



# wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 12:08 PM EST

PDB ID : 4V76  
EMDB ID : EMD-1722  
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post2a)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 17.00 Å (reported)  
Based on initial models : 2HGP, 2K4C, 3I1O, 2WRI

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 : 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) : 2.39

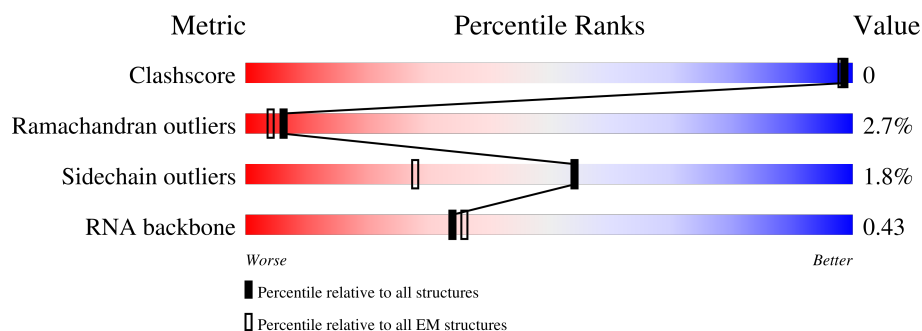
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 17.00 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	AB	220	<div> <div>54%</div> <div>91%</div> <div>9%</div> </div>
2	AC	208	<div> <div>50%</div> <div>90%</div> <div>9%</div> </div>
3	AD	206	<div> <div>52%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
4	AE	152	<div> <div>42%</div> <div>91%</div> <div>9%</div> </div>
5	AF	101	<div> <div>18%</div> <div>87%</div> <div>13%</div> </div>
6	AG	152	<div> <div>25%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
7	AH	130	<div> <div>39%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	AI	128	
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG	177	
30	BH	149	
31	BI	142	
32	BJ	142	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	BK	123	
34	BL	144	
35	BM	136	
36	BN	121	
37	BO	117	
38	BP	115	
39	BQ	118	
40	BR	103	
41	BS	110	
42	BT	94	
43	BU	104	
44	BV	94	
45	BW	80	
46	BX	79	
47	BY	63	
48	BZ	59	
49	B0	57	
50	B1	52	
51	B2	46	
52	B3	65	
53	B4	38	
54	BA	2903	
55	BB	118	
56	B5	234	

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	acetylation	UNP P0A7V0
AB	226	NH2	-	amidation	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	amidation	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total	C	N	O	S	0	1
			1109	689	212	202	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	acetylation	UNP P0A7W1
AE	159	NH2	-	amidation	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	amidation	UNP P02358

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total	C	N	O	S	0	1
			1178	732	227	215	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	acetylation	UNP P02359
AG	152	NH2	-	amidation	UNP P02359

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total	C	N	O	S	0	0
			1025	636	206	180	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	acetylation	UNP P0A7X3

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total	C	N	O	S	0	1
			790	495	151	143	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	acetylation	UNP P0A7R5
AJ	103	NH2	-	amidation	UNP P0A7R5

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total	C	N	O	S	0	0
			880	542	174	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	acetylation	UNP P0A7R9

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	114	Total	C	N	O	S	0	1
			877	541	178	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	amidation	UNP P0A7S9

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	81	Total	C	N	O	S	0	1
			639	400	127	111	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	amidation	UNP P0A7T3

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1
			652	413	122	114	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	acetylation	UNP P0AG63
AQ	83	NH2	-	amidation	UNP P0AG63

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AR	57	Total	C	N	O		0	1
			459	290	87	82			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	18	ACE	-	acetylation	UNP P0A7T7

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	amidation	UNP P0A7T7

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total	C	N	O	S	0	1
			641	410	121	108	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	acetylation	UNP P0A7U3
AS	81	NH2	-	amidation	UNP P0A7U3

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	86	Total	C	N	O	S	0	0
			668	413	137	115	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	acetylation	UNP P0A7U7

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total	C	N	O	S	0	1
			429	267	87	74	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	acetylation	UNP P68679
AU	54	NH2	-	amidation	UNP P68679

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32828	14642	6024	10633	1529		

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

- Molecule 23 is a RNA chain called 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P	0	0
			309	140	46	109	14		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1642	734	297	534	76	1		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	272	Total	C	N	O	S	0	1
			2083	1288	424	364	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	272	NH2	-	amidation	UNP P60422

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

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

- Molecule 31 is a protein called 50S ribosomal protein L11.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	123	Total	C	N	O	S	0	1
			939	587	181	165	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	123	NH2	-	amidation	UNP P0ADY3

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BN	121	Total	C	N	O	S	0	1
			961	593	197	166	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	121	NH2	-	amidation	UNP P0AG44

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BT	94	Total	C	N	O	S	0	1
			739	466	140	131	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	94	NH2	-	amidation	UNP P0ADZ0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BU	103	Total	C	N	O	0	1
			780	492	147	141		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	103	NH2	-	amidation	UNP P60624

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	80	Total	C	N	O	S	0	0
			599	369	120	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	5	ACE	-	acetylation	UNP P0A7L8

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BX	-1	ACE	-	acetylation	UNP P0A7M2

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	B1	52	Total	C	N	O	0	1
			413	265	76	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	acetylation	UNP P0A7N9
B1	53	NH2	-	amidation	UNP P0A7N9

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BA	2903	Total	C	N	O	P	0	0
			62317	27801	11467	20147	2902		

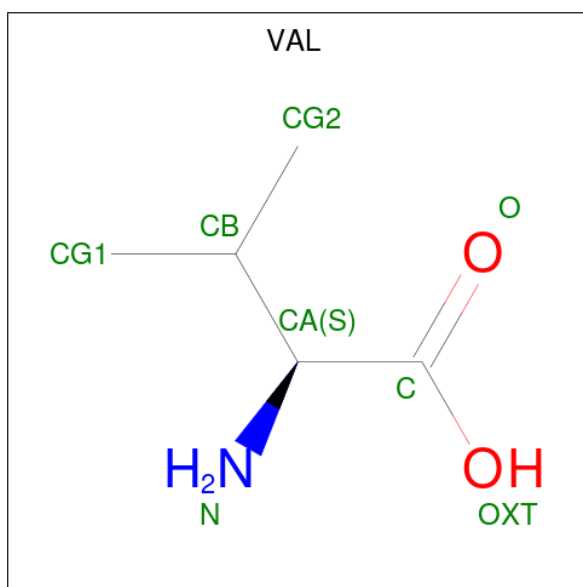
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BB	117	Total	C	N	O	P	0	0
			2504	1116	459	813	116		

- Molecule 56 is a protein called 50S ribosomal protein L1.

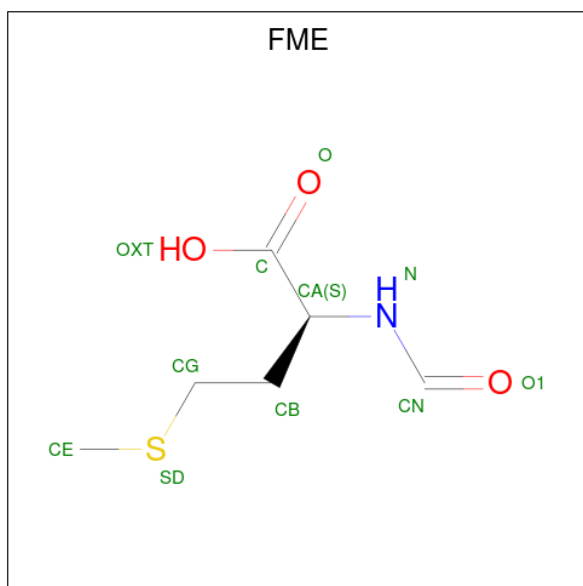
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
57	A1	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



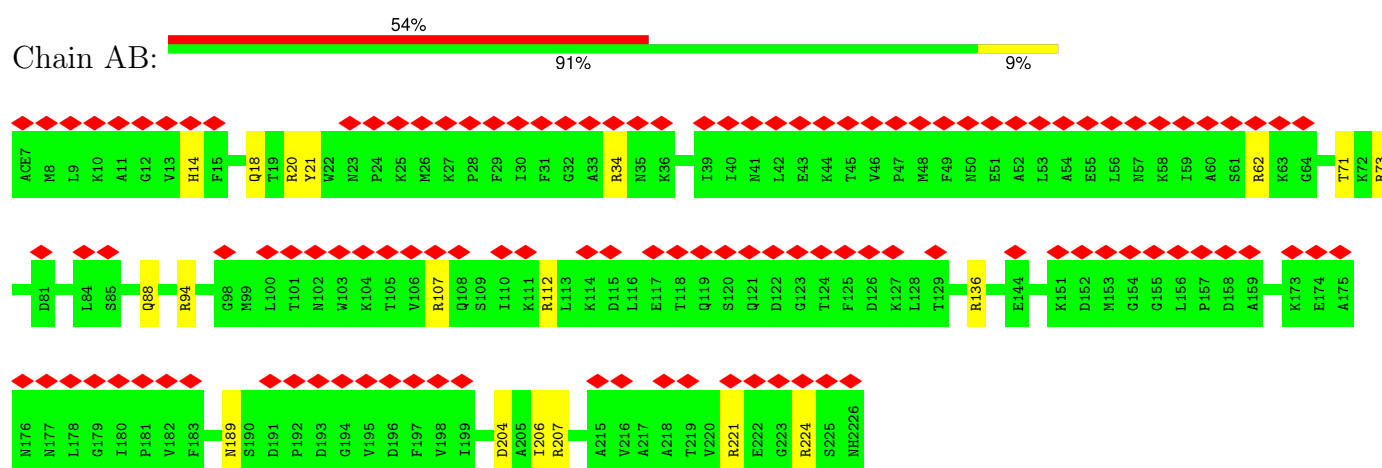
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



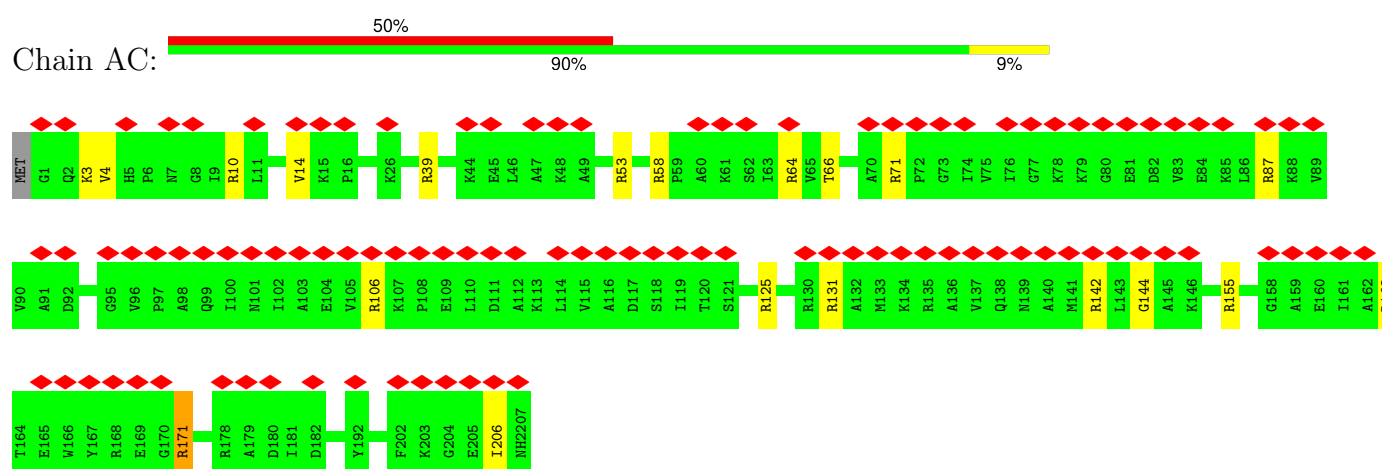
### 3 Residue-property plots

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.

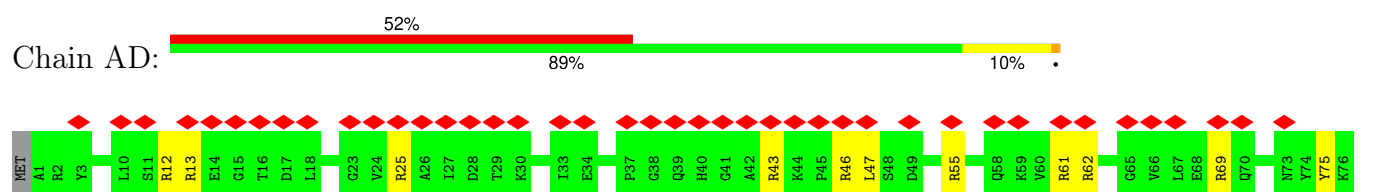
#### • Molecule 1: 30S ribosomal protein S2

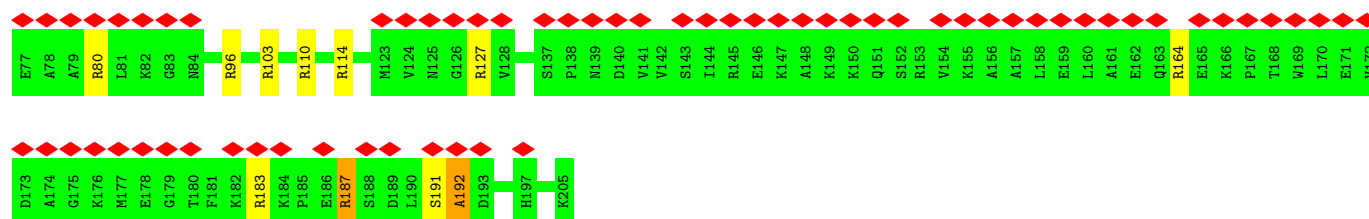


#### • Molecule 2: 30S ribosomal protein S3

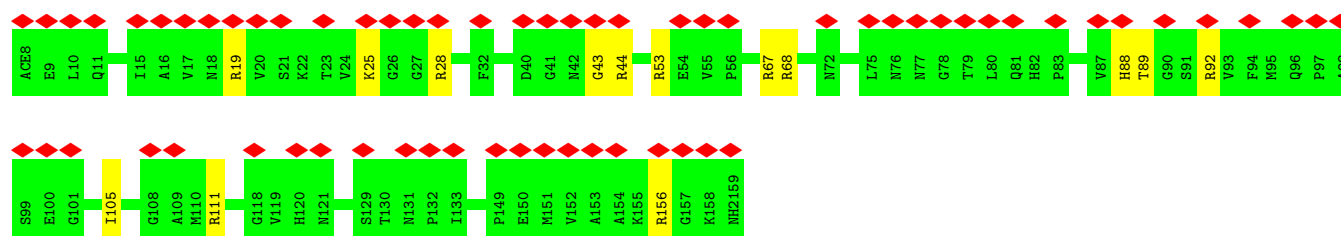
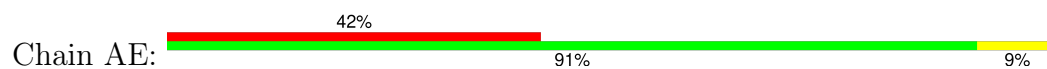


#### • Molecule 3: 30S ribosomal protein S4

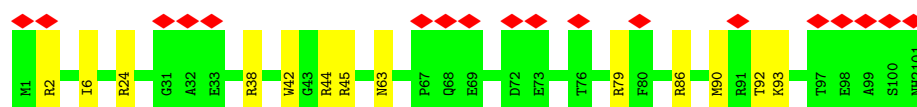
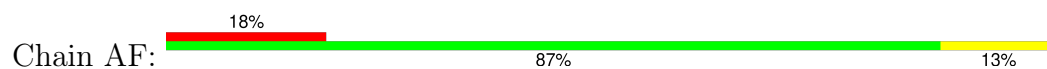




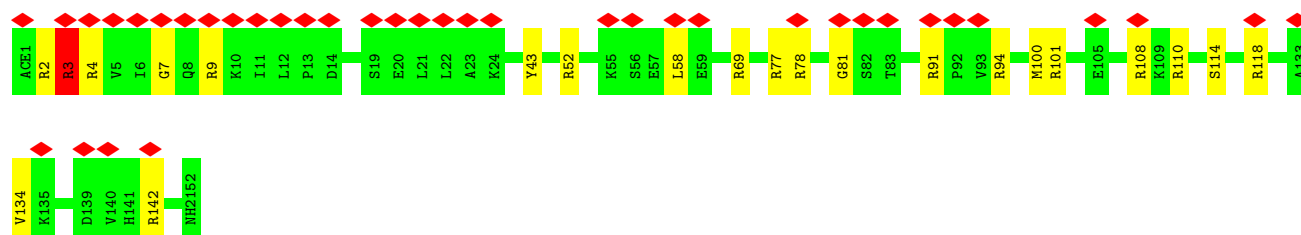
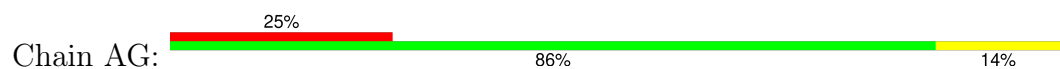
• Molecule 4: 30S ribosomal protein S5



