



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 10:45 PM EST

PDB ID : 4V77
EMDB ID : EMD-2474
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post2b)
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 : 2K4C, 2WRI, 3I1O, 2HGP

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

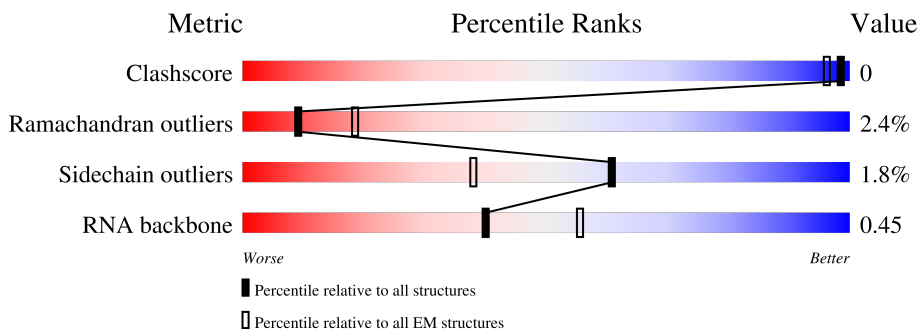
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



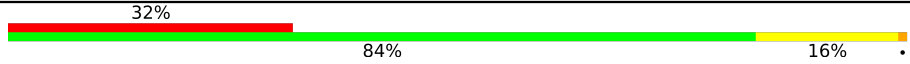

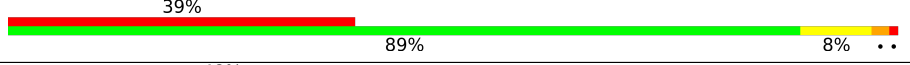
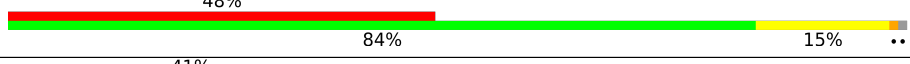
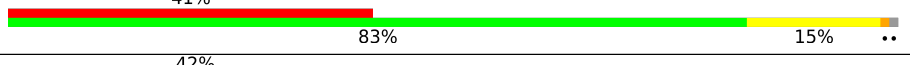
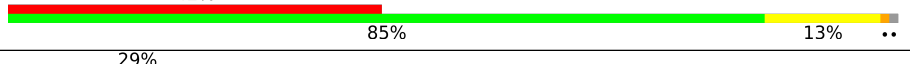
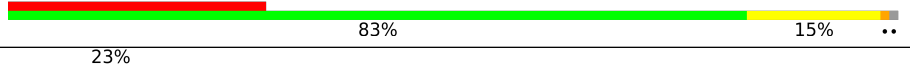

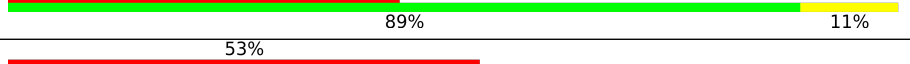
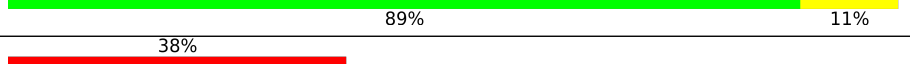
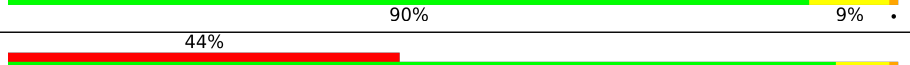

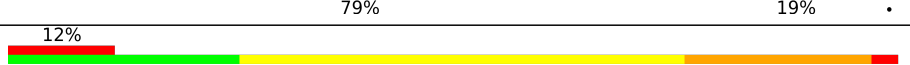
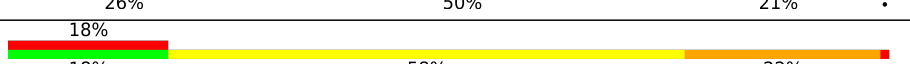
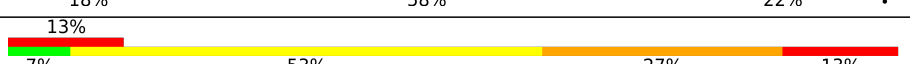
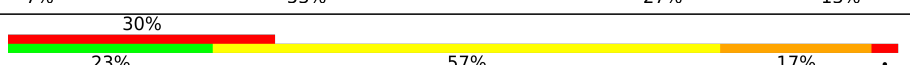

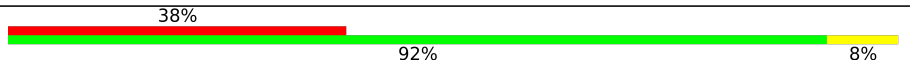
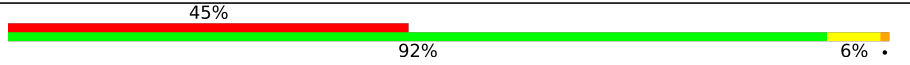

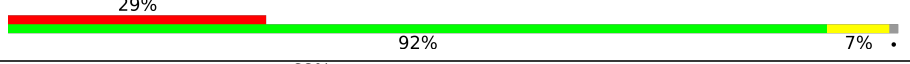
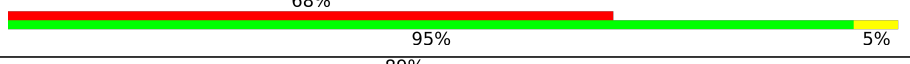
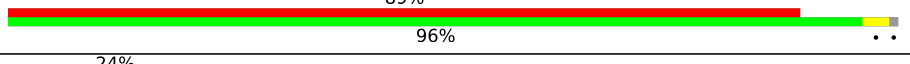


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 style="display: flex; justify-content: space-between;"> 22% 94% 6% </div>
2	AC	208	<div style="display: flex; justify-content: space-between;"> 36% 90% 9% </div>
3	AD	206	<div style="display: flex; justify-content: space-between;"> 33% 87% 12% </div>
4	AE	152	<div style="display: flex; justify-content: space-between;"> 28% 91% 9% </div>
5	AF	101	<div style="display: flex; justify-content: space-between;"> 38% 87% 13% </div>
6	AG	152	<div style="display: flex; justify-content: space-between;"> 50% 88% 12% </div>
7	AH	130	<div style="display: flex; justify-content: space-between;"> 22% 92% 7% </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	46% 88% 10%
34	BL	144	33% 85% 12%
35	BM	136	26% 85% 15%
36	BN	121	29% 88% 12%
37	BO	117	19% 87% 11%
38	BP	115	27% 86% 12%
39	BQ	118	34% 87% 11%
40	BR	103	36% 91% 9%
41	BS	110	43% 92% 8%
42	BT	94	45% 87% 13%
43	BU	104	44% 87% 12%
44	BV	94	33% 91% 9%
45	BW	80	45% 86% 12%
46	BX	79	59% 86% 10%
47	BY	63	41% 92% 8%
48	BZ	59	47% 86% 12%
49	B0	57	39% 84% 14%
50	B1	52	40% 92% 8%
51	B2	46	67% 74% 26%
52	B3	65	60% 86% 12%
53	B4	38	37% 92% 8%
54	BA	2903	18% 22% 52% 22%
55	BB	118	7% 21% 64% 12%
56	B5	234	65% 88% 7% 5%

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
			Total	C	N	O	S		
1	AB	220	1708	1083	306	312	7	0	1

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
			Total	C	N	O	S		
2	AC	207	1625	1028	306	288	3	0	1

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
			Total	C	N	O	S		
3	AD	205	1643	1026	315	298	4	0	0

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

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

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
			Total	C	N	O	S		
5	AF	101	818	515	149	148	6	0	1

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
			Total	C	N	O	S		
6	AG	152	1178	732	227	215	4	0	1

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
			Total	C	N	O	S		
7	AH	129	979	616	173	184	6	0	0

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

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

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
			Total	C	N	O	S		
9	AJ	100	790	495	151	143	1	0	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
			Total	C	N	O	S		
10	AK	118	880	542	174	161	3	0	0

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
			Total	C	N	O	S		
11	AL	123	955	590	196	165	4	0	0

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

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

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
			Total	C	N	O	S		
13	AN	100	805	499	164	139	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AP	81	639	400	127	111	1	0	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
			Total	C	N	O	S		
16	AQ	82	652	413	122	114	3	0	1

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
			Total	C	N	O		
17	AR	57	459	290	87	82	0	1

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
			Total	C	N	O	S		
18	AS	81	641	410	121	108	2	0	1

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
			Total	C	N	O	S		
19	AT	86	668	413	137	115	3	0	0

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
			Total	C	N	O	S		
20	AU	53	429	267	87	74	1	0	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
			Total	C	N	O	P		
21	AA	1530	32828	14642	6024	10633	1529	0	0

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
26	BD	209	1565	979	288	294	4	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
34	BL	143	1045	649	206	189	1	0	0

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

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

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

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

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
			Total	C	N	O		
37	BO	116	892	552	178	162	0	0

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O		
43	BU	103	780	492	147	141	0	1

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
			Total	C	N	O	S		
44	BV	94	753	479	137	134	3	0	0

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

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

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
			Total	C	N	O	S		
46	BX	77	625	388	129	106	2	0	0

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
			Total	C	N	O	S		
47	BY	63	509	313	99	95	2	0	0

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

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

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

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

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

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

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		

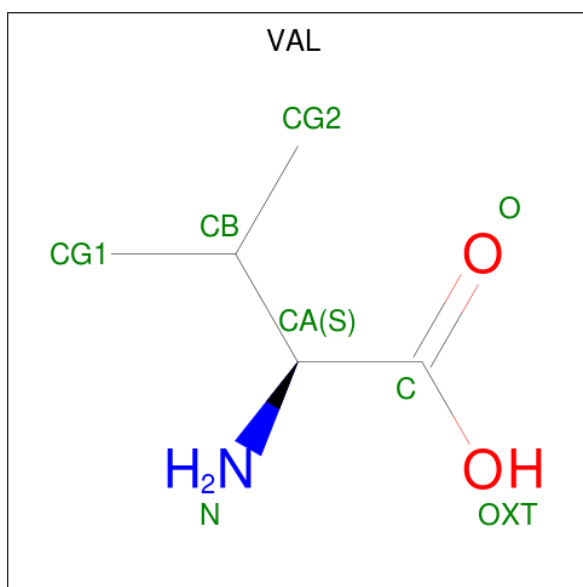
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

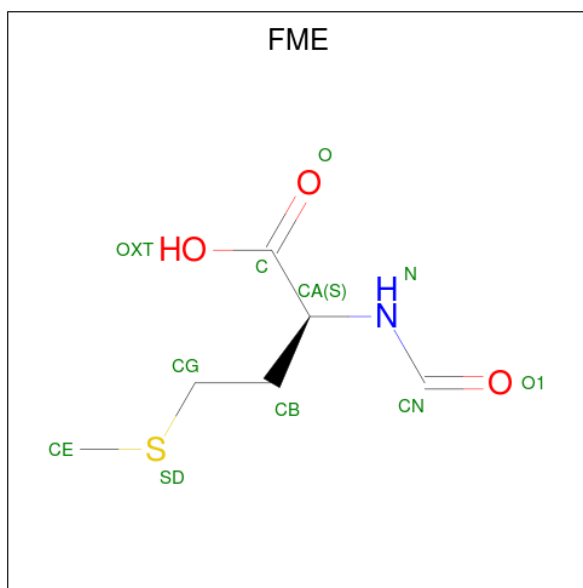
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).

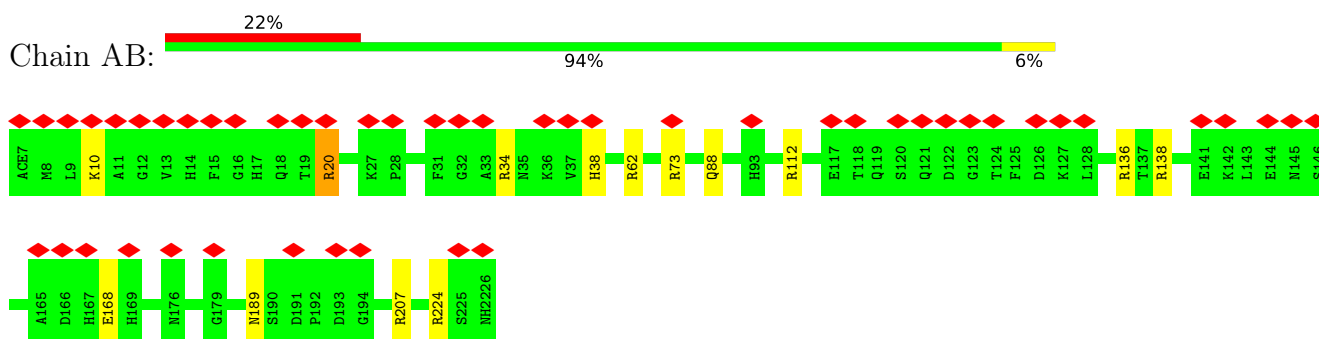


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	BA	1	10	6	1	2	1	0

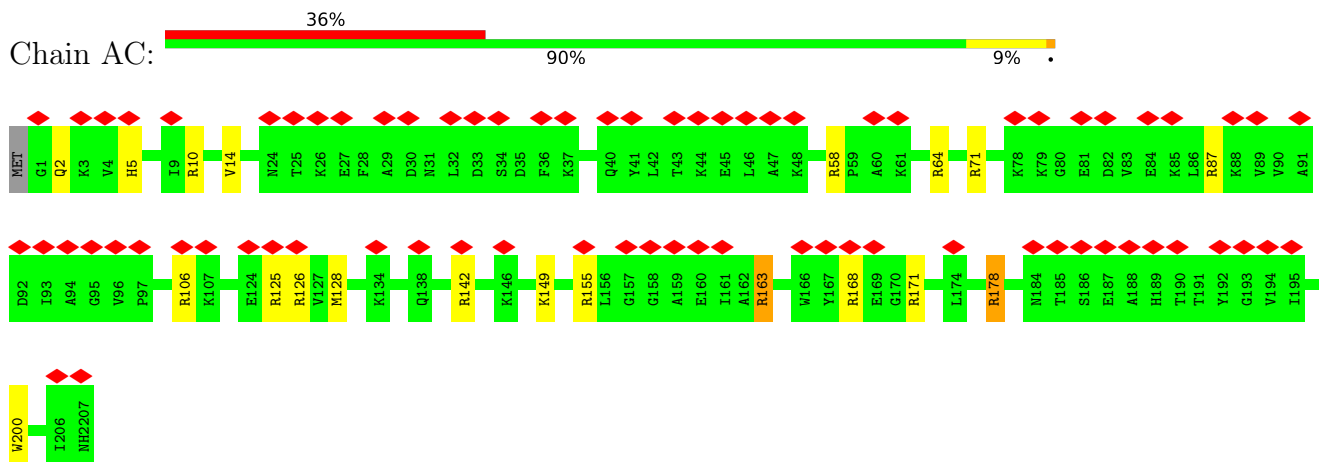
3 Residue-property plots [i](#)

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.

