



wwPDB EM Validation Summary Report ⓘ

Nov 17, 2024 – 09:54 AM EST

PDB ID : 4V72
EMDB ID : EMD-1719
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^fMet complex in hybrid pre-translocation state (pre4)
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 : 13.00 Å (reported)
Based on initial models : 2WRI, 3I1O, 2HGP, 2K4C

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

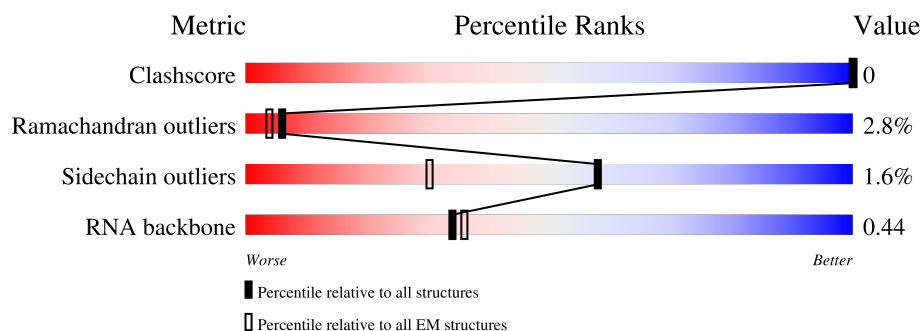
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 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 ≥ 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>29%</div> <div>92%</div> <div>8%</div> </div>
2	AC	208	<div> <div>30%</div> <div>87%</div> <div>12%</div> </div>
3	AD	206	<div> <div>43%</div> <div>87%</div> <div>13%</div> </div>
4	AE	152	<div> <div>28%</div> <div>90%</div> <div>10%</div> </div>
5	AF	101	<div> <div>14%</div> <div>82%</div> <div>18%</div> </div>
6	AG	152	<div> <div>22%</div> <div>86%</div> <div>13%</div> </div>
7	AH	130	<div> <div>32%</div> <div>92%</div> <div>6%</div> </div>

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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	

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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

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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		

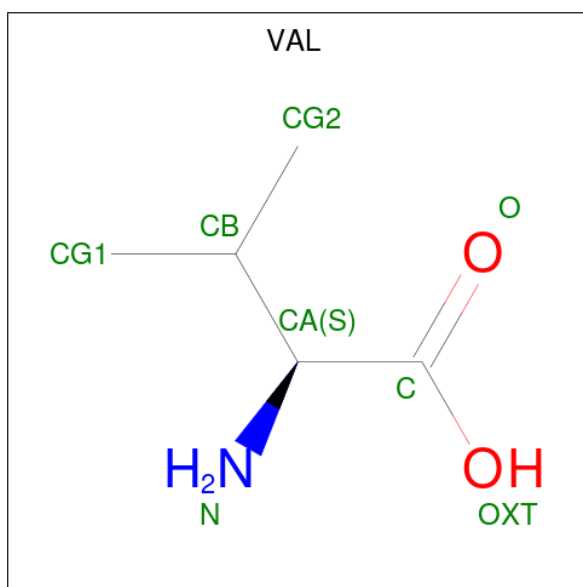
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

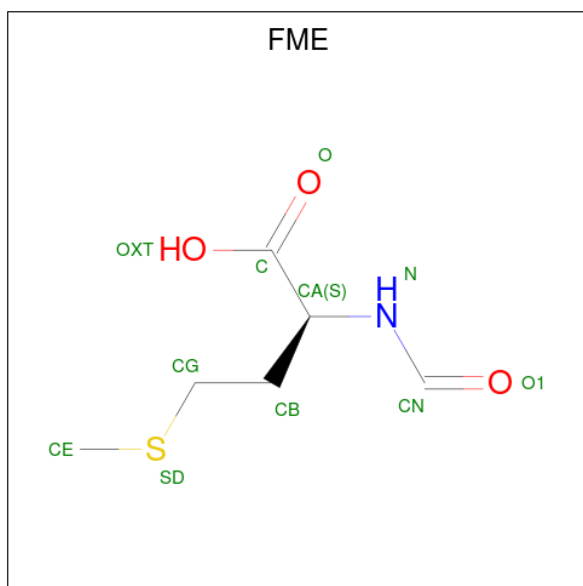
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



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: C₆H₁₁NO₃S).

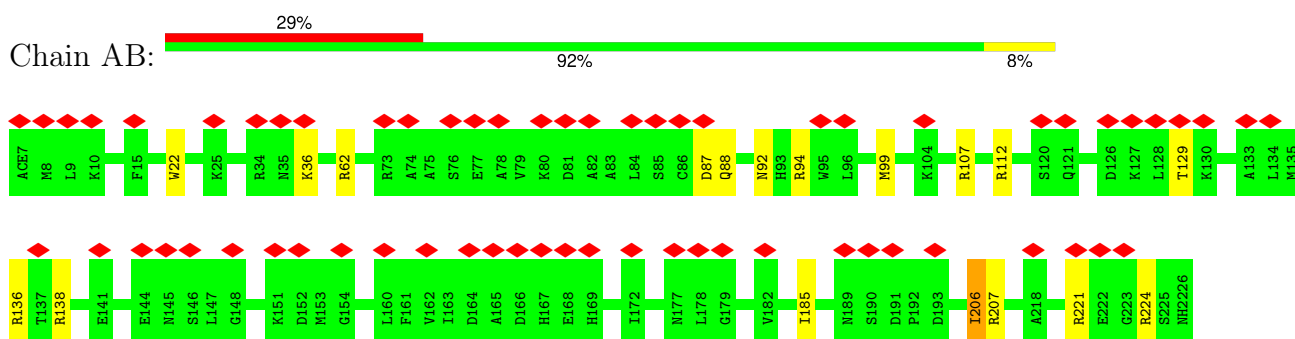


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

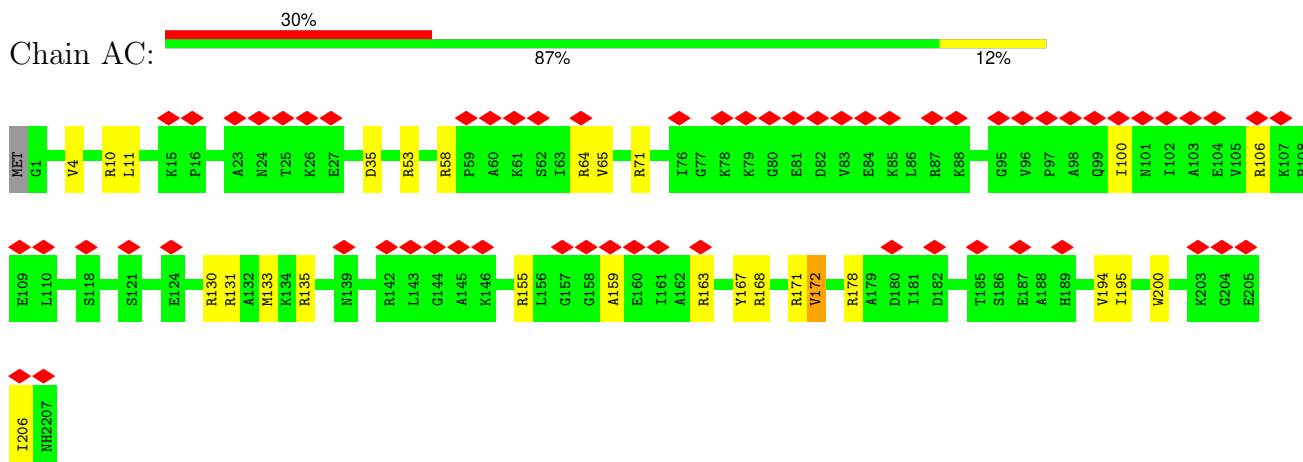
3 Residue-property plots [i](#)

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.

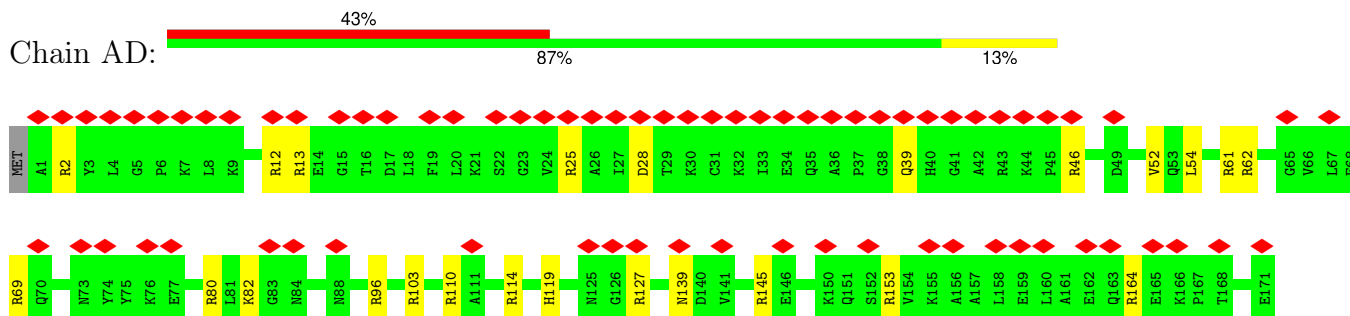
- Molecule 1: 30S ribosomal protein S2

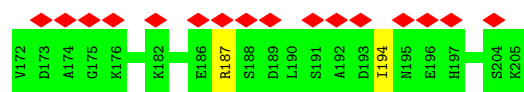


- Molecule 2: 30S ribosomal protein S3

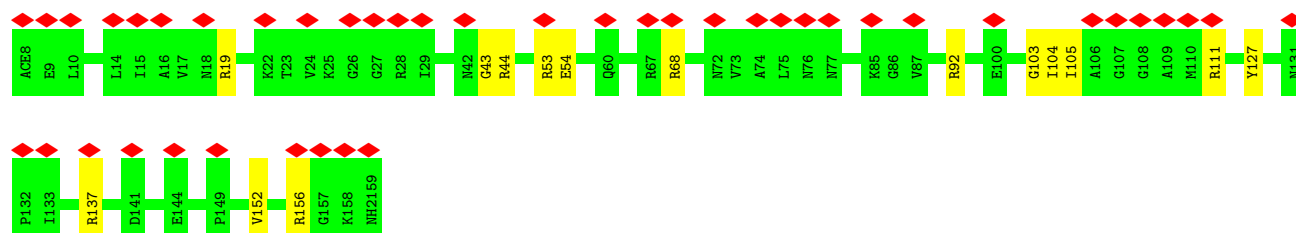
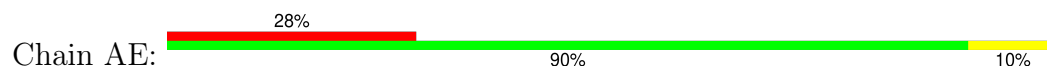


- Molecule 3: 30S ribosomal protein S4

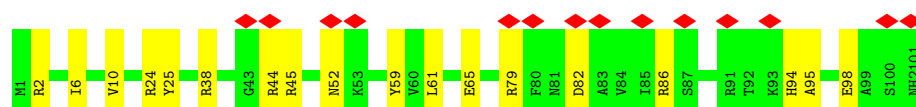
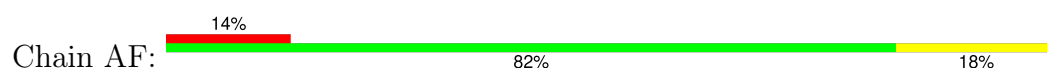




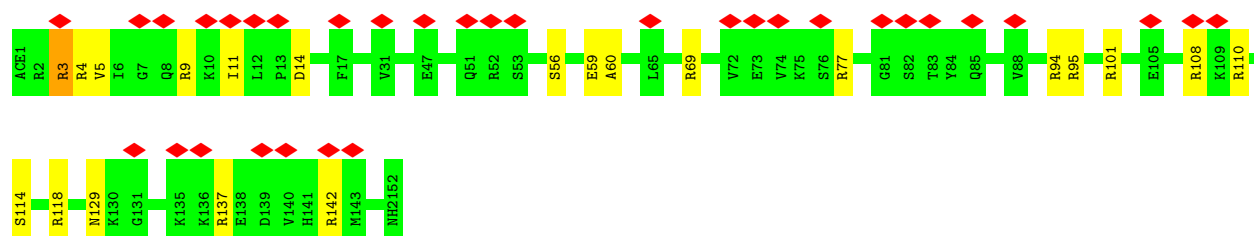
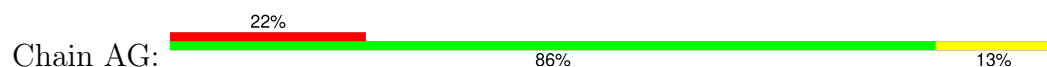
• Molecule 4: 30S ribosomal protein S5



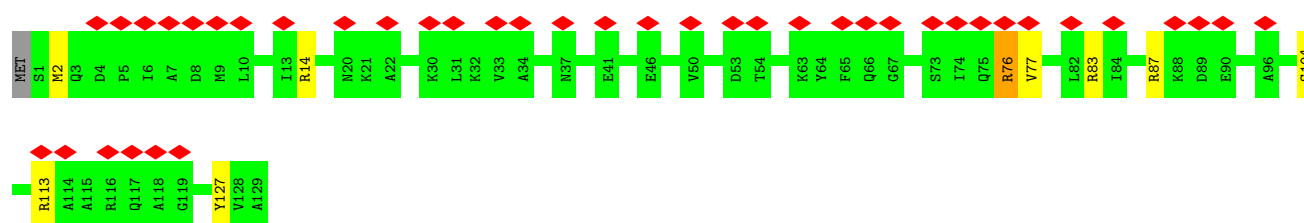
• Molecule 5: 30S ribosomal protein S6



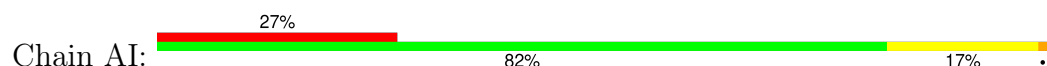
• Molecule 6: 30S ribosomal protein S7

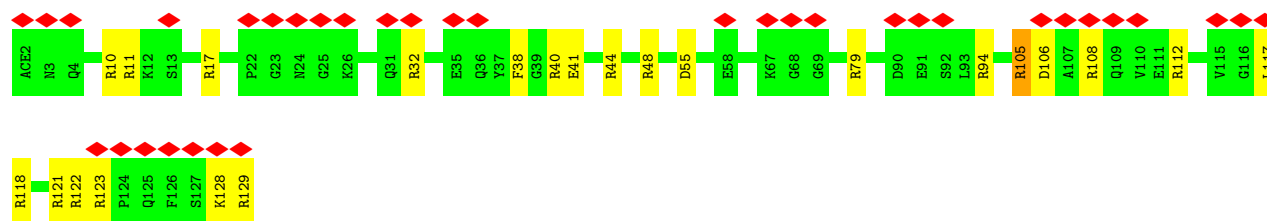


• Molecule 7: 30S ribosomal protein S8

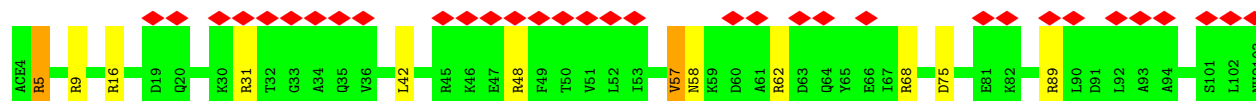
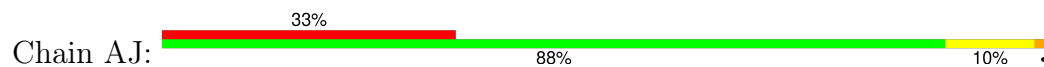


