



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 12:07 PM EST

PDB ID : 4V6Z
EMDB ID : EMD-2472
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in classic pre-translocation state (pre1b)
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 : 12.00 Å (reported)
Based on initial models : 2WRI, 2HGP, 3I1O, 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.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

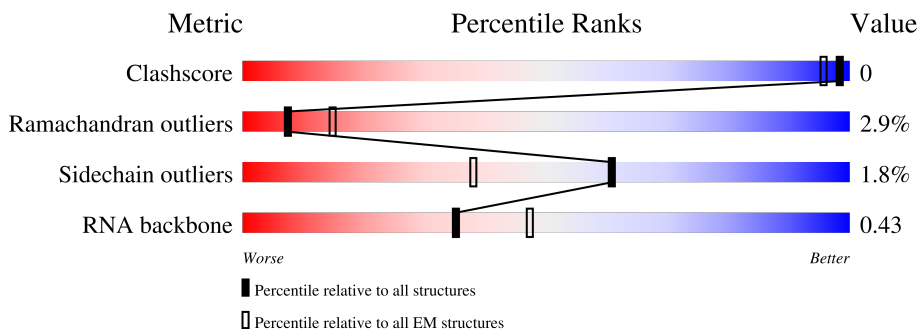
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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	50% 94% 6%
2	AC	208	46% 89% 10%
3	AD	206	51% 88% 11%
4	AE	152	45% 89% 11% .
5	AF	101	26% 87% 12% .
6	AG	152	36% 93% 7%
7	AH	130	43% 92% 7% .

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Mol	Chain	Length	Quality of chain
8	AI	128	25% 88% 11%
9	AJ	100	54% 81% 16%
10	AK	118	26% 90% 8%
11	AL	124	31% 90% 10%
12	AM	115	31% 84% 15%
13	AN	101	60% 85% 14%
14	AO	89	26% 87% 12%
15	AP	81	54% 88% 12%
16	AQ	82	43% 91% 9%
17	AR	57	39% 88% 12%
18	AS	81	31% 91% 9%
19	AT	86	27% 86% 14%
20	AU	53	34% 68% 26% 6%
21	AA	1533	28% 13% 57% 25% 5%
22	A1	76	39% 17% 62% 17%
23	A2	15	33% 33% 47% 20%
24	A3	77	58% 17% 61% 18%
25	BC	273	53% 84% 14%
26	BD	209	51% 88% 11%
27	BE	201	35% 91% 9%
28	BF	179	37% 91% 8%
29	BG	177	53% 89% 8%
30	BH	149	76% 94% 6%
31	BI	142	99% 93% 6%
32	BJ	142	51% 88% 12%

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Mol	Chain	Length	Quality of chain
33	BK	123	51% 87% 11% ..
34	BL	144	33% 81% 17% ..
35	BM	136	54% 89% 11%
36	BN	121	42% 85% 14% .
37	BO	117	11% 88% 11% .
38	BP	115	53% 84% 13% ..
39	BQ	118	43% 88% 10% ..
40	BR	103	31% 89% 11%
41	BS	110	46% 90% 10%
42	BT	94	36% 89% 11%
43	BU	104	39% 91% 7% ..
44	BV	94	34% 93% 7%
45	BW	80	39% 84% 12% .
46	BX	79	49% 84% 13% ..
47	BY	63	40% 92% 8%
48	BZ	59	51% 86% 12% .
49	B0	57	23% 84% 12% ..
50	B1	52	48% 83% 17%
51	B2	46	57% 74% 26%
52	B3	65	51% 91% 6% ..
53	B4	38	45% 87% 13%
54	BA	2903	35% 13% 57% 26% 5%
55	BB	118	23% 9% 57% 31% ..
56	B5	234	60% 90% 5% 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*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
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
			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		

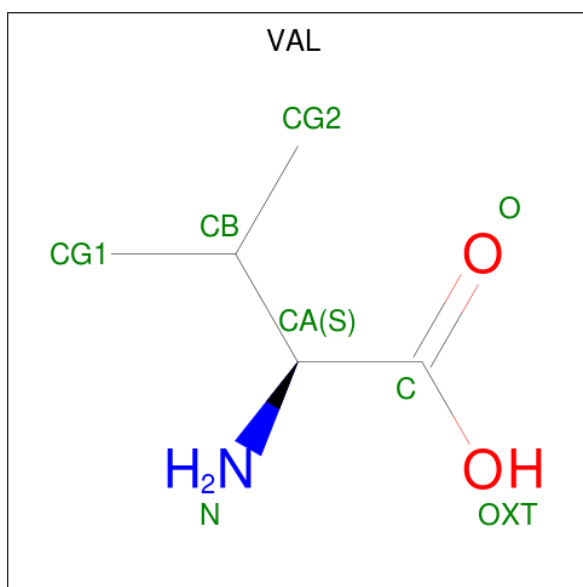
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

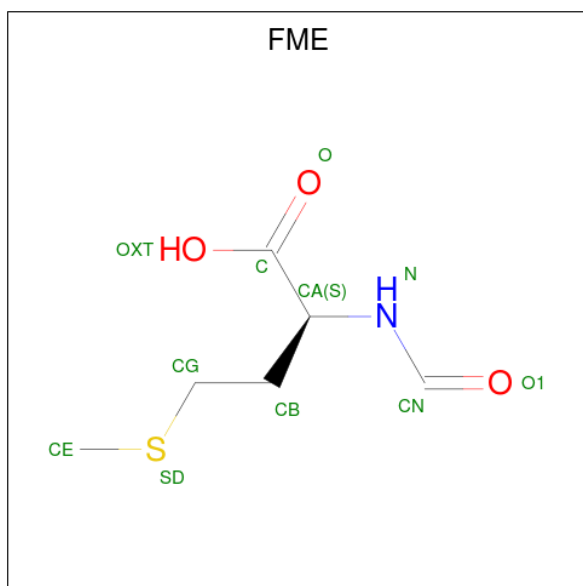
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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).

