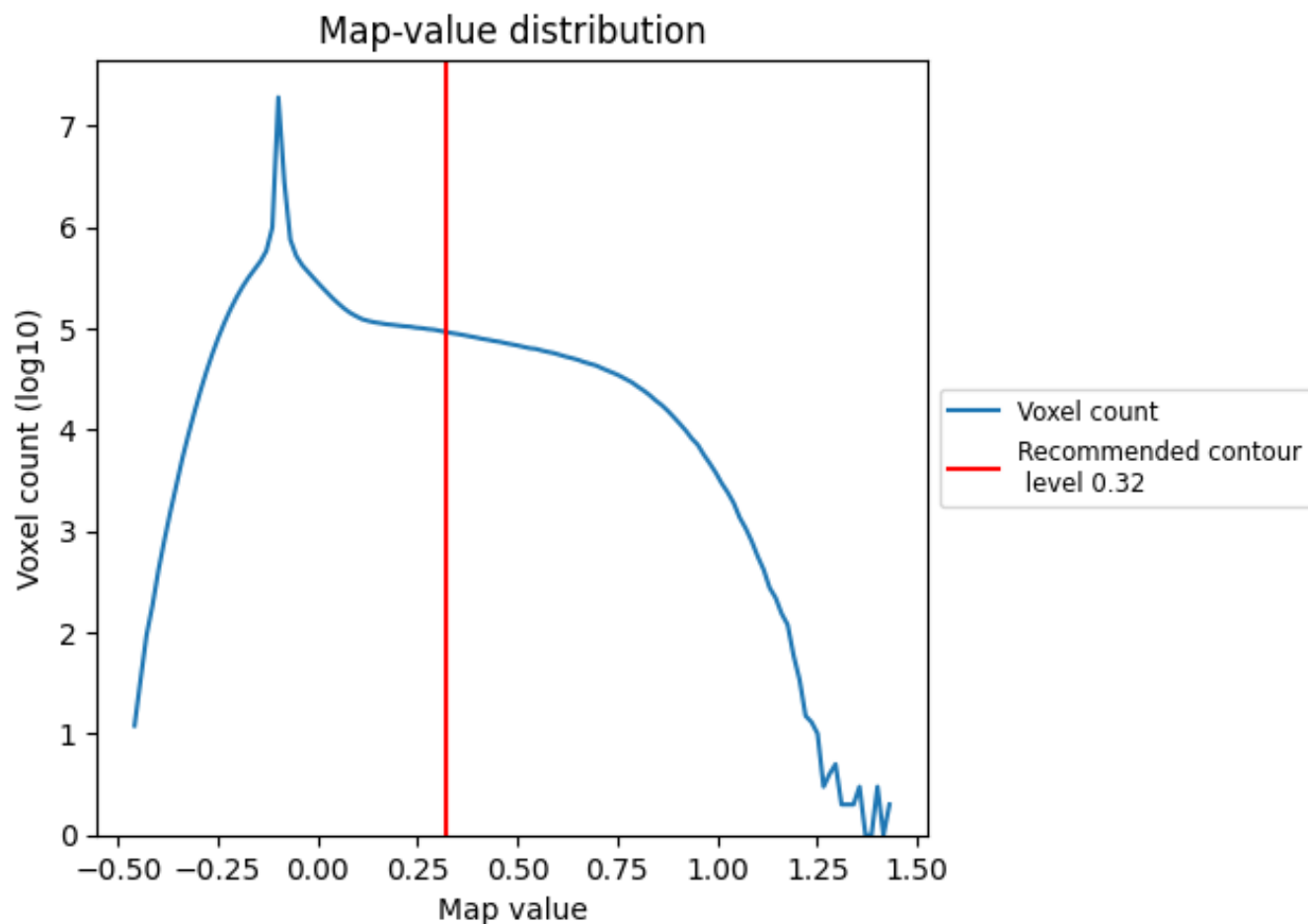
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