• Molecule 8: 30S ribosomal protein S9

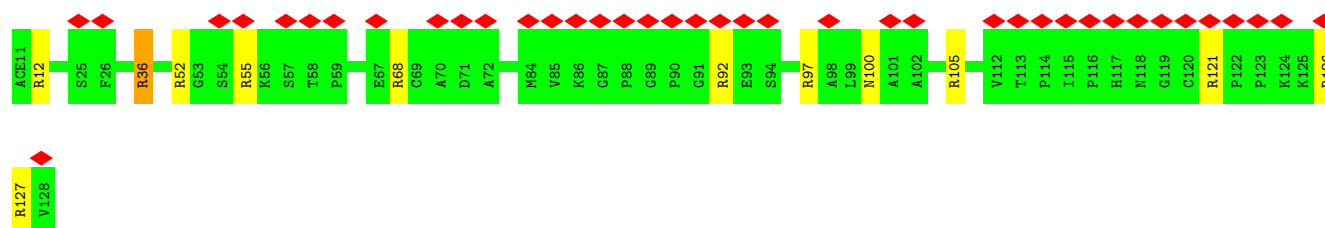
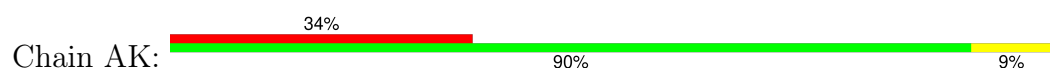




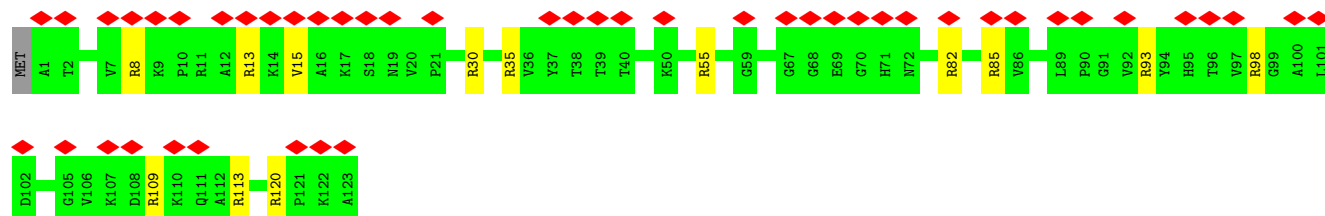
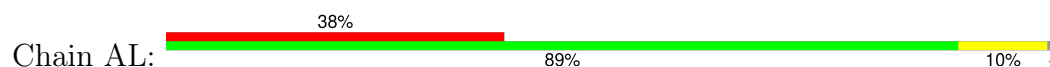
- Molecule 9: 30S ribosomal protein S10



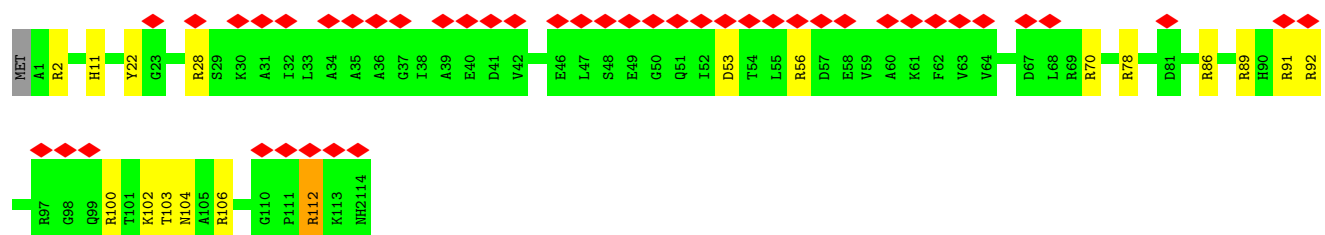
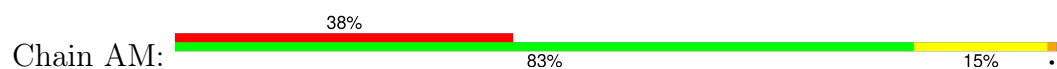
- Molecule 10: 30S ribosomal protein S11



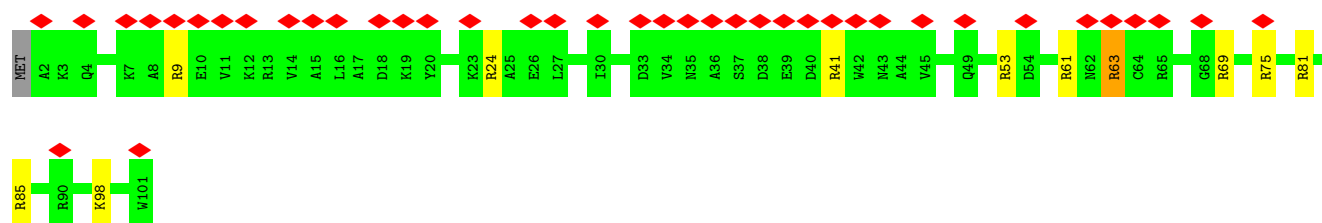
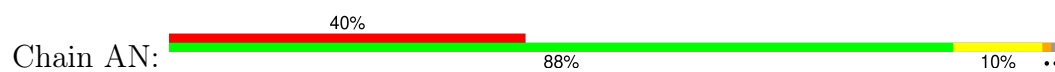
- Molecule 11: 30S ribosomal protein S12



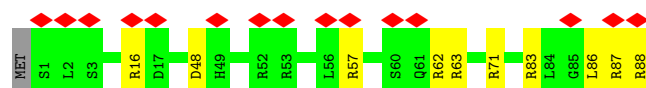
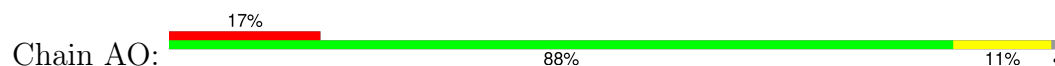
- Molecule 12: 30S ribosomal protein S13



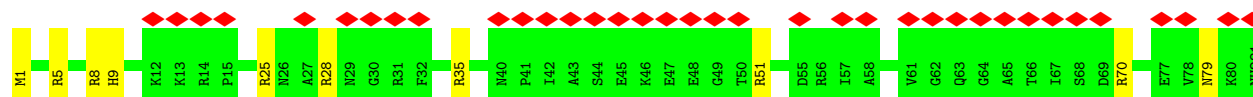
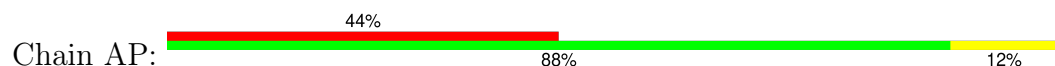
- Molecule 13: 30S ribosomal protein S14



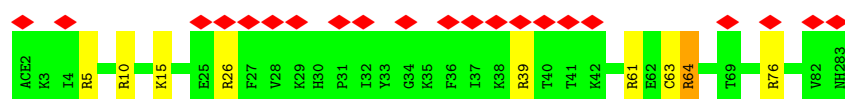
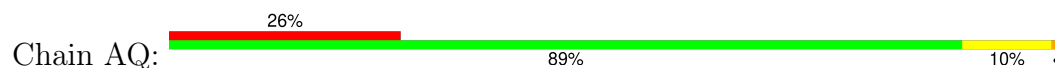
- Molecule 14: 30S ribosomal protein S15



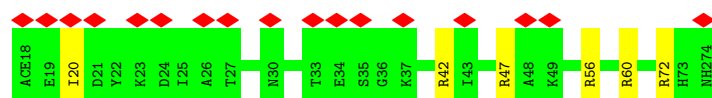
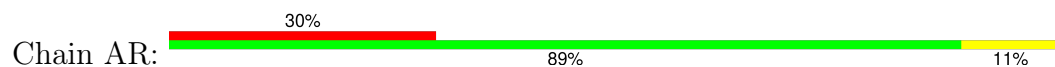
- Molecule 15: 30S ribosomal protein S16



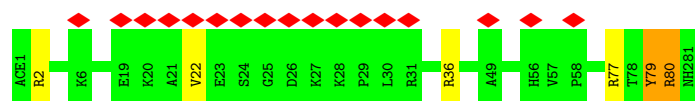
- Molecule 16: 30S ribosomal protein S17



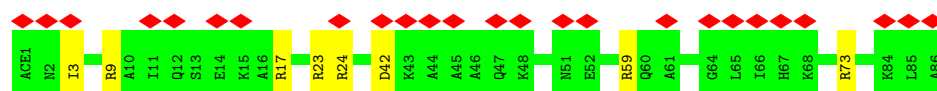
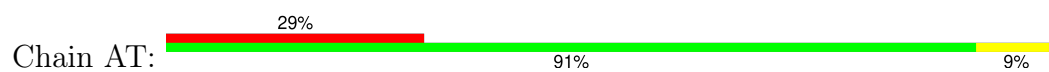
- Molecule 17: 30S ribosomal protein S18



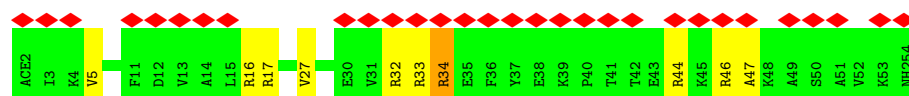
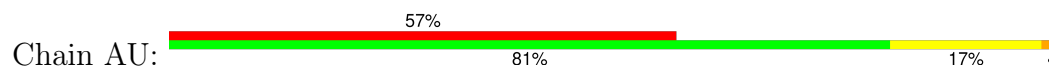
- Molecule 18: 30S ribosomal protein S19



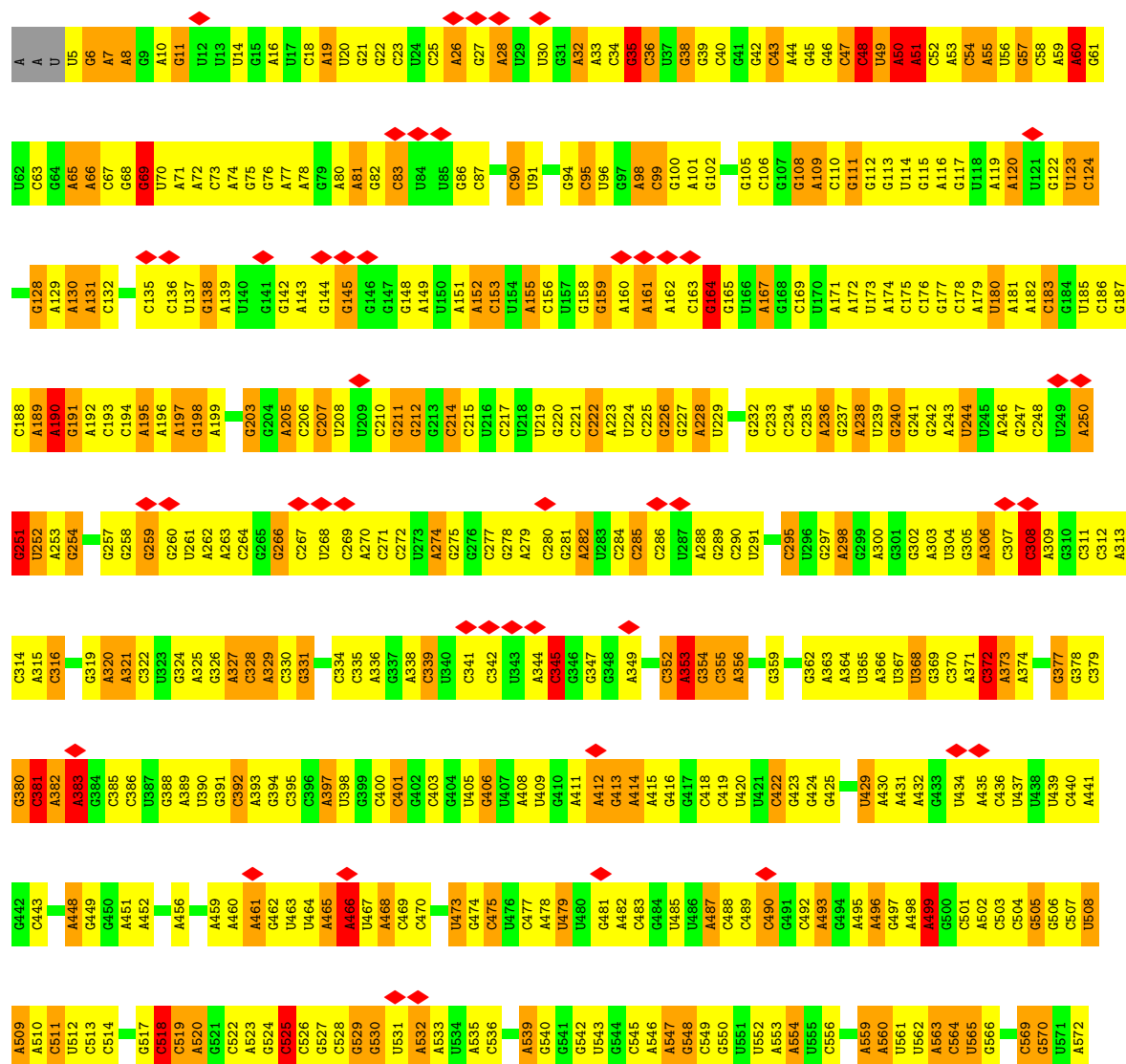
- Molecule 19: 30S ribosomal protein S20