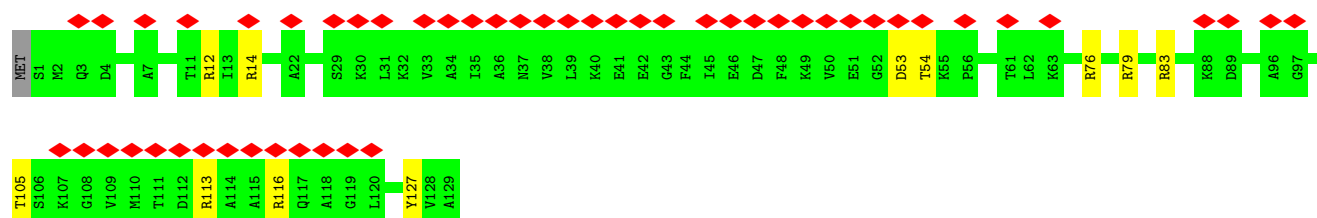
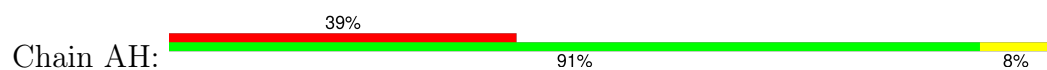
• Molecule 5: 30S ribosomal protein S6



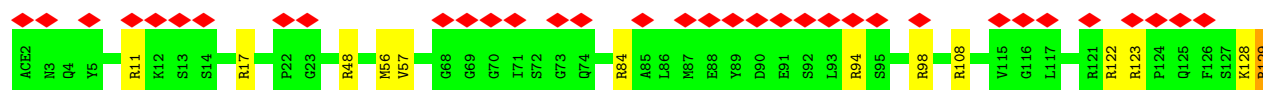
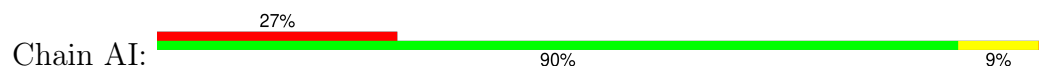
• Molecule 6: 30S ribosomal protein S7



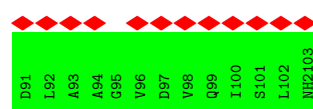
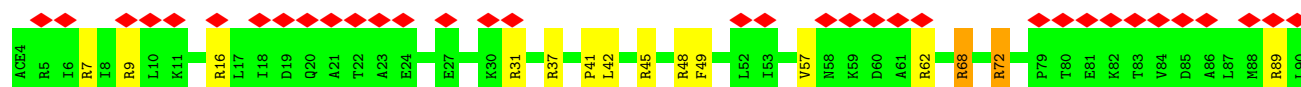
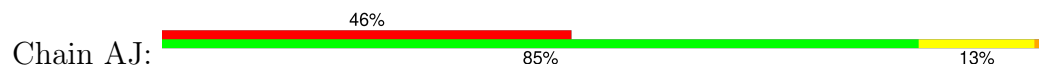
• Molecule 7: 30S ribosomal protein S8



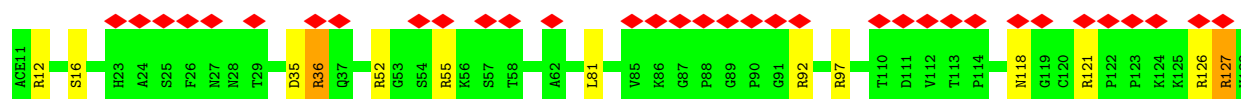
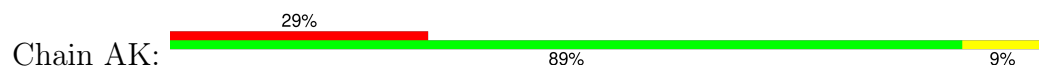
- Molecule 8: 30S ribosomal protein S9



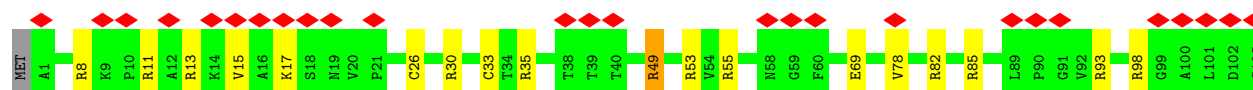
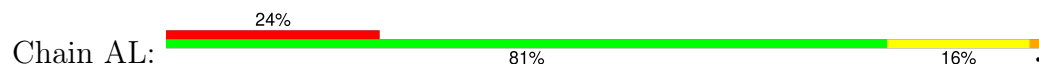
- Molecule 9: 30S ribosomal protein S10



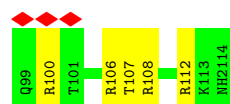
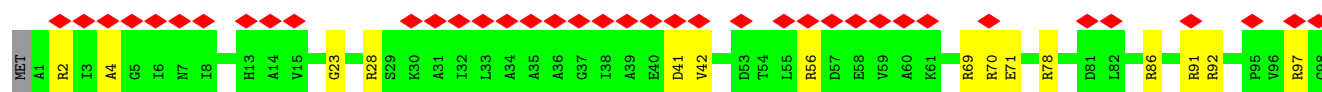
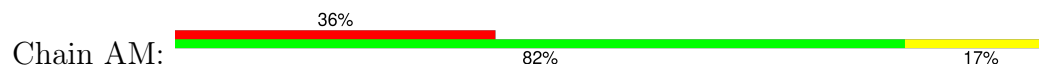
- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12

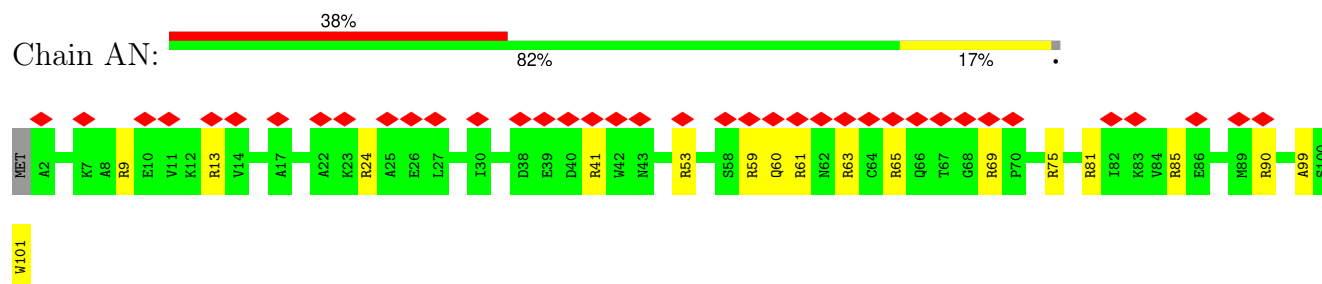


- Molecule 12: 30S ribosomal protein S13



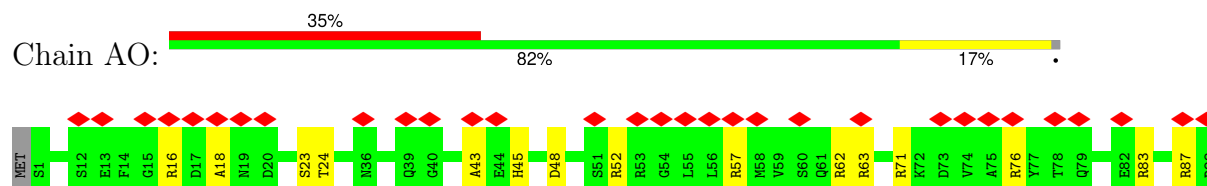
- Molecule 13: 30S ribosomal protein S14

Chain AN:



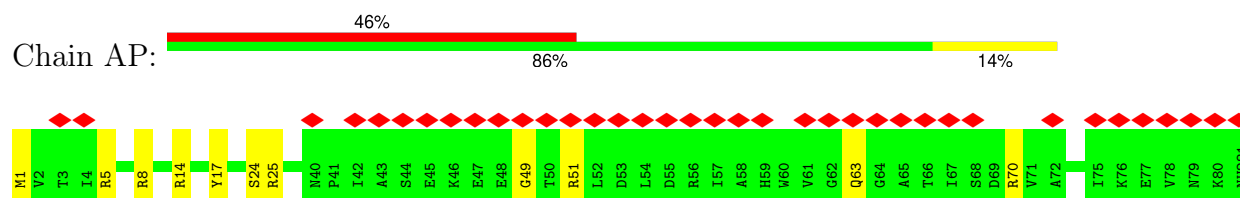
- Molecule 14: 30S ribosomal protein S15

Chain AO:



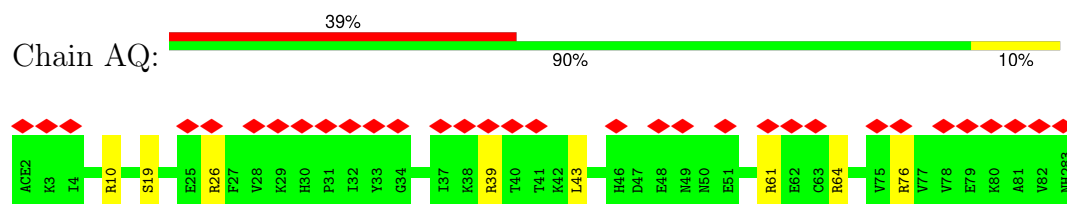
- Molecule 15: 30S ribosomal protein S16

Chain AP:



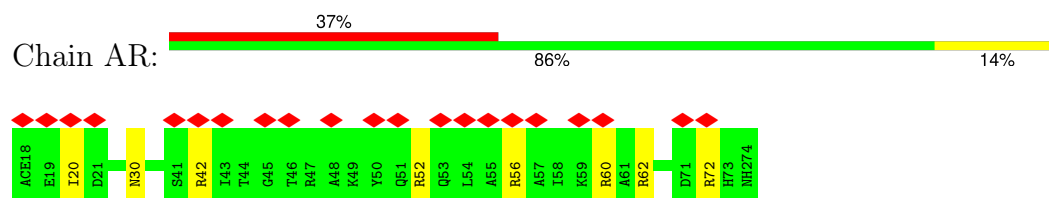
- Molecule 16: 30S ribosomal protein S17

Chain AQ:



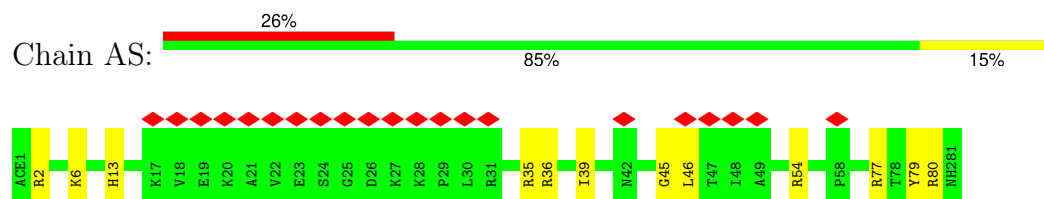
- Molecule 17: 30S ribosomal protein S18

Chain AR:

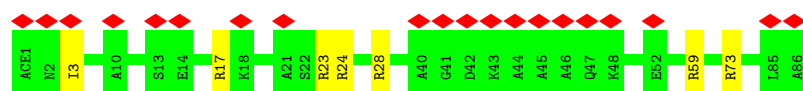


- Molecule 18: 30S ribosomal protein S19

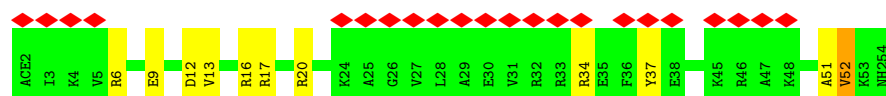
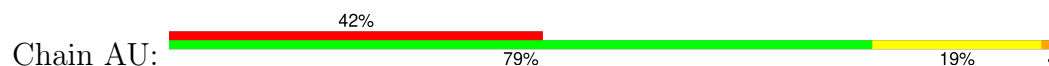
Chain AS:



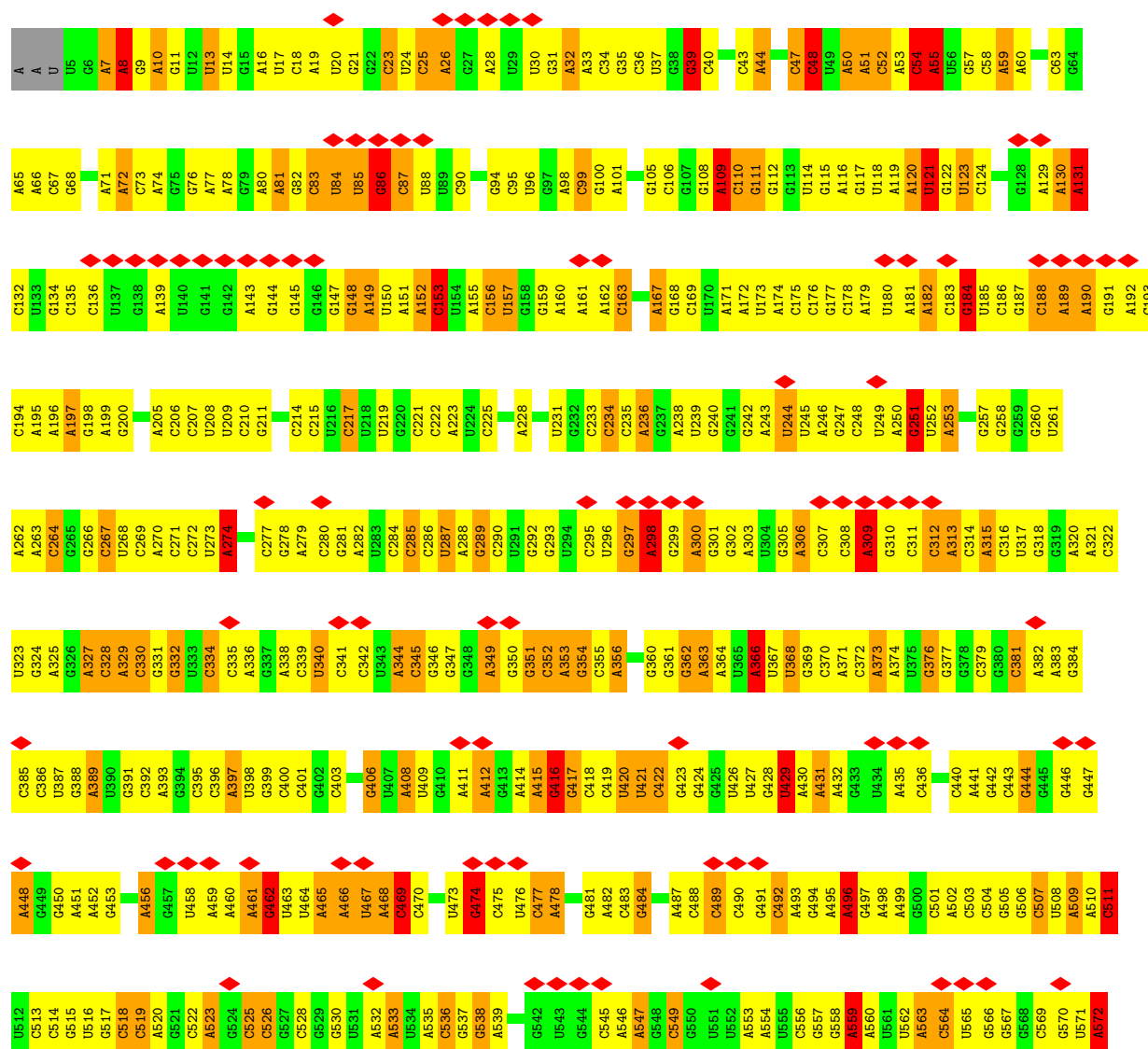
- Molecule 19: 30S ribosomal protein S20