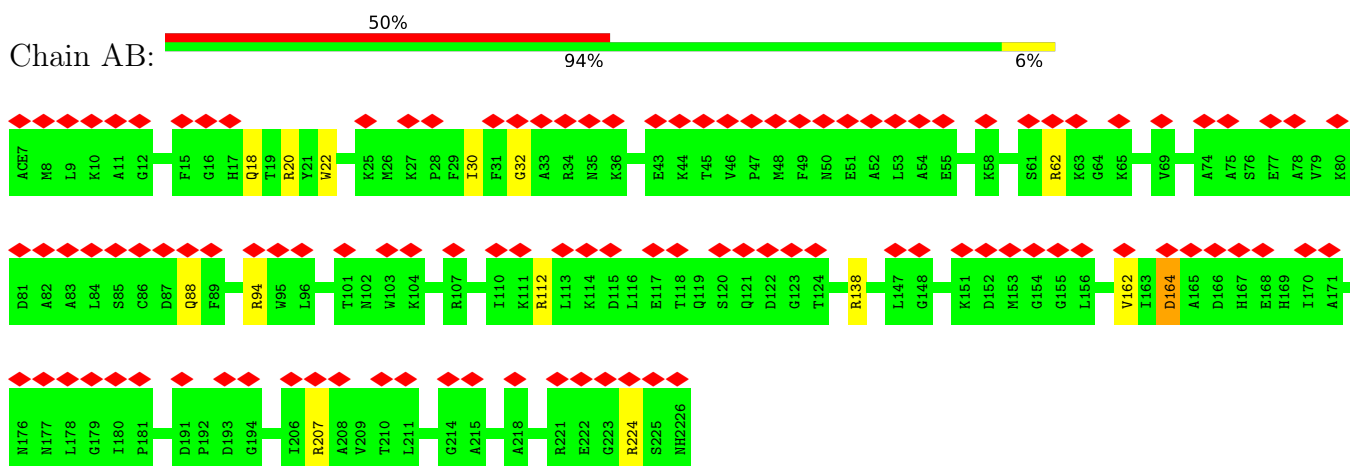


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	BA	1	10	6	1	2	1	0

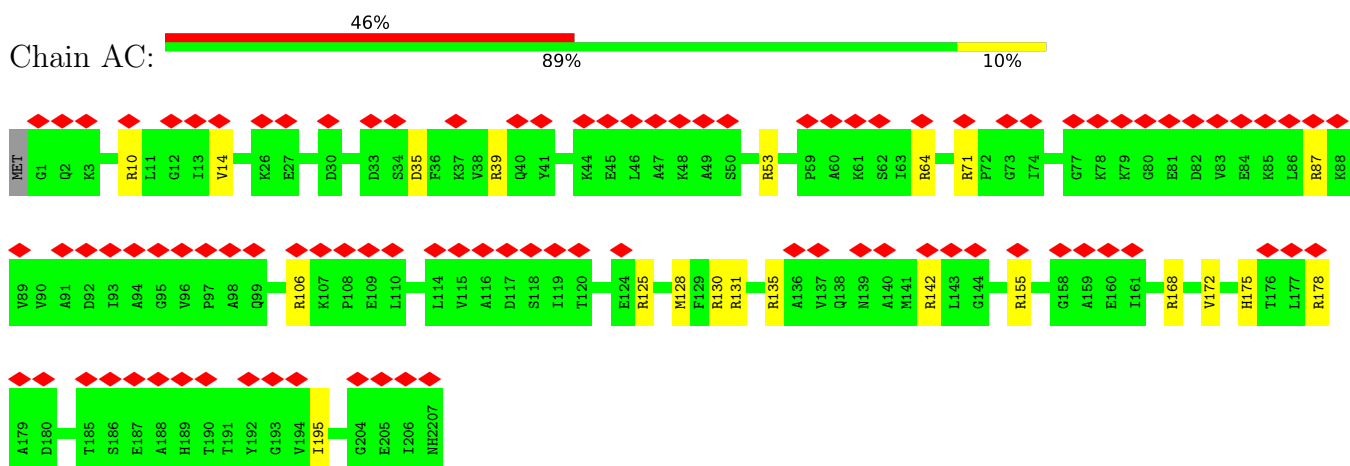
3 Residue-property plots [i](#)

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.