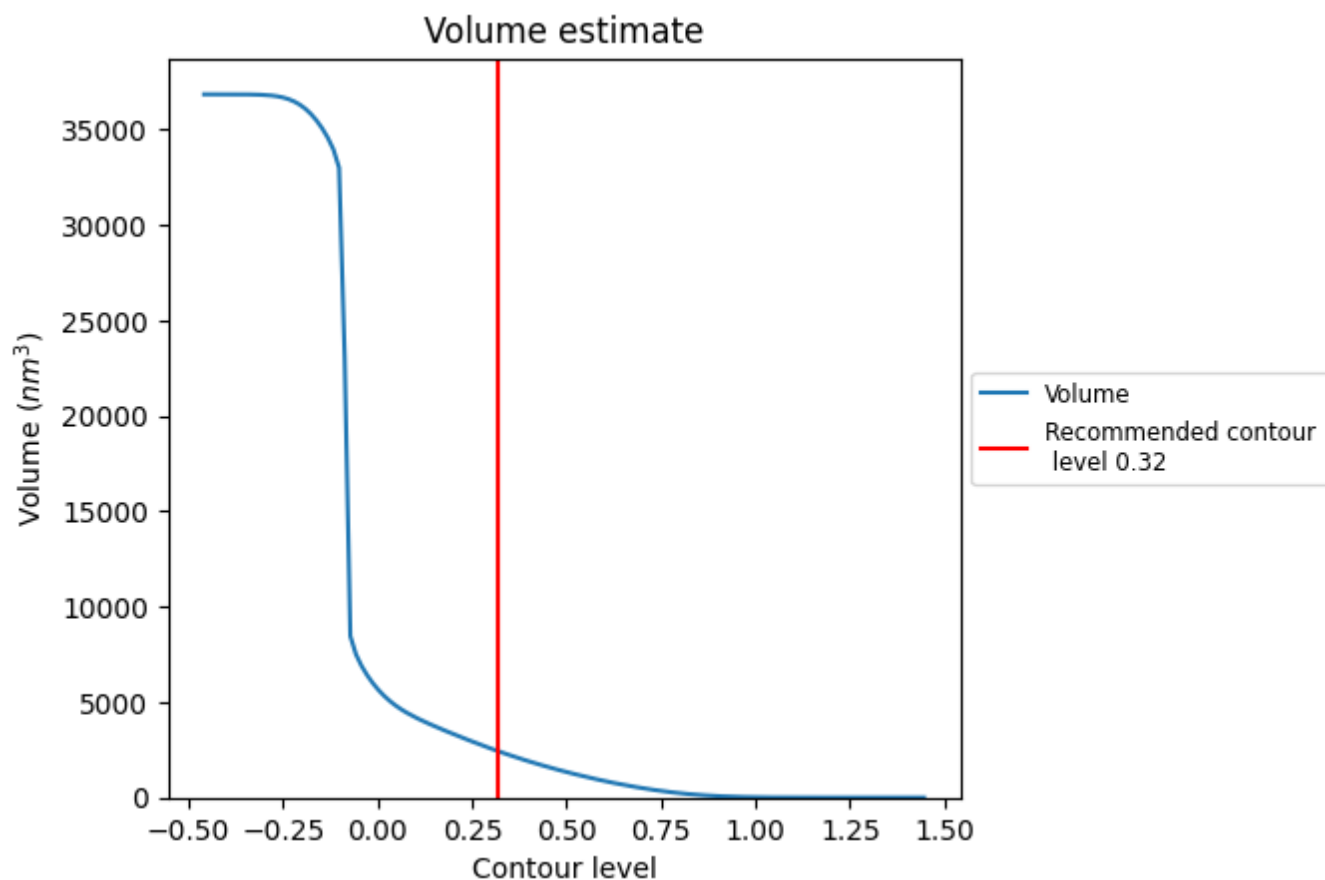
This section contains the results of statistical analysis of the map.