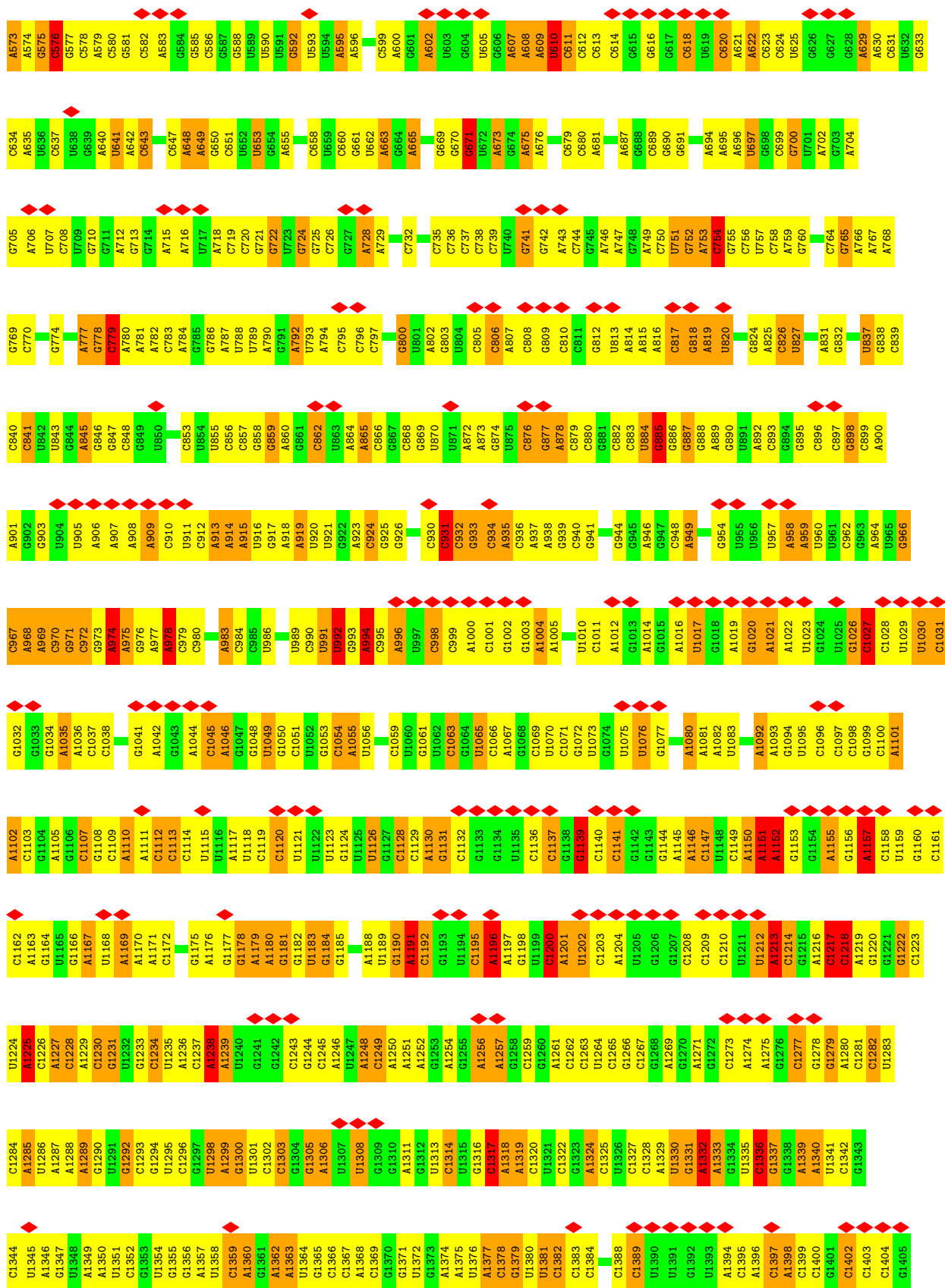


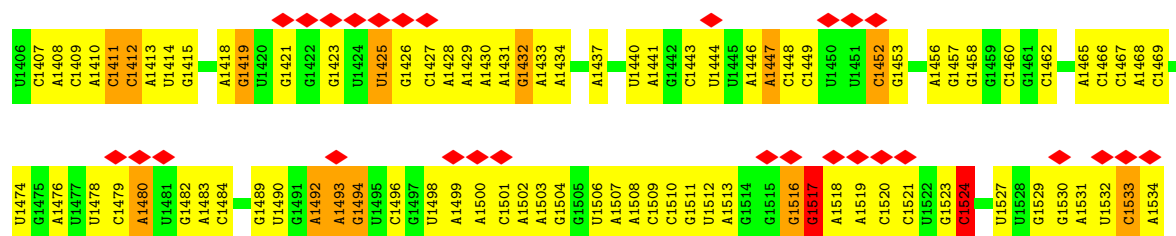
- Molecule 20: 30S ribosomal protein S21



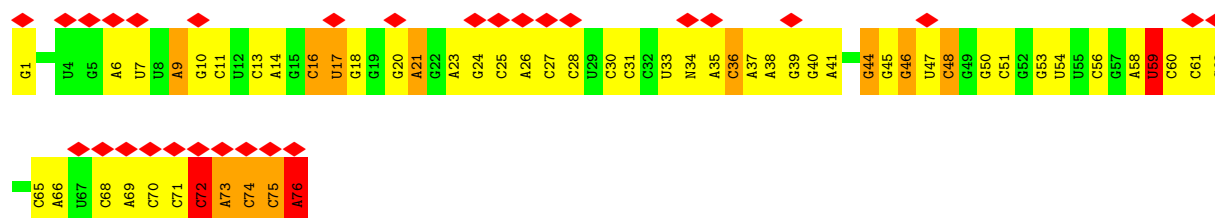
- Molecule 21: 16S ribosomal RNA



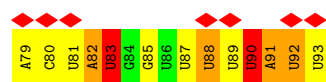
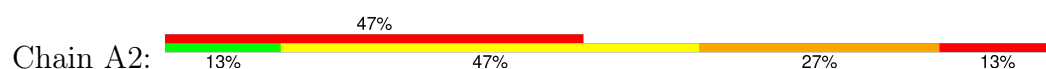




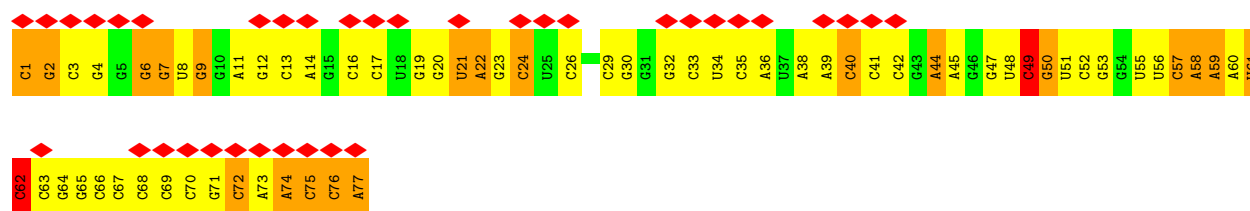
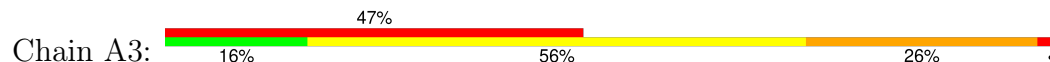
• Molecule 22: fMet-Val-tRNA-Val



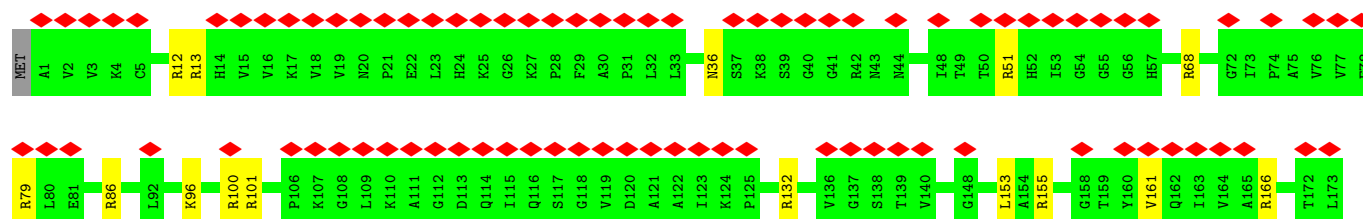
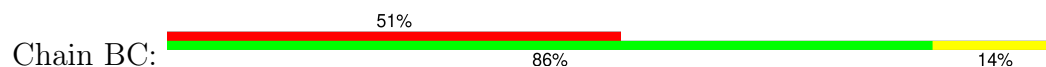
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

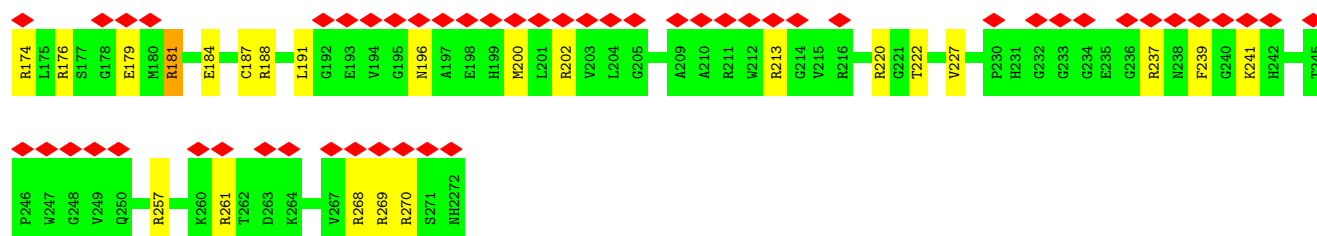


• Molecule 24: tRNA-fMet

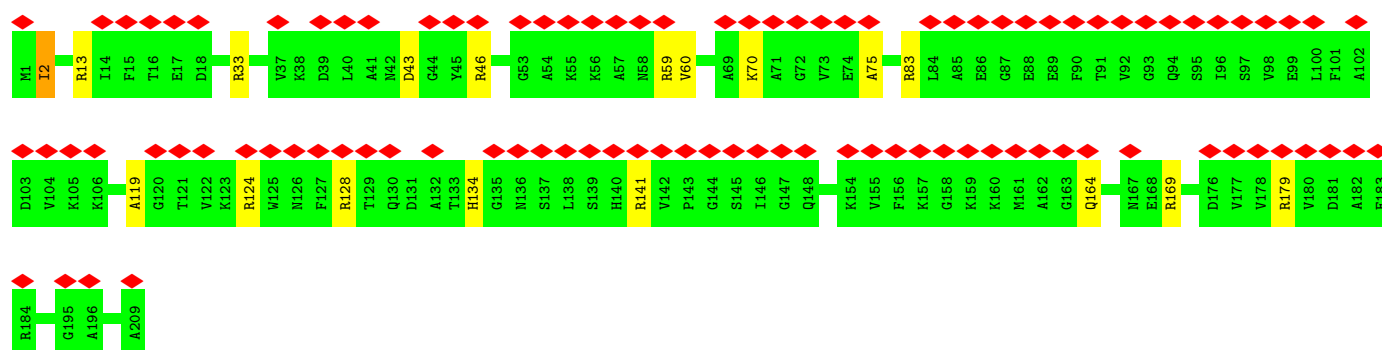


• Molecule 25: 50S ribosomal protein L2

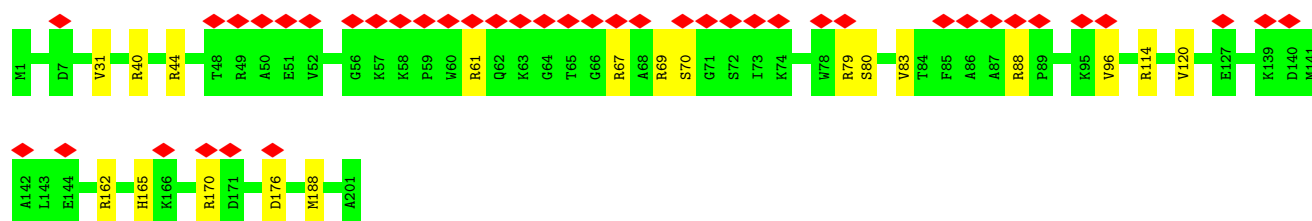




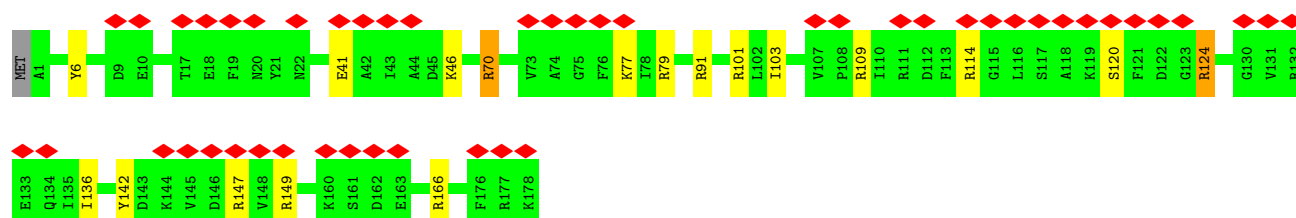
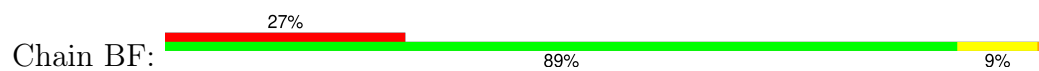
• Molecule 26: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L4



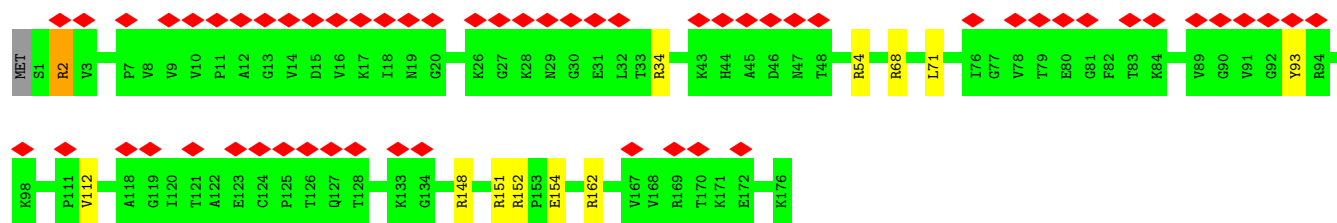
• Molecule 28: 50S ribosomal protein L5



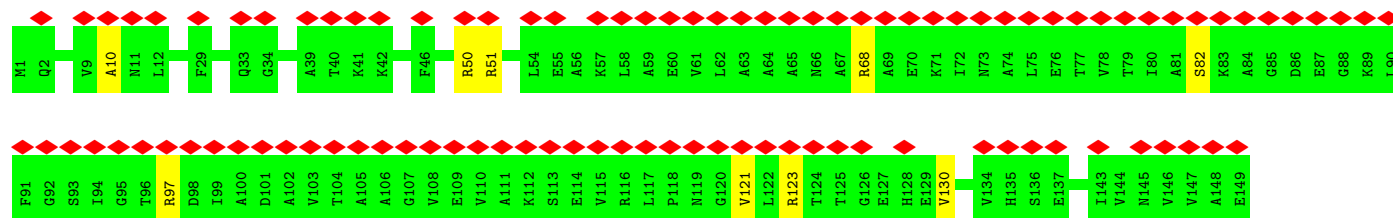
• Molecule 29: 50S ribosomal protein L6



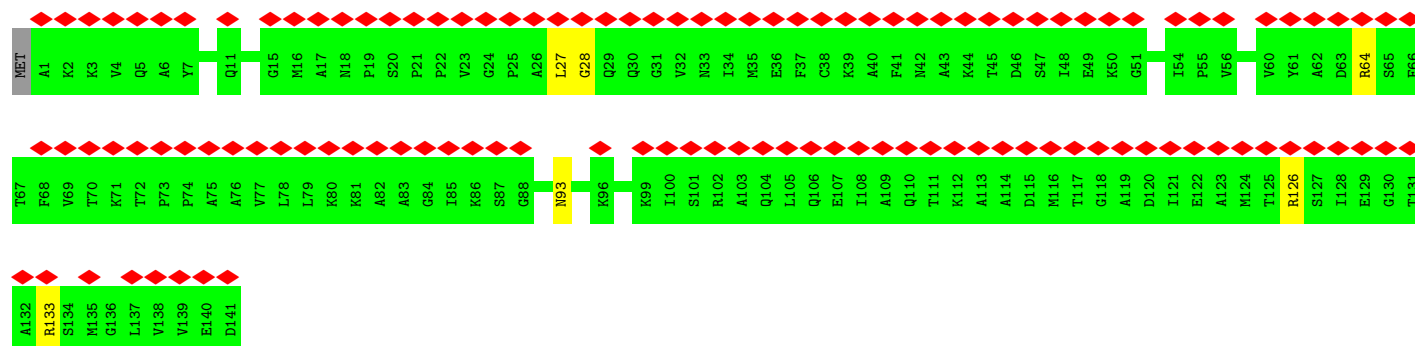
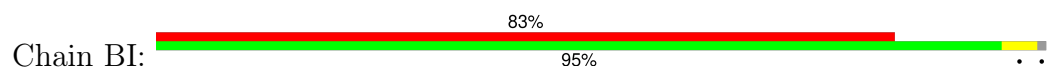