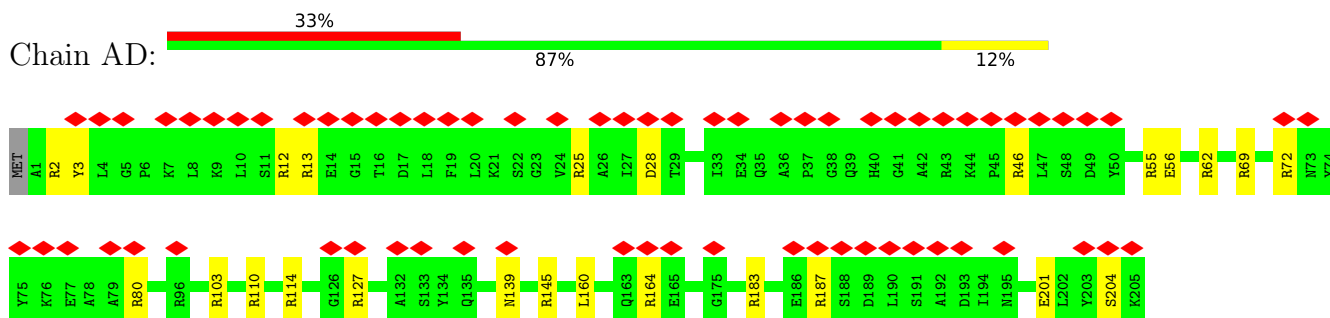
- Molecule 1: 30S ribosomal protein S2



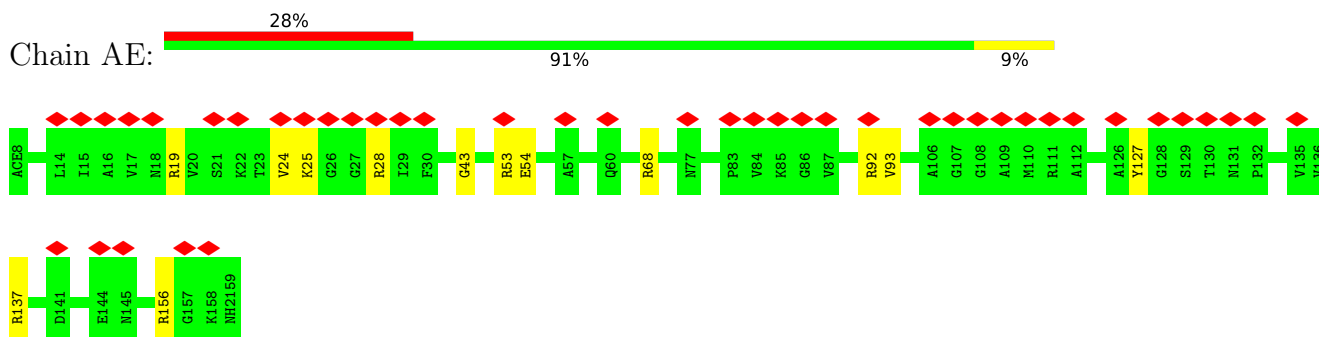
- Molecule 2: 30S ribosomal protein S3



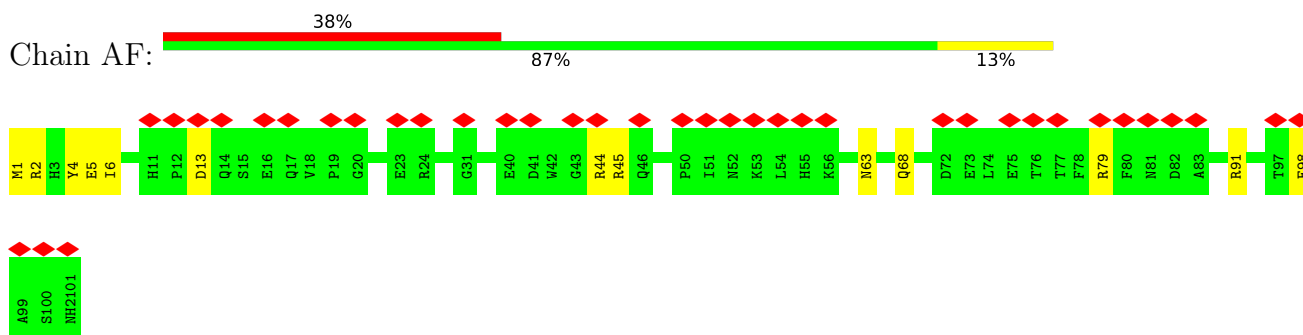
- Molecule 3: 30S ribosomal protein S4



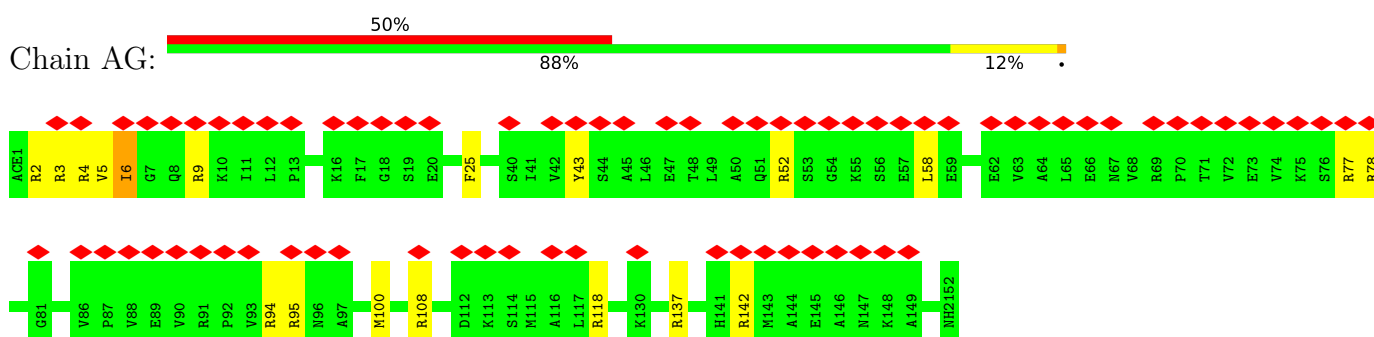
- Molecule 4: 30S ribosomal protein S5



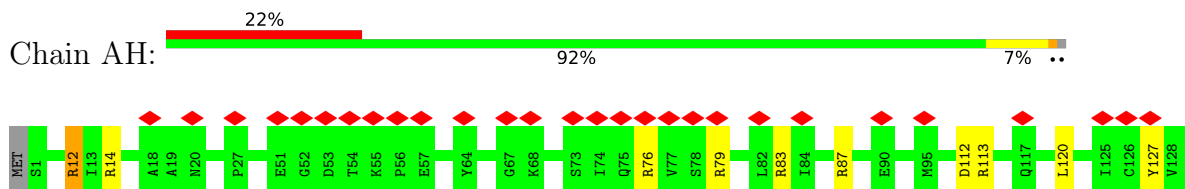
- Molecule 5: 30S ribosomal protein S6



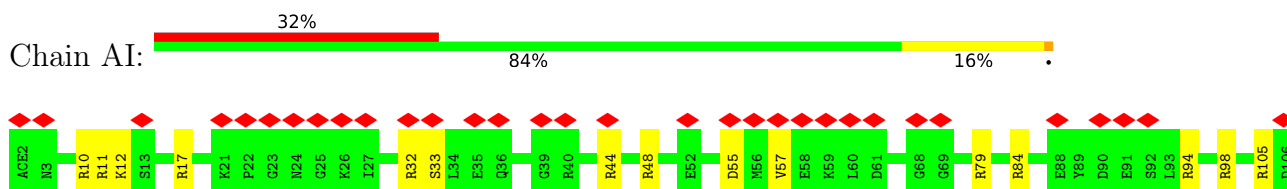
- Molecule 6: 30S ribosomal protein S7

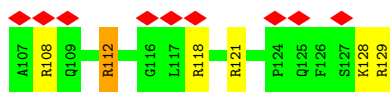


- Molecule 7: 30S ribosomal protein S8

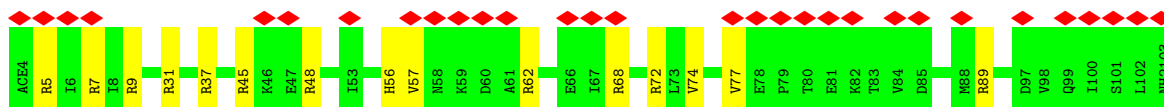
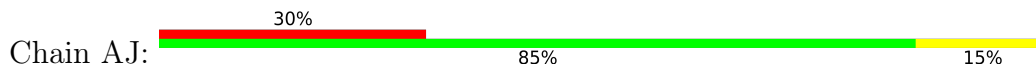


- Molecule 8: 30S ribosomal protein S9

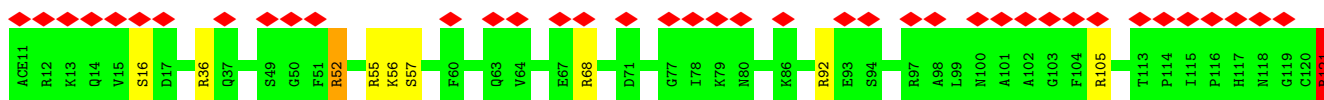
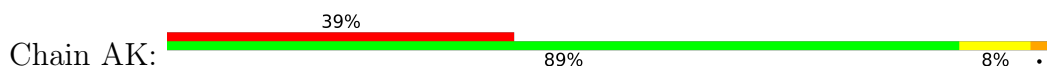




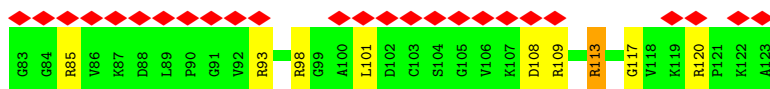
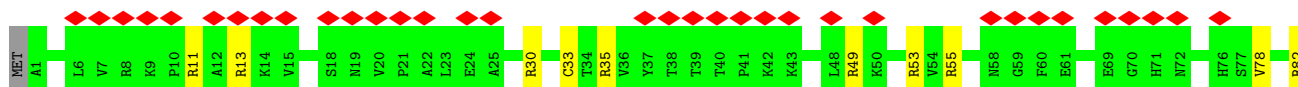
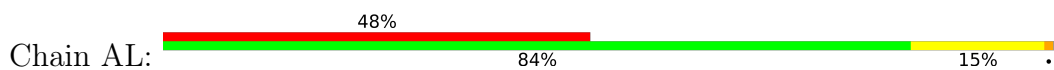
- Molecule 9: 30S ribosomal protein S10



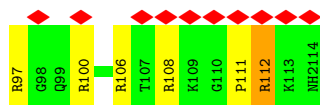
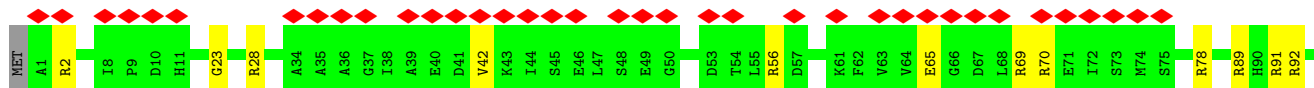
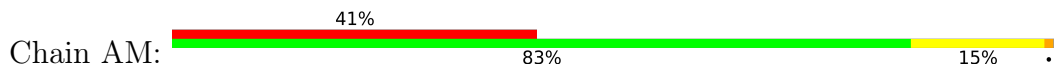
- Molecule 10: 30S ribosomal protein S11



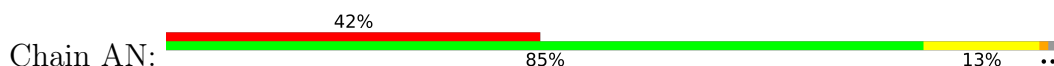
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

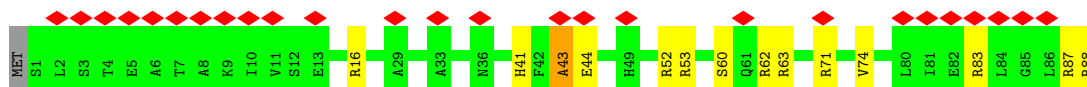
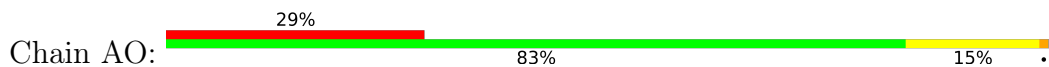


- Molecule 13: 30S ribosomal protein S14

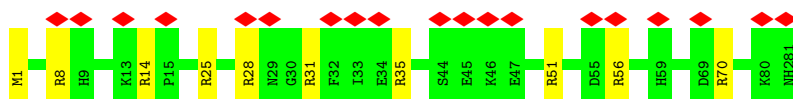
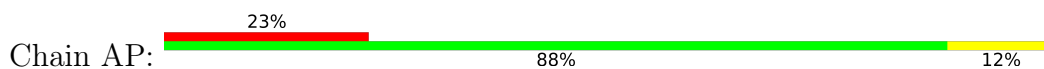




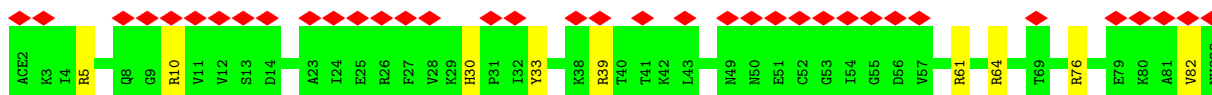
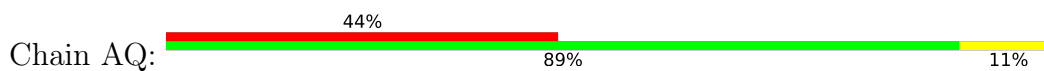
- Molecule 14: 30S ribosomal protein S15



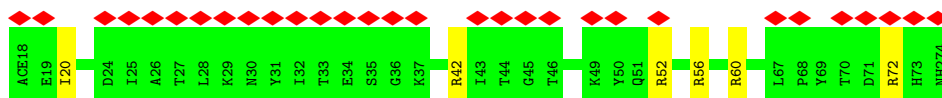
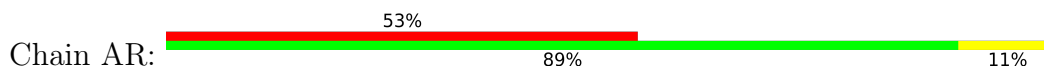
- Molecule 15: 30S ribosomal protein S16



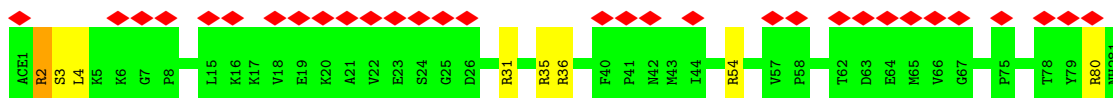
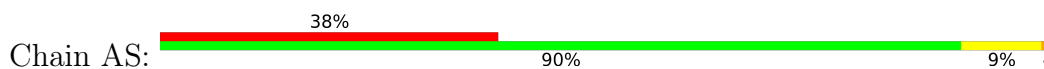
- Molecule 16: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S18

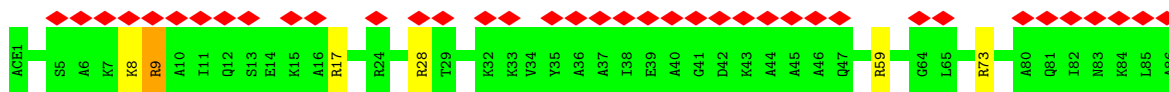


- Molecule 18: 30S ribosomal protein S19

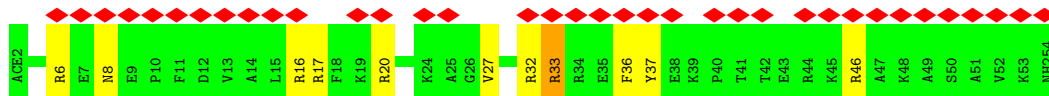
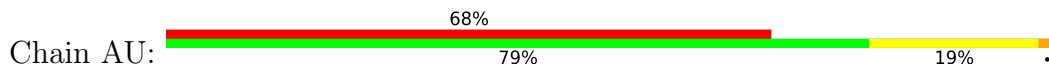