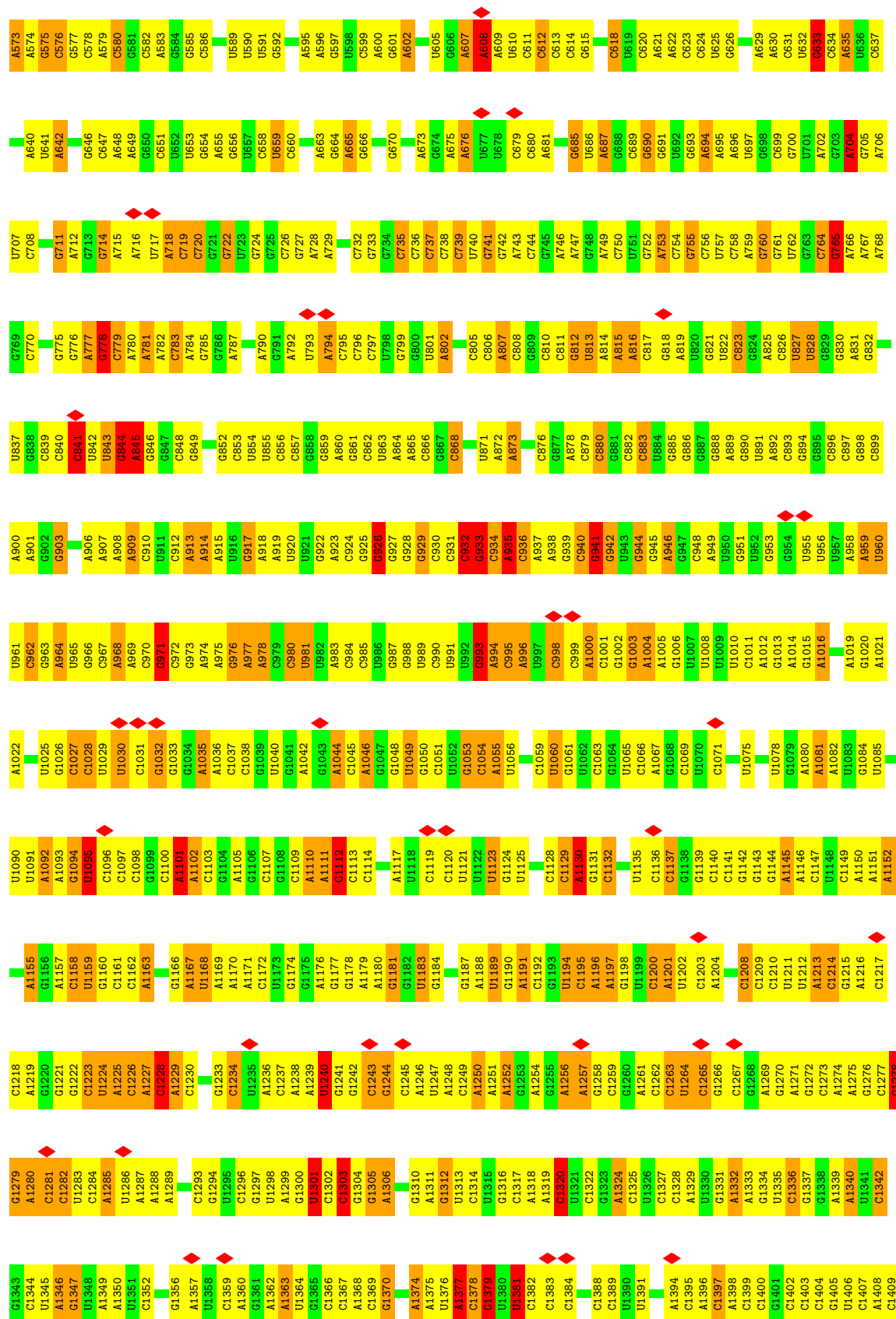


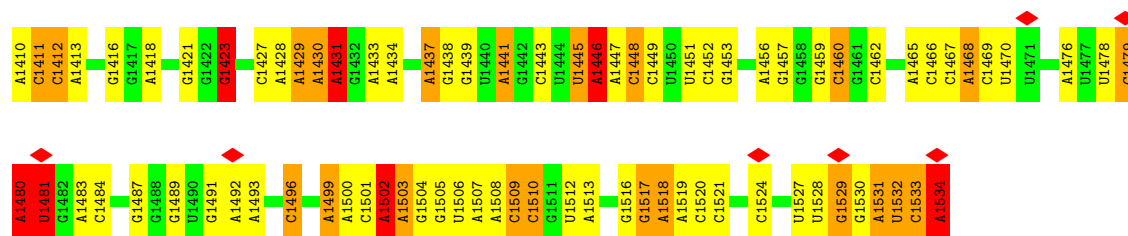
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA



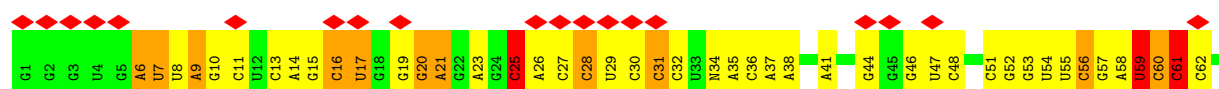




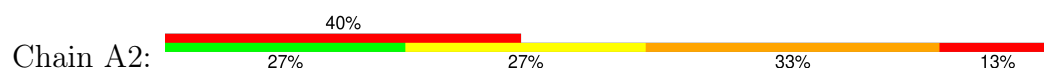
• Molecule 22: fMet-Val-tRNA-Val



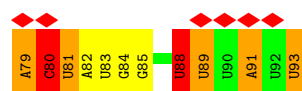
Chain A1:



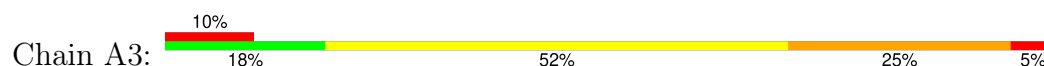
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'



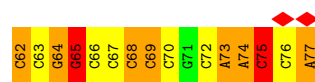
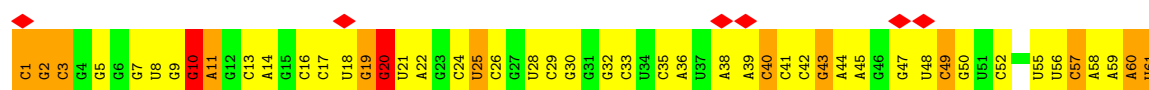
Chain A2:



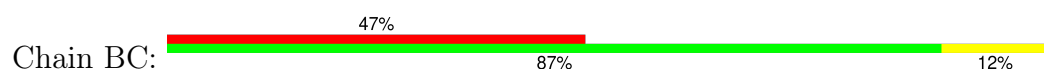
• Molecule 24: tRNA-fMet



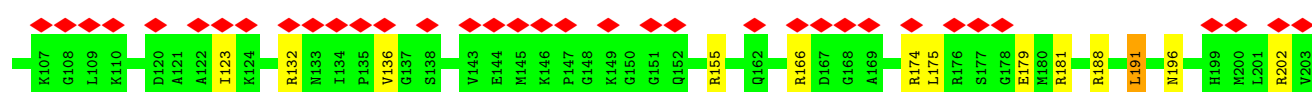
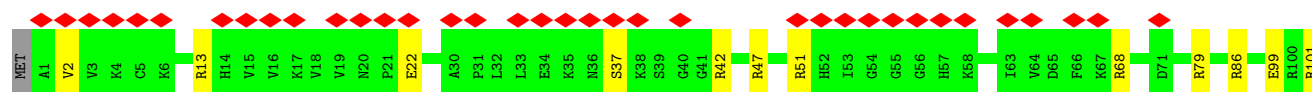
Chain A3:



• Molecule 25: 50S ribosomal protein L2

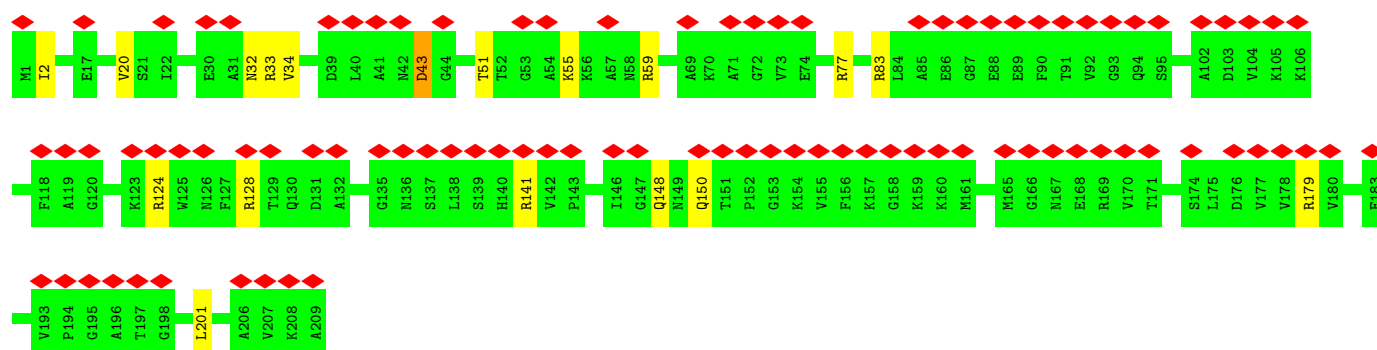


Chain BC:

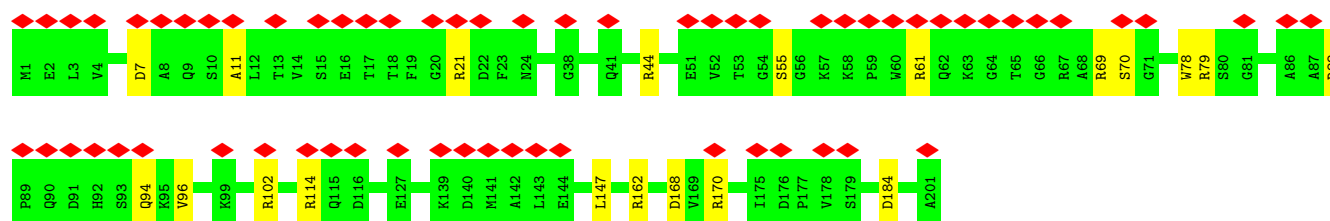
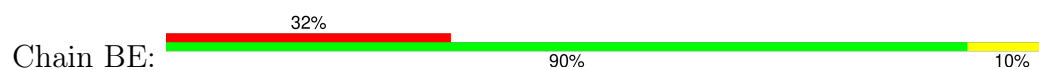




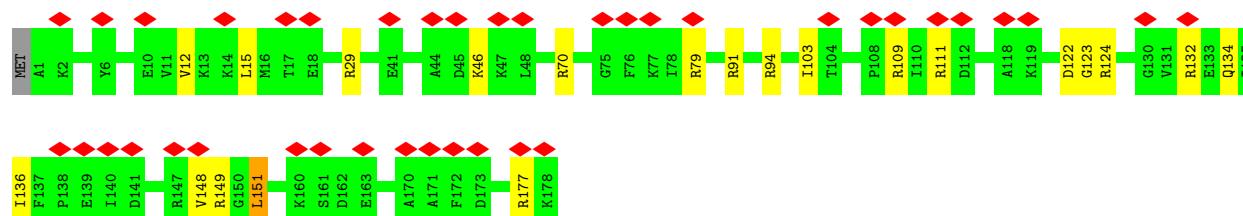
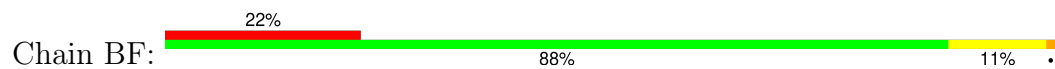
• Molecule 26: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L4

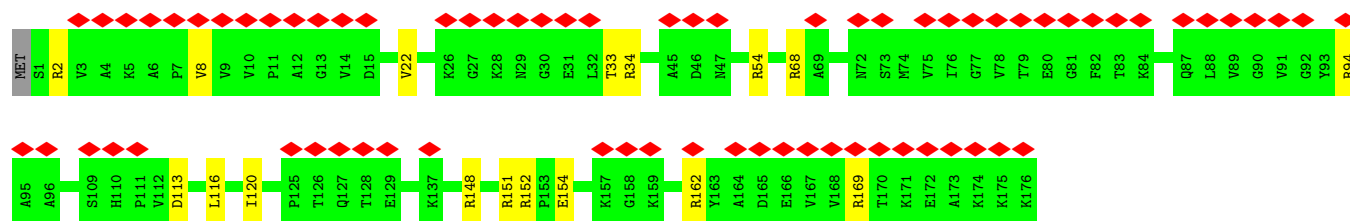


• Molecule 28: 50S ribosomal protein L5

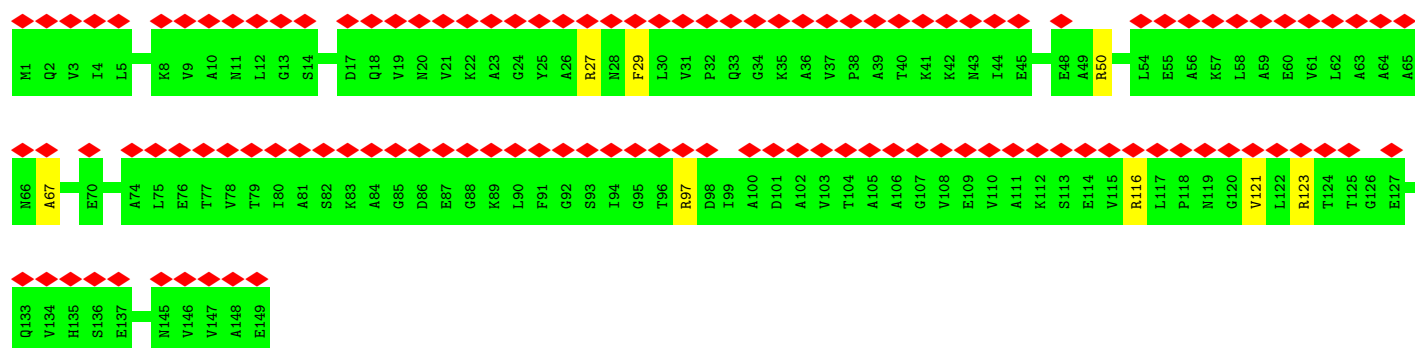
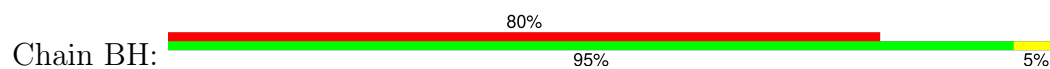


• Molecule 29: 50S ribosomal protein L6

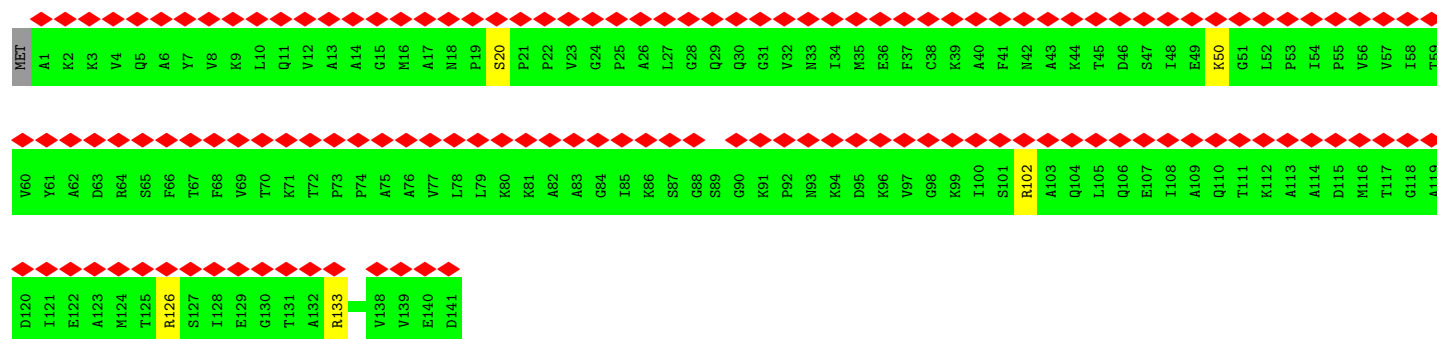




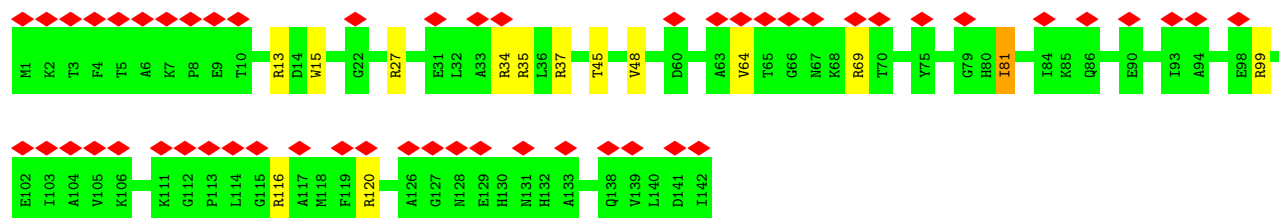
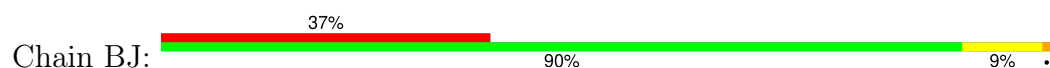
• Molecule 30: 50S ribosomal protein L9