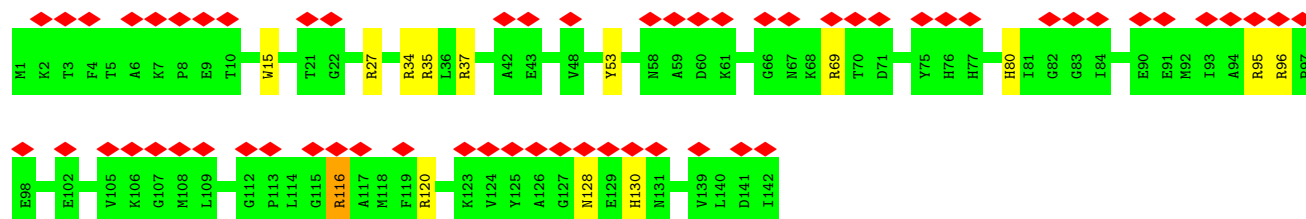
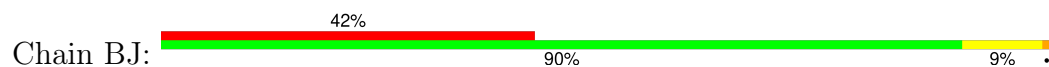
• Molecule 30: 50S ribosomal protein L9



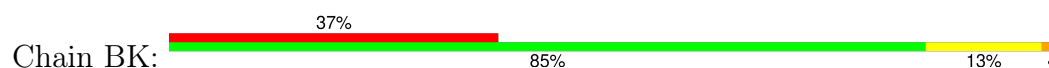
• Molecule 31: 50S ribosomal protein L11

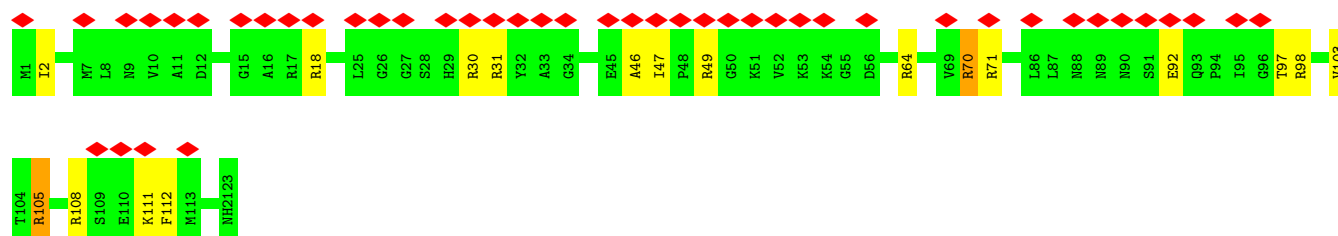


• Molecule 32: 50S ribosomal protein L13

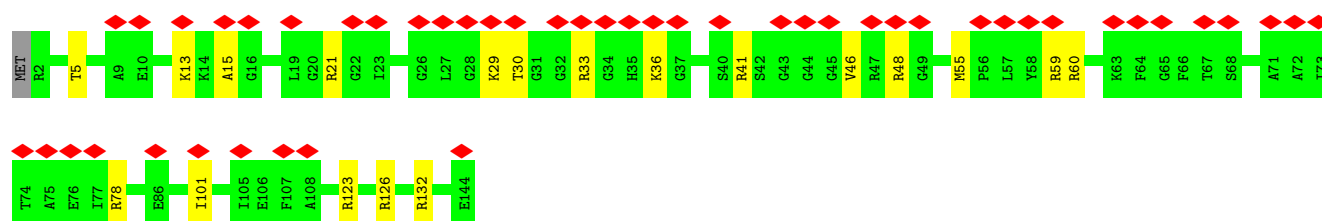
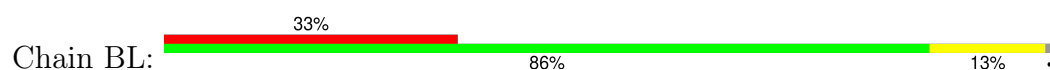


• Molecule 33: 50S ribosomal protein L14

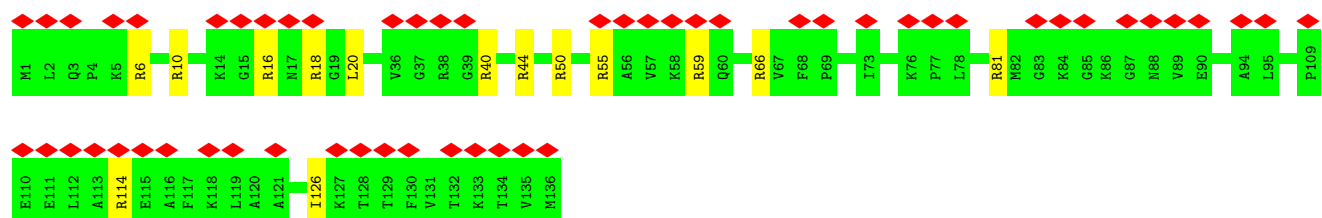
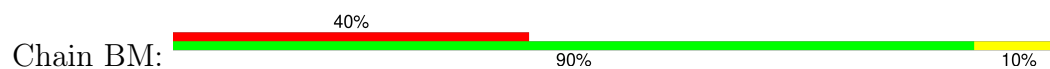




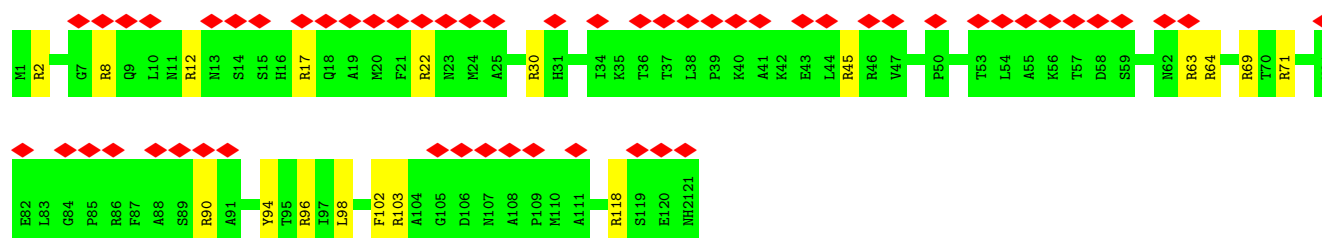
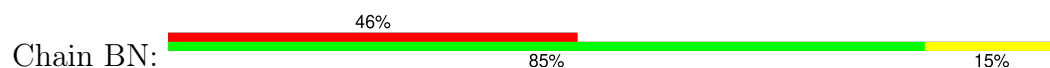
- Molecule 34: 50S ribosomal protein L15



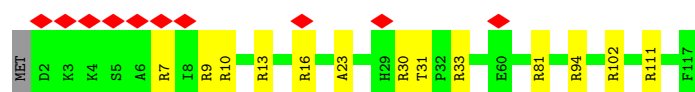
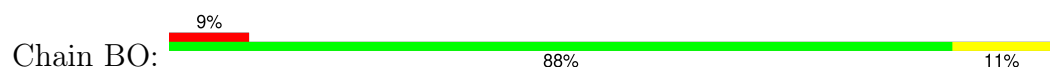
- Molecule 35: 50S ribosomal protein L16




- Molecule 36: 50S ribosomal protein L17

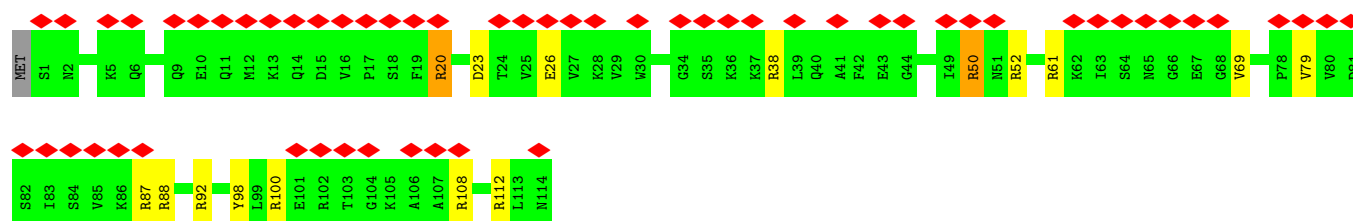


- Molecule 37: 50S ribosomal protein L18




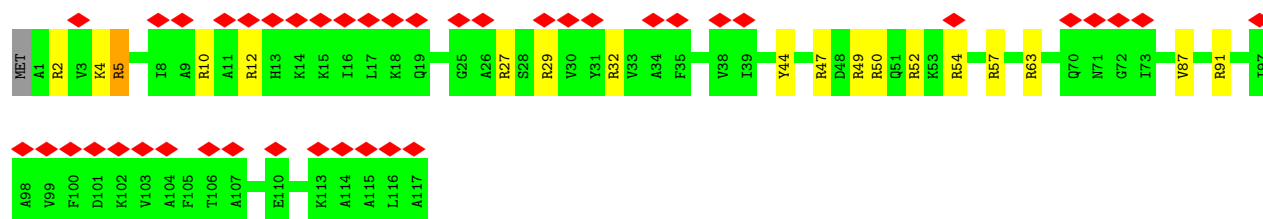
- Molecule 38: 50S ribosomal protein L19

Chain BP: 



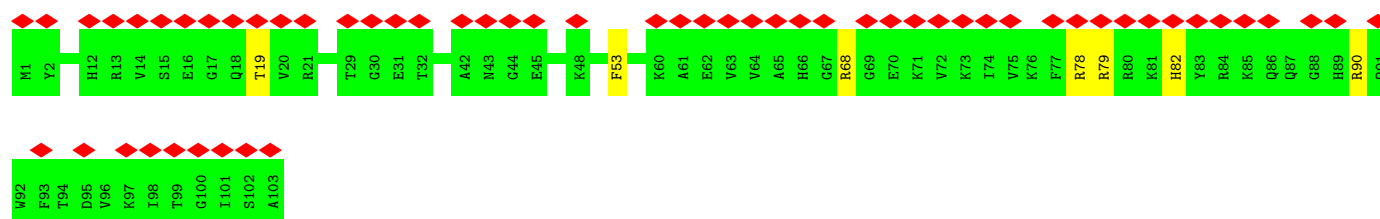
- Molecule 39: 50S ribosomal protein L20

Chain BQ: 




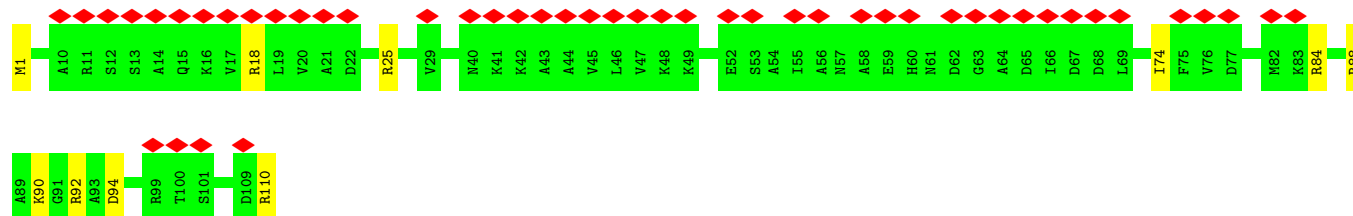
- Molecule 40: 50S ribosomal protein L21

Chain BR: 




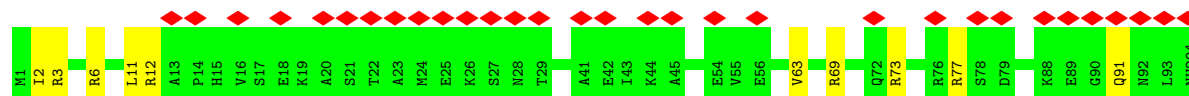
- Molecule 41: 50S ribosomal protein L22

Chain BS: 

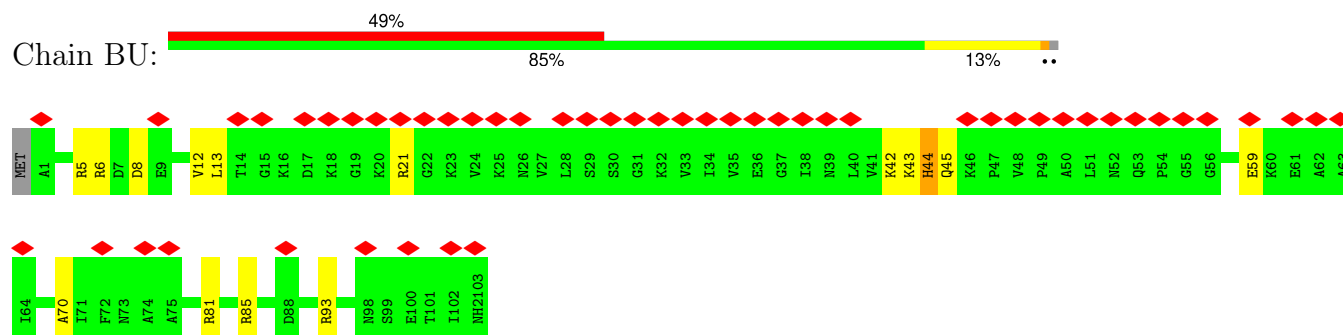


- Molecule 42: 50S ribosomal protein L23

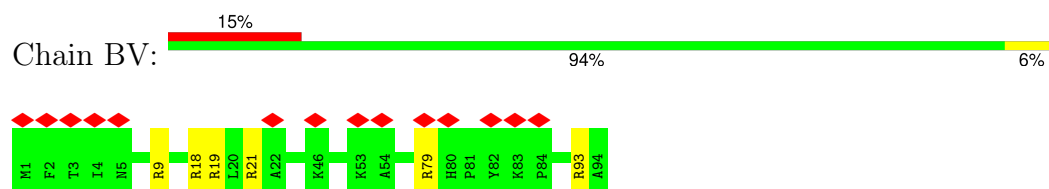
Chain BT: 



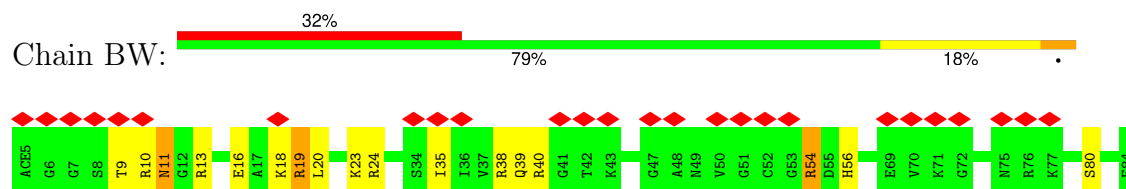
- Molecule 43: 50S ribosomal protein L24



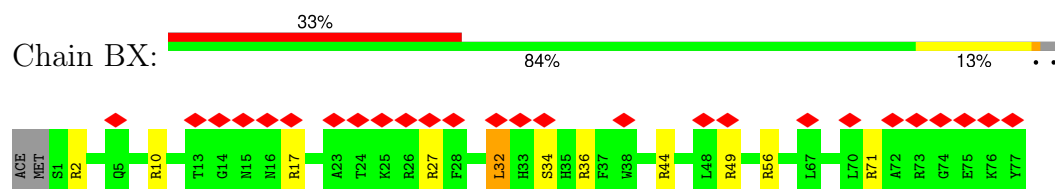
- Molecule 44: 50S ribosomal protein L25



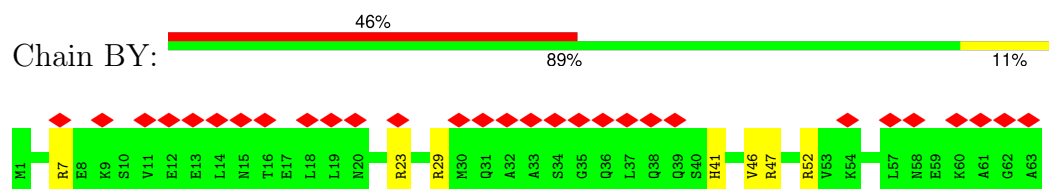
- Molecule 45: 50S ribosomal protein L27



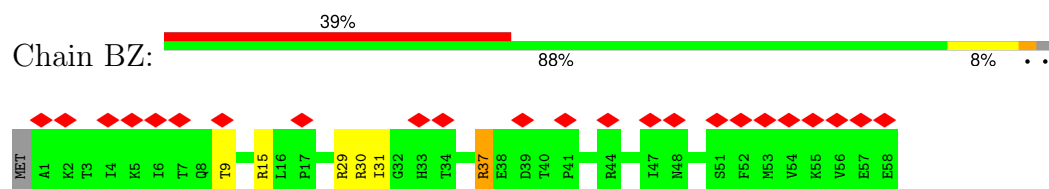
- Molecule 46: 50S ribosomal protein L28



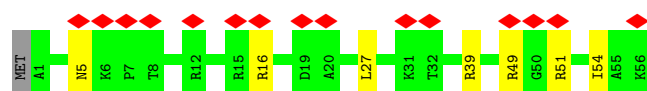
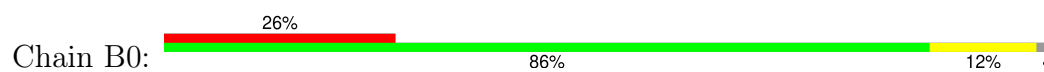
- Molecule 47: 50S ribosomal protein L29



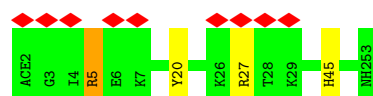
- Molecule 48: 50S ribosomal protein L30