- Molecule 19: 30S ribosomal protein S20

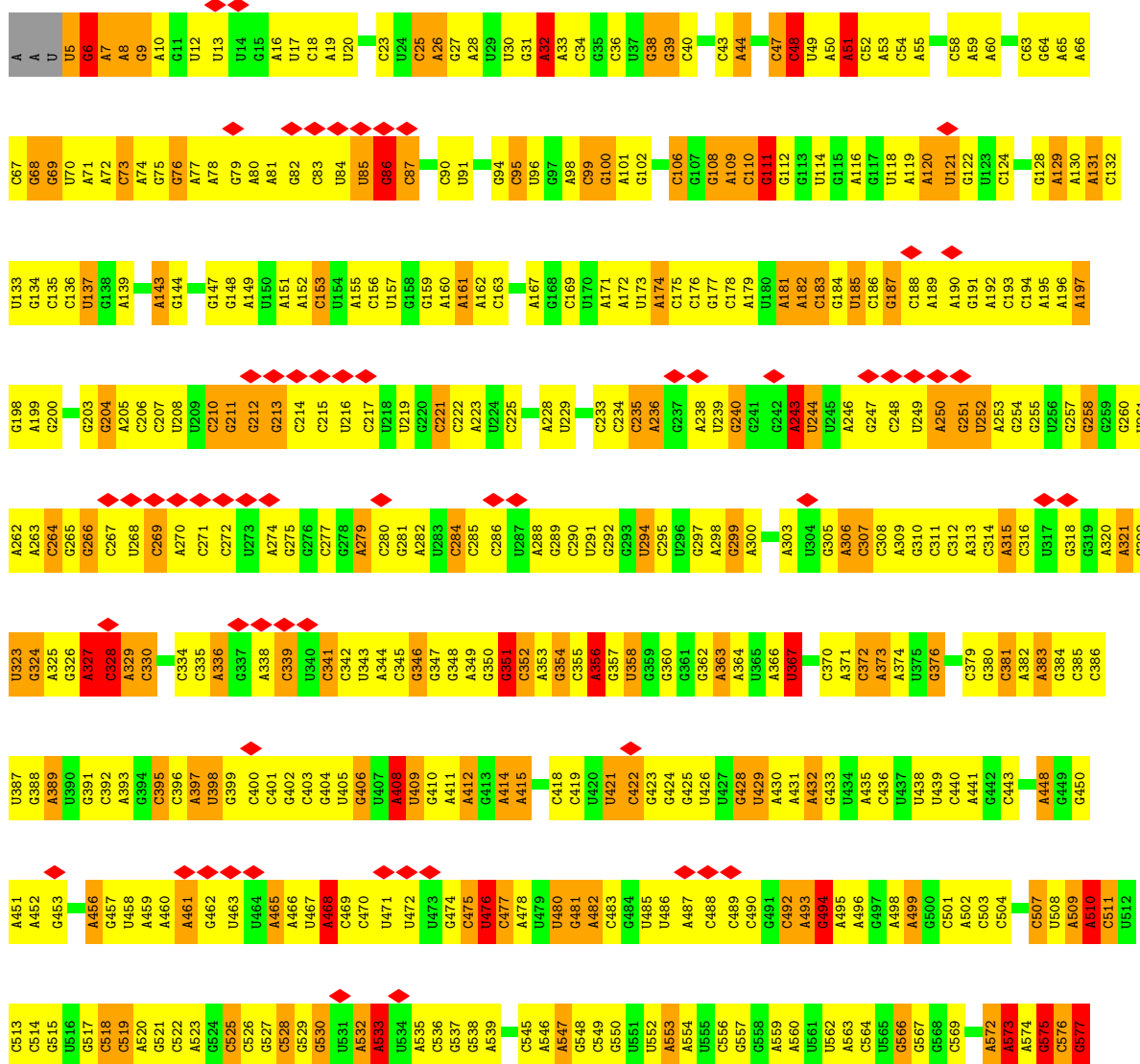


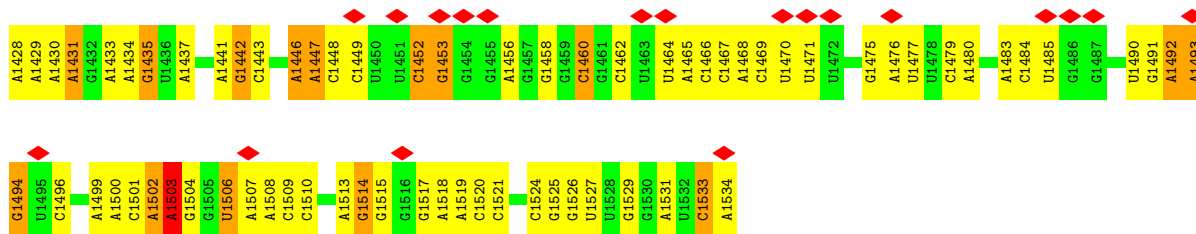


• Molecule 20: 30S ribosomal protein S21

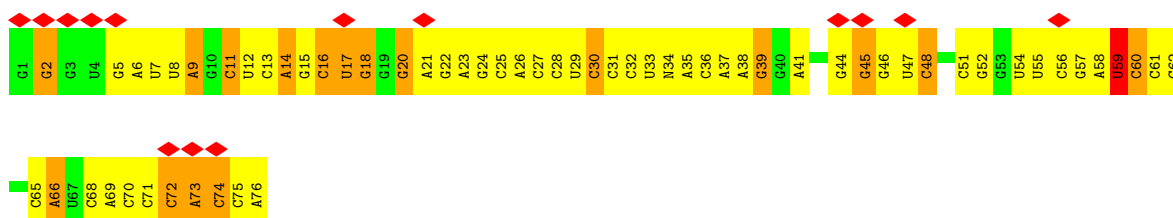


• Molecule 21: 16S ribosomal RNA

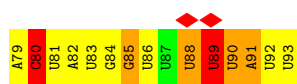




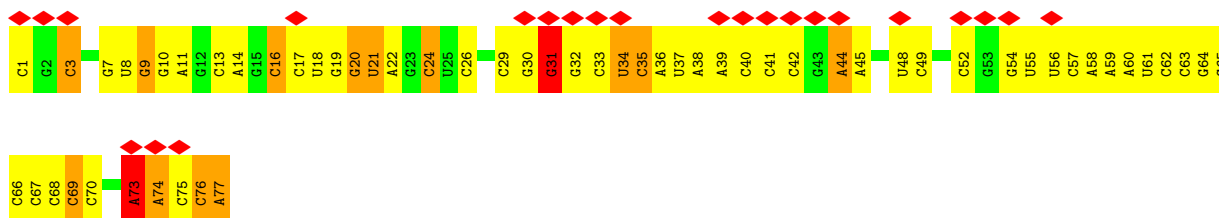
• Molecule 22: fMet-Val-tRNA-Val



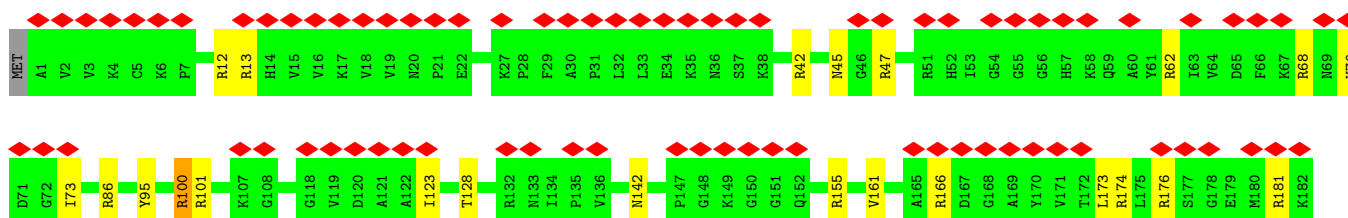
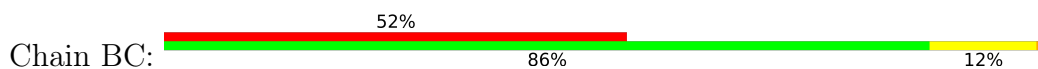
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

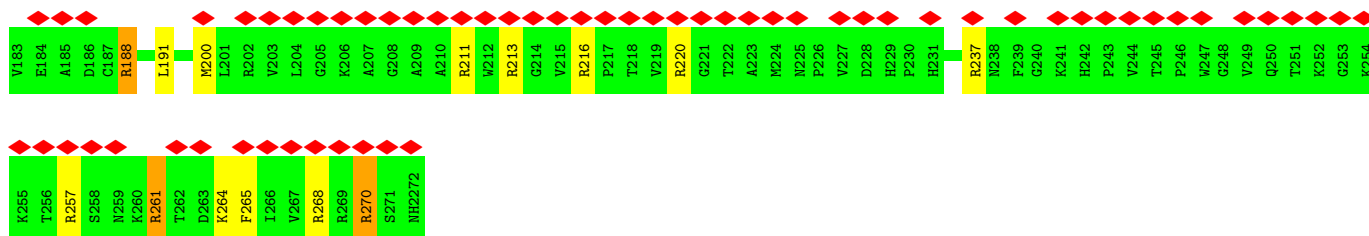


• Molecule 24: tRNA-fMet

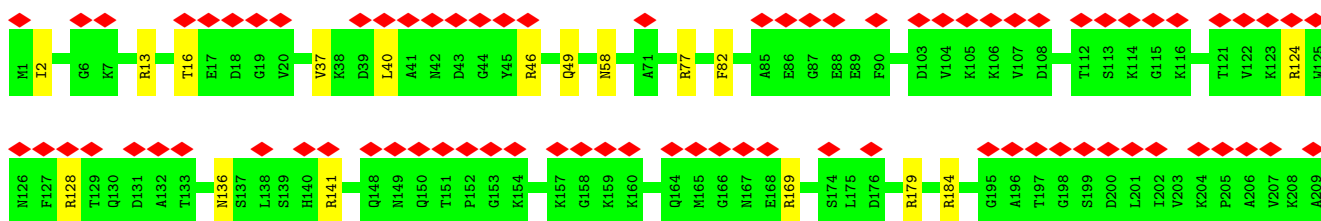
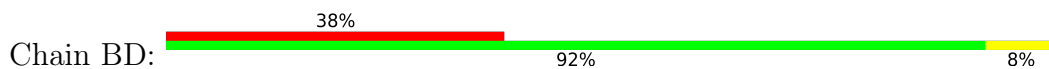


• Molecule 25: 50S ribosomal protein L2

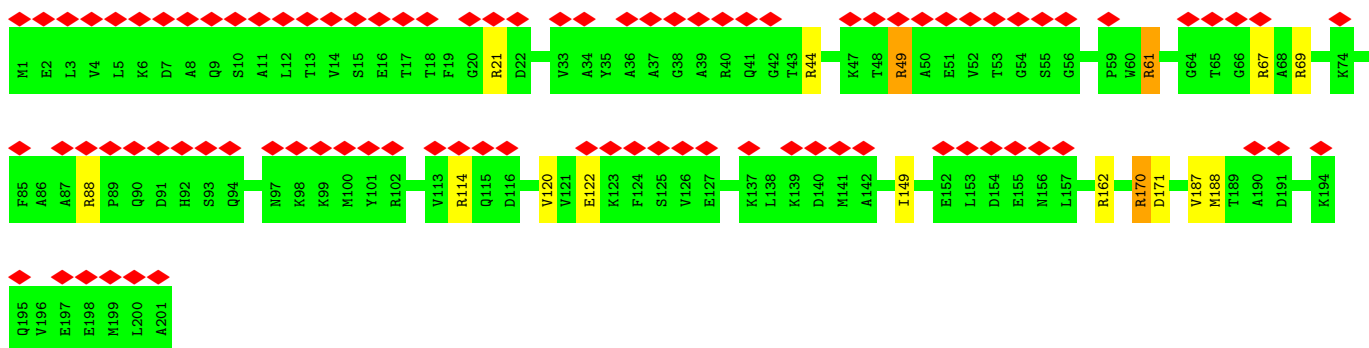




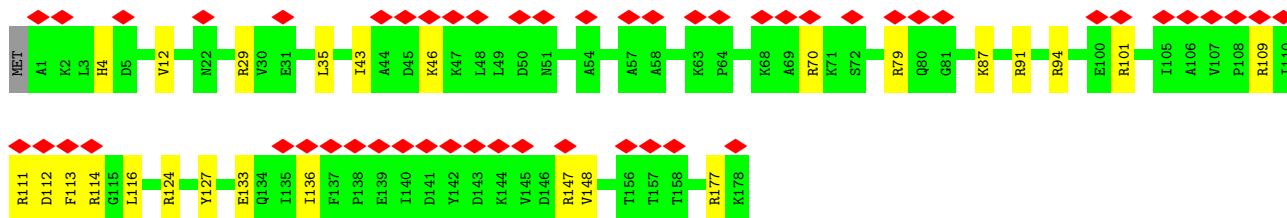
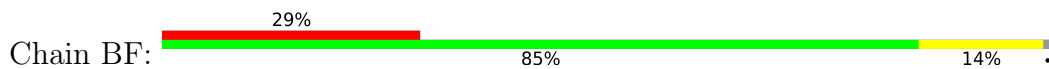
• Molecule 26: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L4

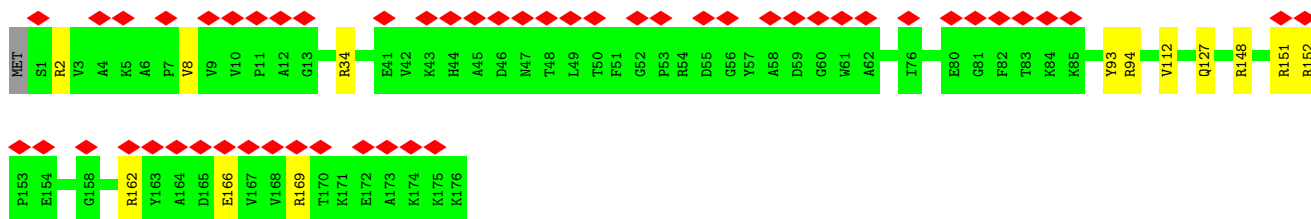


• Molecule 28: 50S ribosomal protein L5

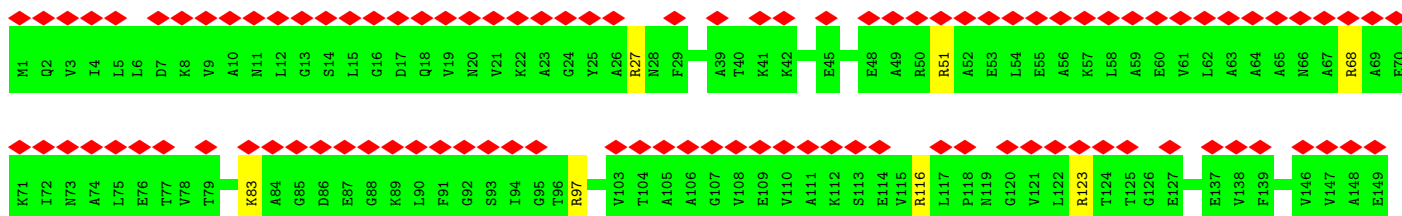


• Molecule 29: 50S ribosomal protein L6





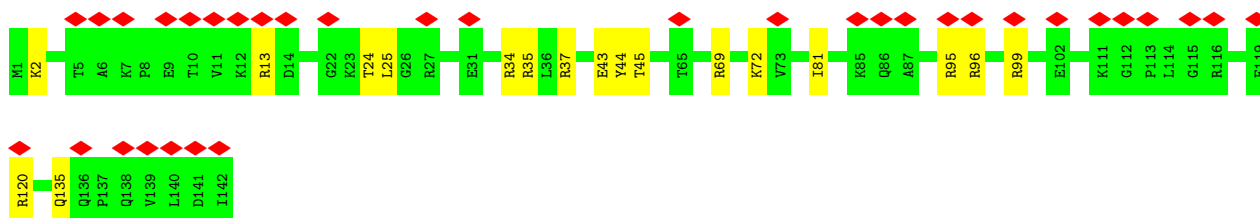
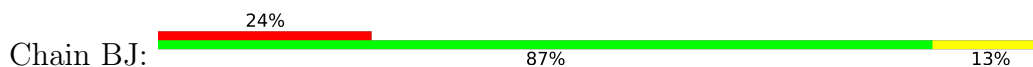
• Molecule 30: 50S ribosomal protein L9