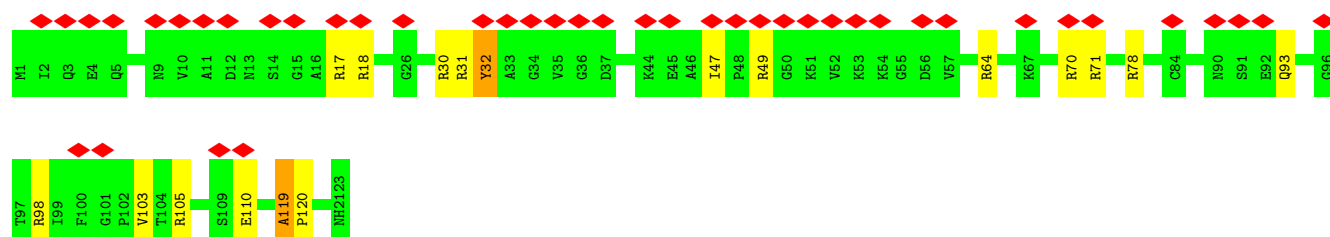
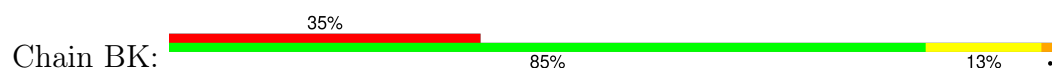
• Molecule 31: 50S ribosomal protein L11



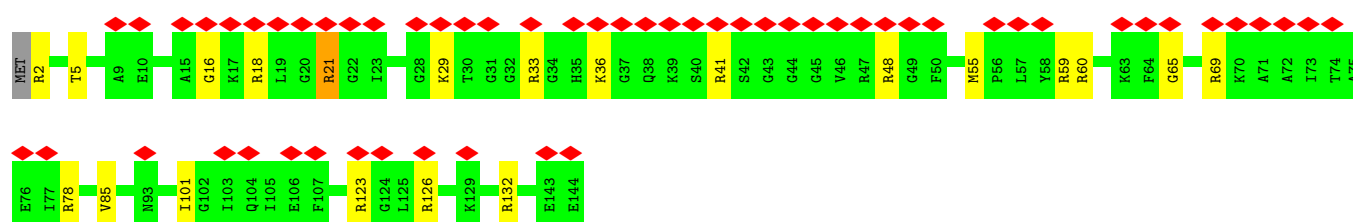
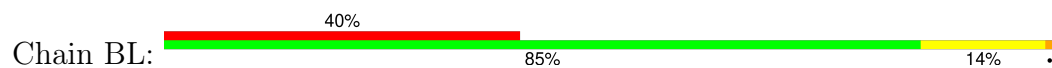
• Molecule 32: 50S ribosomal protein L13



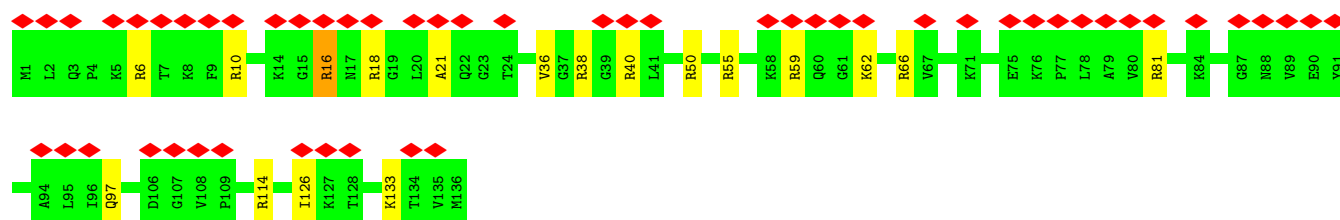
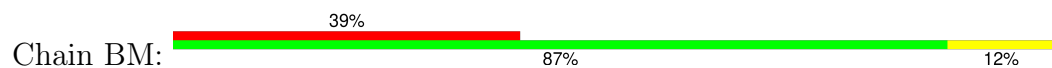
• Molecule 33: 50S ribosomal protein L14



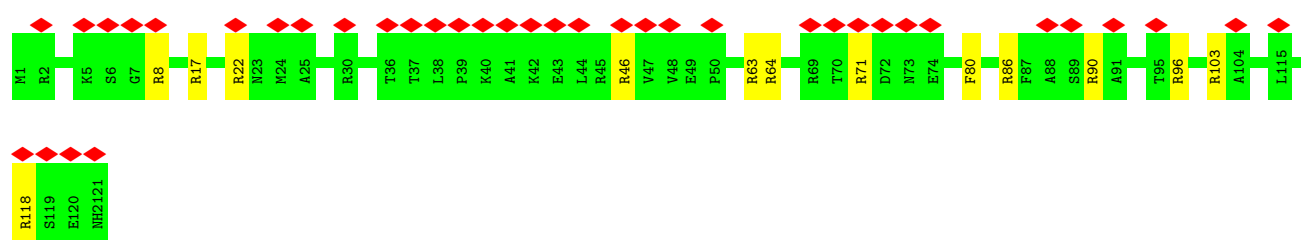
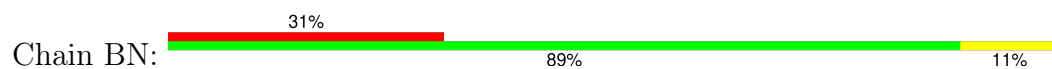
- Molecule 34: 50S ribosomal protein L15



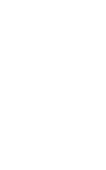
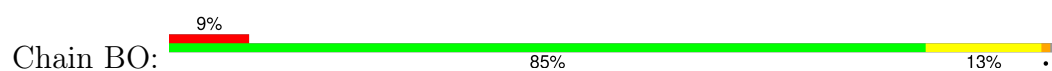
- Molecule 35: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L17

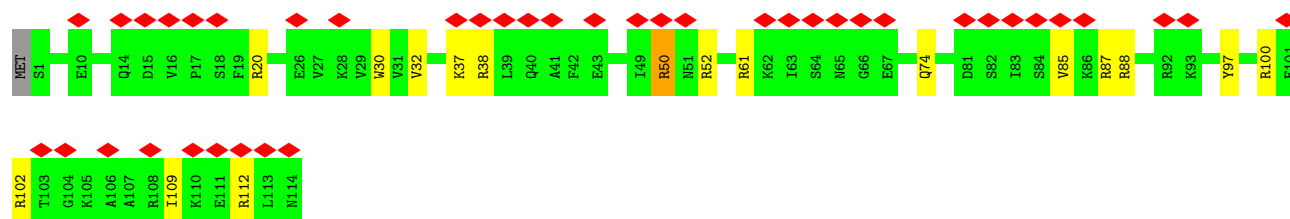
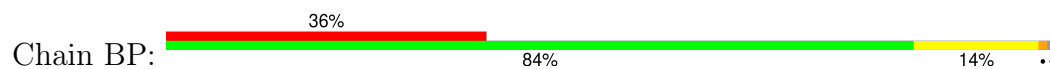


- Molecule 37: 50S ribosomal protein L18

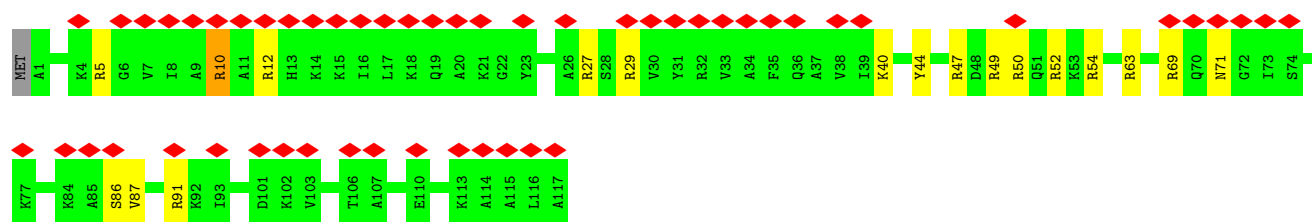
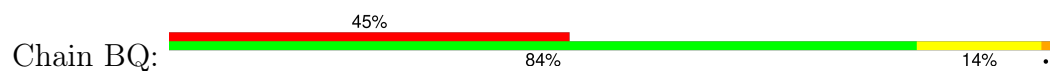




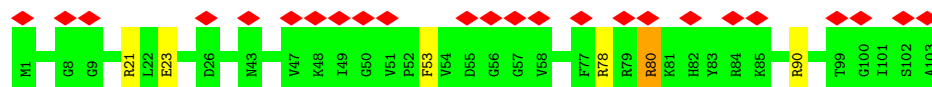
- Molecule 38: 50S ribosomal protein L19



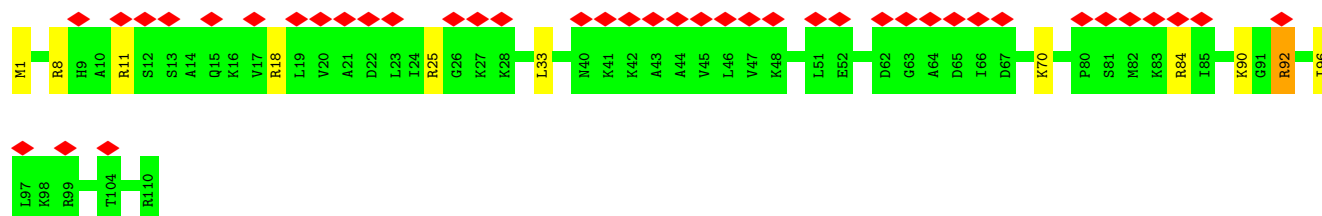
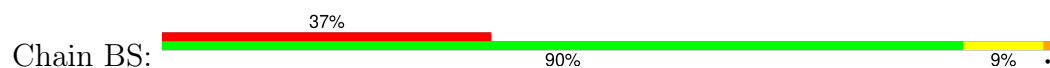
- Molecule 39: 50S ribosomal protein L20



- Molecule 40: 50S ribosomal protein L21

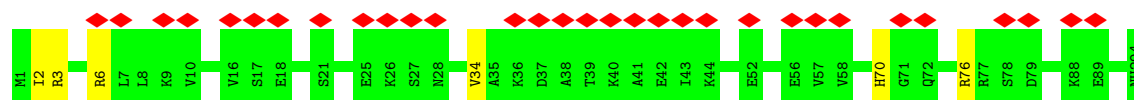


- Molecule 41: 50S ribosomal protein L22

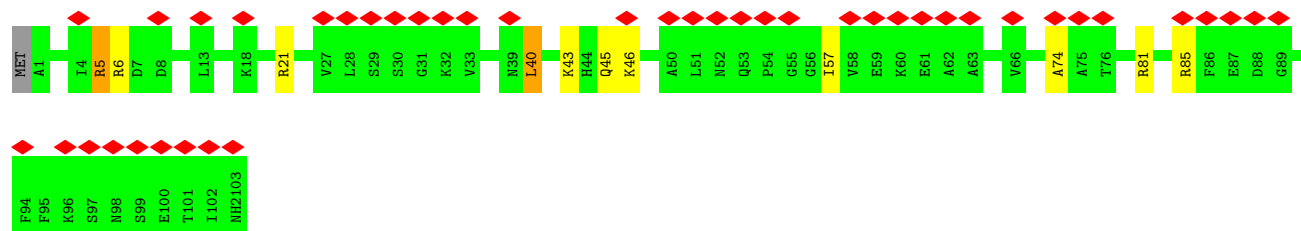
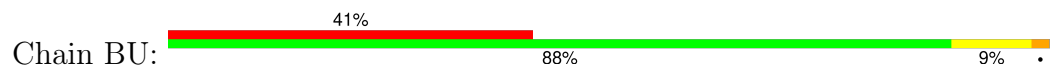


- Molecule 42: 50S ribosomal protein L23

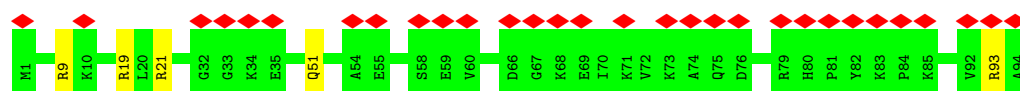




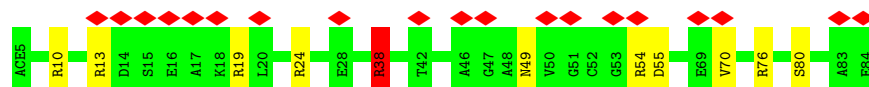
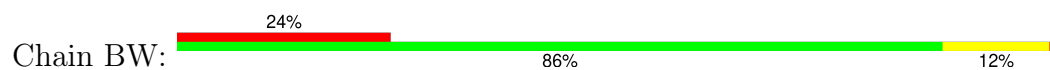
- Molecule 43: 50S ribosomal protein L24



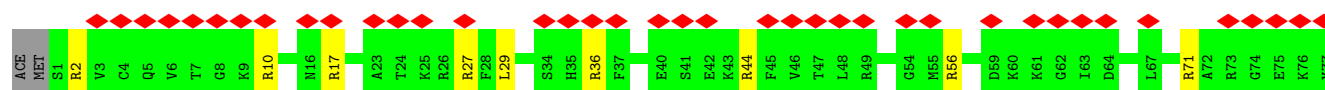
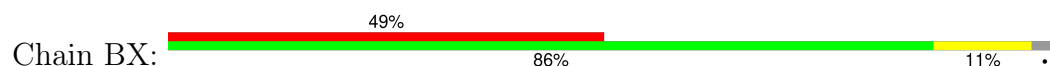
- Molecule 44: 50S ribosomal protein L25



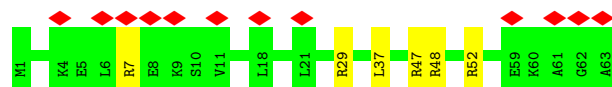
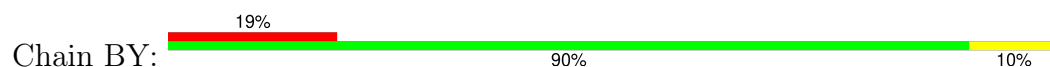
- Molecule 45: 50S ribosomal protein L27