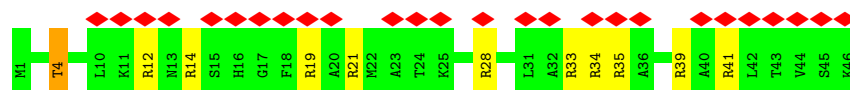
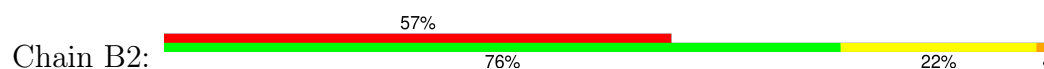
- Molecule 49: 50S ribosomal protein L32



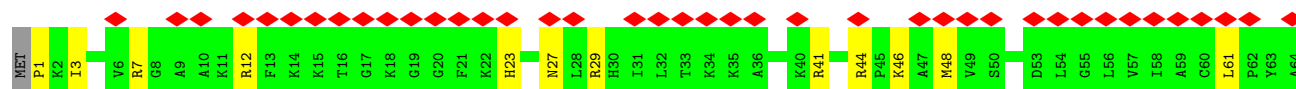
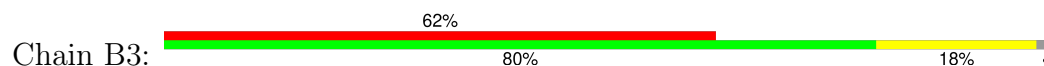
- Molecule 50: 50S ribosomal protein L33



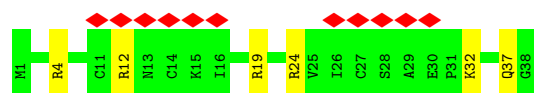
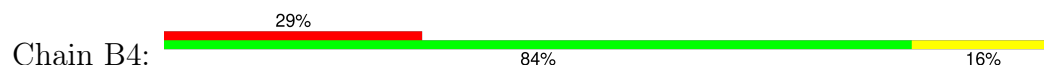
- Molecule 51: 50S ribosomal protein L34



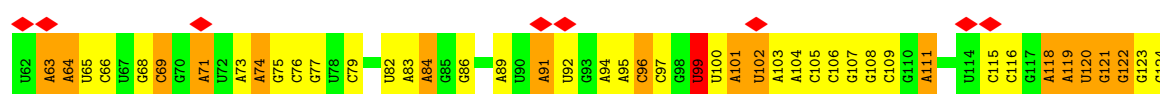
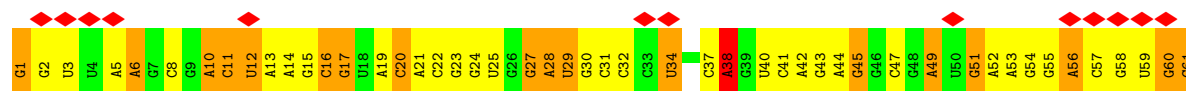
- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36



- Molecule 54: 23S ribosomal RNA

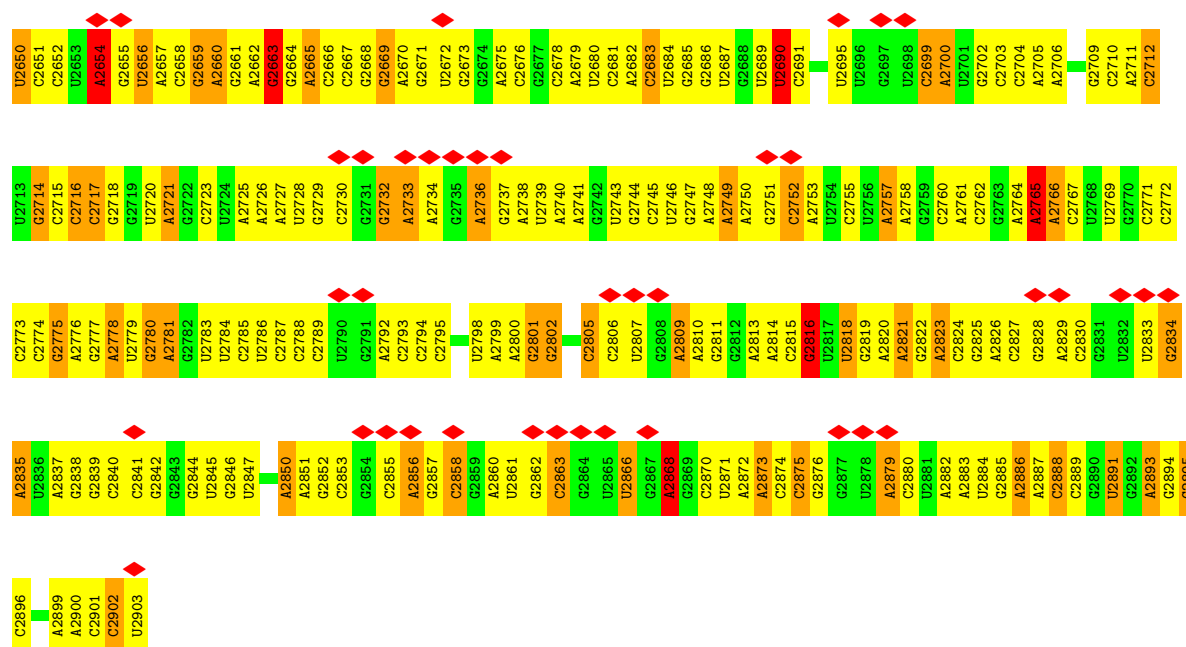




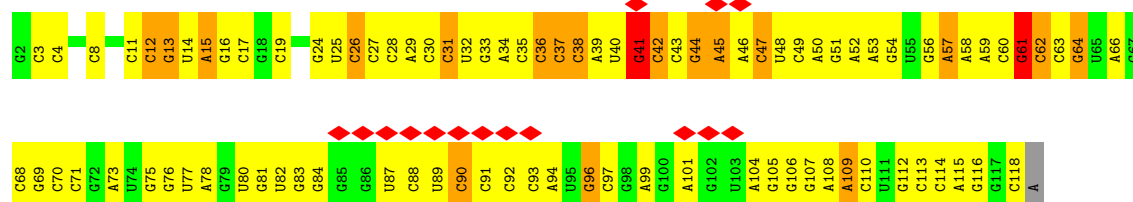
C1771	A1772	C1773	U1774	U1775	U1776	U1777	U1778	U1779	A1780	U1781	U1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	C1790	C1791	C1792	C1793	C1794	C1795	U1796	U1797	U1798	U1799	C1800	A1801	A1802	A1803	C1804	A1805	C1806	A1807	A1808	A1809	A1810	U1811	U1812	U1813	U1814	A1815	C1816	C1817	U1818	A1819	U1820	A1821	C1822	U1823	U1824	U1827	U1828	A1829	C1830	C1831	G1831
G1710	A1711	U1712	A1713	U1714	U1715	U1716	U1717	U1718	U1719	U1722		G1723	G1724	U1725	U1726	U1727	U1728	U1729	U1730	G1731	C1732	G1733	G1734	A1735	U1736	U1737	U1738	U1739	U1740	C1741	U1742	U1743	A1744	A1745	A1746	U1747	C1748	A1749	U1750	U1751	C1752	G1753	A1754	U1755	U1756	A1757	U1758	U1759	C1760	A1761	U1762	U1763	U1764	U1765	U1766	U1767	C1768	U1769	U1770
U1648	U1649	A1650	G1651	A1652	U1653	A1654	A1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	A1664	A1665	U1666	U1667	U1668	A1669	C1670	U1671	U1672	U1673	A1674	U1675	U1676	U1677	U1678	A1679	U1680	U1681	U1682	U1683	U1684	C1685	C1686	U1689	A1690	C1691	C1694	U1695	U1696	U1697	U1698	U1699	A1700	A1701	U1702	U1703	C1704	A1705	U1706	U1707	U1708	U1709		
C1585	A1586		A1590	A1591	C1592	A1593	A1594	C1595	A1596	A1597	A1598	U1599	C1600	U1601	U1602	A1603	C1604	C1605	C1606	C1607	A1608	A1609	A1610	C1611	C1612	G1613	A1614	C1615	A1616	C1617	A1618	U1619	C1620	U1621	U1624	C1625	A1626	U1627	U1628	U1629	A1630	G1631	A1632	U1633	A1634	U1635	U1636	A1637	C1638	C1639	A1640	A1641	U1642	U1643	U1644	U1645	C1646	U1647	
A1525	C1526	U1527	A1528	G1529	U1530	C1531	A1532	C1533	U1534	A1535	C1536	U1537	U1538	U1539	U1540	C1541	U1542	U1543	U1544	U1545	U1546	C1547	U1548	A1549	C1550	U1551	A1552	A1553	U1554	U1555	C1556	C1557	U1558	U1559	U1560	C1561	U1562	U1563	C1564	U1565	U1566	U1567	U1568	A1569	U1570	U1571	A1572	U1573	C1574	U1575	U1576	U1577	U1578	A1579	U1580	G1581	U1582	U1583	U1584
C1463	U1464	U1465	U1466	U1467	U1468	U1469	A1470	U1471	C1472	U1473	U1474	U1475	U1476	A1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	A1490	G1491	U1492	C1493	A1494	U1495	A1496	U1497	C1498	C1499	A1502	A1503	A1504	A1505	U1506	C1507	A1508	A1509	U1510	U1511	U1512	A1515	U1516	U1517	U1518	U1519	U1520	G1521	A1522	U1523	U1524		
U1397	C1398	C1399		U1402	A1403	C1404	U1405	U1406		U1412	A1413	C1414	U1415	U1416	C1417	U1418	A1419	A1420	U1421	U1422	U1423	U1424	U1425	U1426	A1427	U1428	U1429	U1430	A1431	U1432	U1433	A1434	U1435	U1436	U1437	U1438	A1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	C1447	U1448	C1451	U1452	U1453	C1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	
G1334	C1335	A1336	G1338	U1339	U1340	U1341	U1342	U1343	U1344	C1345	U1346	A1347	C1348	C1349	C1350	C1351	U1352	A1353	U1354	C1355	U1356	C1357	U1358	A1359	C1362	C1363	U1364	A1365	U1366	A1367	U1368	C1369	C1370	U1371	U1372	A1373	U1374	U1375	C1376	U1377	U1378	U1379	U1380	G1381	U1382	A1383	A1384	A1385	C1386	U1387		U1391	A1392	A1393	U1394	A1395	U1396		
C1270	U1271		U1273	U1274	A1275	A1276	U1277	C1278	U1283	A1284	A1285	A1286	A1287	U1288	U1289	C1290	C1291	U1292	C1293	U1294	C1295	U1296	C1297	U1298	C1299	G1300	U1301	A1302	G1303	A1304	C1305	C1306	A1307	A1308	C1311	U1312	U1313	U1314	C1315	U1316	U1317	U1318	C1319	C1320	A1321	A1322	C1323	U1324	U1325	U1326	U1327	U1328	U1329	C1330	U1331	U1332	G1333		
C1208	U1209	G1210	U1211	U1212	A1213	A1214	U1215	U1216	U1217	U1218	C1221	U1224	U1225	U1226	U1227	C1228	C1229	A1230	U1231	U1232	C1233	U1234	U1235	U1236	U1237	U1238	U1239	A1240	A1241	U1242	C1243	A1244	U1245	A1246	U1247	U1248	U1249	G1250	C1251	U1252	A1253	U1254	U1255	G1256	U1257	C1258	U1259	A1260	C1261	U1262	U1263	A1264	A1265	U1266	U1267	A1268	U1269		
A1142	A1143	A1144	C1145	C1146	A1147	C1150	A1151	C1152	C1153	U1154	U1155	A1156	U1157	U1158	U1159	U1160	C1161	U1162	U1163	C1164	U1165	U1166	C1167	U1168	A1169	C1170	G1171	C1172	A1175	U1176	U1177	C1178	G1179	U1180	G1185	U1186	U1187	U1188	A1189	U1190	U1191	U1192	G1193	A1194	U1195	C1196	U1197	U1198	U1199	C1200	U1201	A1204	U1205	U1206	C1207	C1208			
U1080	U1081	U1082	U1083	A1084	U1085	A1086	U1087	U1088	A1089	A1090	C1091	C1092	G1093	U1094	U1095	A1096	U1097	A1098	U1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	U1107	U1108	C1109	U1110	A1111	U1112	U1113	C1114	G1115	U1116	C1117	C1118	C1121	G1122	C1123	U1124	U1125	U1126	A1127	G1128	A1129	U1130	G1131	U1132	A1133	A1134	U1135	U1136	G1137	C1140	U1141		
U1018	U1019	A1020	A1021	U1022	U1023	U1024	U1025	U1026	A1027	U1028	A1029	C1030	G1031	A1032	U1033	U1034	U1035	G1038	A1039	A1040	C1043	C1044	C1045	A1046	U1047	A1048	C1049	A1050	U1051	C1052	C1053	A1054	U1055	U1056	A1057	U1058	U1059	U1060	U1061	U1062	G1063	C1064	U1065	U1066	A1067	U1068	A1069	U1070	G1071	C1072	A1073	U1074	C1075	U1076	U1077	U1078	C1079		

U2585	U2586	A2518	U2457	G2397	C2332	A2270	A2205	C2145	G2083	A2019	C1958	U1897	C1832
U2587	A2459	C2521	A2458	G2399	A2335	U2272	C2206	C2146	C2084	A2020	G1959	U1898	C1833
G2588	U2460	U2522	A2461	G2400	U2336	A2273	C2207	G2147	U2085	U2022	C1961	U1899	G1835
A2590	C2462	G2523	U2401	U2402	G2337	A2274	C2208	U2149	U2086	C2023	U1963	A1900	C1836
C2591	C2463	C2524	C2403	C2404	C2338	G2275	U2210	U2150	G2087	G2024	G1964	A1901	C1837
G2592	U2464	G2525	U2405	G2406	C2339	G2276	A2211	U2151	A2088	A2030	C1965	G1839	C1838
G2593	C2465	G2526	C2407	U2408	A2340	G2277	A2212	C2152	A2090	A2031	C1966	G1840	U1841
G2594	C2466	U2527	A2467	G2409	C2341	G2279	C2213	C2153	C2091	G1907	C1967	U1842	U1841
U2596	A2468	U2528	A2468	U2408	C2342	G2280	C2214	A2154	G2092	A2032	G1968	C1843	C1842
A2597	A2469	G2529	A2469	G2410	C2343	A2281	C2215	U2155	G2093	A2033	A1969	C1844	G1845
G2598	G2470	A2530	G2471	A2411	G2345	G2282	U2219	C2156	A2095	U2034	C1970	C1908	C1909
G2599	A2472	G2531	U2473	A2412	A2346	C2283	U2220	G2157	A2096	A2035	U1971	C1910	G1910
G2600	G2473	G2532	U2474	G2413	C2347	A2284	G2221	G2158	C2097	C2036	G1972	U1911	U1911
A2601	U2474	G2533	U2475	G2414	G2348	C2285	G2222	C2160	A2097	G2037	C1973	A1847	A1847
G2602	U2476	G2534	C2476	G2415	G2349	G2286	G2223	G2161	U2098	G2038	C1974	A1948	A1948
U2603	A2477	G2535	A2478	C2416	G2350	A2287	G2224	G2162	U2099	U2039	G1975	C1914	C1914
G2604	U2478	G2536	C2479	C2417	G2351	A2288	G2225	A2163	G2100	G2040	U1976	U1915	U1915
G2605	U2479	C2537	U2480	A2418	A2352	A2289	A2226	C2164	A2101	U2041	A1977	A1916	A1916
C2606	A2481	C2538	G2482	U2419	C2353	G2292	G2227	C2165	C2102	A2042	U1978	U1917	U1917
G2607	U2483	C2539	U2483	G2420	G2354	G2293	A2228	U2166	C2103	C2043	U1979	U1918	U1918
G2608	U2484	C2540	U2484	G2421	G2355	G2294	G2229	U2167	C2104	C2044	G1980	A1919	A1919
U2609	U2485	G2541	U2485	G2422	G2356	C2295	G2230	A2168	A1981	C2045	G1981	C1920	A1858
U2610	U2486	G2542	U2486	U2423	G2357	A2297	U2232	G2169	A2109	G2046	U1982	G1922	G1922
C2611	U2487	G2543	U2487	G2424	G2358	A2298	U2233	U2171	G2110	C2047	C1985	U1923	U1923
C2612	U2488	A2547	U2488	A2425	C2359	A2299	U2236	U2172	G2111	G2048	C1986	C1924	C1924
U2613	U2489	C2551	U2489	A2426	G2360	U2300	G2237	C2173	G2112	C2049	C1987	U1926	U1926
A2614	U2490	U2552	U2490	G2427	G2361	C2301	U2238	C2174	U2113	A2051	G1988	A1927	A1927
U2615	U2491	U2553	U2491	G2428	G2362	G2302	G2239	C2175	G2114	C2052	G1989	C1928	C1928
C2616	U2492	U2554	U2492	A2429	G2363	G2303	U2240	C2176	G2115	A2053	C1990	G1929	G1929
G2619	U2493	U2555	U2493	A2430	G2364	G2304	U2241	C2177	G2116	C2054	U1991	U1931	U1931
C2620	U2494	G2556	U2494	A2431	G2365	U2305	G2242	C2178	U2117	C2055	G1992	A1872	A1872
C2621	U2495	U2557	U2495	A2432	G2366	U2306	G2243	U2180	G2118	A2058	C1993	A1932	A1932
G2624	U2496	U2562	U2496	A2433	G2367	G2307	U2244	U2181	G2119	C2059	C1994	G1933	G1933
G2625	U2497	U2563	U2497	A2434	G2368	G2308	U2245	U2182	G2120	A2060	U1995	C1934	C1934
C2626	U2498	U2564	U2498	A2435	G2369	G2309	G2246	A2183	G2121	G2061	C1996	G1935	G1935
C2627	U2499	U2565	U2499	A2436	C2370	A2309	A2247	A2184	G2122	A2062	C1997	A1936	A1936
C2628	U2500	U2566	U2500	A2437	C2371	G2310	C2248	U2185	G2123	C2063	A1998	A1937	A1937
U2629	G2502	U2567	G2502	U2441	C2372	A2311	U2249	U2186	G2124	C2064	C1999	A1938	A1938
A2632	A2503	U2572	U2503	C2442	C2373	U2312	G2250	U2187	G2125	C2065	C2000	U1939	U1939
G2633	U2504	C2573	U2504	C2443	C2374	G2313	G2251	U2188	G2126	C2066	G2002	U1940	U1940
A2634	G2505	C2574	G2505	C2444	G2375	G2314	G2252	U2189	U2129	U2067	A2003	C1941	C1941
A2635	U2506	U2575	U2506	G2445	C2376	G2315	G2253	G2190	U2130	U2068	G2004	C1942	C1942
C2636	C2507	G2576	C2507	G2446	A2377	G2316	C2254	U2191	U2131	G2069	A2005	U1943	U1943
U2637	G2508	G2577	G2508	G2447	A2378	A2317	G2255	U2192	U2132	A2070	C2006	U1944	U1944
G2638	U2509	U2578	U2509	A2448	U2386	G2318	U2256	U2193	G2133	A2071	U2007	G1945	G1945
A2639	C2510	C2579	C2510	A2449	U2387	G2319	U2257	U2194	A2134	C2072	C2008	U1946	U1946
G2640	U2511	U2580	U2511	A2450	A2388	U2320	U2258	U2195	A2135	U2073	A2009	C1947	C1947
G2644	C2512	C2581	C2512	A2451	G2389	G2321	U2259	U2196	U2136	U2074	G2010	G1948	G1948
G2645	A2513	G2582	A2513	C2452	C2390	U2322	C2260	U2197	G2137	U2075	U2011	G1949	G1949
G2646	U2514	U2583	U2514	C2453	C2391	U2323	C2261	A2198	G2138	U2076	A2012	G1950	G1950
G2647	C2515	G2584	C2515	C2454	C2392	U2324	C2262	U2199	U2139	A2077	C2013	U1951	U1951
C2648	A2516	U2585	A2516	G2455	C2393	G2325	U2263	C2200	G2140	C2078	A2015	A1952	A1952
C2649	C2517	U2586	C2517	G2456	C2394	U2326	U2264	G2201	G2141	A2080	U2016	G1954	G1954
					C2395	C2327	A2267	U2202	A2142	U2081	U2017	U1955	U1955
					G2396	A2328	U2268	U2203	C2143	A2082	G2018	C1956	C1956
						U2329	G2269	G2204	G2144				