• Molecule 31: 50S ribosomal protein L11

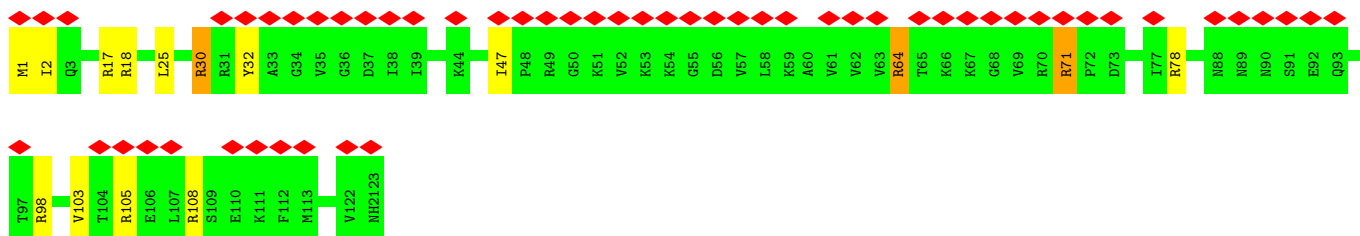


• Molecule 32: 50S ribosomal protein L13

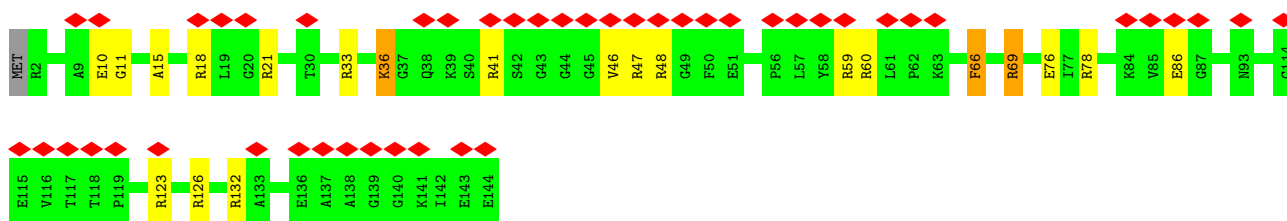
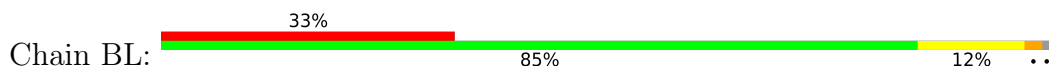


• Molecule 33: 50S ribosomal protein L14

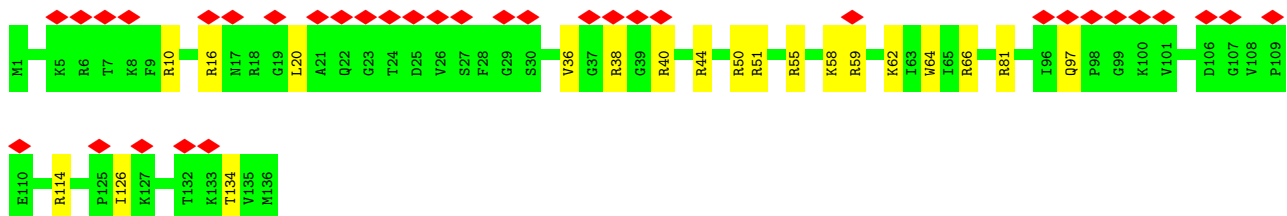
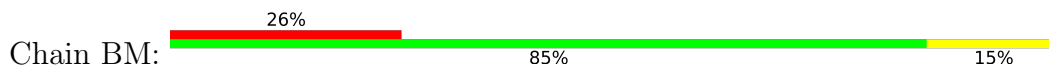




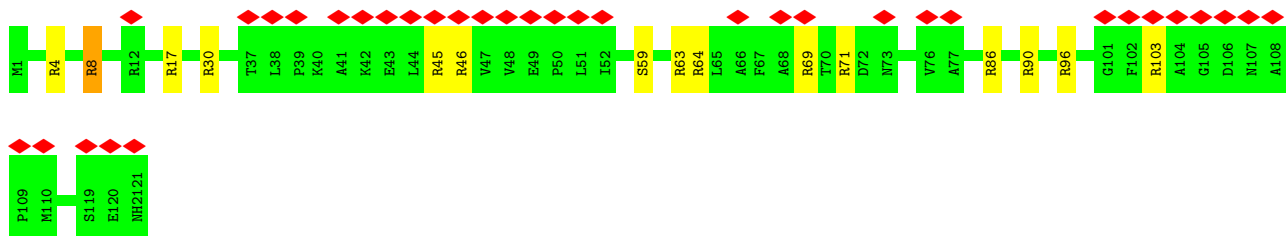
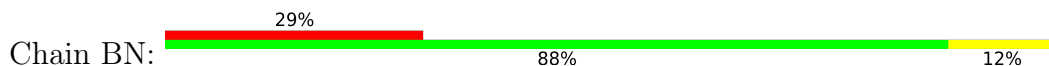
• Molecule 34: 50S ribosomal protein L15



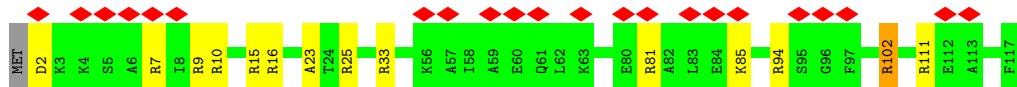
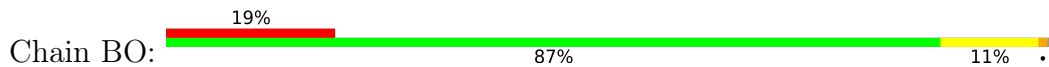
• Molecule 35: 50S ribosomal protein L16



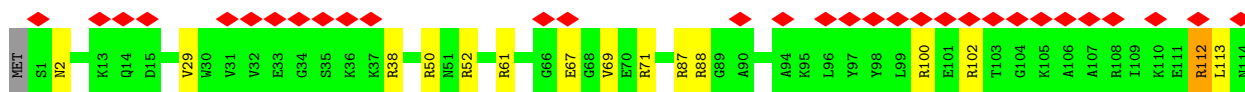
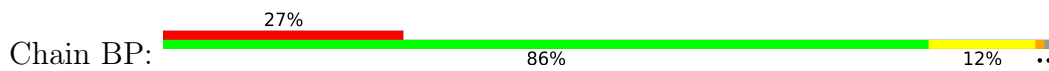
• Molecule 36: 50S ribosomal protein L17



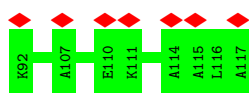
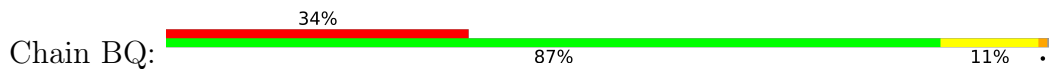
• Molecule 37: 50S ribosomal protein L18



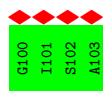
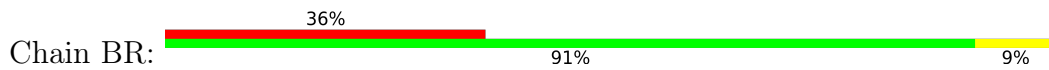
• Molecule 38: 50S ribosomal protein L19



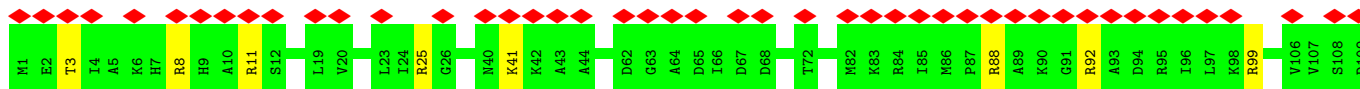
• Molecule 39: 50S ribosomal protein L20



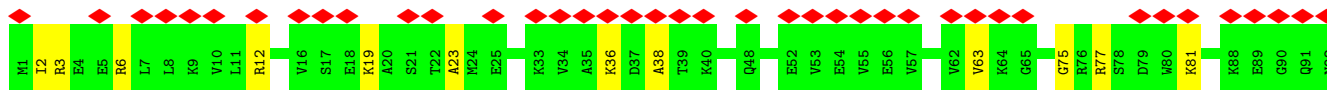
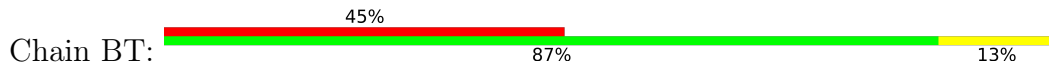
• Molecule 40: 50S ribosomal protein L21



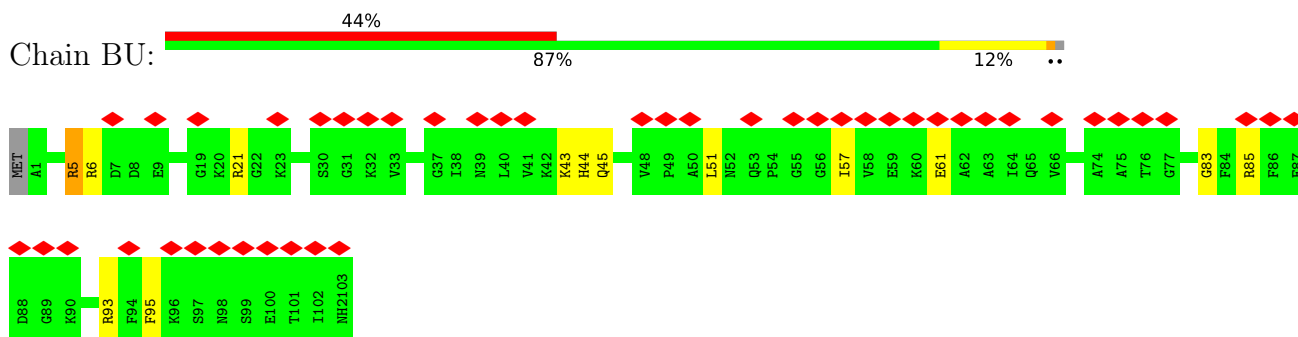
• Molecule 41: 50S ribosomal protein L22



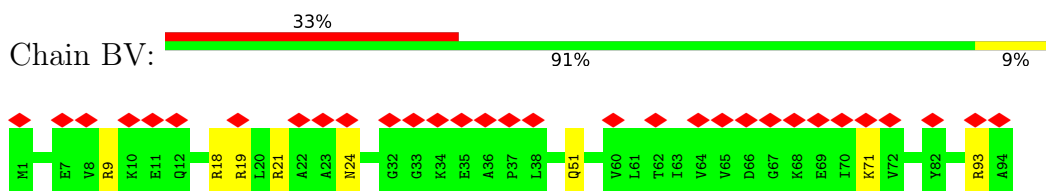
• Molecule 42: 50S ribosomal protein L23



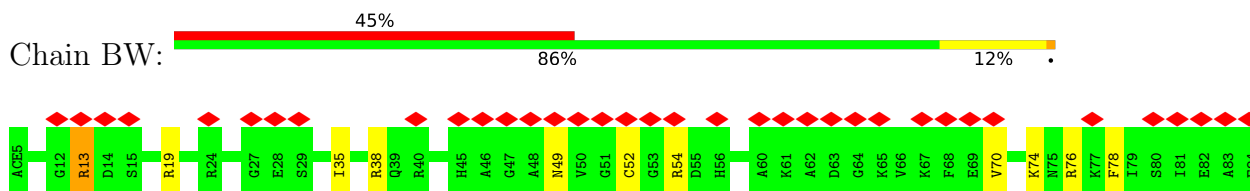
- Molecule 43: 50S ribosomal protein L24



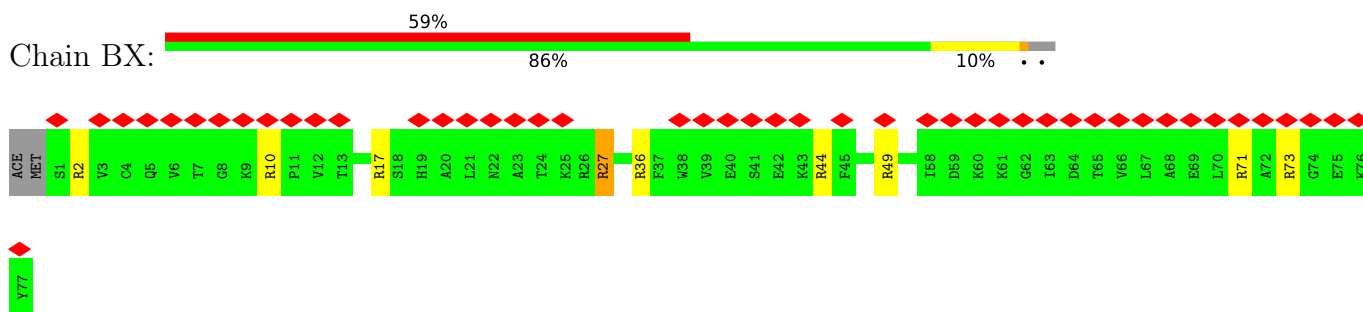
- Molecule 44: 50S ribosomal protein L25



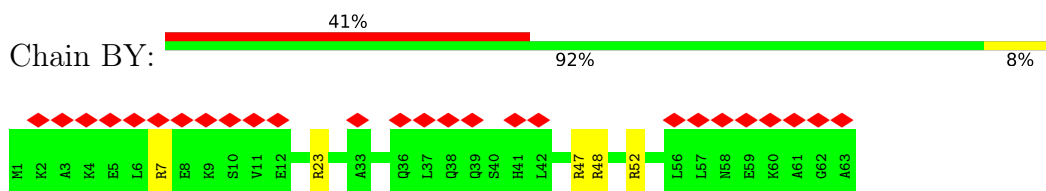
- Molecule 45: 50S ribosomal protein L27



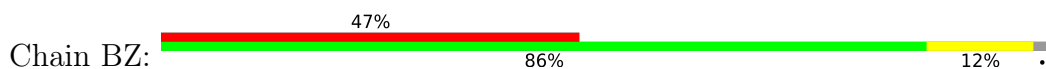
- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L29

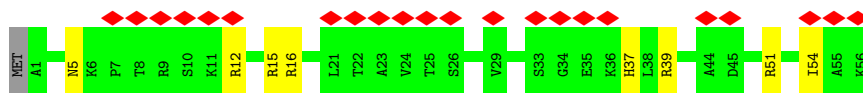
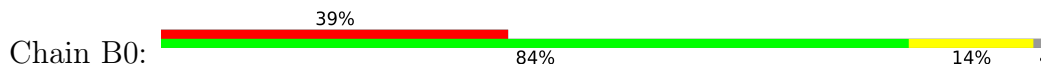


- Molecule 48: 50S ribosomal protein L30

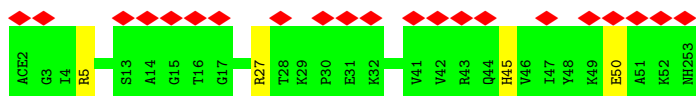
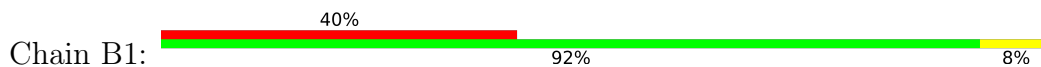




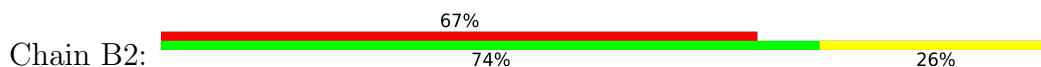
• Molecule 49: 50S ribosomal protein L32



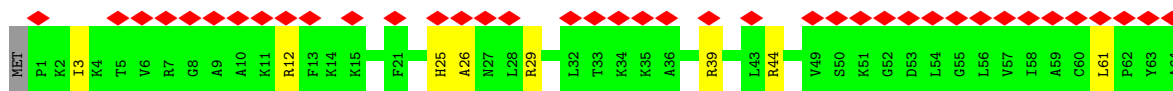
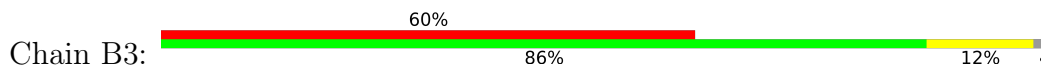
• Molecule 50: 50S ribosomal protein L33