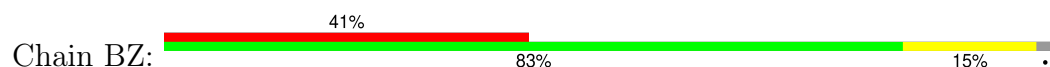
- Molecule 46: 50S ribosomal protein L28

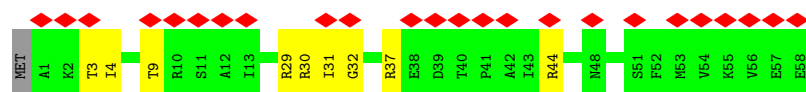


- Molecule 47: 50S ribosomal protein L29

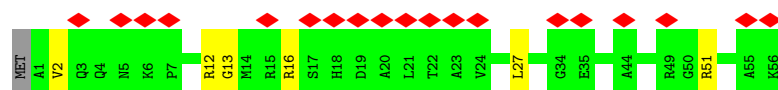
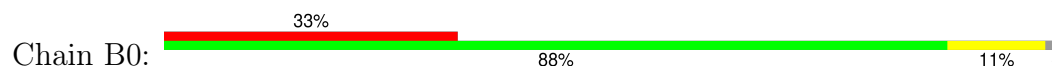


- Molecule 48: 50S ribosomal protein L30

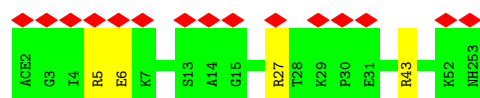




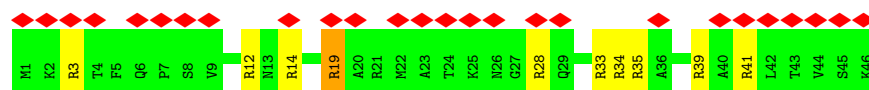
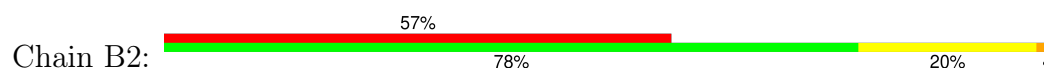
- Molecule 49: 50S ribosomal protein L32



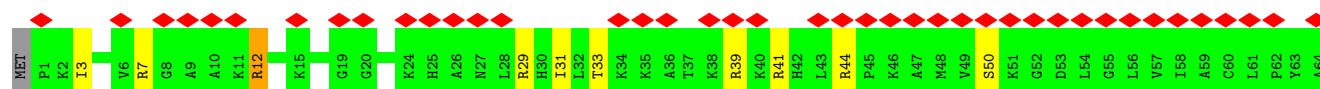
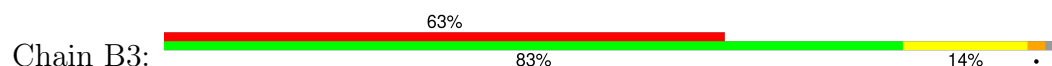
- Molecule 50: 50S ribosomal protein L33



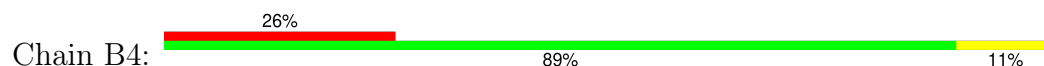
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36



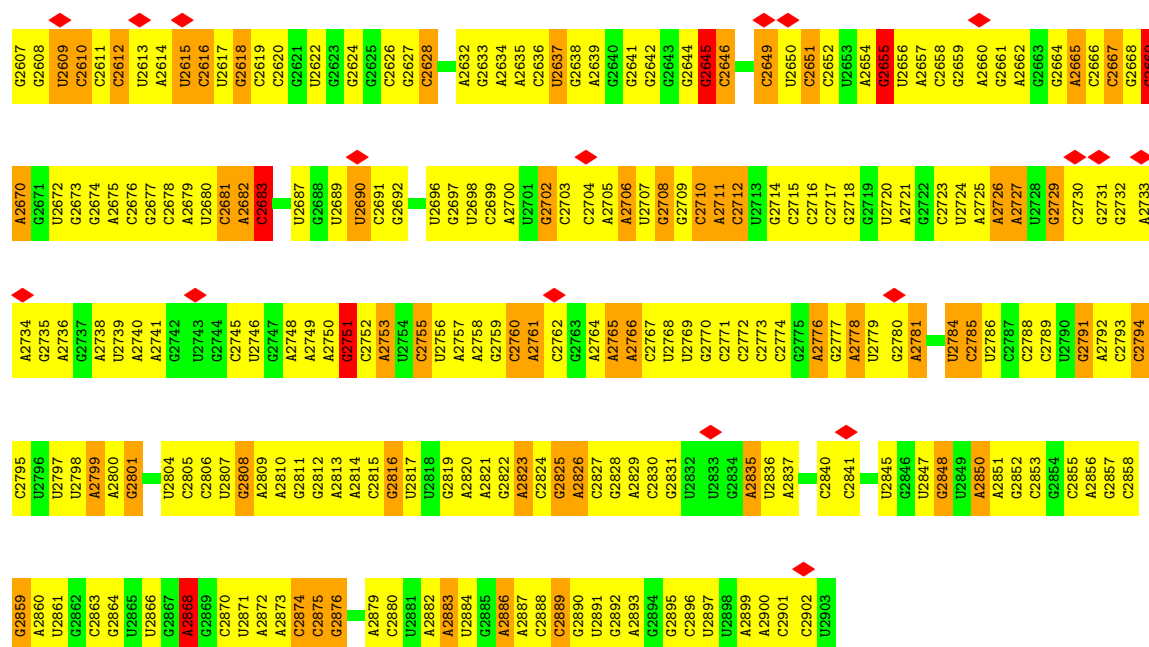
- Molecule 54: 23S ribosomal RNA



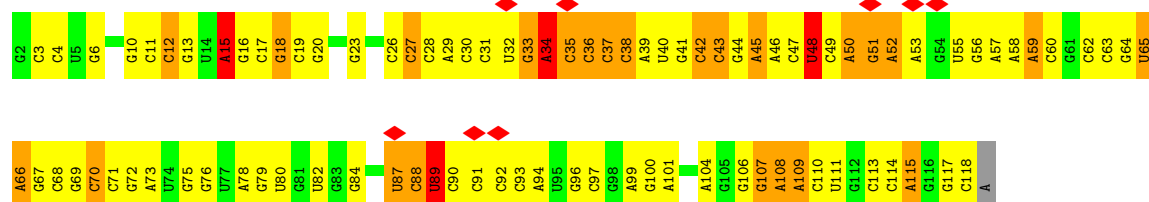


C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	G1738	G1739	G1740	G1741	G1742	G1743	G1744	A1745	A1746	G1747	C1748	A1749	G1750	G1751	C1752	C1753	C1691	C1755	C1756	A1757	C1758	A1759	C1760	C1761	A1762	C1763	C1764	C1765	C1768	C1769	C1770	C1771	A1772	A1773	C1774	C1775	C1776	C1777	C1778	C1779	A1780	C1781	C1782	A1783	A1784	A1785	A1786					
U1662	G1663	A1664	A1665	G1666	G1667	A1668	A1669	C1670	A1671	G1672	G1673	C1674	C1675	A1676	A1677	A1678	A1679	U1680	G1681	G1682	C1683	G1684	C1685	C1686	C1689	A1690	C1692	U1693	C1694	G1695	G1696	G1697	A1698	C1700	A1701	G1702	C1703	C1704	A1705	C1706	G1707	C1708	A1709	C1710	A1711	U1712	A1713	G1714	G1715	G1716	A1717	G1718	G1719	C1782	A1783	G1721	A1722				
C1600	G1601	U1602	A1603	C1604	C1605	C1606	C1607	A1608	A1609	A1610	C1611	C1612	G1613	A1614	C1615	A1616	C1617	A1618	A1619	G1620	U1621	G1622	G1623	U1624	C1625	A1626	G1627	G1628	U1629	A1630	G1631	A1632	G1633	A1634	C1635	U1636	A1637	C1638	C1639	A1640	A1641	C1642	G1643	C1644	G1645	C1646	U1647	U1648	G1649	A1650	G1651	A1652	G1653	A1654	A1655	U1656	U1657	C1658			
U1539	G1540	C1541	U1542	G1543	A1544	A1545	U1546	C1547	A1548	A1549	C1550	A1551	A1552	A1553	U1554	G1555	C1556	C1557	C1558	U1559	G1560	C1561	U1562	U1563	C1564	C1565	A1566	G1567	G1568	A1569	A1570	A1571	A1572	G1573	C1574	C1575	U1576	C1577	U1578	A1579	A1580	G1581	C1582	U1583	A1584	C1585	A1586	U1589	A1590	A1591	C1592	A1593	U1594	C1595	A1596	A1597	U1598	U1599			
C1472	G1473	U1474	U1475	A1476	G1477	G1478	G1479	C1480	U1481	G1482	G1483	C1484	C1485	C1486	C1487	C1488	C1489	A1490	A1491	G1492	C1493	A1494	A1495	A1496	U1497	C1498	C1499	A1500	A1501	A1502	A1503	A1504	A1505	U1506	C1507	A1508	A1509	G1510	G1511	C1512	A1515	C1518	G1519	U1520	G1521	A1522	U1523	G1524	A1525	U1526	G1527	A1528	G1529	G1530	C1531	A1532	U1533	U1534	A1535	C1536	G1537
G1401	U1402	A1403	C1404	U1405	U1406	A1413	A1414	U1415	U1416	C1417	G1418	A1419	A1420	G1421	G1425	G1426	A1427	C1428	C1429	A1431	G1432	A1433	A1434	C1437	U1438	A1439	U1440	G1441	U1442	G1443	G1444	G1445	C1446	C1447	G1450	C1451	G1452	A1453	C1454	G1455	G1456	U1457	U1458	G1459	U1460	C1461	A1462	C1463	G1464	G1465	U1466	A1469	A1470	G1471							
G1338	G1341	A1342	G1343	U1344	C1345	G1346	A1347	C1348	C1349	C1350	C1351	U1352	A1353	A1354	G1355	G1356	C1357	G1358	A1359	G1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	U1372	A1373	C1376	G1377	A1378	U1379	G1382	A1383	A1384	A1385	C1386	A1387	G1388	G1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	C1398	C1399	U1400					
A1274	A1275	A1276	G1277	G1278	G1279	G1280	G1281	U1282	G1283	A1284	A1285	A1286	A1287	G1288	C1289	C1290	C1291	G1292	C1293	U1294	G1295	G1296	C1297	C1298	G1299	G1300	A1301	A1302	G1303	A1304	C1305	C1306	A1307	A1308	G1309	U1312	U1313	C1314	C1315	C1319	C1320	A1321	A1322	C1323	G1324	A1327	A1328	U1329	C1330	A1331	G1332	G1333	G1334	C1335	A1336	G1337					
G1212	A1213	A1214	G1215	G1216	U1219	G1220	C1221	U1222	G1223	U1224	G1225	A1226	G1227	G1228	C1229	A1230	C1233	U1234	G1235	G1236	A1237	G1238	G1239	U1240	A1241	U1242	C1243	A1244	G1245	A1246	G1247	G1248	U1249	G1250	C1251	G1252	A1253	A1254	U1255	G1256	C1257	U1258	G1259	A1260	C1261	A1262	U1263	A1264	A1265	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273				
C1146	A1147	U1148	G1149	C1150	A1151	C1152	C1153	U1154	A1155	A1156	G1157	C1158	U1159	G1160	C1161	C1164	A1165	G1166	G1167	G1168	A1169	C1170	G1171	C1172	U1173	U1174	A1175	U1176	G1177	C1178	U1179	U1180	U1181	G1182	U1183	U1184	G1185	G1186	A1189	A1194	G1195	C1196	G1197	U1198	U1199	C1200	U1201	A1204	A1205	G1206	C1207	C1208	U1209	G1210	C1211						
A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	C1106	G1107	U1108	C1109	A1110	G1111	G1112	U1113	C1114	G1115	G1116	C1117	C1118	U1119	C1120	C1121	G1122	C1123	G1124	G1125	A1126	A1127	G1128	A1129	U1132	A1133	A1134	C1135	G1136	G1137	C1138	G1139	C1140	U1141	A1142	A1143	A1144	C1145			
G1034	G1035	A1036	G1037	A1038	G1039	A1040	G1041	G1042	C1043	C1044	A1045	A1046	G1047	A1048	C985	C986	C987	A988	C989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	C1005	C1006	C1007	A1008	A1009	A1010	G1011	U1012	C1013	A1014	U1015	G1016	U1017	G1018	U1019	A1020	A1021	G1022	U1023											
C961	C962	U963	C964	C965	C968	C969	U970	C971	A972	A973	G974	A975	G976	G977	G978	A979	A980	A981	C982	A983	A984	C985	C986	C987	A988	C989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	C1005	C1006	C1007	A1008	A1009	A1010	G1011	U1012	C1013	A1014	U1015	G1016	U1017	G1018	U1019	A1020	A1021	G1022	U1023				

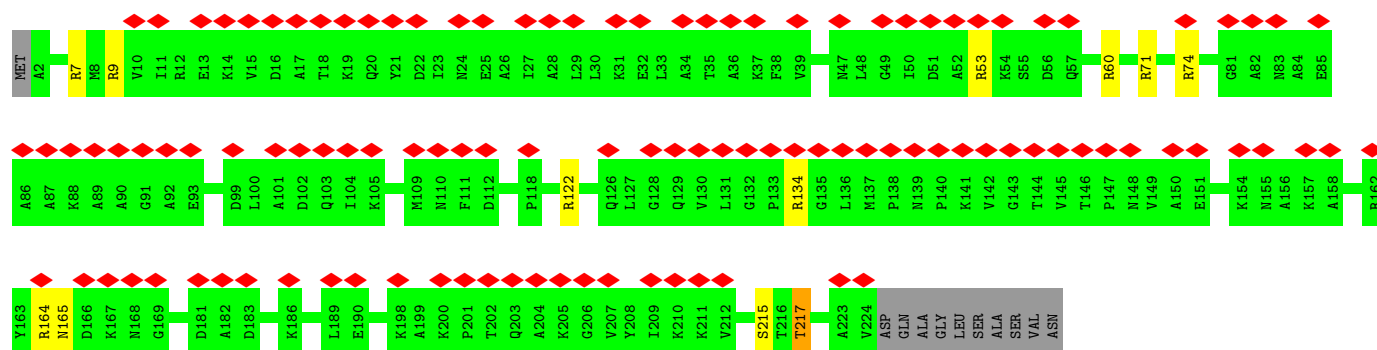
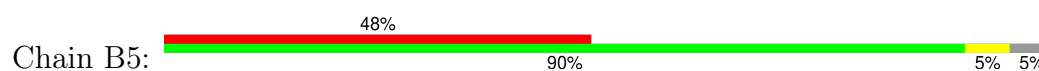




• Molecule 55: 5S ribosomal RNA



• 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	8375	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	194.626	Depositor
Minimum map value	-114.806	Depositor
Average map value	-0.932	Depositor
Map value standard deviation	20.010	Depositor
Recommended contour level	26	Depositor
Map size (\AA)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\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: ACE, 5MU, FME, 4SU, PSU, H2U, 7MG, NH2, OMC, 6MZ, CM0