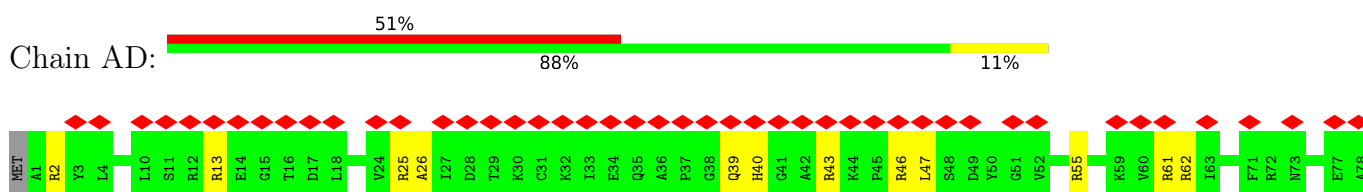
- Molecule 1: 30S ribosomal protein S2

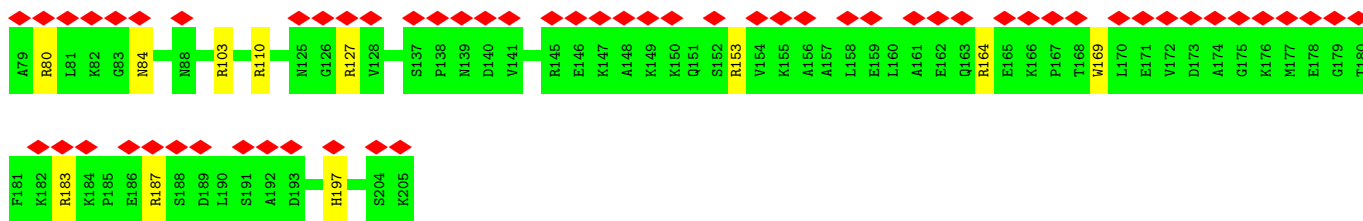


- Molecule 2: 30S ribosomal protein S3



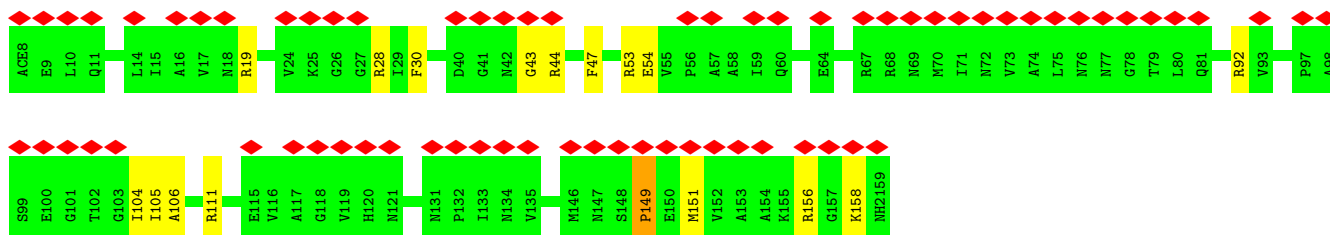
- Molecule 3: 30S ribosomal protein S4





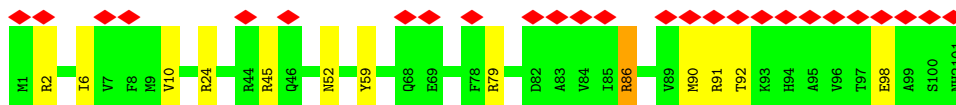
- Molecule 4: 30S ribosomal protein S5

Chain AE: 45% 89% 11%



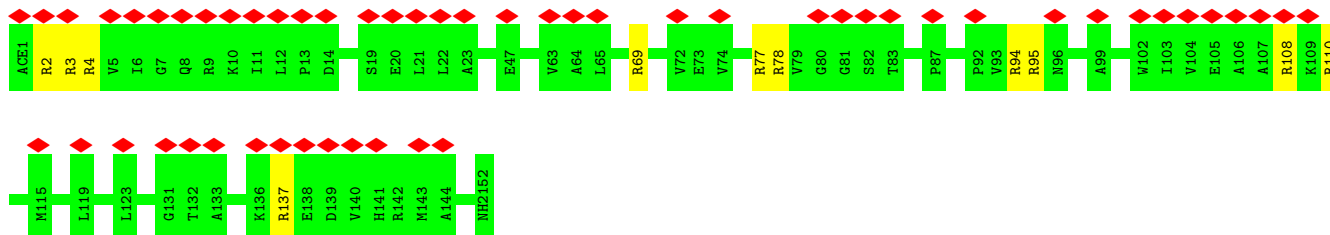
- Molecule 5: 30S ribosomal protein S6

Chain AF: 26% 87% 12%



- Molecule 6: 30S ribosomal protein S7

Chain AG: 36% 93% 7%

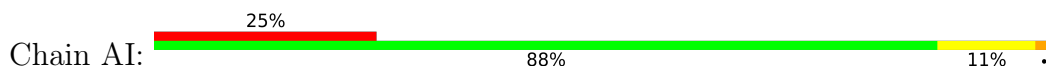


- Molecule 7: 30S ribosomal protein S8

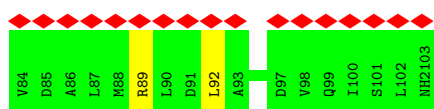
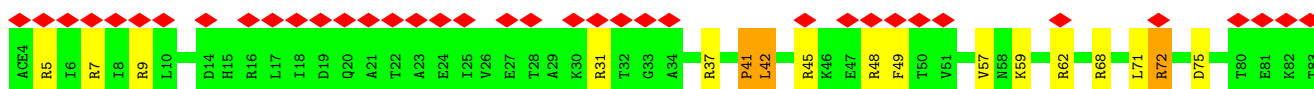