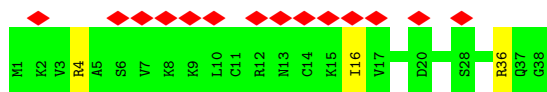
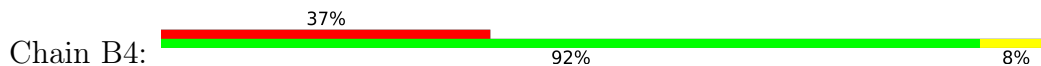
• Molecule 51: 50S ribosomal protein L34



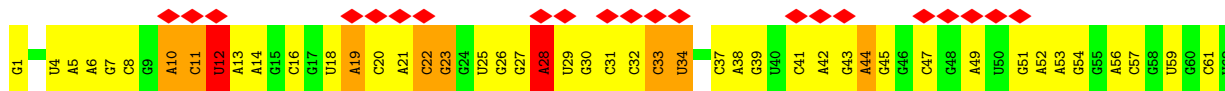
• Molecule 52: 50S ribosomal protein L35

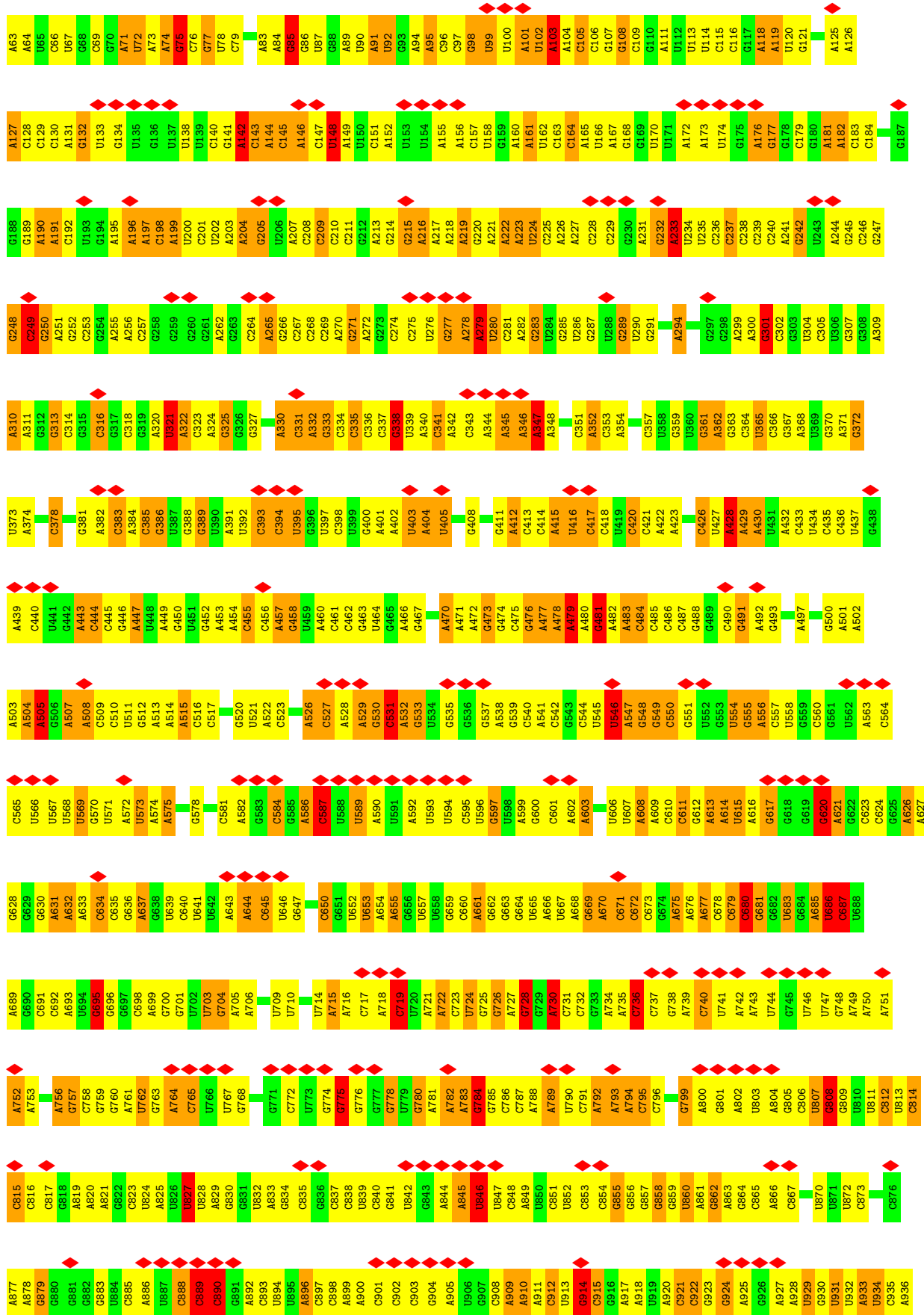


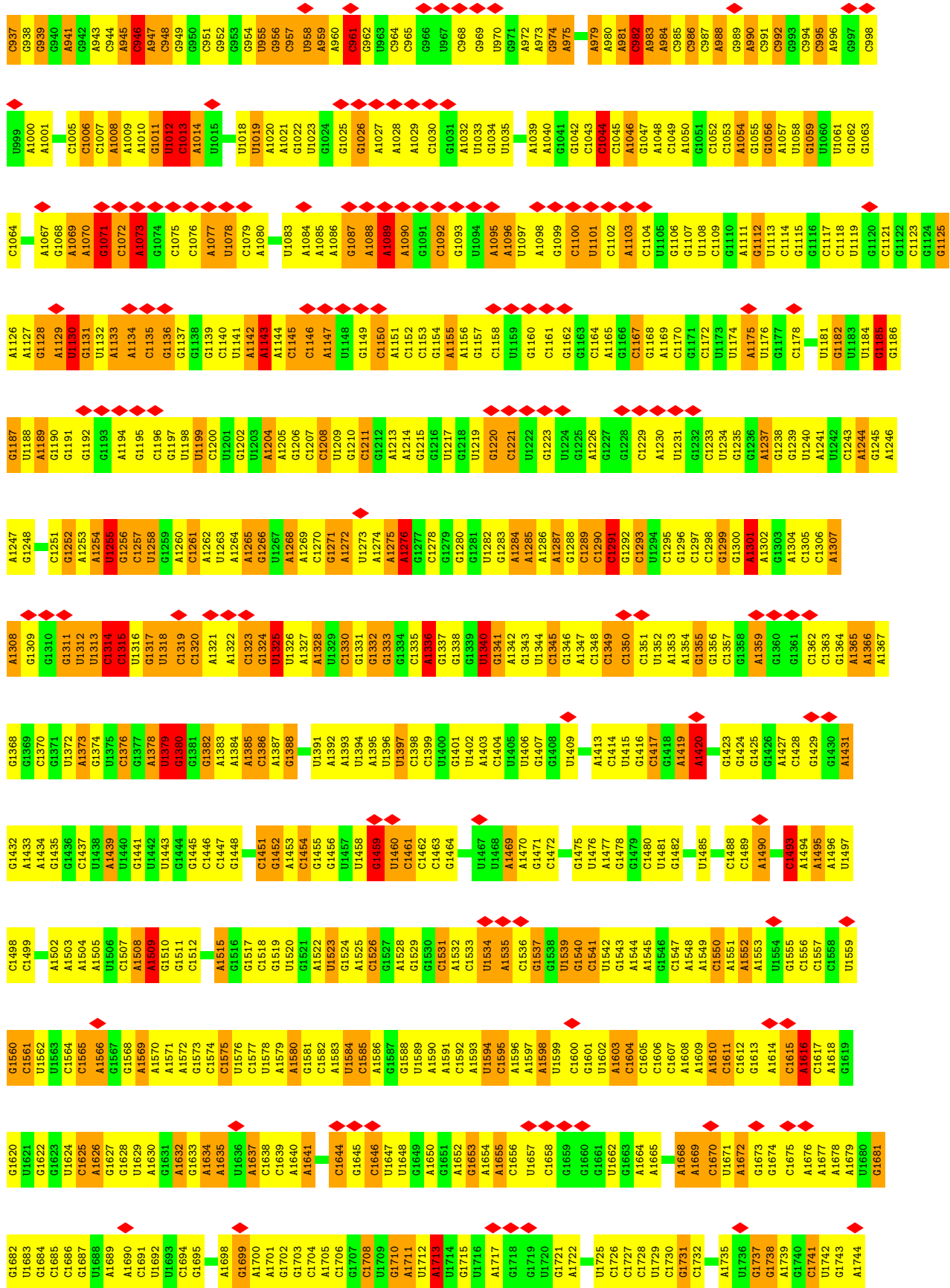
• Molecule 53: 50S ribosomal protein L36