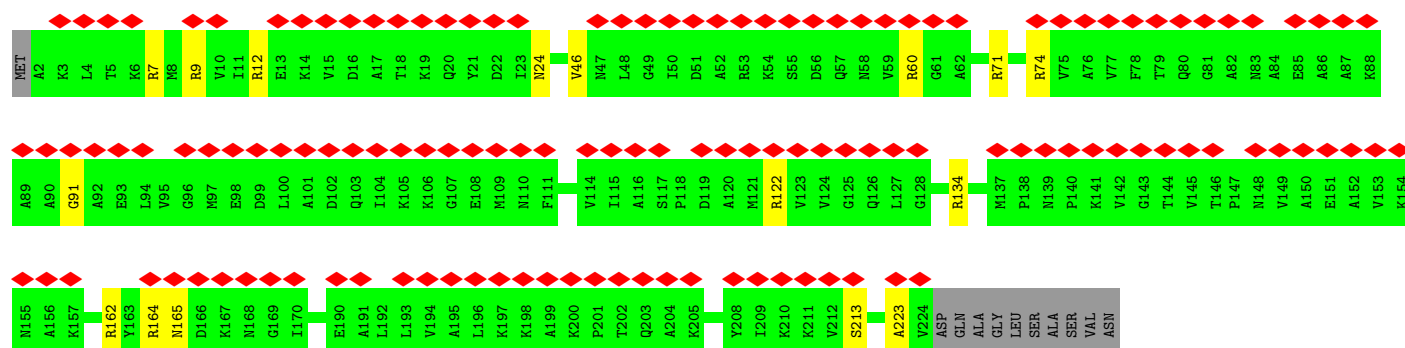
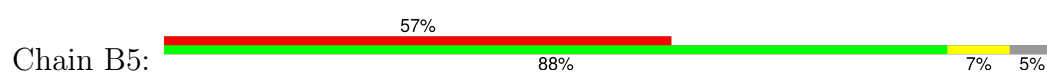




• Molecule 55: 5S ribosomal RNA



• Molecule 56: 50S ribosomal protein L1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5656	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	172.869	Depositor
Minimum map value	-108.132	Depositor
Average map value	-1.067	Depositor
Map value standard deviation	18.681	Depositor
Recommended contour level	22	Depositor
Map size ( $\text{\AA}$ )	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.8, 2.8, 2.8	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, FME, 6MZ, 5MU, NH2, 7MG, H2U, PSU, 4SU, CM0, ACE

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	AB	0.69	0/1736	1.04	13/2340 (0.6%)
2	AC	0.71	0/1651	1.12	15/2225 (0.7%)
3	AD	0.75	0/1665	1.23	21/2227 (0.9%)
4	AE	0.68	0/1119	1.06	8/1506 (0.5%)
5	AF	0.71	0/835	1.13	8/1128 (0.7%)
6	AG	0.73	0/1188	1.19	15/1593 (0.9%)
7	AH	0.69	0/989	1.09	10/1326 (0.8%)
8	AI	0.78	0/1035	1.20	10/1377 (0.7%)
9	AJ	0.72	0/797	1.23	13/1079 (1.2%)
10	AK	0.73	0/894	1.19	10/1207 (0.8%)
11	AL	0.74	0/969	1.23	16/1300 (1.2%)
12	AM	0.74	0/884	1.35	18/1181 (1.5%)
13	AN	0.77	0/817	1.35	14/1088 (1.3%)
14	AO	0.70	0/722	1.26	10/964 (1.0%)
15	AP	0.75	0/648	1.16	7/870 (0.8%)
16	AQ	0.69	0/658	1.15	6/883 (0.7%)
17	AR	0.78	0/463	1.19	6/623 (1.0%)
18	AS	0.74	0/653	1.23	6/879 (0.7%)
19	AT	0.68	0/672	1.06	6/890 (0.7%)
20	AU	0.83	0/431	1.55	6/572 (1.0%)
21	AA	1.57	0/36759	2.22	1953/57346 (3.4%)
22	A1	1.59	0/1668	2.19	92/2595 (3.5%)
23	A2	1.54	0/343	2.27	23/531 (4.3%)
24	A3	1.58	1/1722 (0.1%)	2.19	93/2685 (3.5%)
25	BC	0.72	0/2121	1.26	26/2852 (0.9%)
26	BD	0.66	0/1586	1.19	13/2134 (0.6%)
27	BE	0.66	0/1571	1.13	10/2113 (0.5%)
28	BF	0.73	0/1444	1.17	10/1937 (0.5%)
29	BG	0.68	0/1343	1.18	11/1816 (0.6%)
30	BH	0.64	0/1122	1.12	5/1515 (0.3%)
31	BI	0.63	0/1046	1.07	4/1410 (0.3%)
32	BJ	0.70	0/1152	1.17	10/1551 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BK	0.69	0/947	1.22	10/1268 (0.8%)
34	BL	0.74	0/1054	1.31	10/1403 (0.7%)
35	BM	0.74	0/1093	1.23	12/1460 (0.8%)
36	BN	0.75	0/973	1.41	17/1301 (1.3%)
37	BO	0.71	0/902	1.24	11/1209 (0.9%)
38	BP	0.72	0/929	1.32	15/1242 (1.2%)
39	BQ	0.77	0/960	1.34	18/1278 (1.4%)
40	BR	0.68	0/829	1.10	4/1107 (0.4%)
41	BS	0.64	0/864	1.15	6/1156 (0.5%)
42	BT	0.64	0/744	1.22	7/994 (0.7%)
43	BU	0.68	0/787	1.16	6/1051 (0.6%)
44	BV	0.68	0/766	1.19	8/1025 (0.8%)
45	BW	0.75	0/604	1.28	6/799 (0.8%)
46	BX	0.74	0/635	1.38	9/848 (1.1%)
47	BY	0.66	0/510	1.16	5/677 (0.7%)
48	BZ	0.69	0/453	1.24	3/605 (0.5%)
49	B0	0.73	0/450	1.24	5/599 (0.8%)
50	B1	0.69	0/417	1.04	2/556 (0.4%)
51	B2	0.81	0/380	1.47	11/498 (2.2%)
52	B3	0.72	0/513	1.20	6/676 (0.9%)
53	B4	0.67	0/303	1.22	4/397 (1.0%)
54	BA	1.44	16/69796 (0.0%)	2.22	4183/108888 (3.8%)
55	BB	1.46	0/2800	2.16	142/4367 (3.3%)
56	B5	0.63	0/1673	1.11	10/2255 (0.4%)
All	All	1.31	17/160085 (0.0%)	2.00	6978/239402 (2.9%)

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
3	AD	0	2
4	AE	0	1
8	AI	0	1
9	AJ	0	1
11	AL	0	1
18	AS	0	1
21	AA	0	346
22	A1	0	12
23	A2	0	4
24	A3	0	13

*Continued on next page...*

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
38	BP	0	1
50	B1	0	1
54	BA	0	647
55	BB	0	19
56	B5	0	1
All	All	0	1051

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1784	A	N3-C4	5.88	1.38	1.34
54	BA	2405	G	C2-N2	-5.24	1.29	1.34
54	BA	901	C	C4-N4	-5.22	1.29	1.33
54	BA	192	C	C4-N4	-5.21	1.29	1.33
54	BA	2332	C	C4-N4	-5.19	1.29	1.33

The worst 5 of 6978 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2063	C	N3-C2-O2	-17.09	109.94	121.90
54	BA	614	A	O4'-C1'-N9	14.96	120.17	108.20
22	A1	73	A	N1-C6-N6	-14.17	110.10	118.60
54	BA	548	G	O4'-C1'-N9	12.93	118.55	108.20
54	BA	2114	A	N1-C6-N6	-12.72	110.97	118.60

There are no chirality outliers.

5 of 1051 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	75	TYR	Sidechain
3	AD	96	ARG	Sidechain
4	AE	53	ARG	Sidechain
8	AI	129	ARG	Sidechain
9	AJ	72	ARG	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	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	1	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	3	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	3	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	841	0	0
25	BC	2083	0	2157	1	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	1	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	1	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31298	6	0
55	BB	2504	0	1269	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99612	17	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 0.

The worst 5 of 17 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)
11:AL:69:GLU:H	11:AL:106:VAL:HG13	1.75	0.52
54:BA:1349:C:N4	54:BA:1383:A:H61	2.11	0.49
54:BA:1324:G:H3'	54:BA:1325:U:H5''	1.97	0.46
4:AE:88:HIS:CG	4:AE:89:THR:H	2.32	0.45
33:BK:111:LYS:HE3	33:BK:112:PHE:CZ	2.52	0.45

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	
1	AB	218/220 (99%)	201 (92%)	15 (7%)	2 (1%)	14	52
2	AC	205/208 (99%)	190 (93%)	9 (4%)	6 (3%)	3	23
3	AD	203/206 (98%)	191 (94%)	9 (4%)	3 (2%)	8	40
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	6	32
5	AF	99/101 (98%)	87 (88%)	7 (7%)	5 (5%)	1	15
6	AG	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	2	18
7	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	55
8	AI	126/128 (98%)	110 (87%)	15 (12%)	1 (1%)	16	55
9	AJ	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	2	18
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	14	52
11	AL	121/124 (98%)	110 (91%)	9 (7%)	2 (2%)	7	37
12	AM	112/115 (97%)	92 (82%)	16 (14%)	4 (4%)	3	20
13	AN	98/101 (97%)	92 (94%)	4 (4%)	2 (2%)	6	32
14	AO	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	1	14
15	AP	79/81 (98%)	69 (87%)	6 (8%)	4 (5%)	1	15
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	7	35
18	AS	79/81 (98%)	69 (87%)	7 (9%)	3 (4%)	2	19
19	AT	84/86 (98%)	80 (95%)	3 (4%)	1 (1%)	11	44
20	AU	51/53 (96%)	38 (74%)	9 (18%)	4 (8%)	1	10
25	BC	270/273 (99%)	235 (87%)	27 (10%)	8 (3%)	3	23
26	BD	207/209 (99%)	185 (89%)	16 (8%)	6 (3%)	3	23
27	BE	199/201 (99%)	180 (90%)	11 (6%)	8 (4%)	2	18
28	BF	176/179 (98%)	157 (89%)	13 (7%)	6 (3%)	3	21
29	BG	174/177 (98%)	155 (89%)	18 (10%)	1 (1%)	22	60
30	BH	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	32
31	BI	139/142 (98%)	129 (93%)	9 (6%)	1 (1%)	19	57
32	BJ	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	3	23
33	BK	121/123 (98%)	103 (85%)	13 (11%)	5 (4%)	2	18
34	BL	141/144 (98%)	109 (77%)	24 (17%)	8 (6%)	1	14
35	BM	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	8	40
36	BN	119/121 (98%)	105 (88%)	13 (11%)	1 (1%)	16	55

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	14	52
38	BP	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	3	20
39	BQ	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	4	26
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6	32
41	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	6	32
42	BT	92/94 (98%)	79 (86%)	9 (10%)	4 (4%)	2	17
43	BU	101/104 (97%)	87 (86%)	9 (9%)	5 (5%)	1	16
44	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
45	BW	78/80 (98%)	54 (69%)	15 (19%)	9 (12%)	0	5
46	BX	75/79 (95%)	64 (85%)	8 (11%)	3 (4%)	2	18
47	BY	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	8	38
48	BZ	56/59 (95%)	52 (93%)	1 (2%)	3 (5%)	1	15
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	1	14
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	28
52	B3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	3	21
53	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	24
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	9	41
All	All	5876/6008 (98%)	5259 (90%)	459 (8%)	158 (3%)	6	25

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AM	107	THR
14	AO	45	HIS
20	AU	9	GLU
20	AU	37	TYR
25	BC	181	ARG

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	175 (97%)	5 (3%)	38	57
2	AC	170/171 (99%)	169 (99%)	1 (1%)	84	88
3	AD	172/173 (99%)	172 (100%)	0	100	100
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	70	80
6	AG	123/123 (100%)	119 (97%)	4 (3%)	33	52
7	AH	104/105 (99%)	103 (99%)	1 (1%)	73	82
8	AI	105/105 (100%)	103 (98%)	2 (2%)	52	69
9	AJ	86/86 (100%)	85 (99%)	1 (1%)	67	78
10	AK	90/90 (100%)	85 (94%)	5 (6%)	17	38
11	AL	103/104 (99%)	102 (99%)	1 (1%)	73	82
12	AM	91/92 (99%)	89 (98%)	2 (2%)	47	65
13	AN	83/84 (99%)	82 (99%)	1 (1%)	67	78
14	AO	76/77 (99%)	75 (99%)	1 (1%)	65	77
15	AP	65/65 (100%)	64 (98%)	1 (2%)	60	75
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	40	58
17	AR	48/48 (100%)	47 (98%)	1 (2%)	48	66
18	AS	70/70 (100%)	68 (97%)	2 (3%)	37	56
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	41 (93%)	3 (7%)	13	34
25	BC	216/217 (100%)	211 (98%)	5 (2%)	45	64
26	BD	164/164 (100%)	161 (98%)	3 (2%)	54	71
27	BE	165/165 (100%)	163 (99%)	2 (1%)	67	78
28	BF	149/150 (99%)	145 (97%)	4 (3%)	40	58
29	BG	137/138 (99%)	134 (98%)	3 (2%)	47	65
30	BH	114/114 (100%)	113 (99%)	1 (1%)	75	83
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	56	72
33	BK	103/103 (100%)	100 (97%)	3 (3%)	37	56
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	108 (99%)	1 (1%)	75	83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	73	82
37	BO	86/87 (99%)	84 (98%)	2 (2%)	45	64
38	BP	99/100 (99%)	97 (98%)	2 (2%)	50	68
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	70	80
40	BR	84/84 (100%)	83 (99%)	1 (1%)	67	78
41	BS	93/93 (100%)	91 (98%)	2 (2%)	47	65
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	80 (96%)	3 (4%)	30	50
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	54 (92%)	5 (8%)	8	27
46	BX	67/68 (98%)	66 (98%)	1 (2%)	60	75
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	48	66
49	B0	47/48 (98%)	47 (100%)	0	100	100
50	B1	45/45 (100%)	43 (96%)	2 (4%)	24	45
51	B2	38/38 (100%)	37 (97%)	1 (3%)	41	59
52	B3	51/52 (98%)	47 (92%)	4 (8%)	10	29
53	B4	34/34 (100%)	33 (97%)	1 (3%)	37	56
56	B5	173/181 (96%)	171 (99%)	2 (1%)	67	78
All	All	4842/4870 (99%)	4755 (98%)	87 (2%)	54	71