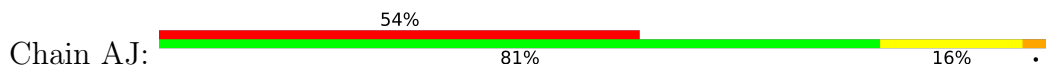
Chain AH: 43% 92% 7%



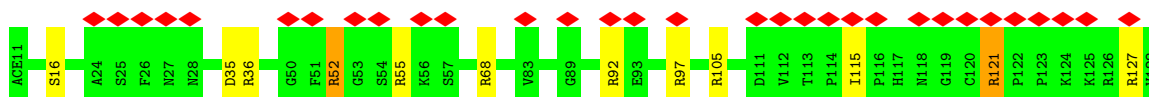
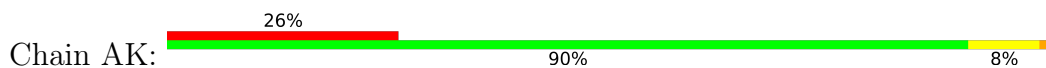
- Molecule 8: 30S ribosomal protein S9



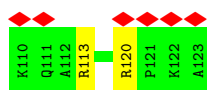
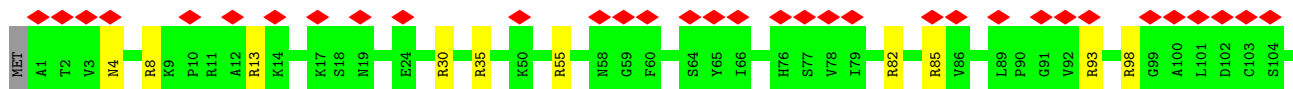
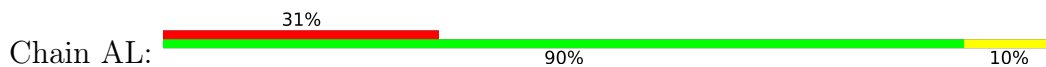
- Molecule 9: 30S ribosomal protein S10



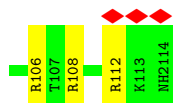
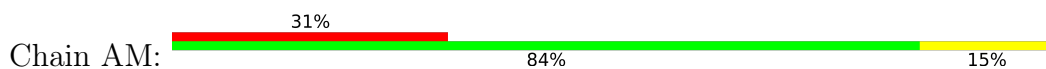
- Molecule 10: 30S ribosomal protein S11



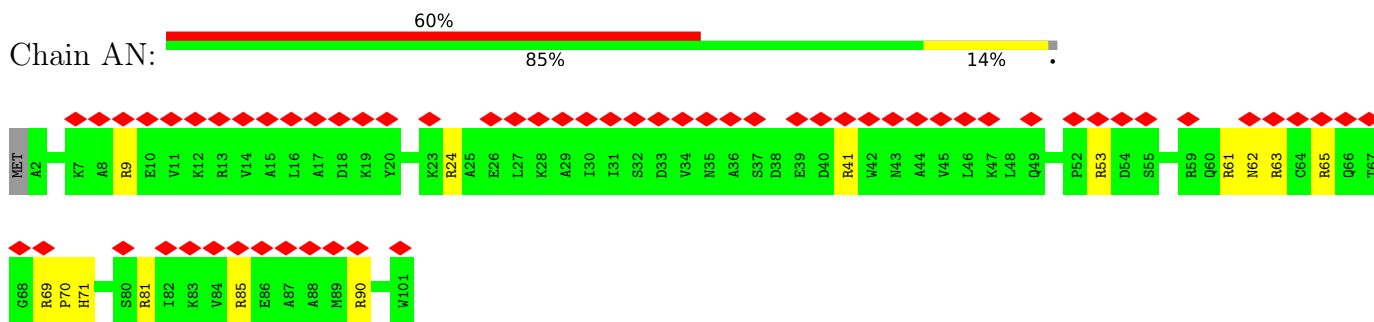
- Molecule 11: 30S ribosomal protein S12



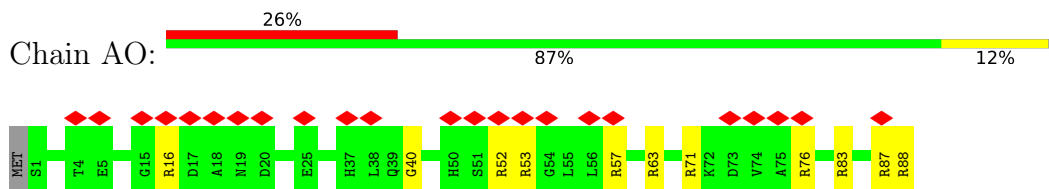
- Molecule 12: 30S ribosomal protein S13