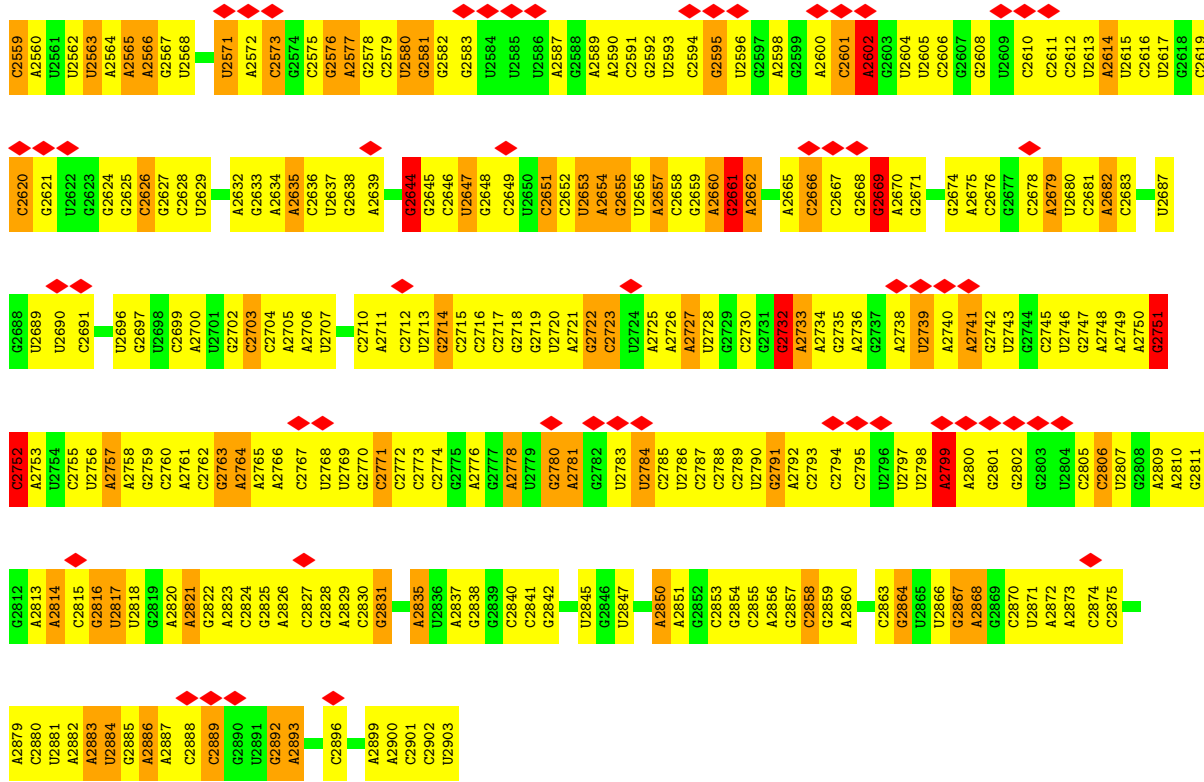
• Molecule 54: 23S ribosomal RNA



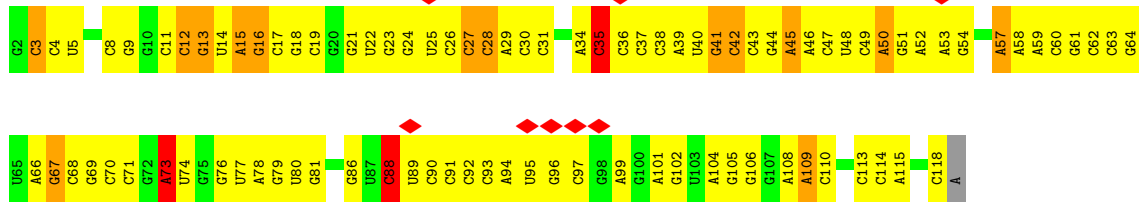




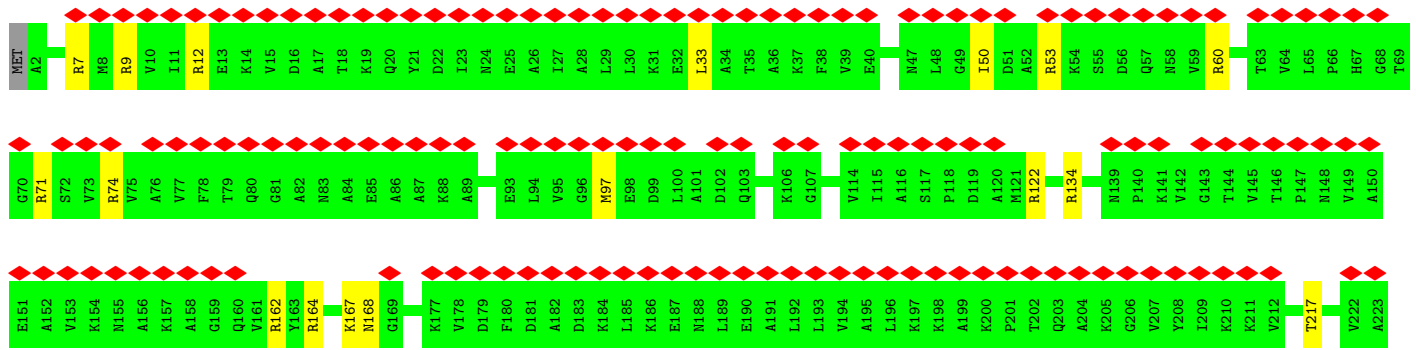
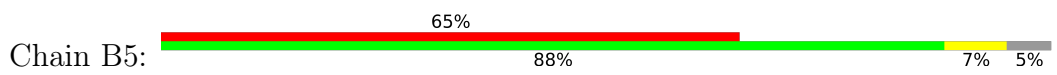
A1745	A1746	A1747	A1748	A1749	A1750	A1751	A1752	A1753	A1754	A1755	A1756	A1757	A1758	A1759	A1760	A1761	A1762	A1763	A1764	A1765	A1766	A1767	A1768	A1769	A1770	A1771	A1772	A1773	A1774	A1775	A1776	A1777	A1778	A1779	A1780	A1781	A1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	A1790	A1791	A1792	A1793	A1794	A1795	A1796	A1797	A1798	A1799	A1800	A1801	A1802	A1803	A1804	A1805
C1806	G1807	A1808	A1809	A1810	G1813	A1814	A1815	A1816	A1819	A1820	A1821	A1822	A1823	A1827	A1828	A1829	A1830	A1831	A1832	A1833	A1834	A1835	A1836	A1837	A1838	A1839	A1840	A1841	A1842	A1843	A1844	A1847	A1848	A1851	A1852	A1853	A1854	A1855	A1856	A1857	A1858	A1859	A1860	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872							
G1873	C1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934			
G1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998
A1999	C1999	C2000	C2001	G2002	A2003	A2004	A2005	C2006	C2008	A2009	G2010	U2011	A2013	A2014	A2015	U2016	U2017	A2018	A2019	A2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	G2035	C2036	A2037	G2038	U2039	G2040	U2041	A2042	C2043	C2044	C2045	G2046	C2047	G2048	G2049	C2050	A2051	A2052	G2053	A2054	C2055	G2056	G2057			
A2058	A2059	A2060	A2061	A2062	A2063	A2064	A2065	A2066	A2067	A2068	A2070	A2071	C2072	U2074	U2075	U2076	A2077	A2078	U2079	A2080	U2081	A2082	C2083	C2084	U2085	U2086	U2087	U2088	A2089	C2089	A2090	A2091	C2092	A2093	A2094	A2095	C2096	A2097	U2098	U2099	G2100	A2101	C2102	C2103	C2104	U2105	U2106	G2107	A2108	U2109	G2110	U2111	A2112	U2113	A2114	U2115	A2116	U2117	U2118	
U2118	A2119	G2120	G2121	U2122	A2126	A2127	A2128	A2129	U2132	G2133	A2134	A2135	U2137	G2138	U2139	G2140	G2141	G2142	G2143	G2144	G2145	C2146	A2147	G2148	U2149	C2150	U2151	G2152	C2153	A2154	U2155	G2156	A2157	A2158	A2159	C2160	A2161	C2162	A2163	A2164	C2165	G2166	A2169	A2170	A2171	A2172	A2173	C2174	C2175	C2176	C2177	C2178	C2179	U2180	U2181					
U2182	A2183	A2184	U2185	G2186	U2187	U2188	U2189	G2190	A2191	U2194	U2195	C2196	A2197	A2198	A2199	C2200	G2201	U2202	U2203	G2204	A2205	C2206	G2208	G2209	U2210	A2211	A2212	U2213	C2214	C2215	G2216	G2217	G2218	U2219	U2220	G2221	C2222	A2225	C2226	A2227	G2228	U2229	G2232	U2233	G2234	G2235	U2236	G2237	G2238	G2239	U2240	A2241	C2242	U2243	U2244					
A2247	C2248	U2249	G2250	G2251	C2254	G2255	G2256	U2257	C2258	U2259	C2260	C2261	U2262	C2263	C2264	U2265	A2266	A2267	A2268	G2269	A2270	G2271	U2272	A2273	A2274	C2275	G2276	G2277	A2278	A2281	C2282	C2283	A2284	C2285	G2286	A2287	A2288	U2291	G2294	C2295	U2296	A2297	A2298	U2299	C2300	C2301	U2302	G2303	G2304	C2305	C2306	G2307	C2308	A2309						
C2310	A2311	U2312	C2313	A2314	G2315	G2316	A2317	U2320	U2321	A2322	A2323	U2324	G2325	C2326	A2327	A2328	U2329	C2330	G2331	A2332	A2333	U2334	A2335	A2336	G2337	C2338	C2339	G2340	G2341	C2342	U2343	U2344	G2345	A2346	A2347	C2350	G2351	A2352	G2353	C2354	G2355	U2356	G2357	A2358	C2359	G2360	G2361	C2362	G2363	C2364	G2365	A2366	C2367	G2368	A2369	G2370	C2371	U2372		
G2372	G2373	C2374	G2375	A2376	A2377	A2378	G2379	C2380	A2381	G2382	G2383	U2384	G2385	A2386	U2387	A2388	G2389	U2390	G2391	A2392	U2393	C2394	C2395	G2396	U2398	G2399	G2400	U2401	U2402	C2403	U2404	G2405	A2406	A2407	U2408	G2409	G2410	A2411	A2412	C2416	C2417	A2418	U2419	C2420	G2421	C2422	U2423	C2424	A2425	A2426	C2427	G2428	G2429	A2430	U2431	U2432	A2433			
A2434	A2435	G2436	G2437	U2438	A2439	C2440	U2441	C2442	C2443	G2444	G2445	G2446	G2447	A2448	U2449	A2450	A2451	C2452	A2453	C2456	U2457	G2458	A2459	U2460	A2461	C2462	C2463	G2464	C2465	C2466	C2467	A2468	A2469	G2470	A2471	U2472	U2473	U2474	C2475	A2476	U2477	U2478	U2479	C2480	G2481	A2482	C2483	G2484	C2485	C2486	G2487	G2488	U2489	U2490	U2491	U2492	U2493	U2494	G2495	
C2495	C2496	A2497	C2498	C2499	U2500	C2501	C2502	U2504	C2505	U2506	G2507	G2508	C2509	C2510	U2511	C2512	A2513	U2514	C2515	A2516	C2517	A2518	U2519	C2520	A2521	C2522	G2524	C2527	U2528	C2529	A2530	A2531	G2532	U2533	A2534	C2535	C2538	C2539	C2540	A2541	A2542	G2543	G2544	C2545	U2546	A2547	U2548	C2551	U2552	C2553	U2554	U2555	U2556	C2557	C2558					



• Molecule 55: 5S ribosomal RNA



• Molecule 56: 50S ribosomal protein L1



◆

V224
ASP
GLN
ALA
GLY
LEU
SER
ALA
SER
VAL
ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3085	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
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	161000	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	181.278	Depositor
Minimum map value	-113.496	Depositor
Average map value	-0.658	Depositor
Map value standard deviation	18.679	Depositor
Recommended contour level	25.0	Depositor
Map size (\AA)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.8, 2.8, 2.8	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, FME, 7MG, 4SU, NH2, ACE, PSU, 6MZ, 5MU, OMC, 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	1.05	12/2340 (0.5%)
2	AC	0.72	0/1651	1.12	14/2225 (0.6%)
3	AD	0.77	0/1665	1.23	21/2227 (0.9%)
4	AE	0.70	0/1119	1.09	9/1506 (0.6%)
5	AF	0.74	0/835	1.09	5/1128 (0.4%)
6	AG	0.75	0/1188	1.21	17/1593 (1.1%)
7	AH	0.70	0/989	1.10	9/1326 (0.7%)
8	AI	0.81	0/1035	1.28	20/1377 (1.5%)
9	AJ	0.72	0/797	1.21	14/1079 (1.3%)
10	AK	0.74	0/894	1.20	12/1207 (1.0%)
11	AL	0.76	0/969	1.32	18/1300 (1.4%)
12	AM	0.76	0/884	1.23	16/1181 (1.4%)
13	AN	0.79	0/817	1.32	12/1088 (1.1%)
14	AO	0.73	0/722	1.12	9/964 (0.9%)
15	AP	0.76	0/648	1.22	9/870 (1.0%)
16	AQ	0.71	0/658	1.14	6/883 (0.7%)
17	AR	0.81	0/463	1.28	6/623 (1.0%)
18	AS	0.78	0/653	1.29	8/879 (0.9%)
19	AT	0.71	0/672	1.08	6/890 (0.7%)
20	AU	0.83	0/431	1.48	10/572 (1.7%)
21	AA	1.52	2/36759 (0.0%)	2.21	1934/57346 (3.4%)
22	A1	1.53	0/1668	2.22	92/2595 (3.5%)
23	A2	1.51	0/343	2.43	24/531 (4.5%)
24	A3	1.53	0/1722	2.18	82/2685 (3.1%)
25	BC	0.75	0/2121	1.27	26/2852 (0.9%)
26	BD	0.68	0/1586	1.11	8/2134 (0.4%)
27	BE	0.68	0/1571	1.12	9/2113 (0.4%)
28	BF	0.76	0/1444	1.21	13/1937 (0.7%)
29	BG	0.69	0/1343	1.13	10/1816 (0.6%)
30	BH	0.67	0/1122	1.08	6/1515 (0.4%)
31	BI	0.66	0/1046	1.02	3/1410 (0.2%)
32	BJ	0.72	0/1152	1.19	11/1551 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.73	0/947	1.28	10/1268 (0.8%)
34	BL	0.74	0/1054	1.32	14/1403 (1.0%)
35	BM	0.75	0/1093	1.22	14/1460 (1.0%)
36	BN	0.77	0/973	1.31	14/1301 (1.1%)
37	BO	0.75	0/902	1.25	11/1209 (0.9%)
38	BP	0.73	0/929	1.20	10/1242 (0.8%)
39	BQ	0.79	0/960	1.30	14/1278 (1.1%)
40	BR	0.72	0/829	1.19	7/1107 (0.6%)
41	BS	0.65	0/864	1.13	7/1156 (0.6%)
42	BT	0.68	0/744	1.21	5/994 (0.5%)
43	BU	0.70	0/787	1.14	6/1051 (0.6%)
44	BV	0.72	0/766	1.18	6/1025 (0.6%)
45	BW	0.75	0/604	1.27	5/799 (0.6%)
46	BX	0.76	0/635	1.32	10/848 (1.2%)
47	BY	0.67	0/510	1.24	6/677 (0.9%)
48	BZ	0.68	0/453	1.21	4/605 (0.7%)
49	B0	0.72	0/450	1.18	5/599 (0.8%)
50	B1	0.72	0/417	1.04	2/556 (0.4%)
51	B2	0.80	0/380	1.47	10/498 (2.0%)
52	B3	0.71	0/513	1.20	5/676 (0.7%)
53	B4	0.70	0/303	1.17	2/397 (0.5%)
54	BA	1.40	0/69796	2.22	4069/108888 (3.7%)
55	BB	1.40	0/2800	2.18	144/4367 (3.3%)
56	B5	0.66	0/1673	1.12	11/2255 (0.5%)
All	All	1.28	2/160085 (0.0%)	2.00	6842/239402 (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
1	AB	0	1
2	AC	0	1
5	AF	0	1
10	AK	0	1
14	AO	0	1
21	AA	0	350
22	A1	0	16
23	A2	0	5
24	A3	0	17
26	BD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	BE	0	1
37	BO	0	1
54	BA	0	705
55	BB	0	21
All	All	0	1122

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1382	C	C4-N4	-5.09	1.29	1.33
21	AA	476	U	C5'-C4'	5.08	1.57	1.51

The worst 5 of 6842 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1932	A	N1-C6-N6	-13.19	110.69	118.60
54	BA	371	A	N1-C6-N6	-12.55	111.07	118.60
21	AA	1239	A	N1-C6-N6	-12.45	111.13	118.60
54	BA	2432	A	N1-C6-N6	-12.35	111.19	118.60
54	BA	1635	A	N1-C6-N6	-12.24	111.26	118.60

There are no chirality outliers.

5 of 1122 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	20	ARG	Sidechain
2	AC	178	ARG	Sidechain
5	AF	4	TYR	Sidechain
10	AK	121	ARG	Peptide
14	AO	43	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AC	1625	0	1699	1	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	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	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	1	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	1	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	2	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	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	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	1	0
43	BU	780	0	834	0	0

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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	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	1	0
53	B4	302	0	343	0	0
54	BA	62317	0	31345	4	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	14	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 14 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)
54:BA:889:C:H1'	54:BA:890:C:C6	2.44	0.52
42:BT:19:LYS:HA	42:BT:23:ALA:HB3	1.92	0.52
21:AA:577:G:H1'	21:AA:816:A:C4	2.49	0.47
2:AC:149:LYS:HE3	2:AC:200:TRP:CZ3	2.50	0.46
54:BA:680:C:H2'	54:BA:681:G:C8	2.52	0.44

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%)	202 (93%)	16 (7%)	0	100	100
2	AC	205/208 (99%)	190 (93%)	13 (6%)	2 (1%)	15	55
3	AD	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	15	55
4	AE	150/152 (99%)	135 (90%)	10 (7%)	5 (3%)	4	26
5	AF	99/101 (98%)	87 (88%)	8 (8%)	4 (4%)	3	23
6	AG	150/152 (99%)	134 (89%)	14 (9%)	2 (1%)	12	48
7	AH	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AI	126/128 (98%)	119 (94%)	4 (3%)	3 (2%)	6	33
9	AJ	98/100 (98%)	93 (95%)	3 (3%)	2 (2%)	7	38
10	AK	116/118 (98%)	105 (90%)	8 (7%)	3 (3%)	5	31
11	AL	121/124 (98%)	106 (88%)	10 (8%)	5 (4%)	3	23
12	AM	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	3	25
13	AN	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	7	38
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3	25
15	AP	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
16	AQ	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	5	32
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	8	40
18	AS	79/81 (98%)	69 (87%)	10 (13%)	0	100	100
19	AT	84/86 (98%)	72 (86%)	10 (12%)	2 (2%)	6	33
20	AU	51/53 (96%)	36 (71%)	11 (22%)	4 (8%)	1	13
25	BC	270/273 (99%)	244 (90%)	22 (8%)	4 (2%)	10	46
26	BD	207/209 (99%)	182 (88%)	19 (9%)	6 (3%)	4	29
27	BE	199/201 (99%)	185 (93%)	7 (4%)	7 (4%)	3	25
28	BF	176/179 (98%)	149 (85%)	16 (9%)	11 (6%)	1	17
29	BG	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	14	52
30	BH	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	22	63
31	BI	139/142 (98%)	125 (90%)	14 (10%)	0	100	100
32	BJ	140/142 (99%)	125 (89%)	10 (7%)	5 (4%)	3	25
33	BK	121/123 (98%)	106 (88%)	9 (7%)	6 (5%)	2	20
34	BL	141/144 (98%)	118 (84%)	15 (11%)	8 (6%)	1	18
35	BM	134/136 (98%)	128 (96%)	2 (2%)	4 (3%)	4	28
36	BN	119/121 (98%)	105 (88%)	13 (11%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	17	57
38	BP	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	3	25
39	BQ	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
40	BR	101/103 (98%)	88 (87%)	11 (11%)	2 (2%)	7	38
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	8	38
42	BT	92/94 (98%)	75 (82%)	13 (14%)	4 (4%)	2	22
43	BU	101/104 (97%)	85 (84%)	9 (9%)	7 (7%)	1	15
44	BV	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	14	52
45	BW	78/80 (98%)	60 (77%)	13 (17%)	5 (6%)	1	16
46	BX	75/79 (95%)	67 (89%)	7 (9%)	1 (1%)	12	48
47	BY	61/63 (97%)	53 (87%)	8 (13%)	0	100	100
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	19
49	B0	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	8	38
50	B1	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	23
51	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	2	22
52	B3	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	9	44
53	B4	36/38 (95%)	28 (78%)	7 (19%)	1 (3%)	5	30
56	B5	221/234 (94%)	205 (93%)	13 (6%)	3 (1%)	11	46
All	All	5876/6008 (98%)	5257 (90%)	478 (8%)	141 (2%)	9	33

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	AG	5	VAL
11	AL	108	ASP
19	AT	9	ARG
26	BD	2	ILE
27	BE	69	ARG

5.3.2 Protein sidechains [i](#)

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%)	176 (98%)	4 (2%)	52	71
2	AC	170/171 (99%)	167 (98%)	3 (2%)	59	77
3	AD	172/173 (99%)	168 (98%)	4 (2%)	50	70
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	84 (97%)	3 (3%)	37	60
6	AG	123/123 (100%)	120 (98%)	3 (2%)	49	69
7	AH	104/105 (99%)	101 (97%)	3 (3%)	42	64
8	AI	105/105 (100%)	103 (98%)	2 (2%)	57	75
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	86 (96%)	4 (4%)	28	53
11	AL	103/104 (99%)	102 (99%)	1 (1%)	76	86
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	49	69
14	AO	76/77 (99%)	74 (97%)	2 (3%)	46	66
15	AP	65/65 (100%)	64 (98%)	1 (2%)	65	80
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%)	68 (97%)	2 (3%)	42	64
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%)	207 (96%)	9 (4%)	30	54
26	BD	164/164 (100%)	161 (98%)	3 (2%)	59	77
27	BE	165/165 (100%)	163 (99%)	2 (1%)	71	83
28	BF	149/150 (99%)	147 (99%)	2 (1%)	69	81
29	BG	137/138 (99%)	135 (98%)	2 (2%)	65	80
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	78	87
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	46	66
33	BK	103/103 (100%)	100 (97%)	3 (3%)	42	64
34	BL	102/103 (99%)	99 (97%)	3 (3%)	42	64
35	BM	109/109 (100%)	107 (98%)	2 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	76	86
37	BO	86/87 (99%)	85 (99%)	1 (1%)	71	83
38	BP	99/100 (99%)	97 (98%)	2 (2%)	55	74
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	52	71
40	BR	84/84 (100%)	83 (99%)	1 (1%)	71	83
41	BS	93/93 (100%)	93 (100%)	0	100	100
42	BT	80/80 (100%)	78 (98%)	2 (2%)	47	68
43	BU	83/84 (99%)	81 (98%)	2 (2%)	49	69
44	BV	78/78 (100%)	76 (97%)	2 (3%)	46	66
45	BW	59/59 (100%)	57 (97%)	2 (3%)	37	60
46	BX	67/68 (98%)	67 (100%)	0	100	100
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%)	45 (96%)	2 (4%)	29	53
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	50 (98%)	1 (2%)	55	74
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	60	78
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	61	77