### 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.

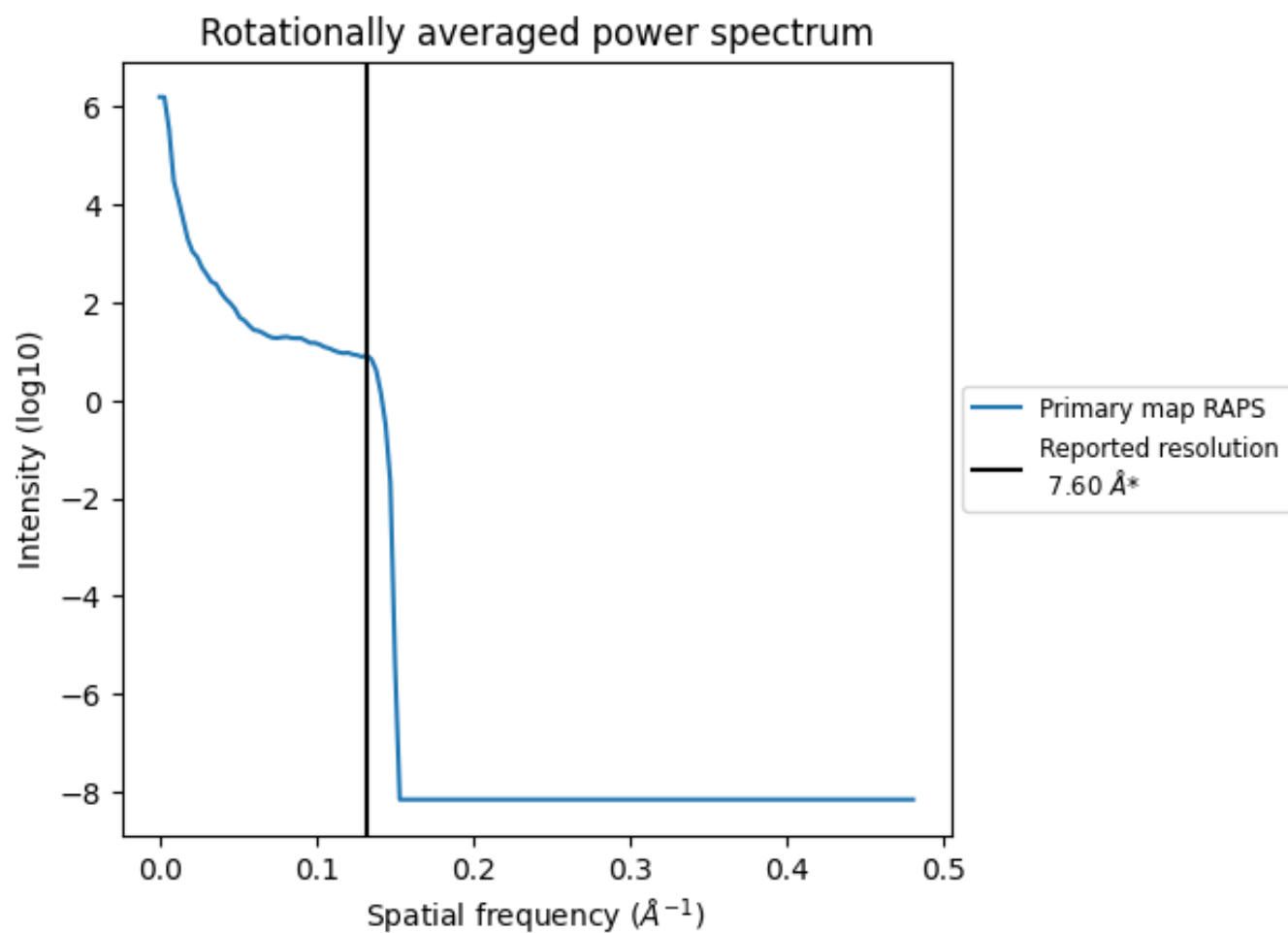
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2426 nm<sup>3</sup>; this corresponds to an approximate mass of 2192 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 0.132 Å<sup>-1</sup>