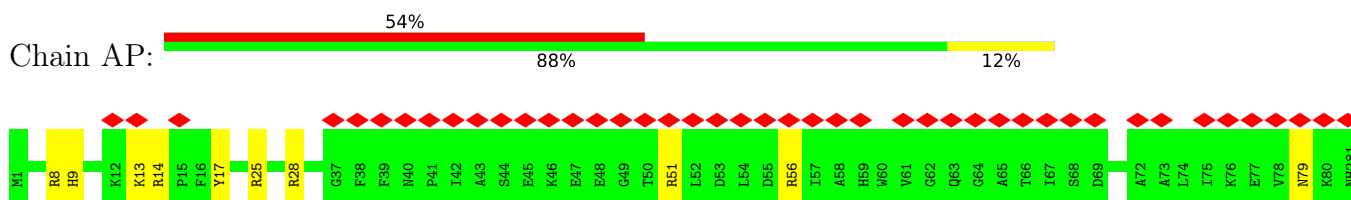
- Molecule 13: 30S ribosomal protein S14



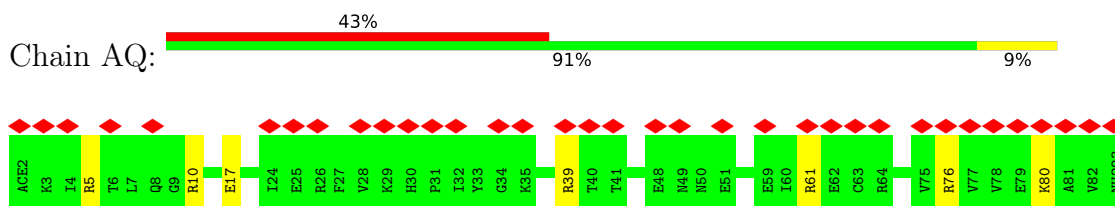
- Molecule 14: 30S ribosomal protein S15



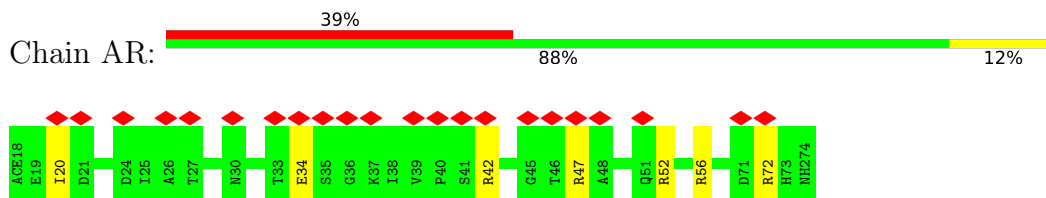
- Molecule 15: 30S ribosomal protein S16



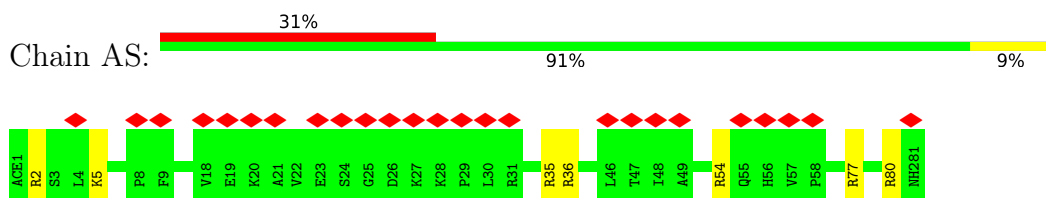
- Molecule 16: 30S ribosomal protein S17



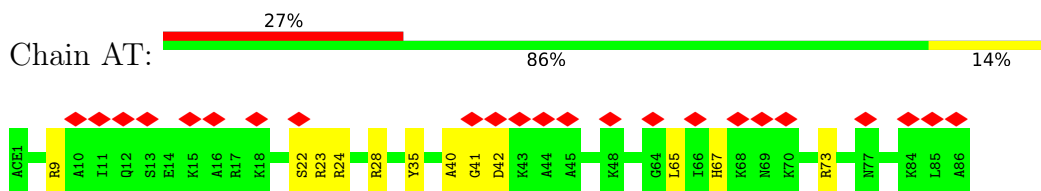
- Molecule 17: 30S ribosomal protein S18



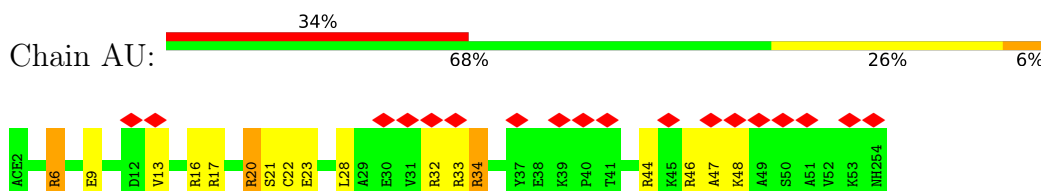
- Molecule 18: 30S ribosomal protein S19



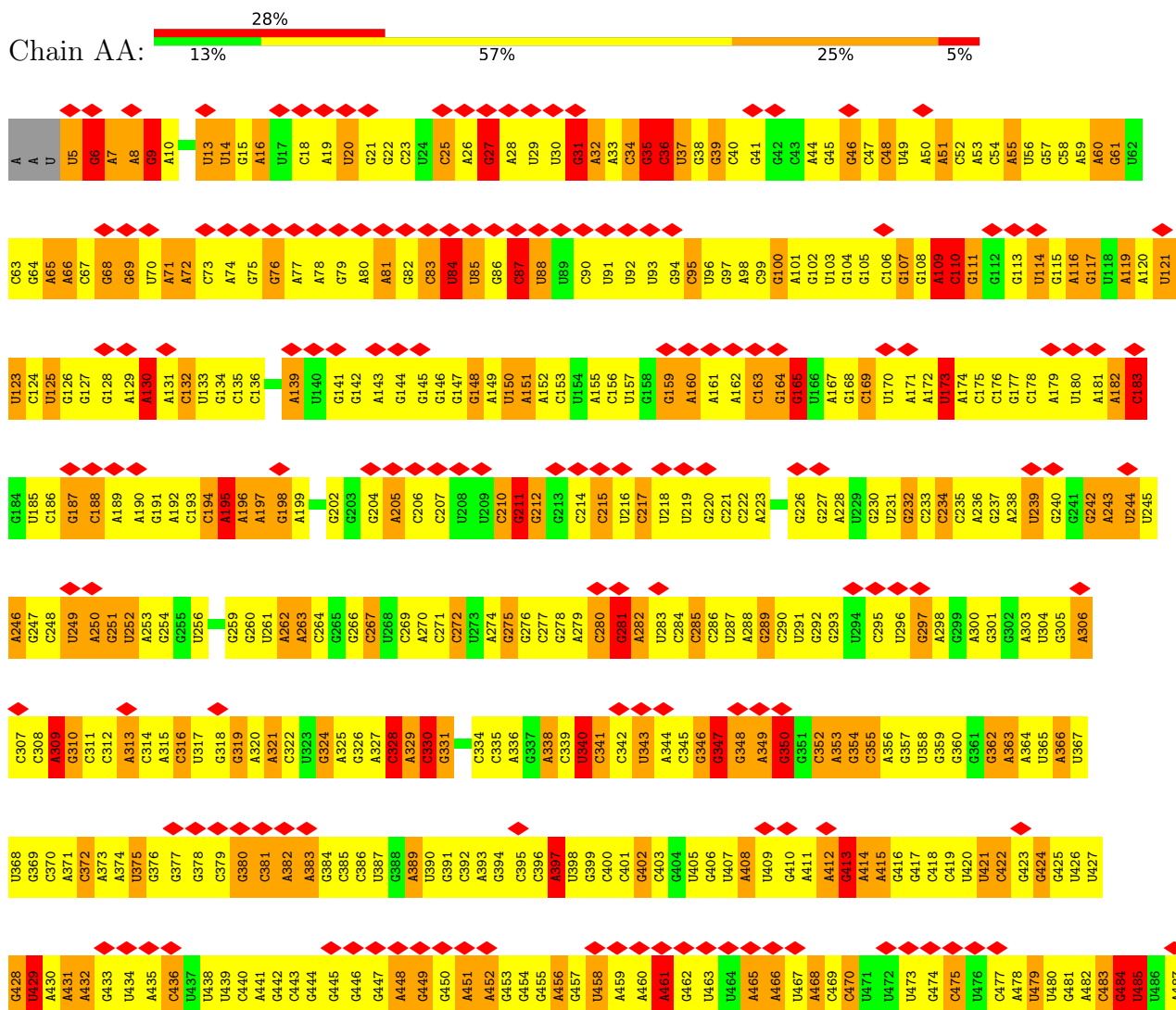
• Molecule 19: 30S ribosomal protein S20