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	0.72	0/1736	1.06	11/2340 (0.5%)
2	AC	0.75	0/1651	1.13	14/2225 (0.6%)
3	AD	0.78	0/1665	1.20	20/2227 (0.9%)
4	AE	0.70	0/1119	1.01	8/1506 (0.5%)
5	AF	0.74	0/835	1.16	8/1128 (0.7%)
6	AG	0.74	0/1188	1.21	15/1593 (0.9%)
7	AH	0.71	0/989	1.03	6/1326 (0.5%)
8	AI	0.82	0/1035	1.31	19/1377 (1.4%)
9	AJ	0.71	0/797	1.18	8/1079 (0.7%)
10	AK	0.75	0/894	1.17	11/1207 (0.9%)
11	AL	0.78	0/969	1.24	13/1300 (1.0%)
12	AM	0.75	0/884	1.29	13/1181 (1.1%)
13	AN	0.78	0/817	1.22	10/1088 (0.9%)
14	AO	0.73	0/722	1.14	9/964 (0.9%)
15	AP	0.78	0/648	1.21	7/870 (0.8%)
16	AQ	0.69	0/658	1.21	11/883 (1.2%)
17	AR	0.83	0/463	1.23	7/623 (1.1%)
18	AS	0.76	0/653	1.17	7/879 (0.8%)
19	AT	0.70	0/672	1.11	7/890 (0.8%)
20	AU	0.83	0/431	1.39	7/572 (1.2%)
21	AA	1.52	2/36759 (0.0%)	2.22	1945/57346 (3.4%)
22	A1	1.52	0/1668	2.16	80/2595 (3.1%)
23	A2	1.51	0/343	2.27	22/531 (4.1%)
24	A3	1.54	0/1722	2.21	92/2685 (3.4%)
25	BC	0.76	0/2121	1.32	27/2852 (0.9%)
26	BD	0.69	0/1586	1.14	10/2134 (0.5%)
27	BE	0.68	0/1571	1.18	13/2113 (0.6%)
28	BF	0.76	0/1444	1.15	11/1937 (0.6%)
29	BG	0.69	0/1343	1.16	9/1816 (0.5%)
30	BH	0.67	0/1122	1.14	6/1515 (0.4%)
31	BI	0.67	0/1046	1.04	3/1410 (0.2%)
32	BJ	0.75	0/1152	1.20	9/1551 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.72	0/947	1.25	11/1268 (0.9%)
34	BL	0.75	0/1054	1.38	15/1403 (1.1%)
35	BM	0.76	0/1093	1.25	14/1460 (1.0%)
36	BN	0.77	0/973	1.28	13/1301 (1.0%)
37	BO	0.75	0/902	1.25	13/1209 (1.1%)
38	BP	0.74	0/929	1.26	12/1242 (1.0%)
39	BQ	0.82	0/960	1.35	17/1278 (1.3%)
40	BR	0.72	0/829	1.14	6/1107 (0.5%)
41	BS	0.66	0/864	1.18	6/1156 (0.5%)
42	BT	0.67	0/744	1.15	4/994 (0.4%)
43	BU	0.69	0/787	1.16	5/1051 (0.5%)
44	BV	0.74	0/766	1.13	4/1025 (0.4%)
45	BW	0.76	0/604	1.33	9/799 (1.1%)
46	BX	0.76	0/635	1.27	9/848 (1.1%)
47	BY	0.69	0/510	1.26	6/677 (0.9%)
48	BZ	0.70	0/453	1.24	5/605 (0.8%)
49	B0	0.74	0/450	1.17	3/599 (0.5%)
50	B1	0.72	0/417	1.15	4/556 (0.7%)
51	B2	0.83	0/380	1.65	11/498 (2.2%)
52	B3	0.75	0/513	1.25	5/676 (0.7%)
53	B4	0.71	0/303	1.34	5/397 (1.3%)
54	BA	1.40	0/69796	2.21	4043/108888 (3.7%)
55	BB	1.41	0/2800	2.18	152/4367 (3.5%)
56	B5	0.67	0/1673	1.09	10/2255 (0.4%)
All	All	1.28	2/160085 (0.0%)	2.00	6820/239402 (2.8%)

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
2	AC	0	1
6	AG	0	1
7	AH	0	1
21	AA	0	369
22	A1	0	10
23	A2	0	4
24	A3	0	19
37	BO	0	1
52	B3	0	1
54	BA	0	715

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	28
All	All	0	1150

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1533	C	C4-N4	-5.16	1.29	1.33
21	AA	942	G	C5'-C4'	5.05	1.57	1.51

The worst 5 of 6820 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	704	A	N1-C6-N6	-13.07	110.76	118.60
54	BA	1274	A	N1-C6-N6	-12.32	111.21	118.60
34	BL	41	ARG	NE-CZ-NH1	12.26	126.43	120.30
54	BA	910	A	N1-C6-N6	-12.23	111.26	118.60
21	AA	913	A	N1-C6-N6	-12.01	111.40	118.60

There are no chirality outliers.

5 of 1150 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	6	G	Sidechain
21	AA	7	A	Sidechain
2	AC	172	VAL	Peptide
6	AG	3	ARG	Sidechain
7	AH	76	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AF	818	0	808	2	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	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	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	2	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	1	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	0	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	2	0
39	BQ	947	0	1022	1	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	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BY	509	0	543	0	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	31345	1	0
55	BB	2504	0	1271	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	99663	11	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 11 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)
28:BF:151:LEU:HD13	28:BF:151:LEU:H	1.75	0.51
9:AJ:57:VAL:HG23	9:AJ:58:ASN:H	1.77	0.50
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.30	0.50
21:AA:565:U:H2'	21:AA:566:G:C8	2.48	0.47
21:AA:940:C:H2'	21:AA:941:G:C8	2.50	0.46

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%)	198 (91%)	16 (7%)	4 (2%)	7	35
2	AC	205/208 (99%)	188 (92%)	8 (4%)	9 (4%)	2	17
3	AD	203/206 (98%)	182 (90%)	18 (9%)	3 (2%)	8	40
4	AE	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	2	18
5	AF	99/101 (98%)	84 (85%)	9 (9%)	6 (6%)	1	13
6	AG	150/152 (99%)	130 (87%)	14 (9%)	6 (4%)	2	18
7	AH	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	55
8	AI	126/128 (98%)	115 (91%)	9 (7%)	2 (2%)	8	38
9	AJ	98/100 (98%)	92 (94%)	2 (2%)	4 (4%)	2	18
10	AK	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	14	52
11	AL	121/124 (98%)	107 (88%)	13 (11%)	1 (1%)	16	55
12	AM	112/115 (97%)	98 (88%)	9 (8%)	5 (4%)	2	17
13	AN	98/101 (97%)	87 (89%)	10 (10%)	1 (1%)	13	49
14	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	11	44
15	AP	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	10	43
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	26
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	7	35
18	AS	79/81 (98%)	67 (85%)	9 (11%)	3 (4%)	2	19
19	AT	84/86 (98%)	78 (93%)	4 (5%)	2 (2%)	5	27
20	AU	51/53 (96%)	33 (65%)	14 (28%)	4 (8%)	1	10
25	BC	270/273 (99%)	237 (88%)	25 (9%)	8 (3%)	3	23
26	BD	207/209 (99%)	181 (87%)	17 (8%)	9 (4%)	2	17
27	BE	199/201 (99%)	180 (90%)	12 (6%)	7 (4%)	3	20
28	BF	176/179 (98%)	161 (92%)	8 (4%)	7 (4%)	2	18
29	BG	174/177 (98%)	158 (91%)	11 (6%)	5 (3%)	3	23
30	BH	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	6	32
31	BI	139/142 (98%)	132 (95%)	7 (5%)	0	100	100
32	BJ	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	3	20
33	BK	121/123 (98%)	103 (85%)	12 (10%)	6 (5%)	1	16
34	BL	141/144 (98%)	122 (86%)	10 (7%)	9 (6%)	1	13
35	BM	134/136 (98%)	121 (90%)	8 (6%)	5 (4%)	2	20
36	BN	119/121 (98%)	101 (85%)	17 (14%)	1 (1%)	16	55

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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%)	99 (88%)	10 (9%)	3 (3%)	4	25
39	BQ	115/118 (98%)	105 (91%)	7 (6%)	3 (3%)	4	26
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6	32
41	BS	108/110 (98%)	96 (89%)	8 (7%)	4 (4%)	2	20
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	5	29
43	BU	101/104 (97%)	79 (78%)	16 (16%)	6 (6%)	1	13
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	4	26
46	BX	75/79 (95%)	69 (92%)	6 (8%)	0	100	100
47	BY	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	8	38
48	BZ	56/59 (95%)	47 (84%)	4 (7%)	5 (9%)	0	9
49	B0	54/57 (95%)	50 (93%)	2 (4%)	2 (4%)	2	20
50	B1	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	6	32
51	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
52	B3	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	1	12
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	205 (93%)	15 (7%)	1 (0%)	25	64
All	All	5876/6008 (98%)	5258 (90%)	453 (8%)	165 (3%)	6	24

5 of 165 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	206	ILE
2	AC	4	VAL
3	AD	54	LEU
4	AE	105	ILE
5	AF	59	TYR

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%)	166 (98%)	4 (2%)	44	62
3	AD	172/173 (99%)	168 (98%)	4 (2%)	45	64
4	AE	113/113 (100%)	112 (99%)	1 (1%)	75	83
5	AF	87/87 (100%)	85 (98%)	2 (2%)	45	64
6	AG	123/123 (100%)	121 (98%)	2 (2%)	58	73
7	AH	104/105 (99%)	102 (98%)	2 (2%)	52	69
8	AI	105/105 (100%)	100 (95%)	5 (5%)	21	43
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	88 (98%)	2 (2%)	47	65
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	90 (99%)	1 (1%)	70	80
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%)	63 (97%)	2 (3%)	35	54
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	212 (98%)	4 (2%)	52	69
26	BD	164/164 (100%)	161 (98%)	3 (2%)	54	71
27	BE	165/165 (100%)	161 (98%)	4 (2%)	44	62
28	BF	149/150 (99%)	146 (98%)	3 (2%)	50	68
29	BG	137/138 (99%)	134 (98%)	3 (2%)	47	65
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	107 (98%)	2 (2%)	54	71
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	75	83
33	BK	103/103 (100%)	102 (99%)	1 (1%)	73	82
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	107 (98%)	2 (2%)	54	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	100 (100%)	0	100	100
37	BO	86/87 (99%)	83 (96%)	3 (4%)	31	51
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%)	79 (99%)	1 (1%)	65	77
43	BU	83/84 (99%)	81 (98%)	2 (2%)	44	62
44	BV	78/78 (100%)	77 (99%)	1 (1%)	65	77
45	BW	59/59 (100%)	55 (93%)	4 (7%)	13	34
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%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	48	66
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	37 (97%)	1 (3%)	41	59
52	B3	51/52 (98%)	50 (98%)	1 (2%)	50	68
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	56	72
All	All	4842/4870 (99%)	4763 (98%)	79 (2%)	58	73

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	BO	117	PHE
45	BW	80	SER
38	BP	85	VAL
43	BU	40	LEU
52	B3	33	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	AF	14	GLN

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Mol	Chain	Res	Type
27	BE	46	GLN
35	BM	97	GLN
37	BO	29	HIS
49	B0	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	229 (14%)	86 (5%)
22	A1	73/76 (96%)	14 (19%)	5 (6%)
23	A2	15/15 (100%)	5 (33%)	4 (26%)
24	A3	76/77 (98%)	17 (22%)	6 (7%)
54	BA	2902/2903 (99%)	457 (15%)	117 (4%)
55	BB	116/118 (98%)	18 (15%)	4 (3%)
All	All	4711/4722 (99%)	740 (15%)	222 (4%)

5 of 740 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	27	G
21	AA	28	A
21	AA	32	A
21	AA	35	G

5 of 222 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	276	U
55	BB	107	G
54	BA	989	G
55	BB	51	G
54	BA	2428	G

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	22,23	21,26,27	1.30	2 (9%)	26,37,40	1.36	3 (11%)
24	5MU	A3	55	24	19,22,23	0.71	0	27,32,35	1.33	3 (11%)
24	OMC	A3	33	24	19,22,23	0.68	0	25,31,34	1.12	1 (4%)
22	PSU	A1	55	22	18,21,22	0.82	0	21,30,33	1.36	3 (14%)
24	PSU	A3	56	24	18,21,22	0.82	0	21,30,33	1.10	2 (9%)
22	6MZ	A1	37	22	17,25,26	1.01	1 (5%)	15,36,39	1.59	3 (20%)
24	4SU	A3	8	24	18,21,22	1.49	1 (5%)	25,30,33	0.83	1 (4%)
22	5MU	A1	54	22	19,22,23	0.68	0	27,32,35	1.21	2 (7%)
24	H2U	A3	21	24	18,21,22	1.36	2 (11%)	19,30,33	1.23	3 (15%)
22	4SU	A1	7	22	18,21,22	1.41	2 (11%)	25,30,33	1.08	3 (12%)
22	7MG	A1	46	22	23,26,27	4.09	2 (8%)	27,39,42	1.51	2 (7%)

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

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

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	-19.21	1.33	1.45
24	A3	8	4SU	C5-C4	-5.26	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	7	4SU	C5-C4	-5.02	1.36	1.42
22	A1	34	CM0	O5-C5	-4.72	1.25	1.36
24	A3	21	H2U	C2-N3	-3.46	1.31	1.38

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	6.08	111.97	103.37
22	A1	34	CM0	C7-O5-C5	4.47	123.17	117.48
22	A1	55	PSU	C6-C5-C4	3.73	120.69	118.17
22	A1	37	6MZ	C9-N6-C6	3.47	126.07	122.85
24	A3	33	OMC	O2-C2-N3	-3.45	116.89	122.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	O5-C7-C8-O9
22	A1	34	CM0	O5-C7-C8-O8
22	A1	55	PSU	O4'-C1'-C5-C6

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	$\# Z > 2$
58	FME	BA	3001	57	8,9,10	0.67	0	8,9,11	1.24	1 (12%)
57	VAL	A1	101	58,22	4,6,7	0.77	0	6,7,9	1.82	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	FME	BA	3001	57	-	1/7/9/11	-
57	VAL	A1	101	58,22	-	0/5/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
57	A1	101	VAL	O-C-CA	-4.11	114.21	124.77
58	BA	3001	FME	C-CA-N	2.48	114.28	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.

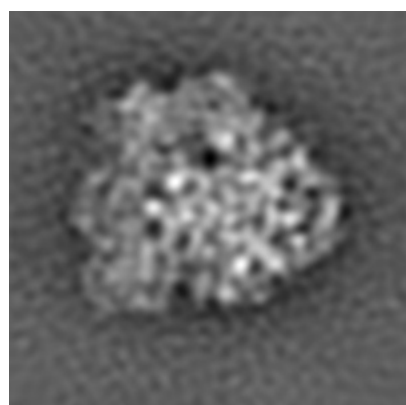
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1719. These allow visual inspection of the internal detail of the map and identification of artifacts.