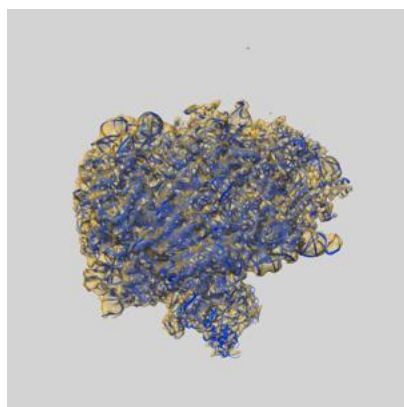
## 8 Fourier-Shell correlation

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

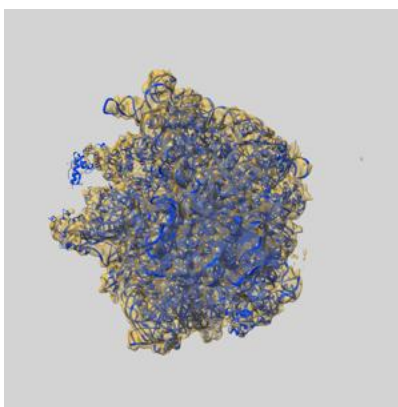
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5800 and PDB model 4V7D. Per-residue inclusion information can be found in section [3](#) on page [15](#).

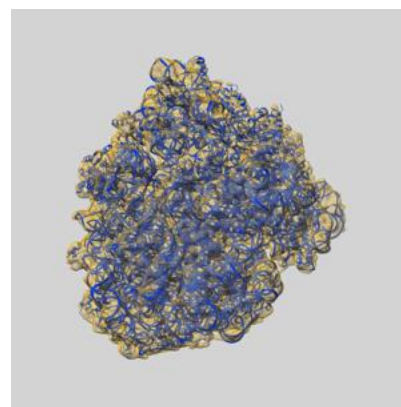
### 9.1 Map-model overlay [i](#)