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	BM	126	ILE
45	BW	11	ASN
37	BO	30	ARG
41	BS	1	MET
46	BX	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
26	BD	173	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
27	BE	165	HIS
50	B1	18	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	244 (15%)	92 (6%)
22	A1	73/76 (96%)	11 (15%)	2 (2%)
23	A2	14/15 (93%)	6 (42%)	3 (21%)
24	A3	77/77 (100%)	18 (23%)	8 (10%)
54	BA	2902/2903 (99%)	468 (16%)	130 (4%)
55	BB	116/118 (98%)	17 (14%)	3 (2%)
All	All	4711/4722 (99%)	764 (16%)	238 (5%)

5 of 764 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	10	A
21	AA	13	U
21	AA	14	U

5 of 238 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	271	G
54	BA	2450	A
54	BA	980	A
54	BA	2373	G
55	BB	15	A

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	CM0	A1	34	23,22	21,26,27	1.35	2 (9%)	26,37,40	1.57	3 (11%)
24	PSU	A3	56	24	18,21,22	0.95	0	21,30,33	1.27	2 (9%)
22	6MZ	A1	37	22	17,25,26	1.00	0	15,36,39	1.56	3 (20%)
24	4SU	A3	8	24	18,21,22	1.44	2 (11%)	25,30,33	0.87	1 (4%)
22	7MG	A1	46	22	23,26,27	4.01	2 (8%)	27,39,42	1.48	1 (3%)
22	4SU	A1	7	22	18,21,22	1.42	2 (11%)	25,30,33	1.00	2 (8%)
22	5MU	A1	54	22	19,22,23	0.72	0	27,32,35	1.39	3 (11%)
24	5MU	A3	55	24	19,22,23	0.68	0	27,32,35	1.34	3 (11%)
24	H2U	A3	21	24	18,21,22	1.35	2 (11%)	19,30,33	1.23	3 (15%)
22	PSU	A1	55	22	18,21,22	0.79	0	21,30,33	1.06	0
24	OMC	A3	33	24	19,22,23	0.74	0	25,31,34	0.98	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	23,22	-	3/12/30/31	0/2/2/2
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
22	6MZ	A1	37	22	-	2/5/27/28	0/3/3/3
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
22	PSU	A1	55	22	-	1/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-18.86	1.33	1.45
24	A3	8	4SU	C5-C4	-5.18	1.36	1.42
22	A1	7	4SU	C5-C4	-5.05	1.36	1.42
22	A1	34	CM0	O5-C5	-4.87	1.25	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C4-N3	-3.27	1.32	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	5.74	111.49	103.37
22	A1	34	CM0	C7-O5-C5	5.63	124.65	117.48
22	A1	37	6MZ	C9-N6-C6	3.87	126.44	122.85
22	A1	54	5MU	C5M-C5-C6	-3.73	117.80	122.85
24	A3	55	5MU	C5M-C5-C6	-3.63	117.94	122.85

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	37	6MZ	C5-C6-N6-C9
22	A1	37	6MZ	N1-C6-N6-C9
22	A1	46	7MG	C4'-C5'-O5'-P
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands 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
57	VAL	A1	101	58,22	4,6,7	0.65	0	6,7,9	0.91	0
58	FME	BA	3001	57	8,9,10	0.73	0	8,9,11	1.77	2 (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
57	VAL	A1	101	58,22	-	0/5/6/8	-
58	FME	BA	3001	57	-	1/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	CA-N-CN	3.33	127.95	122.82
58	BA	3001	FME	C-CA-N	2.64	114.59	109.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	FME	O1-CN-N-CA

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](#)

There are no chain breaks in this entry.

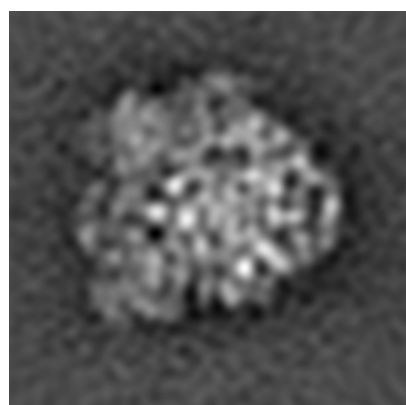
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1722. These allow visual inspection of the internal detail of the map and identification of artifacts.

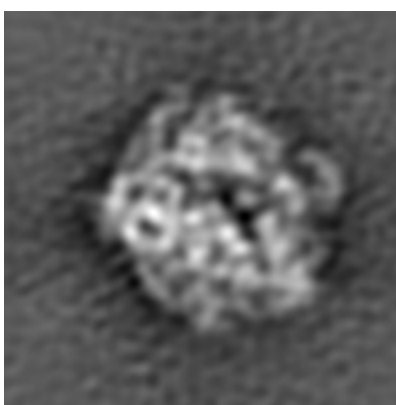
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

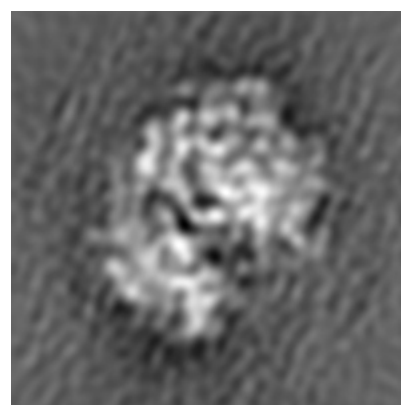
#### 6.1.1 Primary map



X



Y

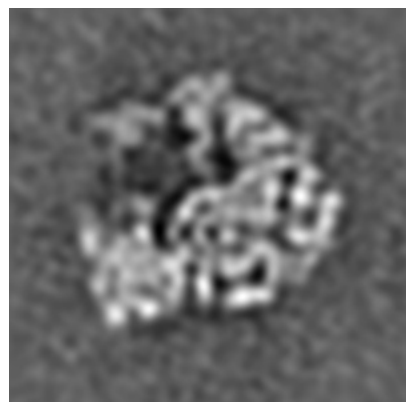


Z

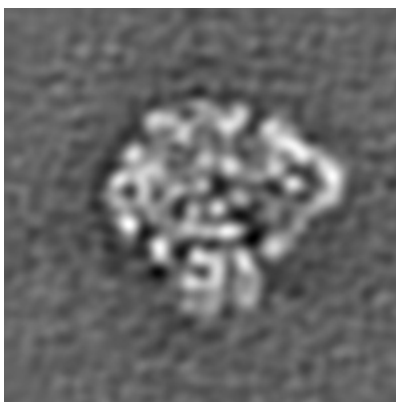
The images above show the map projected in three orthogonal directions.

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

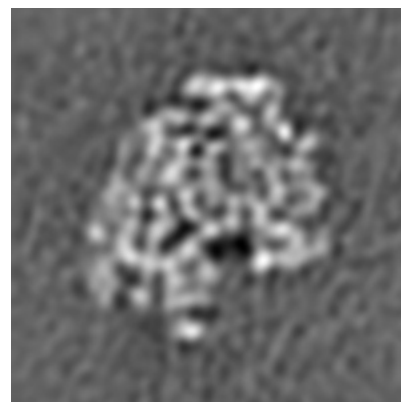
#### 6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64



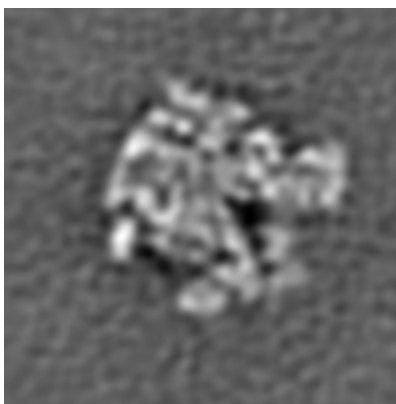
The images above show central slices of the map in three orthogonal directions.

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

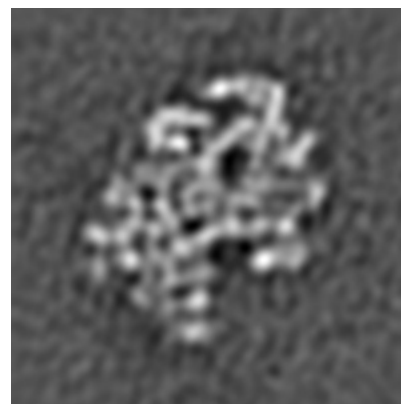
### 6.3.1 Primary map



X Index: 62



Y Index: 69

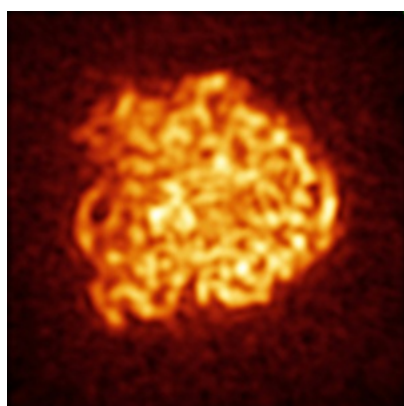


Z Index: 61

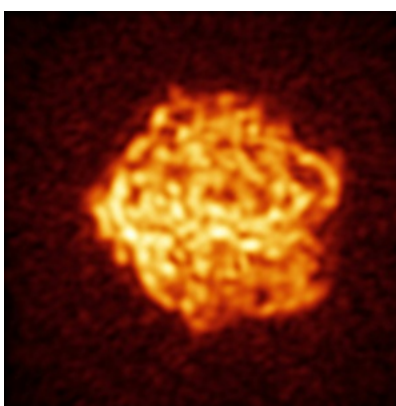
The images above show the largest variance slices of the map in three orthogonal directions.

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

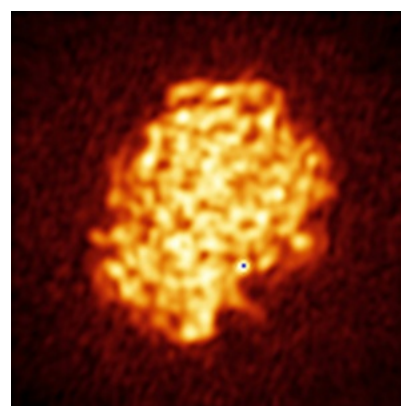
### 6.4.1 Primary map



X



Y

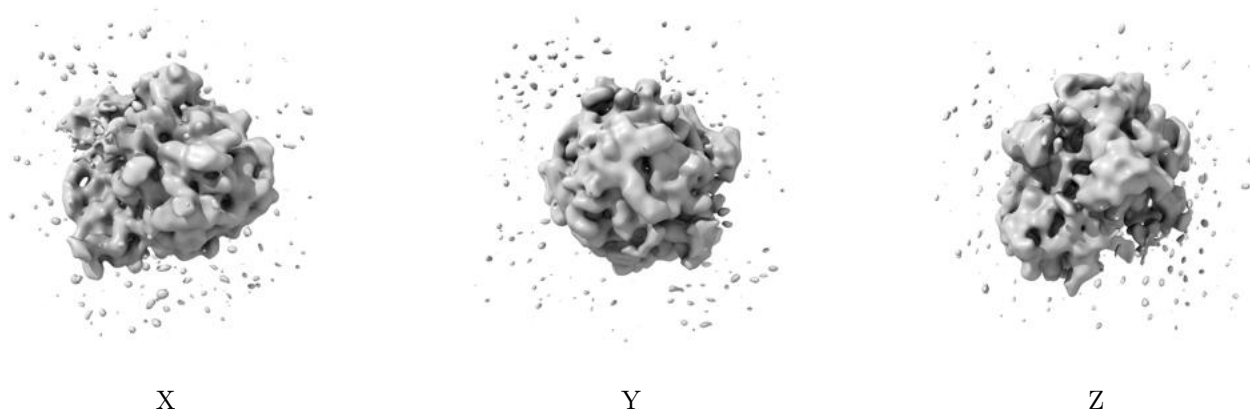


Z

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 22.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

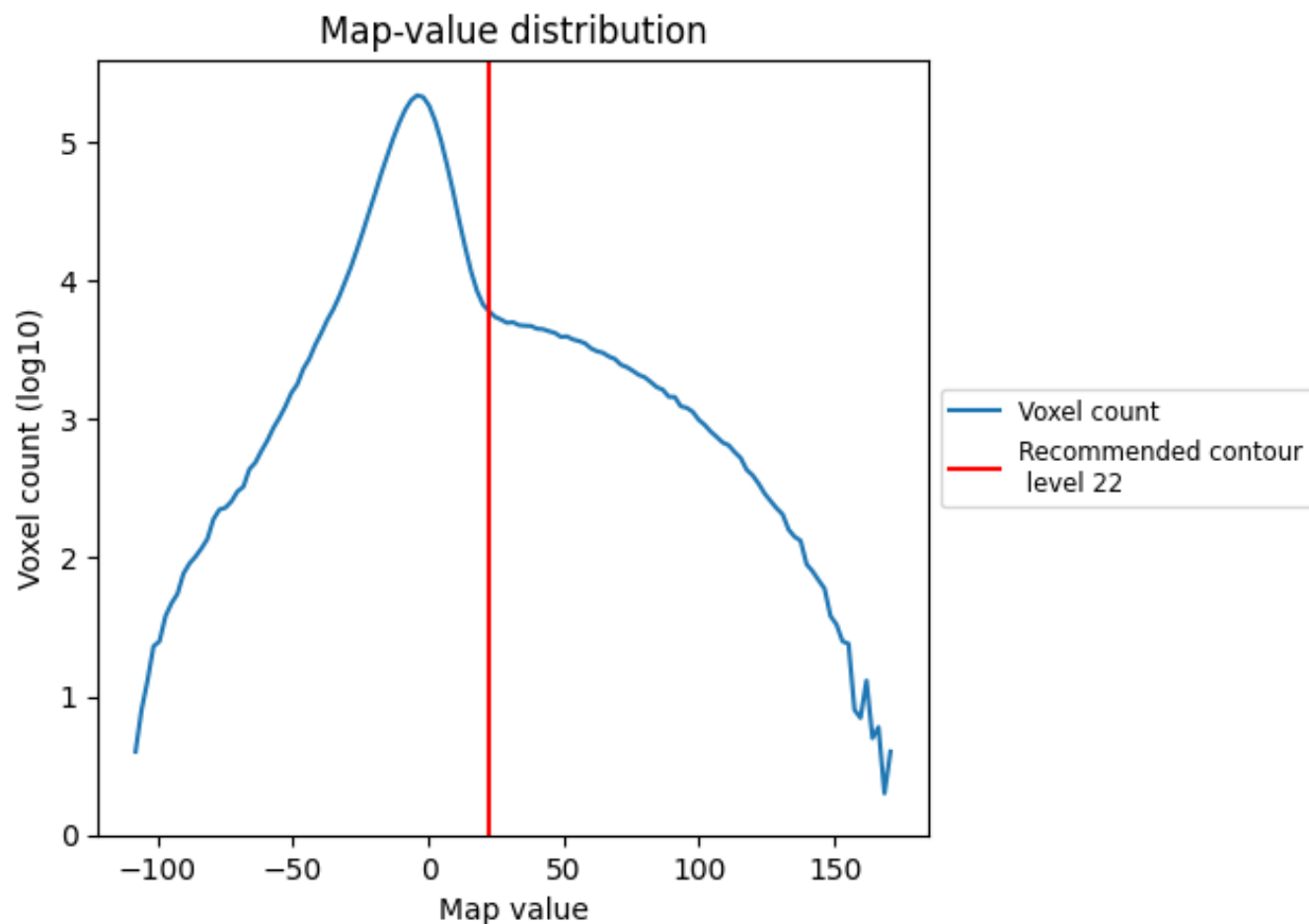
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