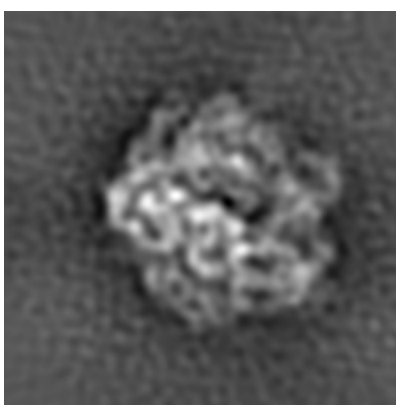
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

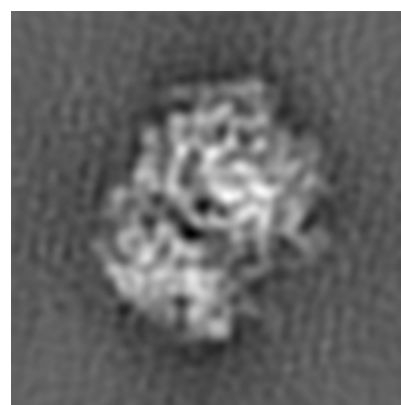
6.1.1 Primary map



X



Y

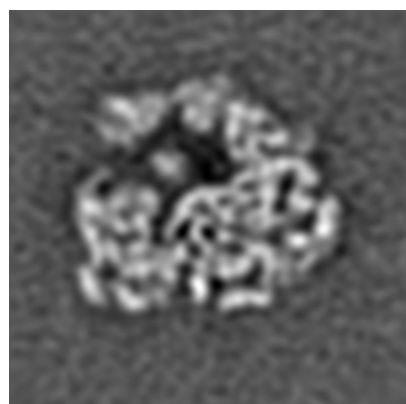


Z

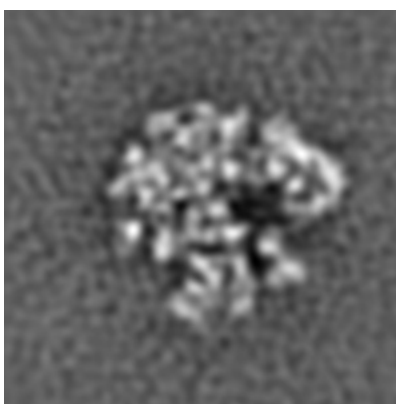
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

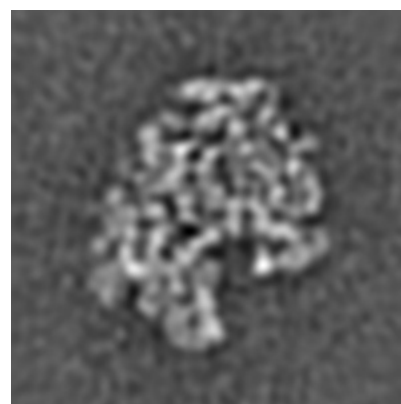
6.2.1 Primary map



X Index: 64



Y Index: 64

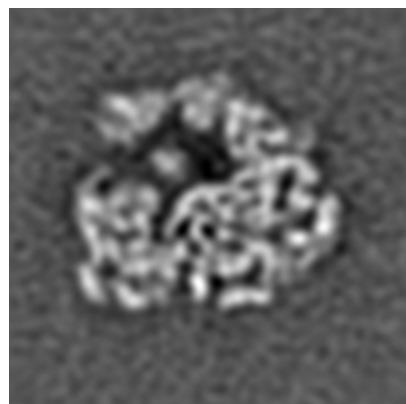


Z Index: 64

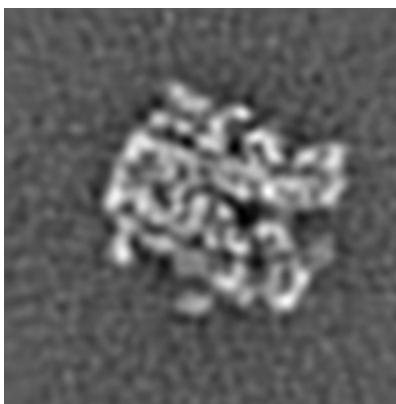
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

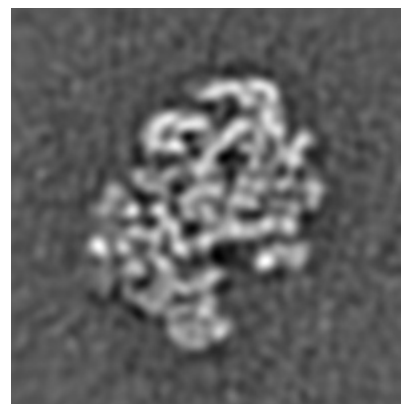
6.3.1 Primary map



X Index: 64



Y Index: 69

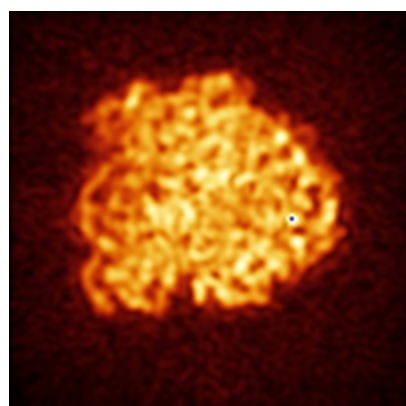


Z Index: 61

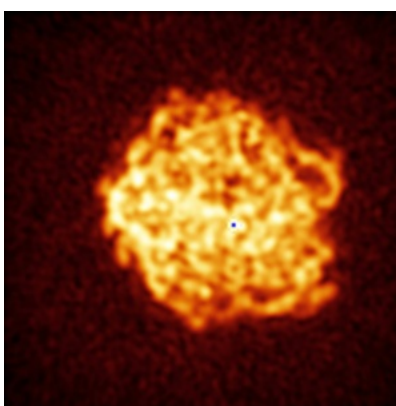
The images above show the largest variance slices of the map in three orthogonal directions.

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

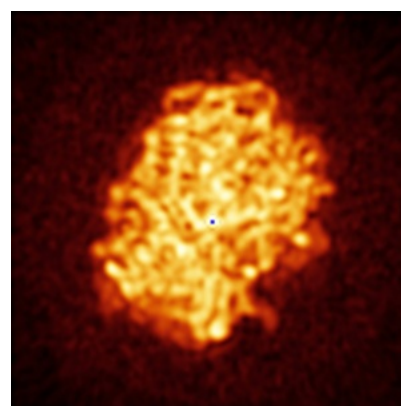
6.4.1 Primary map



X



Y

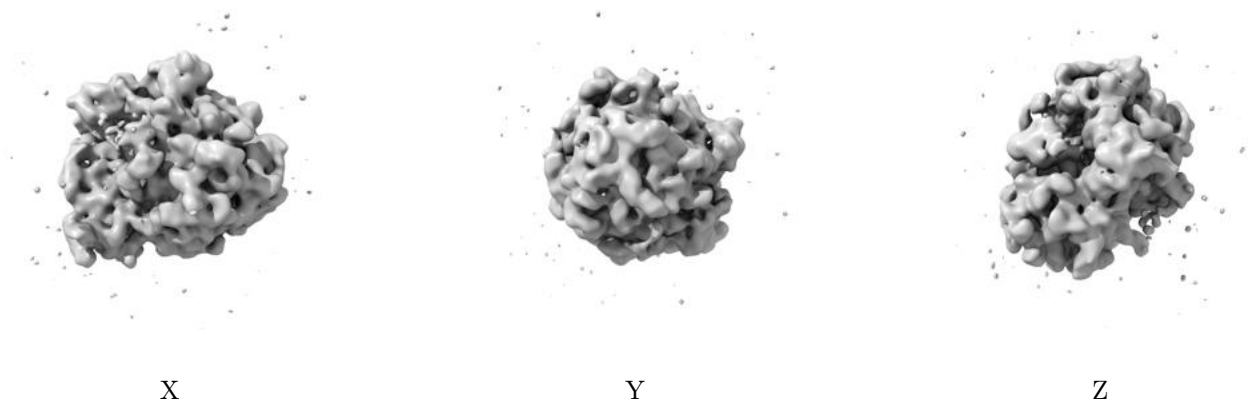


Z

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

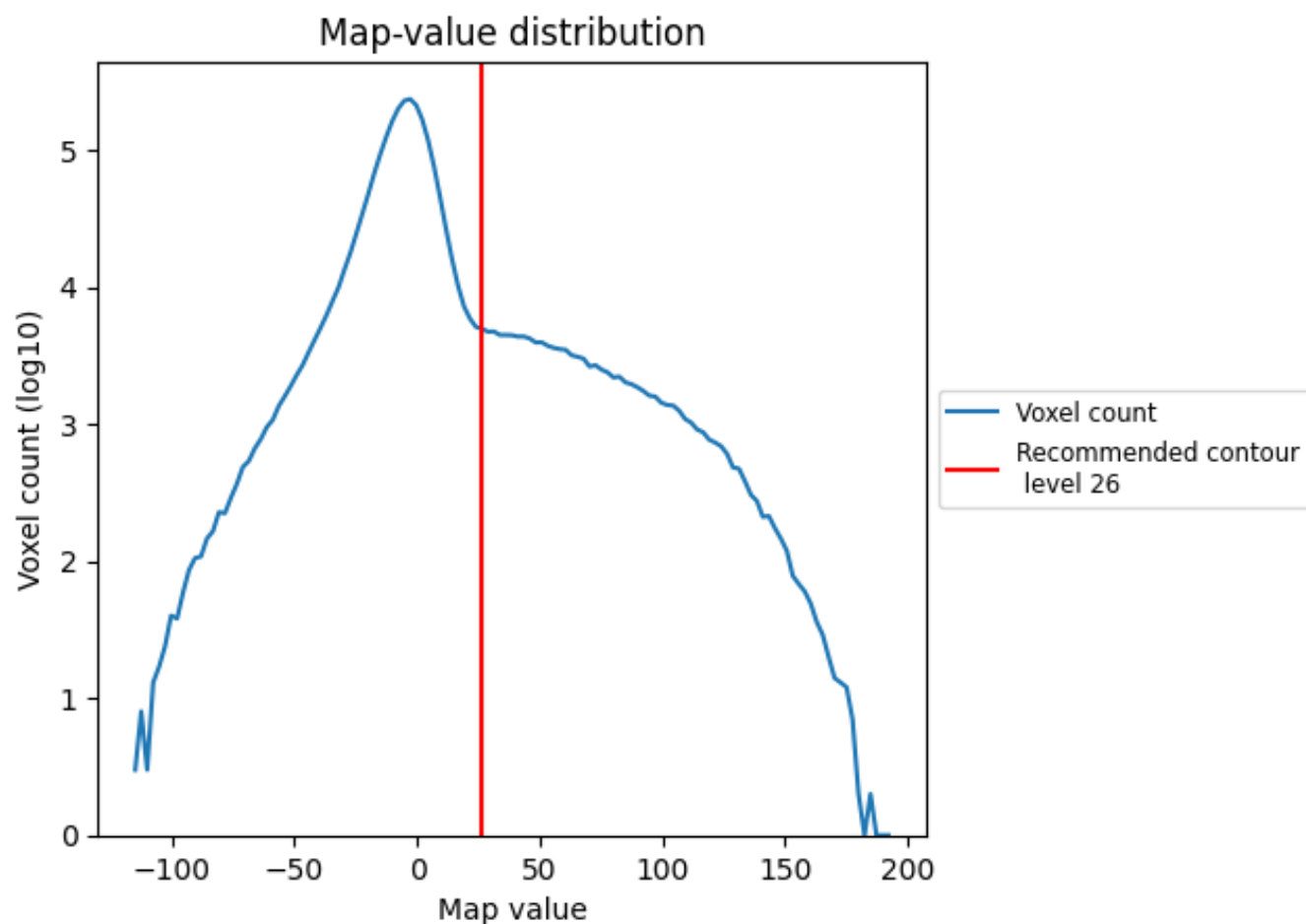
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

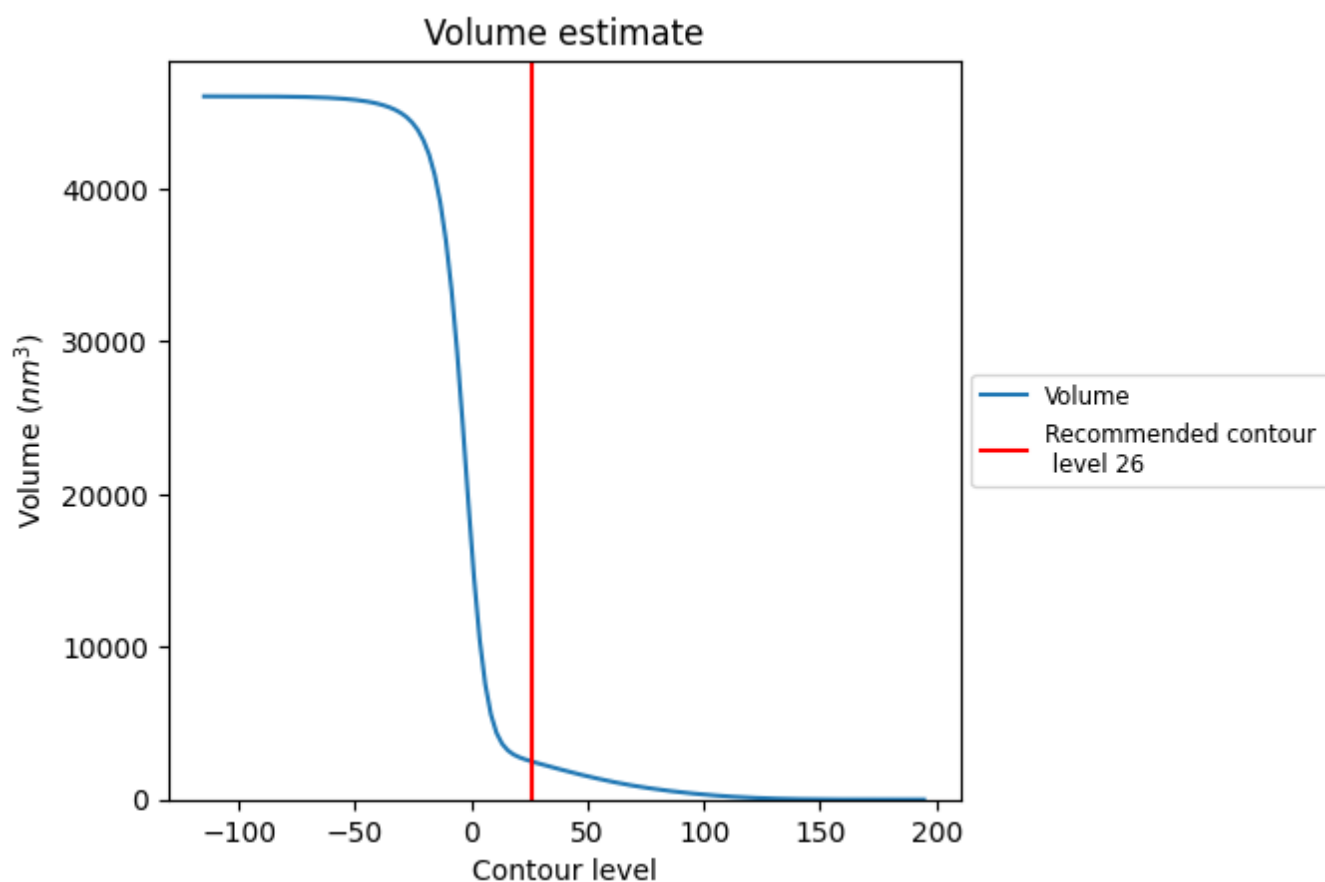
This section contains the results of statistical analysis of the map.