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	BK	30	ARG
42	BT	2	ILE
34	BL	36	LYS
37	BO	2	ASP
44	BV	24	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
13	AN	62	ASN

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Mol	Chain	Res	Type
26	BD	134	HIS
34	BL	99	ASN
38	BP	55	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	240 (15%)	90 (5%)
22	A1	73/76 (96%)	9 (12%)	2 (2%)
23	A2	14/15 (93%)	7 (50%)	2 (14%)
24	A3	76/77 (98%)	9 (11%)	5 (6%)
54	BA	2902/2903 (99%)	458 (15%)	137 (4%)
55	BB	116/118 (98%)	12 (10%)	3 (2%)
All	All	4711/4722 (99%)	735 (15%)	239 (5%)

5 of 735 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	32	A
21	AA	39	G

5 of 239 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	549	G
54	BA	2442	C
54	BA	1071	G
54	BA	2431	U
55	BB	14	U

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

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	6MZ	A1	37	22	18,25,26	0.89	0	16,36,39	1.71	2 (12%)
22	CM0	A1	34	22,23	22,26,27	1.33	2 (9%)	28,37,40	0.93	0
22	5MU	A1	54	22	19,22,23	0.81	0	28,32,35	1.45	4 (14%)
24	PSU	A3	56	24	18,21,22	0.89	0	22,30,33	1.09	2 (9%)
24	4SU	A3	8	24	18,21,22	1.40	1 (5%)	26,30,33	0.87	1 (3%)
24	H2U	A3	21	24	18,21,22	1.31	2 (11%)	21,30,33	1.38	3 (14%)
22	4SU	A1	7	22	18,21,22	1.34	1 (5%)	26,30,33	0.96	2 (7%)
22	7MG	A1	46	22	22,26,27	4.82	2 (9%)	29,39,42	1.47	1 (3%)
24	5MU	A3	55	24	19,22,23	0.76	0	28,32,35	1.33	3 (10%)
22	PSU	A1	55	22	18,21,22	0.81	0	22,30,33	1.06	2 (9%)
24	OMC	A3	33	24	19,22,23	0.76	0	26,31,34	1.04	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	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	CM0	A1	34	22,23	-	3/12/30/31	0/2/2/2
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
24	PSU	A3	56	24	-	2/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	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
24	5MU	A3	55	24	-	0/7/25/26	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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-22.33	1.33	1.46
24	A3	8	4SU	C5-C4	-4.91	1.36	1.42
22	A1	34	CM0	O5-C5	-4.83	1.25	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	7	4SU	C5-C4	-4.79	1.36	1.42
24	A3	21	H2U	C4-N3	-3.48	1.31	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	5.73	111.57	103.38
22	A1	37	6MZ	C9-N6-C6	4.72	126.93	122.87
22	A1	37	6MZ	C2-N1-C6	4.11	120.11	116.59
22	A1	54	5MU	C5M-C5-C6	-3.97	117.55	122.85
24	A3	21	H2U	N3-C2-N1	3.78	120.65	116.65

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	22,58	4,6,7	0.66	0	6,7,9	0.83	0
58	FME	BA	3001	57	8,9,10	0.78	0	7,9,11	2.09	3 (42%)

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	22,58	-	3/5/6/8	-
58	FME	BA	3001	57	-	0/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
58	BA	3001	FME	CA-N-CN	3.70	128.52	122.82
58	BA	3001	FME	C-CA-N	3.08	115.29	109.73
58	BA	3001	FME	O-C-CA	-2.56	118.07	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A1	101	VAL	O-C-CA-CB
57	A1	101	VAL	C-CA-CB-CG1
57	A1	101	VAL	C-CA-CB-CG2

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.

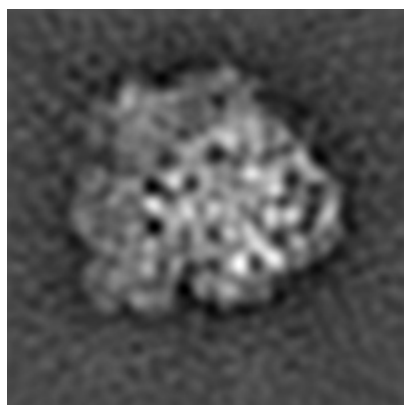
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2474. These allow visual inspection of the internal detail of the map and identification of artifacts.

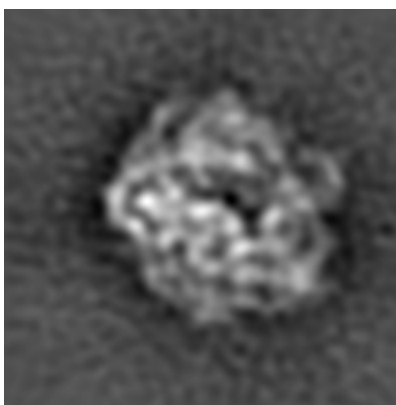
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

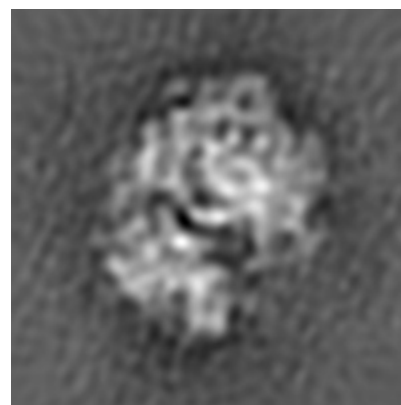
6.1.1 Primary map



X



Y

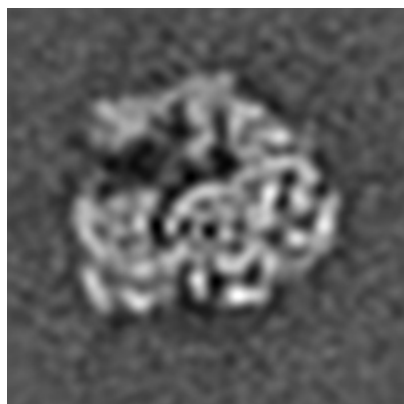


Z

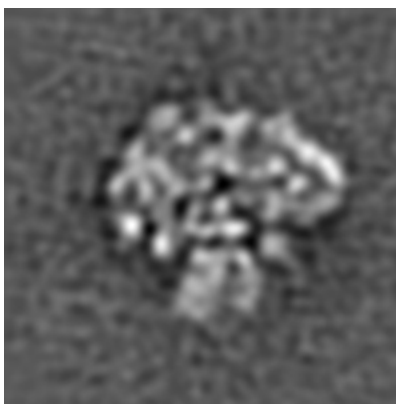
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

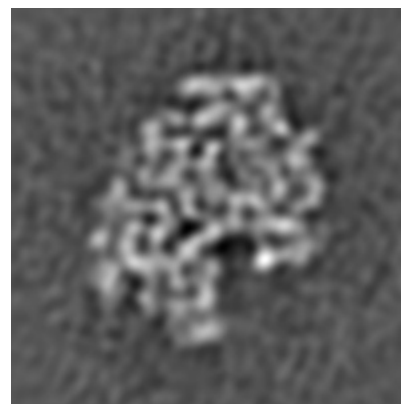
6.2.1 Primary map



X Index: 64



Y Index: 64

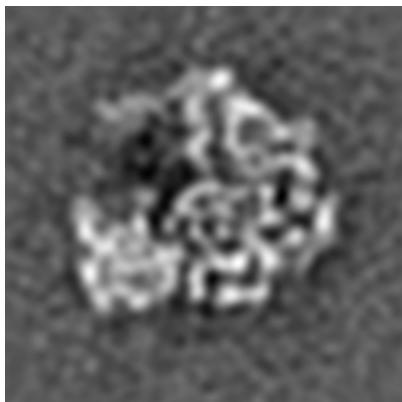


Z Index: 64

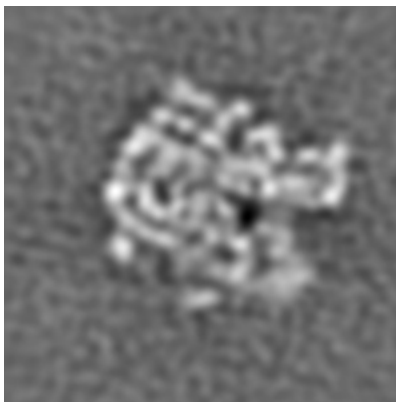
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

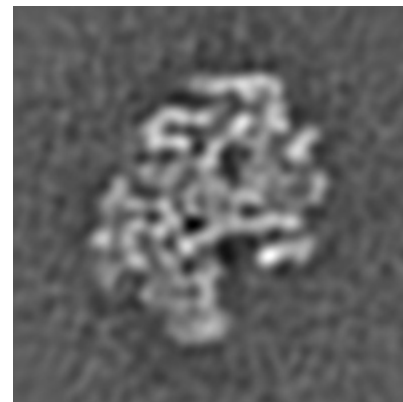
6.3.1 Primary map



X Index: 66



Y Index: 70

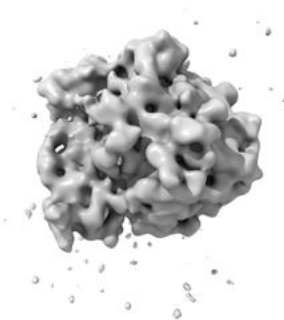


Z Index: 62

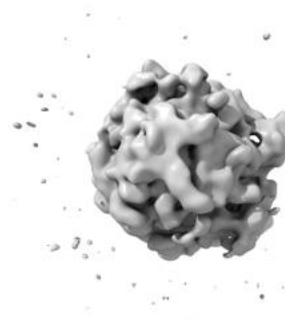
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

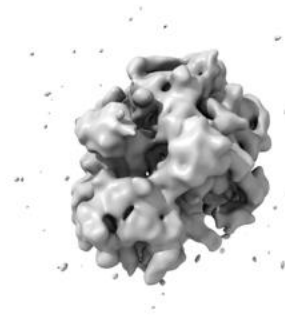
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 25.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