X



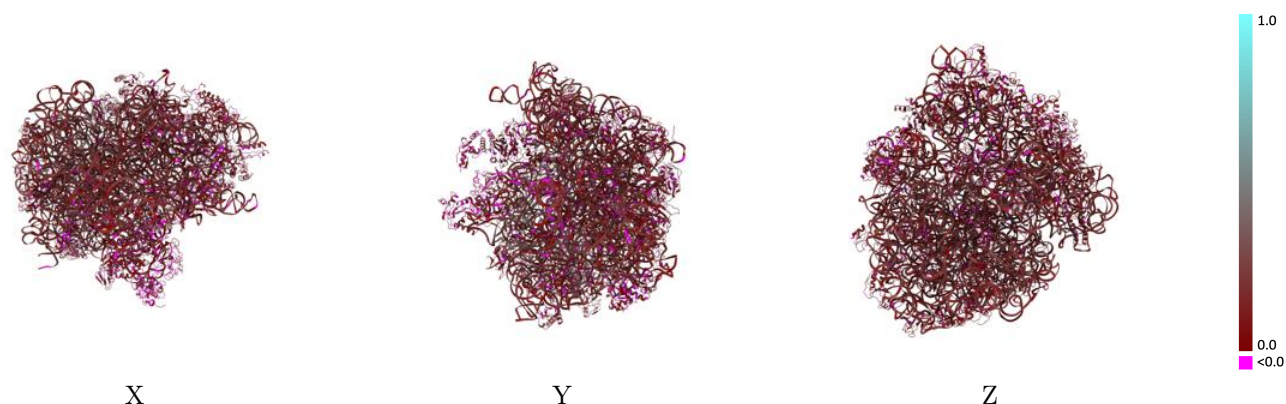
Y



Z

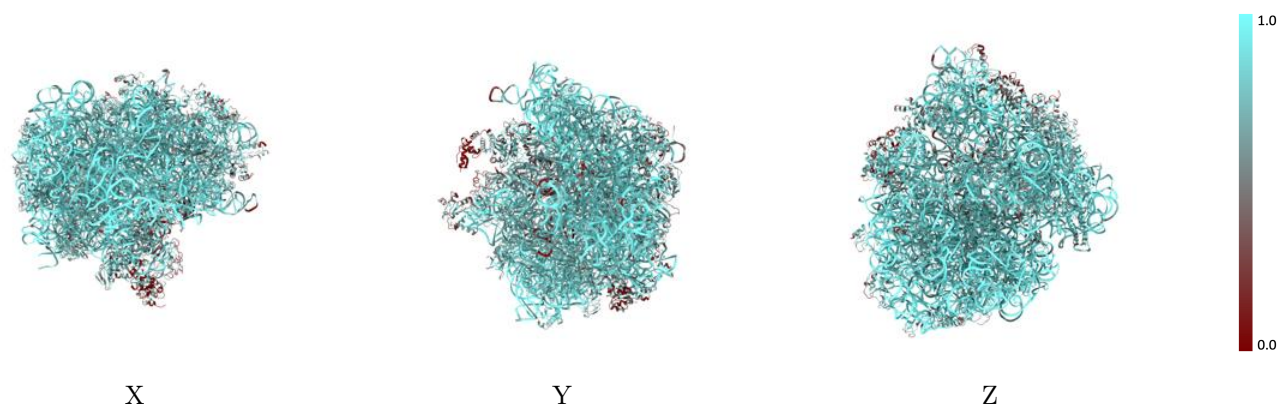
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