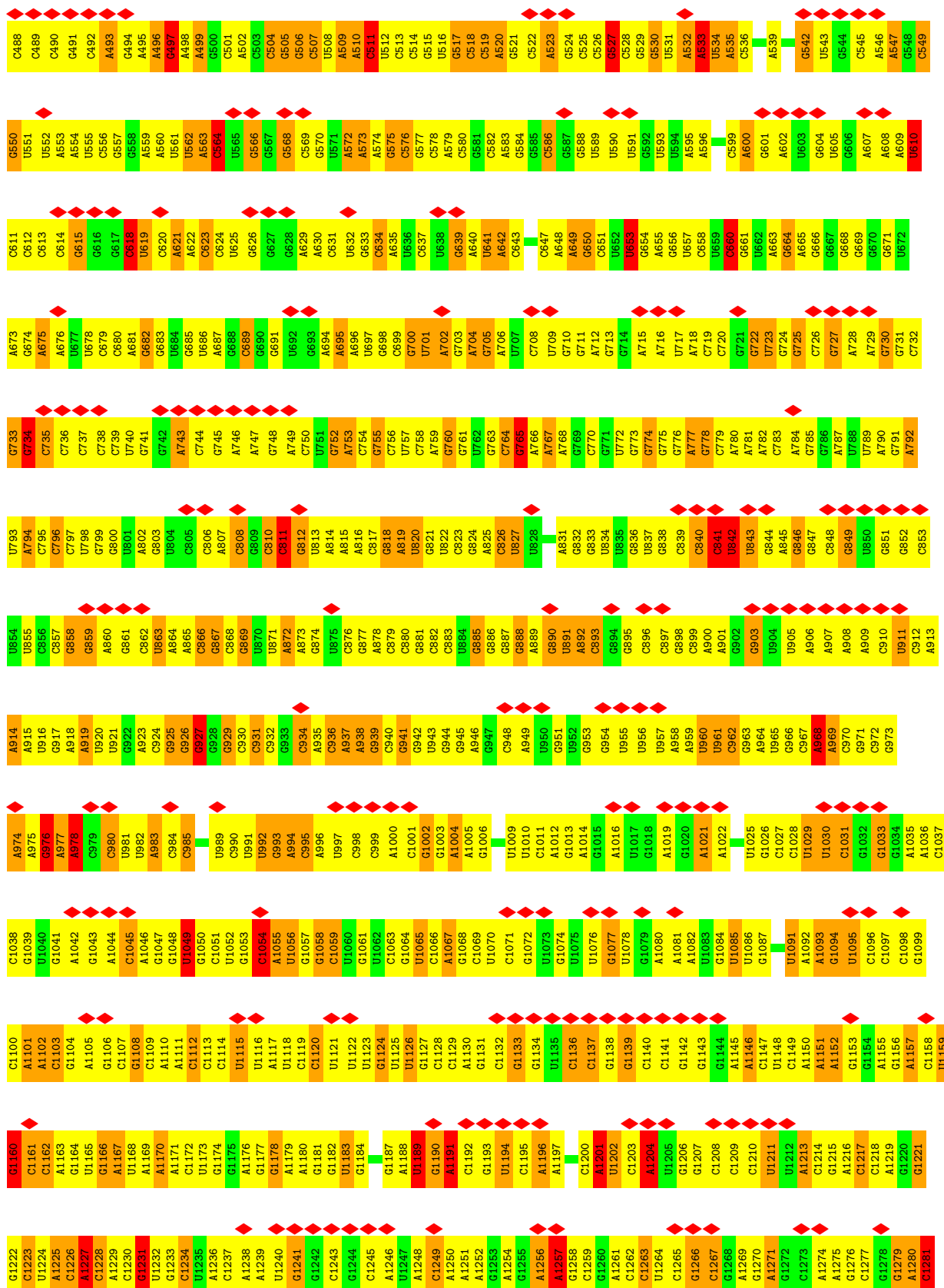


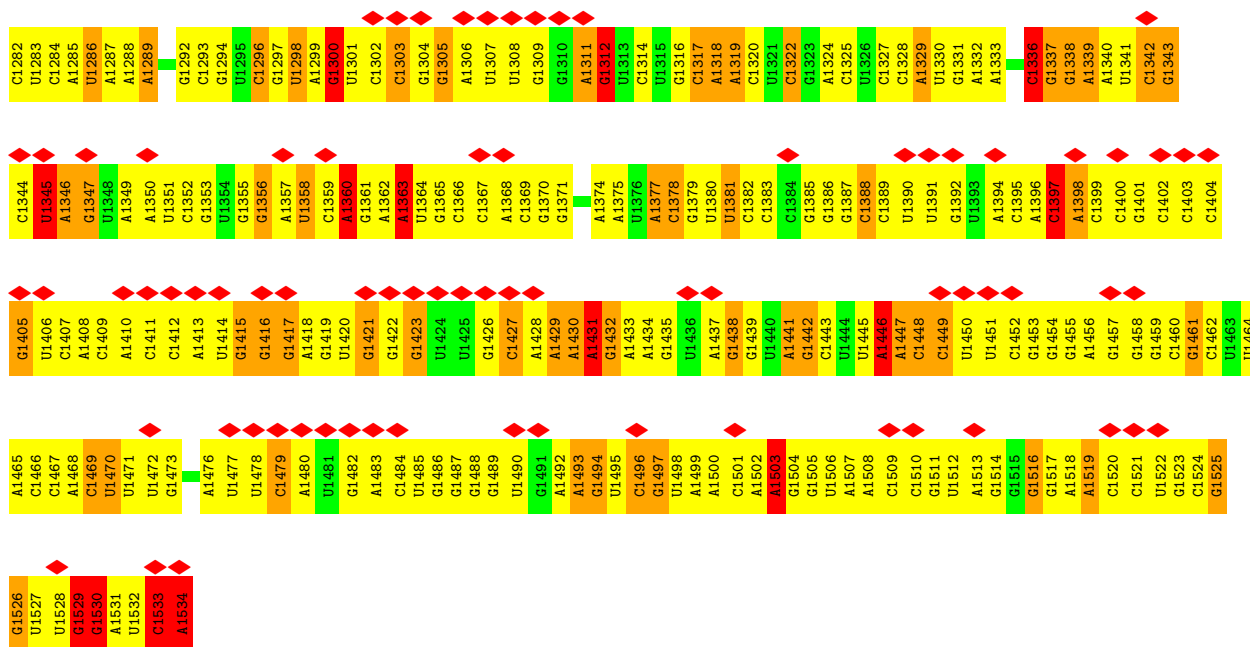
• Molecule 20: 30S ribosomal protein S21



• Molecule 21: 16S ribosomal RNA







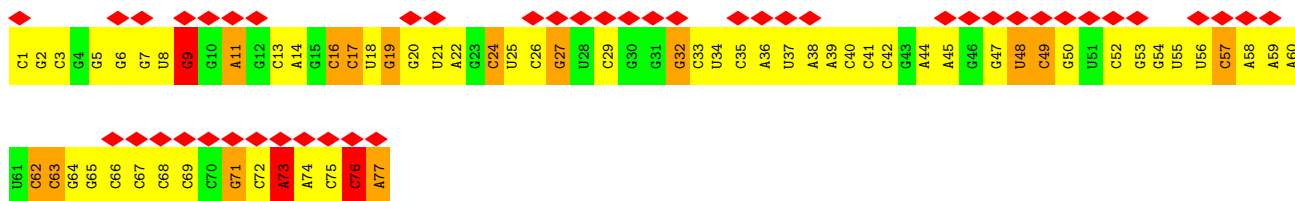
• Molecule 22: fMet-Val-tRNA-Val



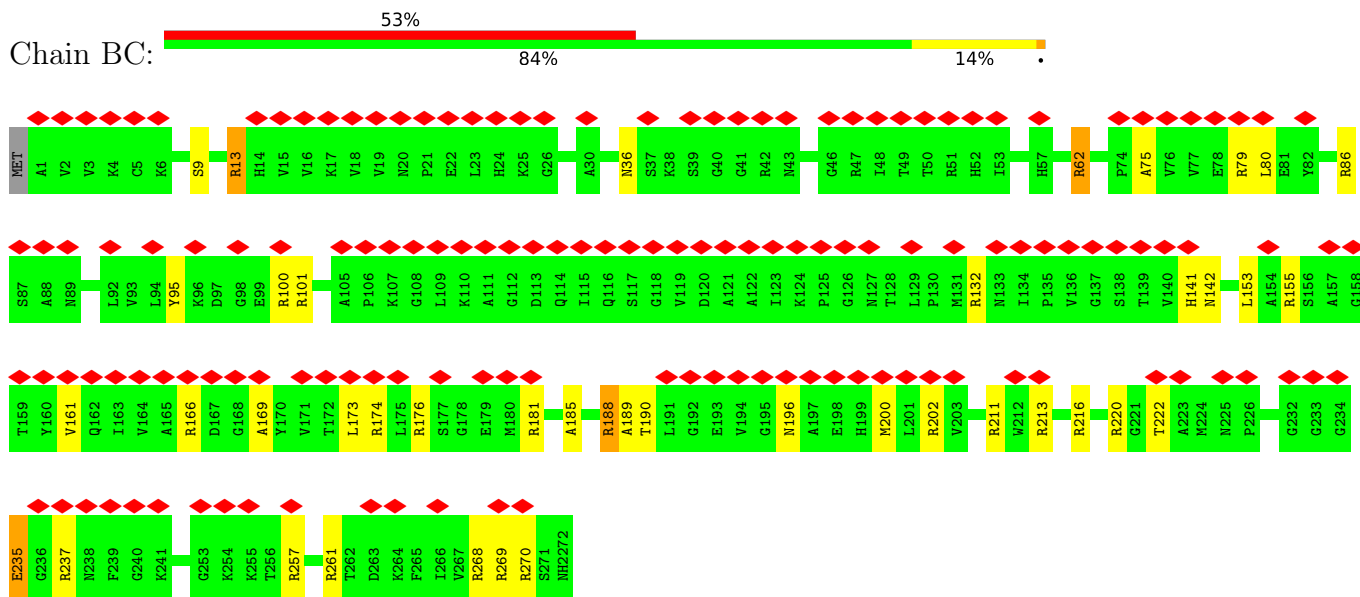
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'