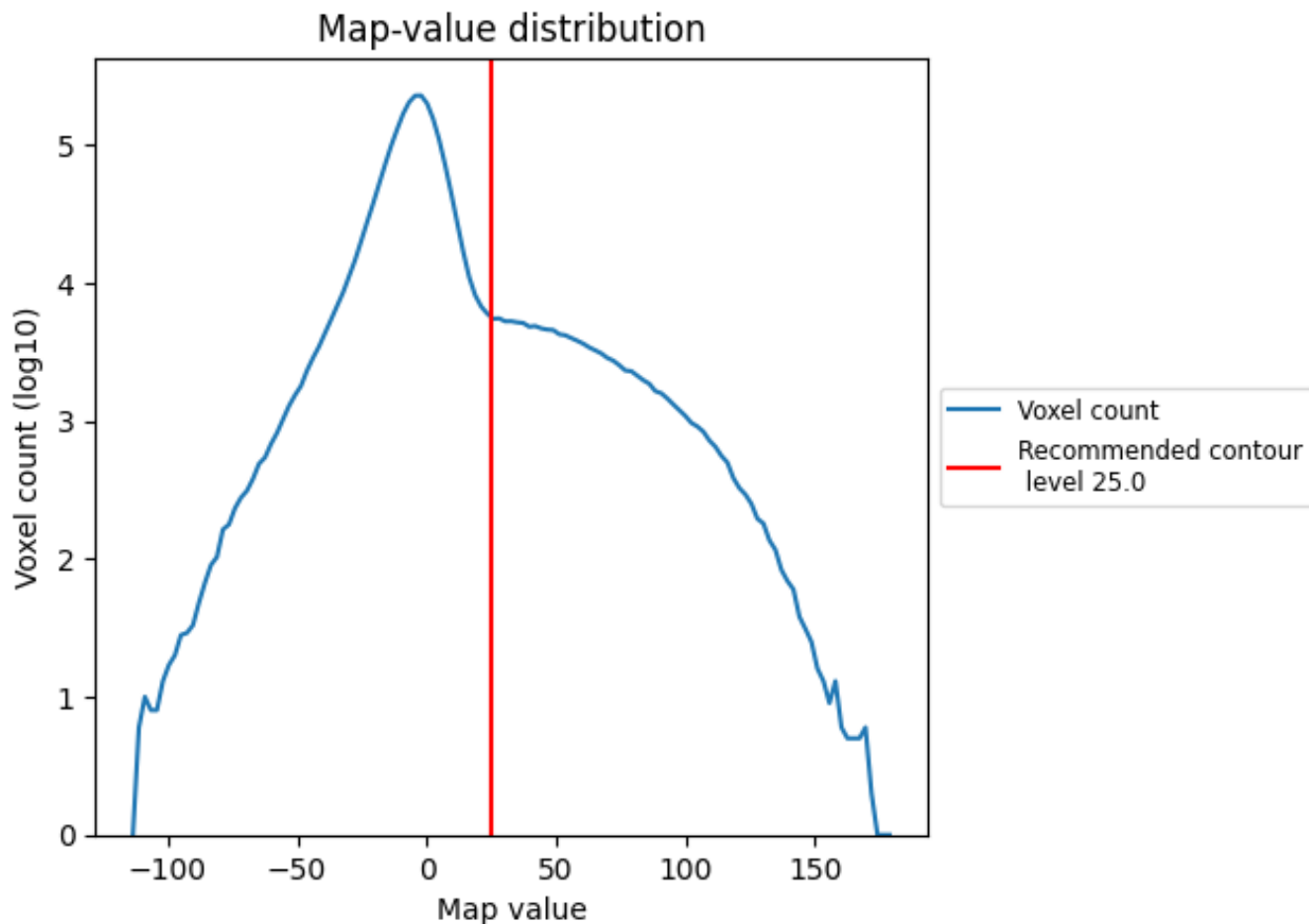
6.5 Mask visualisation

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

7 Map analysis [i](#)

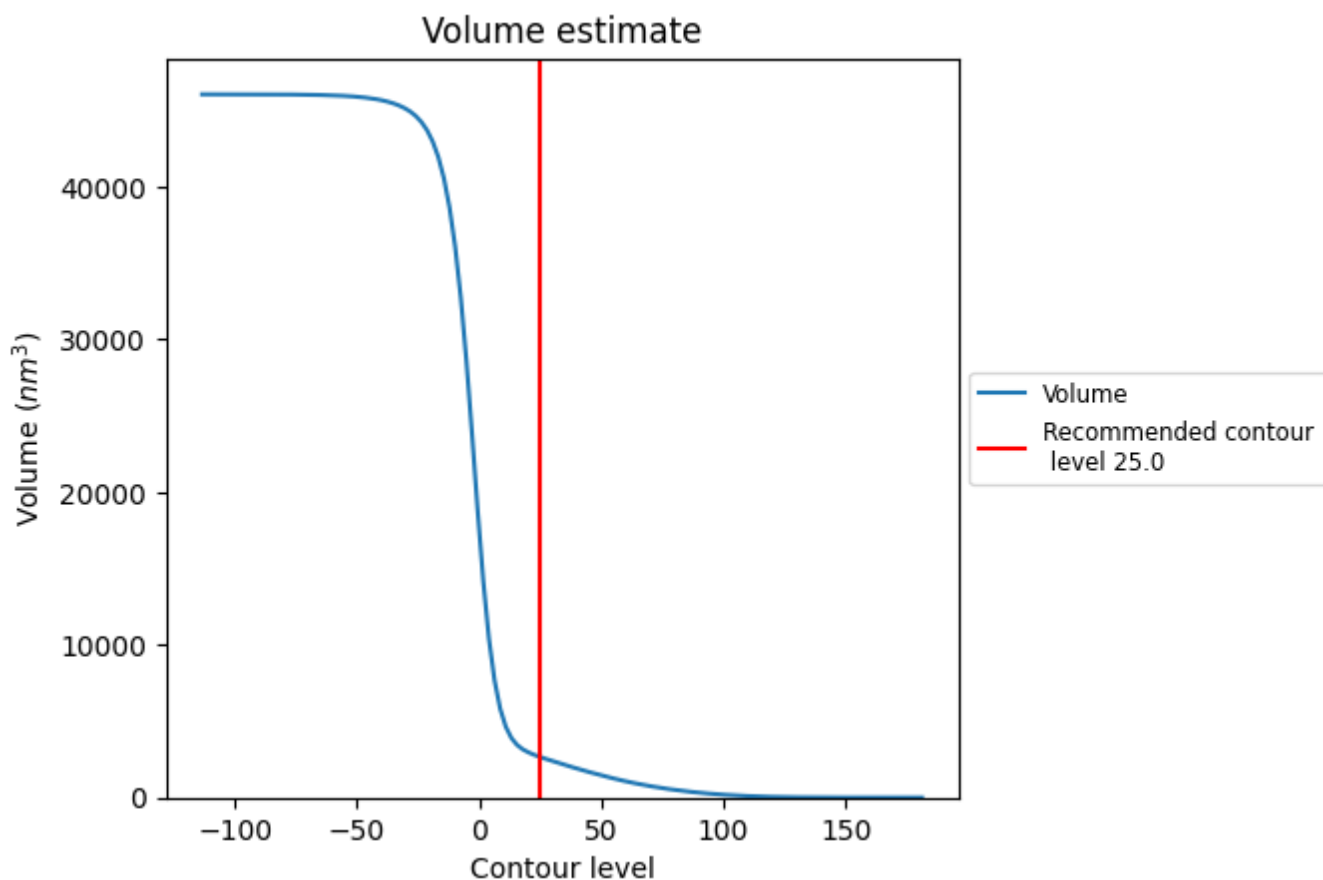
This section contains the results of statistical analysis of the map.

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.

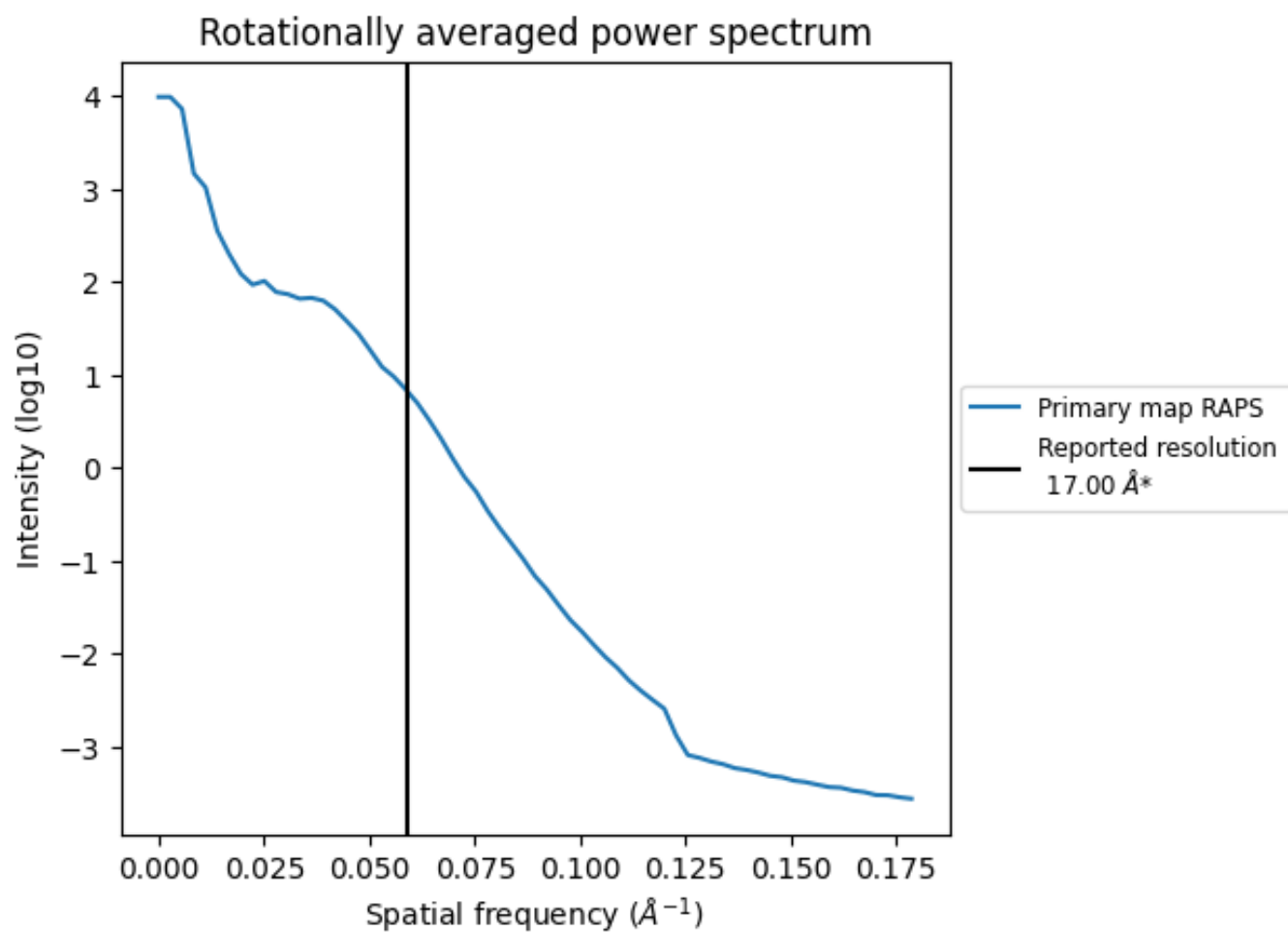
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2652 nm³; this corresponds to an approximate mass of 2396 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.059 Å⁻¹

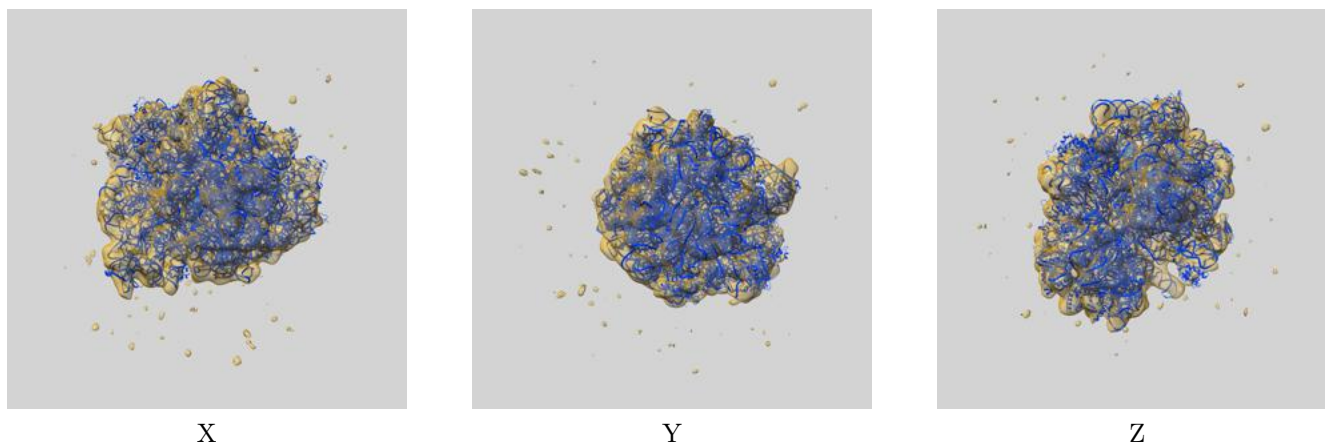
8 Fourier-Shell correlation

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-2474 and PDB model 4V77. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



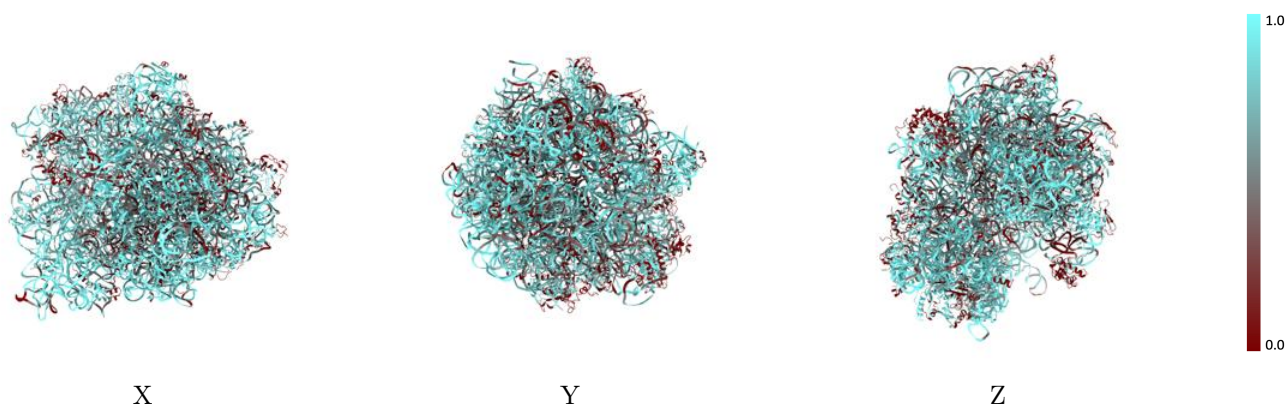
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



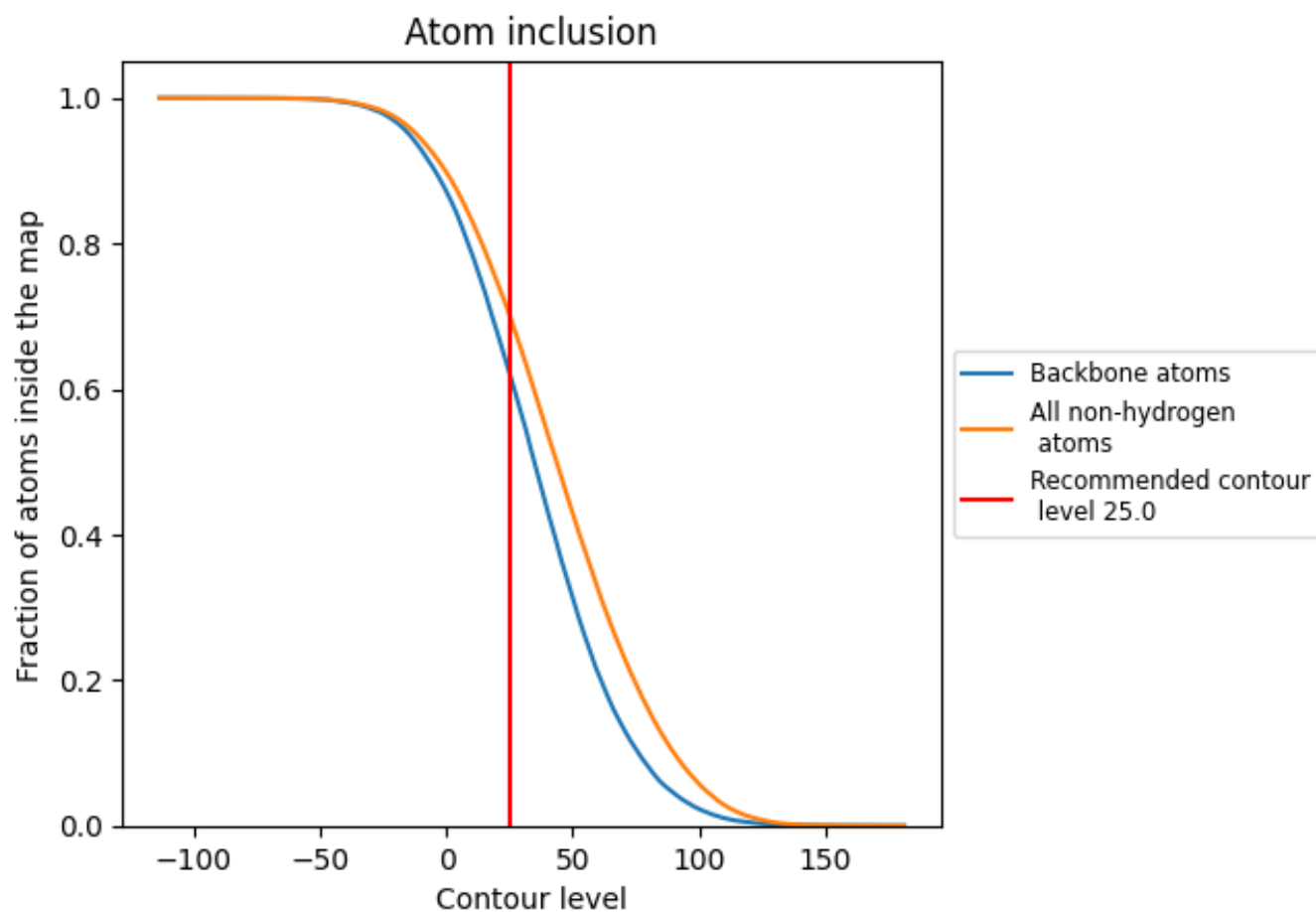
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (25.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 70% 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 (25.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7018	 0.0510
A1	 0.6818	 0.0680
A2	 0.7443	 0.0280
A3	 0.6279	 0.0530
AA	 0.8007	 0.0680
AB	 0.7336	 0.0570
AC	 0.5909	 0.0360
AD	 0.6314	 0.0310
AE	 0.6602	 0.0460
AF	 0.5960	 0.0460
AG	 0.4904	 0.0510
AH	 0.7063	 0.0440
AI	 0.6116	 0.0210
AJ	 0.6675	 0.0170
AK	 0.5544	 0.0260
AL	 0.4647	 0.0100
AM	 0.5692	 0.0430
AN	 0.5297	 0.0330
AO	 0.6623	 0.0380
AP	 0.7407	 0.0380
AQ	 0.5291	 0.0380
AR	 0.4829	 0.0190
AS	 0.6122	 0.0230
AT	 0.5153	 0.0100
AU	 0.2714	 -0.0160
B0	 0.5841	 0.0160
B1	 0.6337	 0.0630
B2	 0.3324	 -0.0150
B3	 0.3849	 -0.0630
B4	 0.5890	 0.0060
B5	 0.2970	 0.0180
BA	 0.7467	 0.0580
BB	 0.8690	 0.0750
BC	 0.4373	 -0.0000
BD	 0.5923	 0.0220



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Chain	Atom inclusion	Q-score
BE	 0.5349	 0.0300
BF	 0.6732	 0.0450
BG	 0.6646	 0.0410
BH	 0.2920	 0.0370
BI	 0.1037	 0.0440
BJ	 0.7136	 0.0300
BK	 0.4847	 0.0160
BL	 0.6112	 0.0320
BM	 0.7198	 0.0300
BN	 0.6555	 0.0120
BO	 0.7555	 0.0270
BP	 0.6971	 0.0500
BQ	 0.6211	 -0.0020
BR	 0.6336	 0.0470
BS	 0.5323	 0.0040
BT	 0.5311	 0.0060
BU	 0.5286	 0.0040
BV	 0.6369	 0.0370
BW	 0.5223	 0.0220
BX	 0.3877	 0.0040
BY	 0.5412	 0.0280
BZ	 0.4897	 0.0450