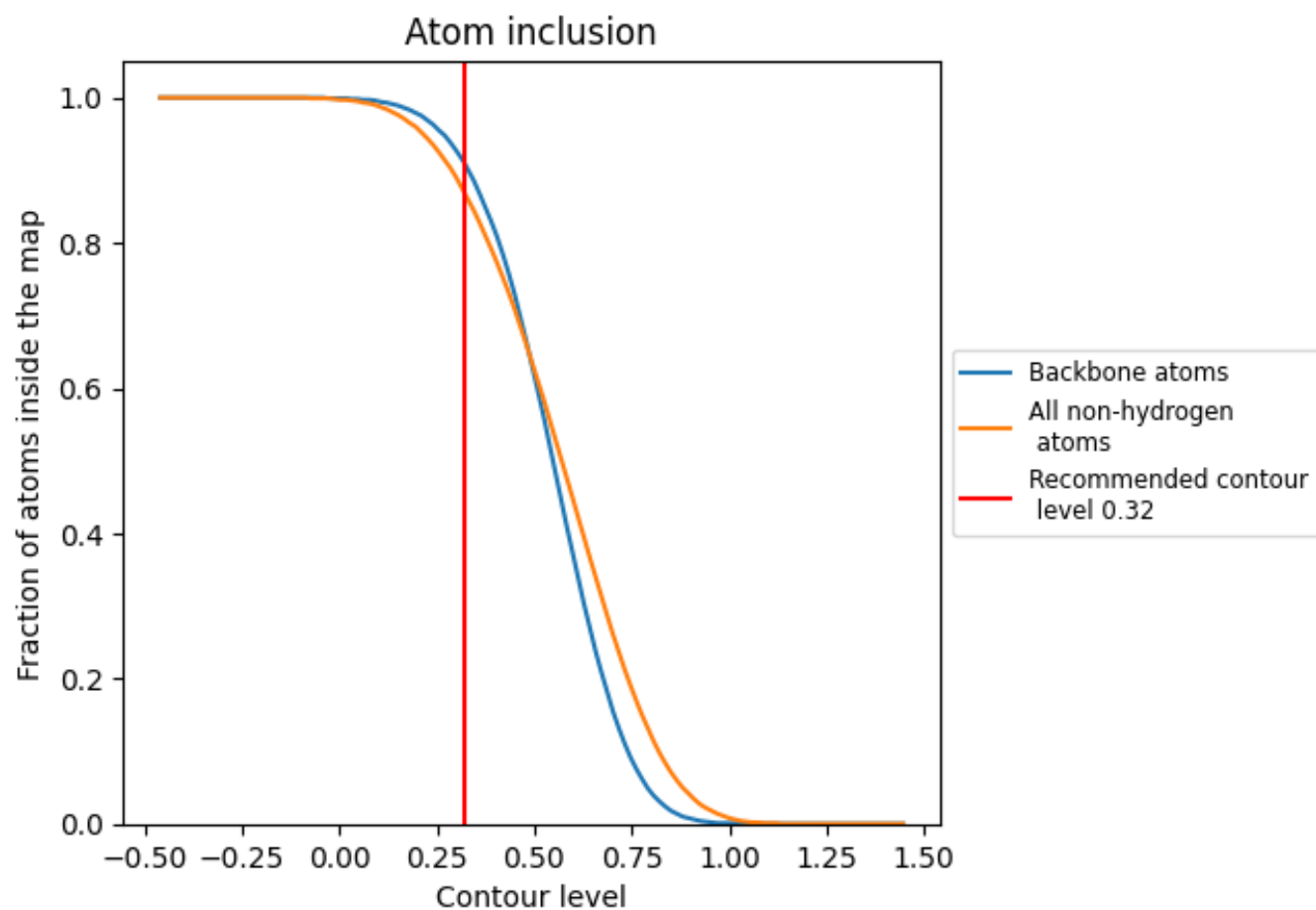
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.32).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.1650
A1	 0.7920	 0.1180
A2	 0.7360	 0.1450
A3	 0.8080	 0.1500
A4	 0.7940	 0.1300
A5	 0.5940	 0.1250
A6	 0.8700	 0.1170
A7	 0.8370	 0.1190
A8	 0.9080	 0.1140
AA	 0.9670	 0.1910
AB	 0.9650	 0.1950
AC	 0.4190	 0.0720
AD	 0.8420	 0.1300
AE	 0.7700	 0.1160
AF	 0.7720	 0.1260
AG	 0.7630	 0.1320
AH	 0.7340	 0.1370
AI	 0.5170	 0.1440
AJ	 0.4470	 0.0660
AK	 0.3950	 0.0440
AL	 0.0370	 0.0920
AM	 0.8230	 0.1330
AN	 0.7240	 0.1470
AO	 0.7960	 0.1330
AP	 0.7630	 0.1340
AQ	 0.8530	 0.1200
AR	 0.8260	 0.1340
AS	 0.7380	 0.1500
AT	 0.8630	 0.1040
AU	 0.7820	 0.1270
AV	 0.7610	 0.1260
AW	 0.7940	 0.1480
AX	 0.7550	 0.1260
AY	 0.7750	 0.1620
AZ	 0.8280	 0.1160



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Chain	Atom inclusion	Q-score
BA	 0.9510	 0.1840
BB	 0.5560	 0.1370
BC	 0.6490	 0.1310
BD	 0.7590	 0.1180
BE	 0.7440	 0.1380
BF	 0.6530	 0.1410
BG	 0.7030	 0.1420
BH	 0.7530	 0.1460
BI	 0.7780	 0.1070
BJ	 0.6020	 0.0740
BK	 0.7570	 0.1390
BL	 0.7630	 0.1320
BM	 0.7060	 0.1400
BN	 0.7940	 0.1140
BO	 0.7450	 0.1460
BP	 0.8520	 0.1390
BQ	 0.7590	 0.1300
BR	 0.7180	 0.1290
BS	 0.7390	 0.1200
BT	 0.7970	 0.1540
BU	 0.5860	 0.1290
BV	 0.6990	 0.1090
BW	 0.9400	 0.2020
BX	 0.8390	 0.1410
BY	 0.8960	 0.1980
BZ	 0.5310	 0.0990