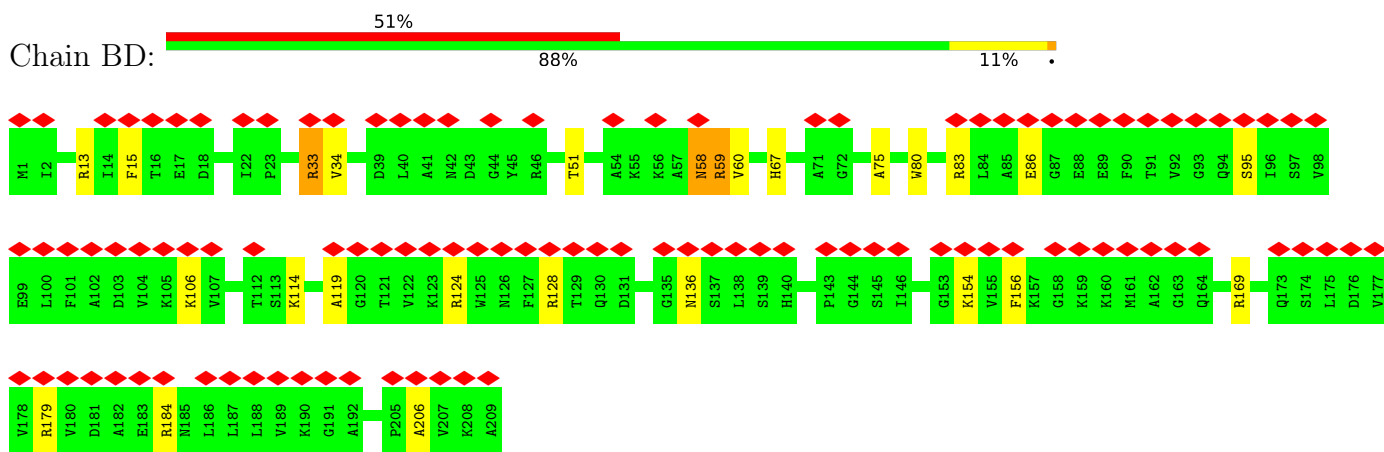
• Molecule 24: tRNA-fMet



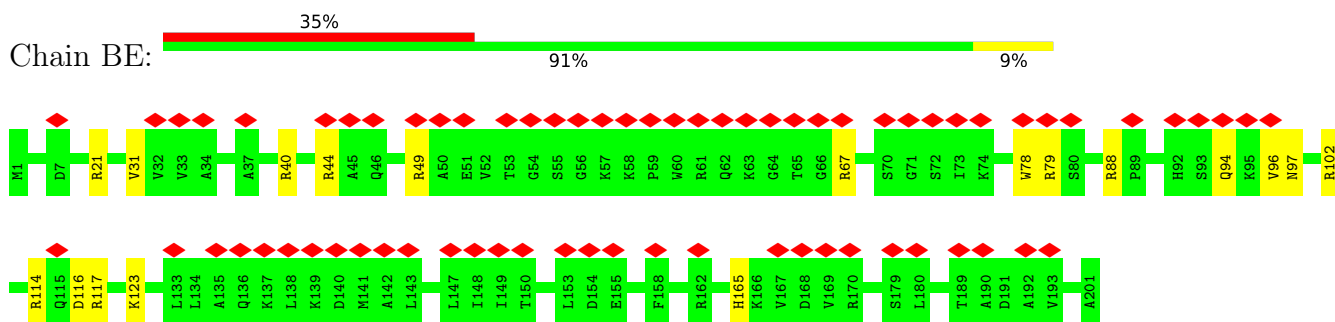
• Molecule 25: 50S ribosomal protein L2



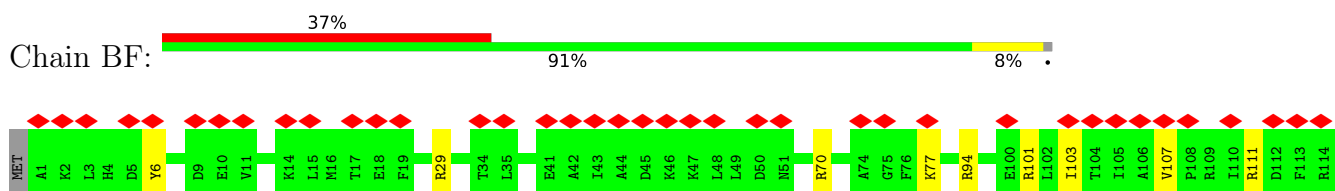
• Molecule 26: 50S ribosomal protein L3

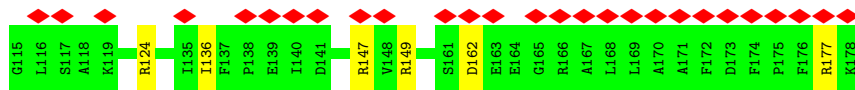


• Molecule 27: 50S ribosomal protein L4

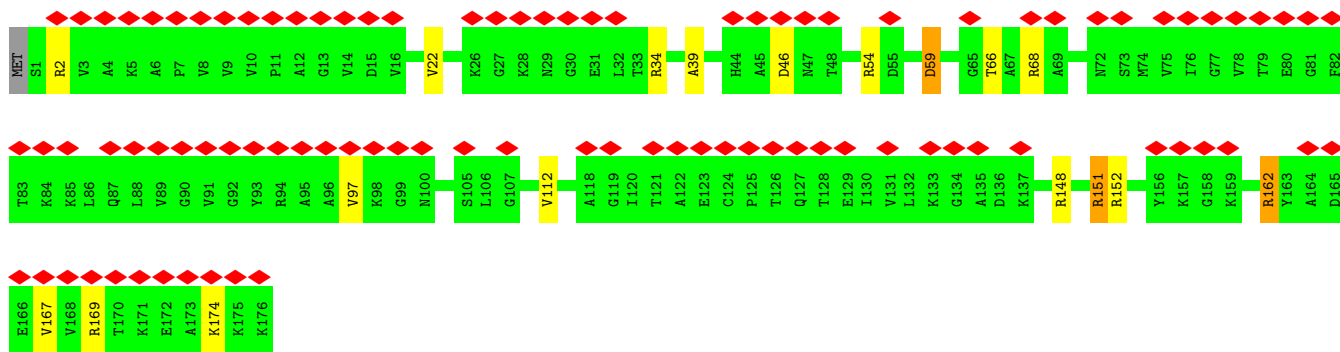
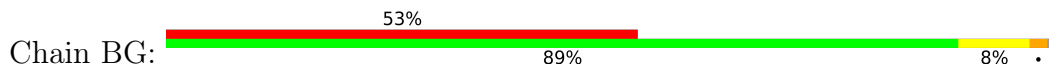


• Molecule 28: 50S ribosomal protein L5

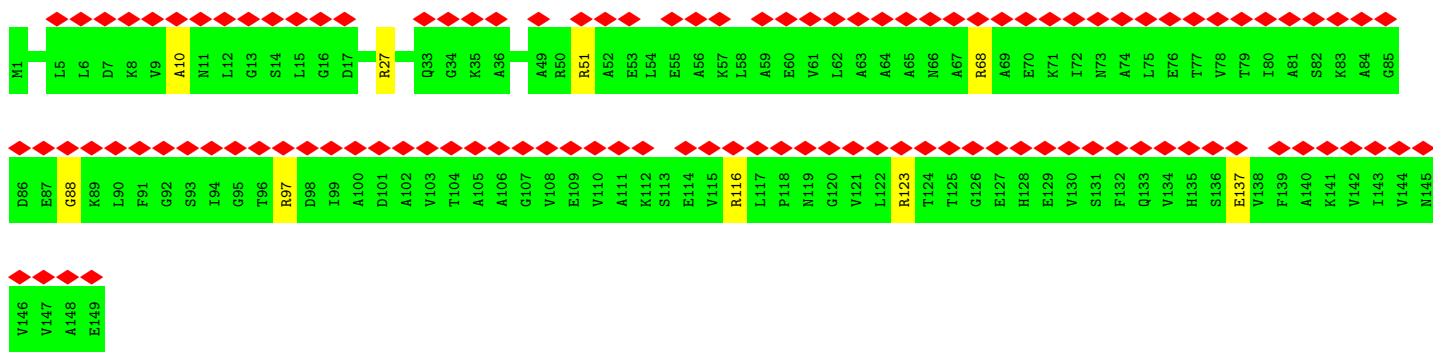
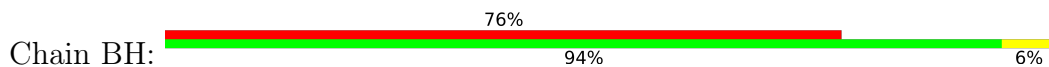