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.

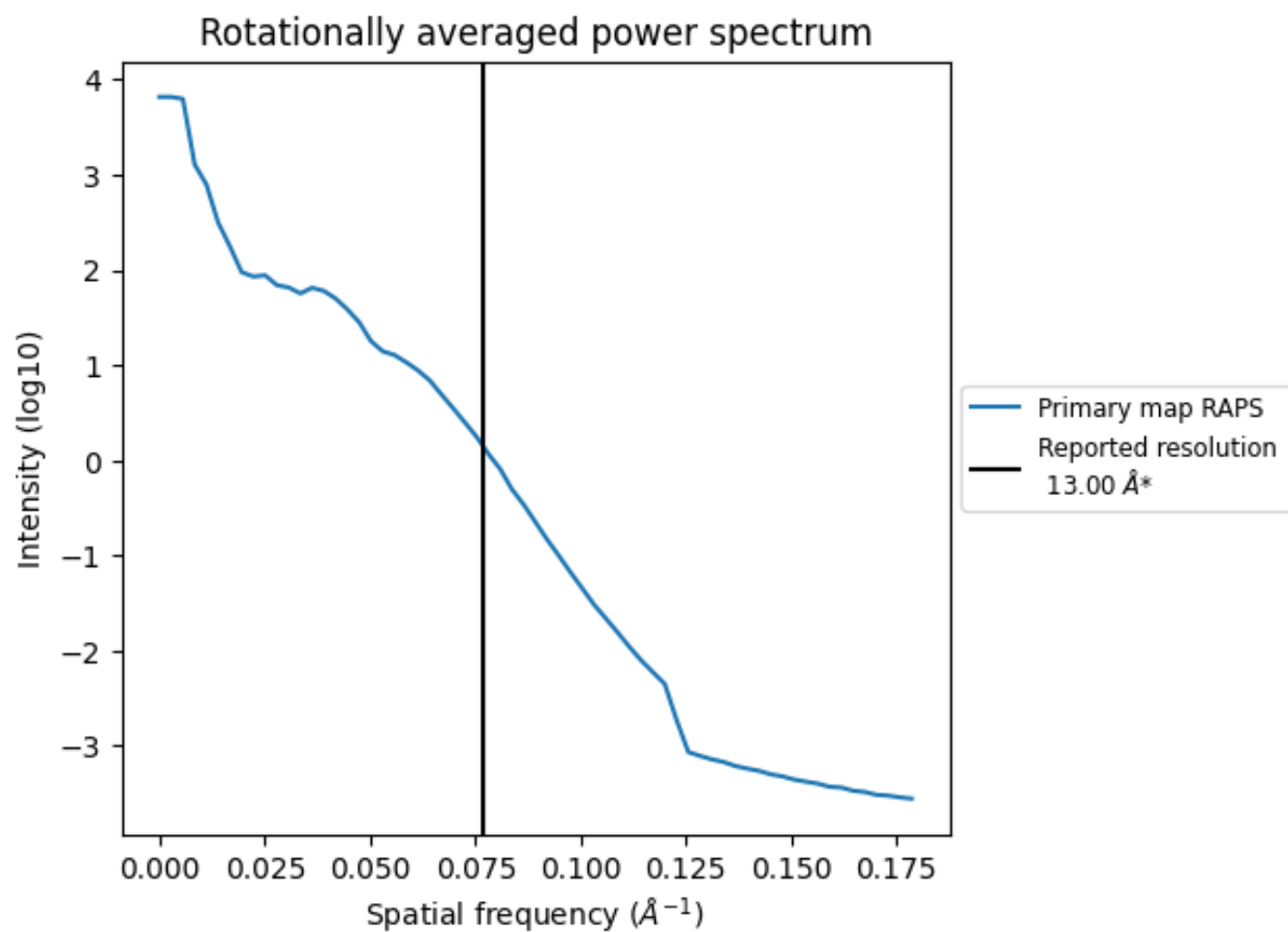
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2493 nm³; this corresponds to an approximate mass of 2252 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 0.077 Å⁻¹

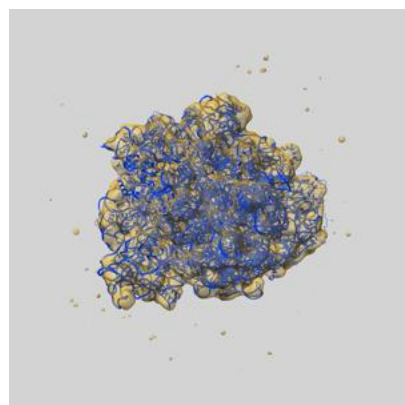
8 Fourier-Shell correlation

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

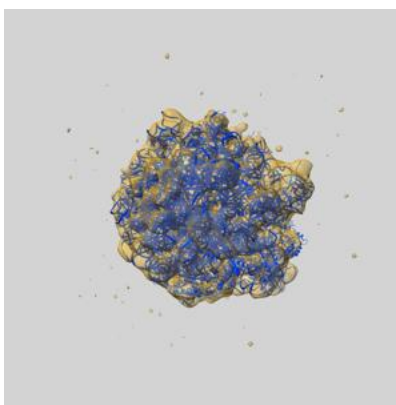
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1719 and PDB model 4V72. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

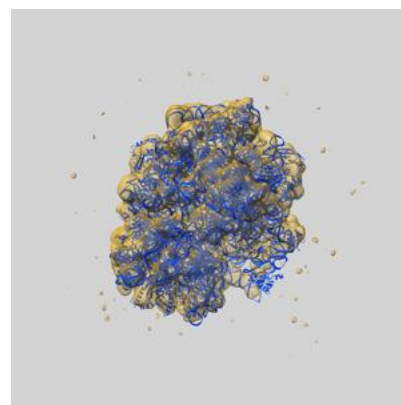
9.1 Map-model overlay [i](#)



X



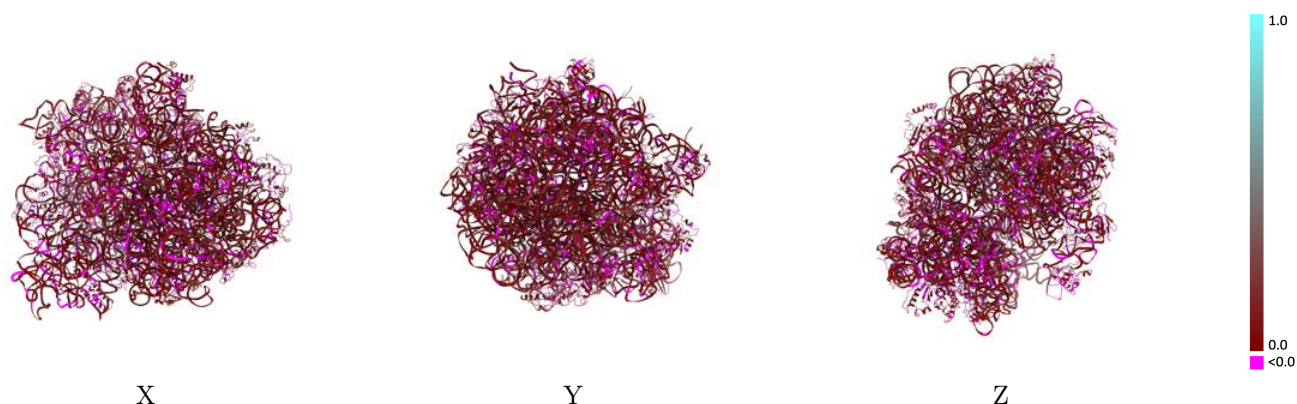
Y



Z

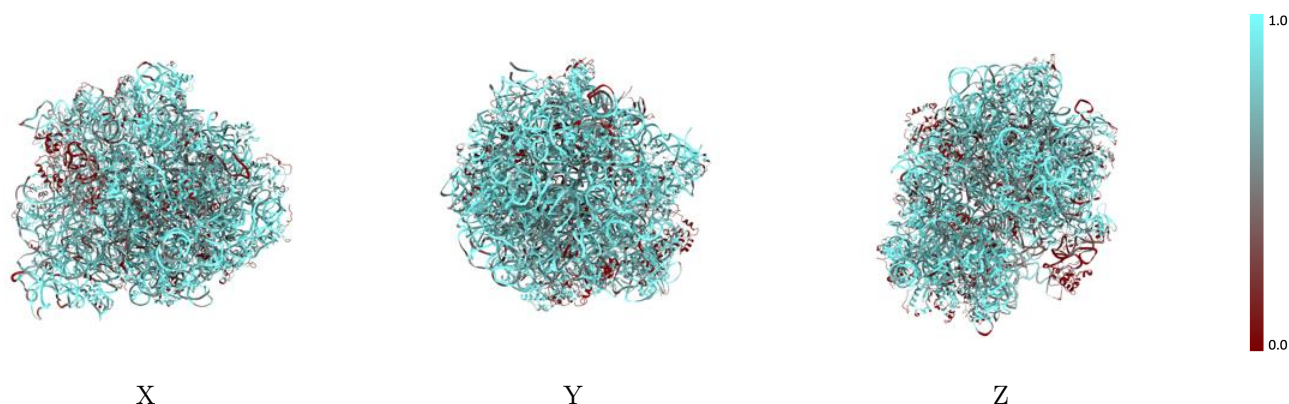
The images above show the 3D surface view of the map at the recommended contour level 26.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



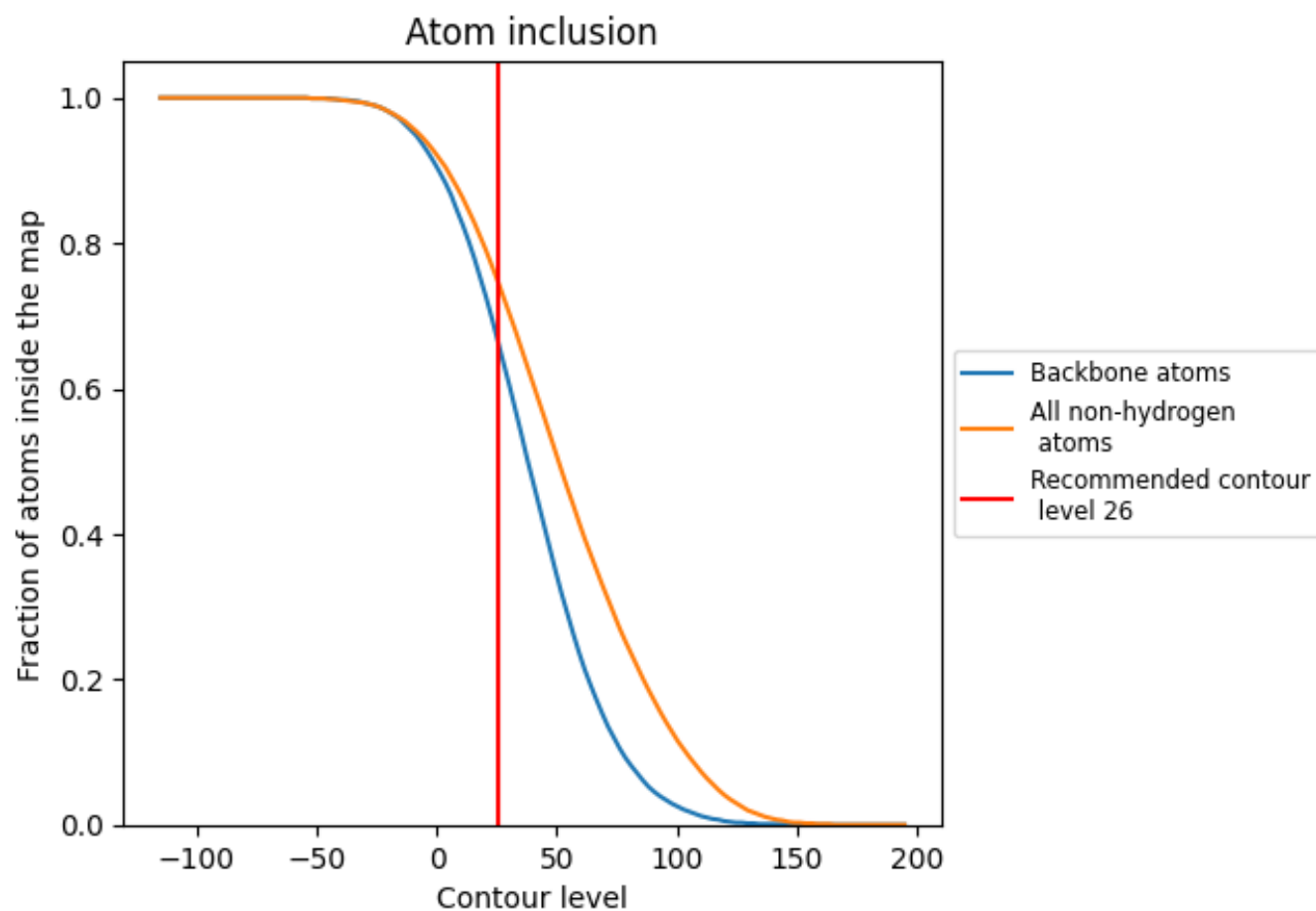
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (26).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 74% 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 (26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.0720
A1	 0.5900	 0.0670
A2	 0.5790	 0.0370
A3	 0.7360	 0.0960
AA	 0.8330	 0.0830
AB	 0.6480	 0.0790
AC	 0.6660	 0.0570
AD	 0.5620	 0.0410
AE	 0.6770	 0.0650
AF	 0.8080	 0.0820
AG	 0.7020	 0.0440
AH	 0.6150	 0.0490
AI	 0.6990	 0.0370
AJ	 0.6320	 0.0230
AK	 0.6220	 0.0360
AL	 0.5580	 0.0380
AM	 0.5750	 0.0250
AN	 0.5580	 0.0390
AO	 0.7460	 0.0500
AP	 0.5490	 0.0060
AQ	 0.6850	 0.0690
AR	 0.6860	 0.0420
AS	 0.7710	 0.0290
AT	 0.6640	 0.0250
AU	 0.3940	 -0.0080
B0	 0.6220	 0.0360
B1	 0.6810	 0.0480
B2	 0.3720	 0.0240
B3	 0.3320	 -0.0140
B4	 0.6440	 0.0190
B5	 0.4540	 0.0460
BA	 0.8100	 0.0890
BB	 0.8630	 0.0810
BC	 0.4930	 0.0310
BD	 0.5310	 0.0370



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Chain	Atom inclusion	Q-score
BE	 0.6160	 0.0380
BF	 0.7380	 0.0570
BG	 0.5690	 0.0360
BH	 0.2130	 0.0390
BI	 0.0290	 0.0230
BJ	 0.5760	 0.0310
BK	 0.5640	 0.0400
BL	 0.5720	 0.0130
BM	 0.5190	 0.0400
BN	 0.6150	 0.0260
BO	 0.8580	 0.0500
BP	 0.5770	 0.0500
BQ	 0.5120	 0.0270
BR	 0.7130	 0.0580
BS	 0.5730	 0.0520
BT	 0.6360	 0.0350
BU	 0.5640	 0.0190
BV	 0.6640	 0.0480
BW	 0.6860	 0.0440
BX	 0.4230	 0.0510
BY	 0.7450	 0.0880
BZ	 0.5450	 0.0230