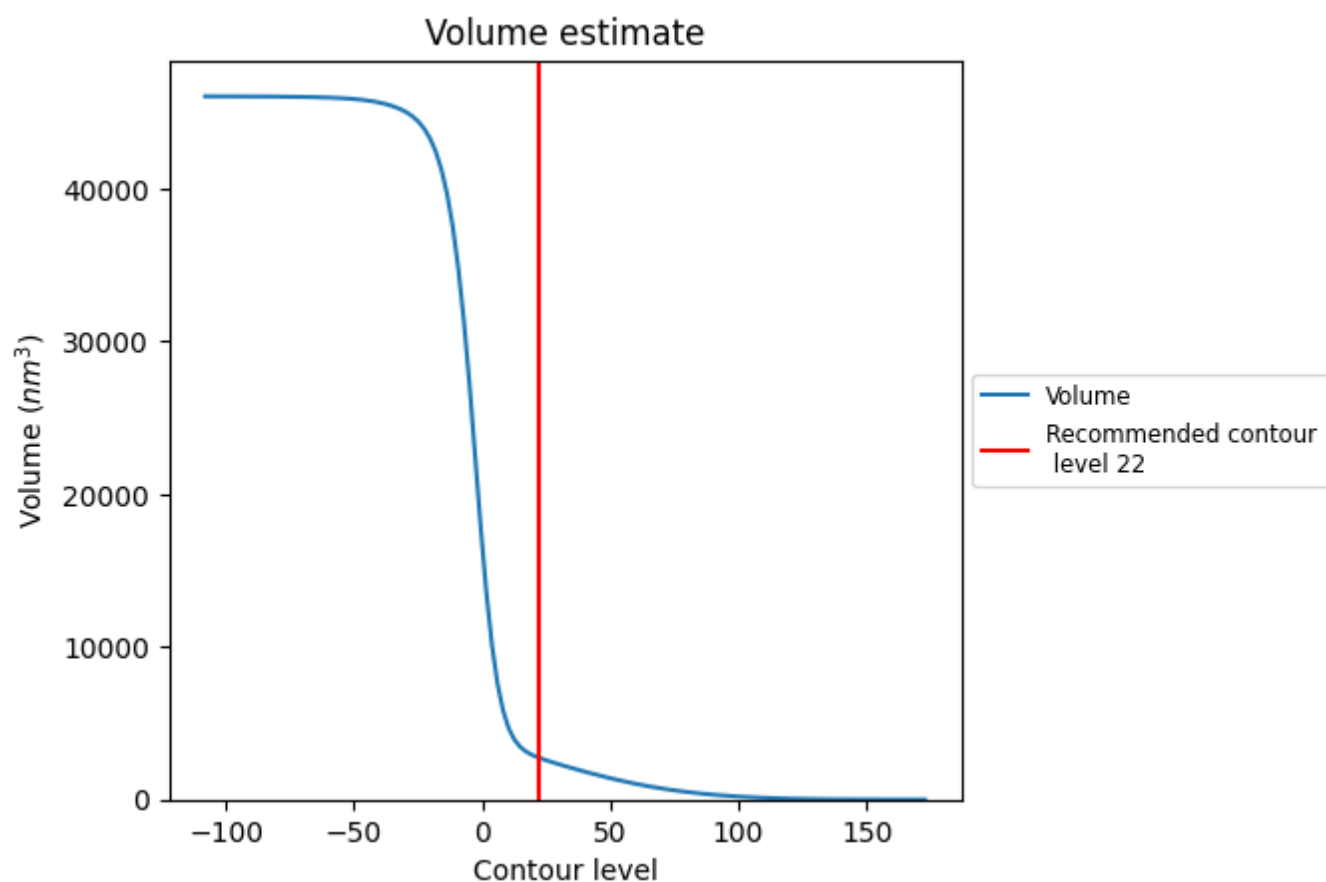
This section contains the results of statistical analysis of the map.

### 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.

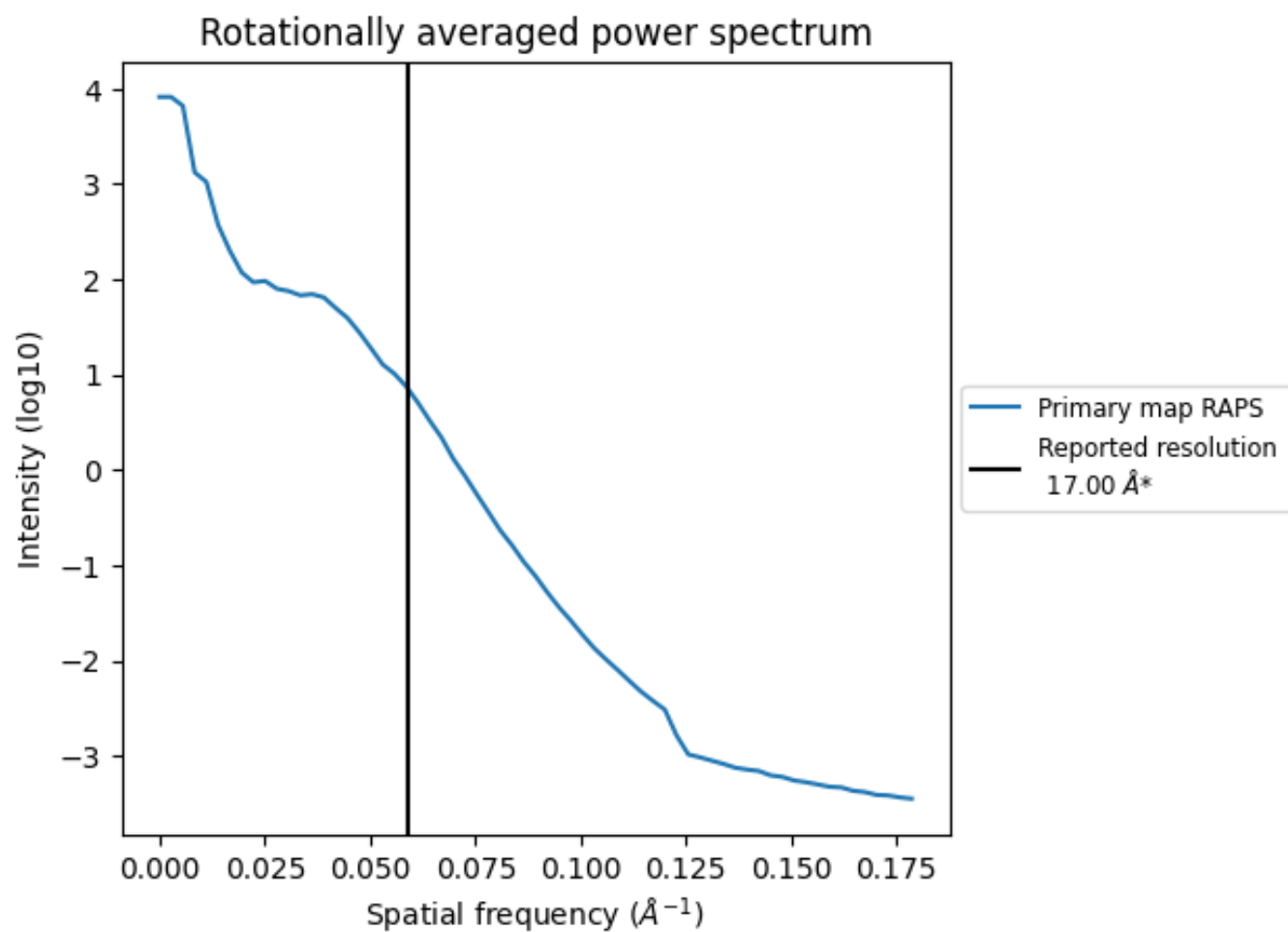
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2749 nm<sup>3</sup>; this corresponds to an approximate mass of 2483 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 0.059 Å<sup>-1</sup>

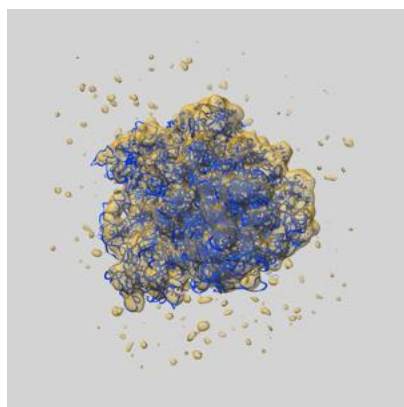
## 8 Fourier-Shell correlation

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

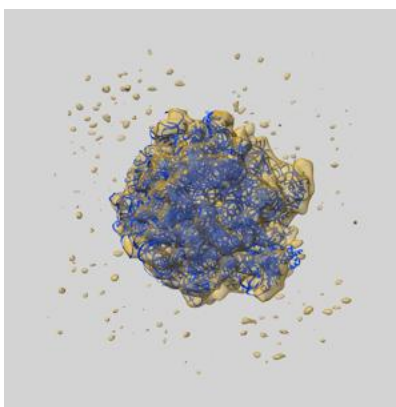
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1722 and PDB model 4V76. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

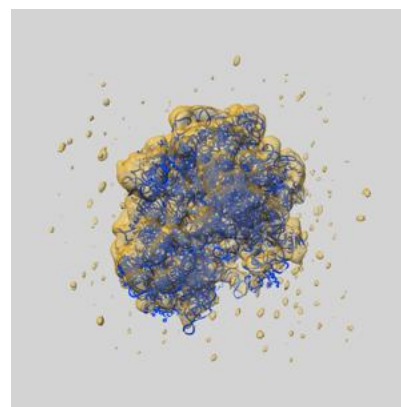
### 9.1 Map-model overlay [i](#)



X



Y



Z

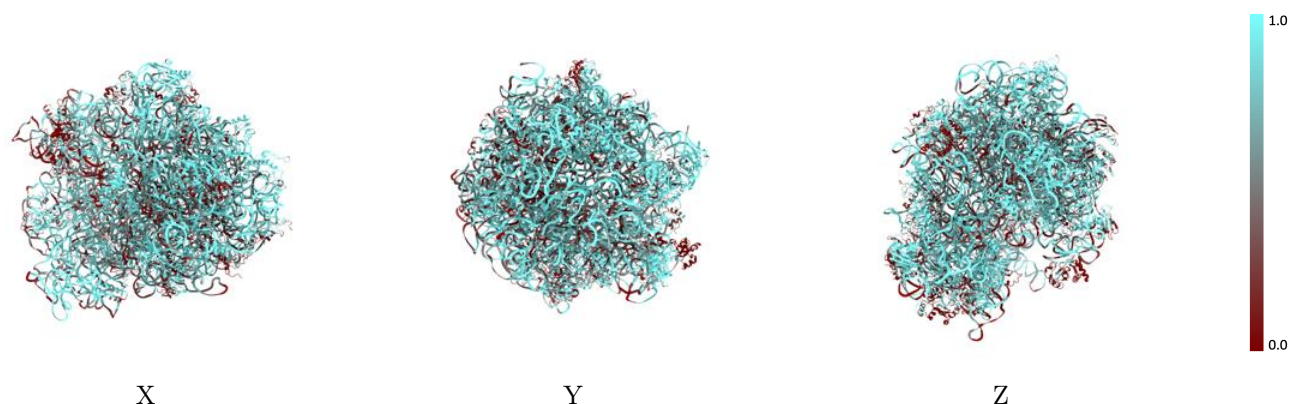
The images above show the 3D surface view of the map at the recommended contour level 22.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

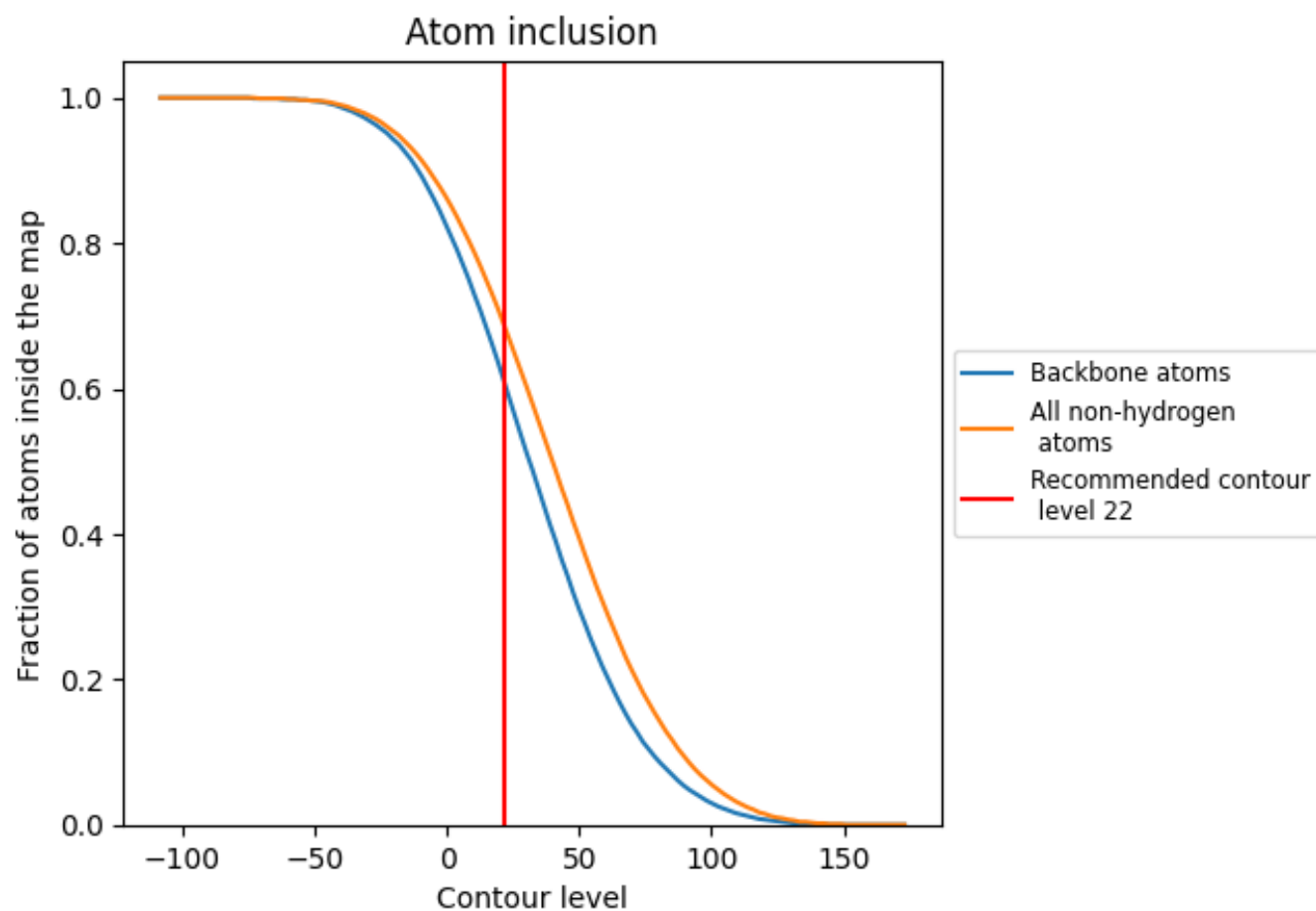
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (22).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 68% 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 (22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6840	 0.0370
A1	 0.5760	 0.0450
A2	 0.4820	 -0.0220
A3	 0.5150	 0.0290
AA	 0.7520	 0.0460
AB	 0.4450	 0.0190
AC	 0.4720	 0.0350
AD	 0.4490	 0.0100
AE	 0.5510	 0.0400
AF	 0.8170	 0.0540
AG	 0.7100	 0.0210
AH	 0.5710	 0.0210
AI	 0.7320	 0.0200
AJ	 0.5130	 0.0170
AK	 0.6700	 0.0270
AL	 0.7000	 0.0340
AM	 0.6070	 0.0290
AN	 0.5880	 0.0120
AO	 0.6320	 0.0260
AP	 0.5300	 0.0040
AQ	 0.5400	 0.0080
AR	 0.6060	 -0.0260
AS	 0.7400	 0.0290
AT	 0.7300	 -0.0140
AU	 0.5670	 -0.0090
B0	 0.7010	 0.0580
B1	 0.7720	 0.0440
B2	 0.3780	 -0.0020
B3	 0.3770	 -0.0360
B4	 0.6780	 0.0220
B5	 0.3780	 0.0000
BA	 0.7390	 0.0460
BB	 0.7890	 0.0500
BC	 0.4730	 0.0120
BD	 0.5070	 0.0100



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
BE	 0.7430	 0.0260
BF	 0.6980	 0.0560
BG	 0.6350	 0.0470
BH	 0.3300	 0.0120
BI	 0.1420	 0.0320
BJ	 0.5140	 0.0170
BK	 0.5770	 0.0300
BL	 0.6140	 -0.0030
BM	 0.5580	 0.0190
BN	 0.5220	 -0.0100
BO	 0.8640	 0.0310
BP	 0.4820	 0.0120
BQ	 0.6350	 0.0180
BR	 0.4180	 -0.0060
BS	 0.5270	 -0.0100
BT	 0.6200	 0.0130
BU	 0.5060	 0.0190
BV	 0.7520	 0.0480
BW	 0.6600	 0.0160
BX	 0.5940	 0.0040
BY	 0.5410	 0.0370
BZ	 0.5400	 0.0060