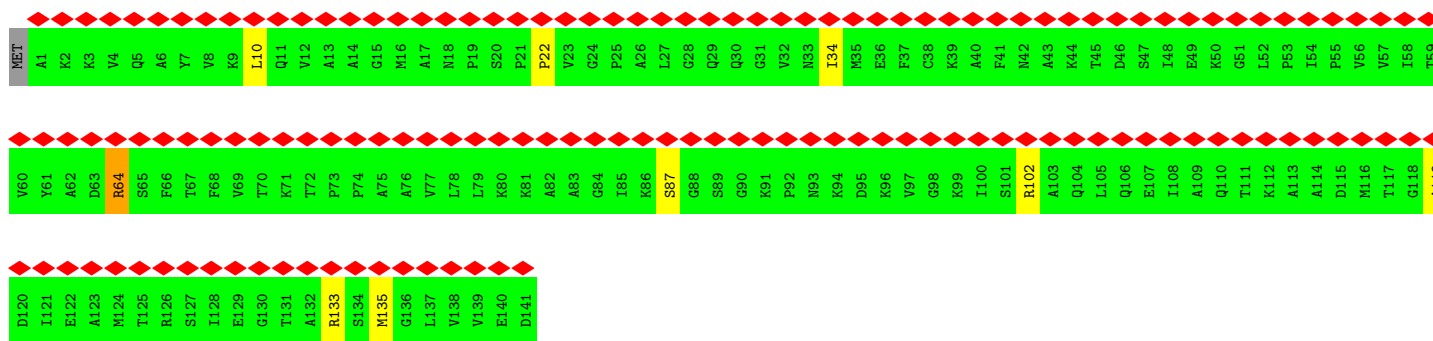
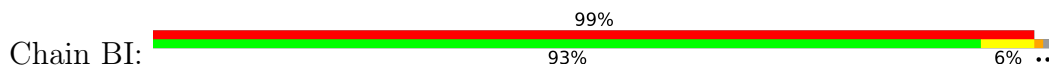
• Molecule 29: 50S ribosomal protein L6



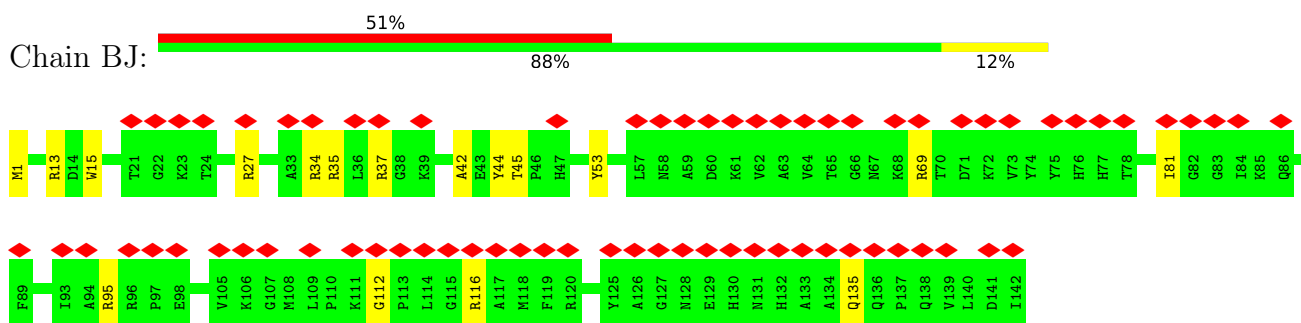
• Molecule 30: 50S ribosomal protein L9



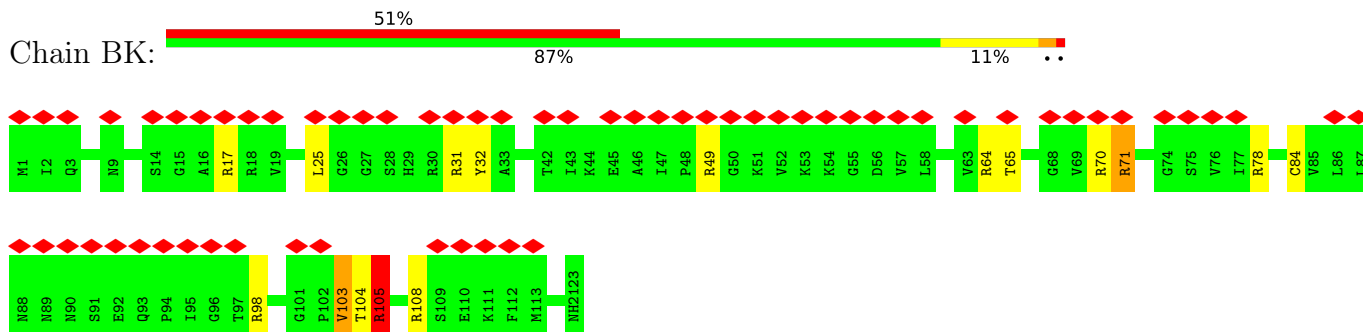
• Molecule 31: 50S ribosomal protein L11



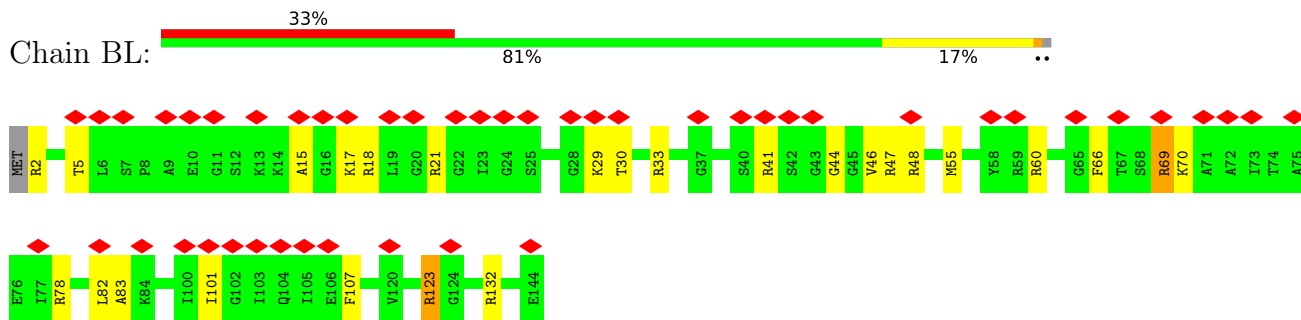
• Molecule 32: 50S ribosomal protein L13



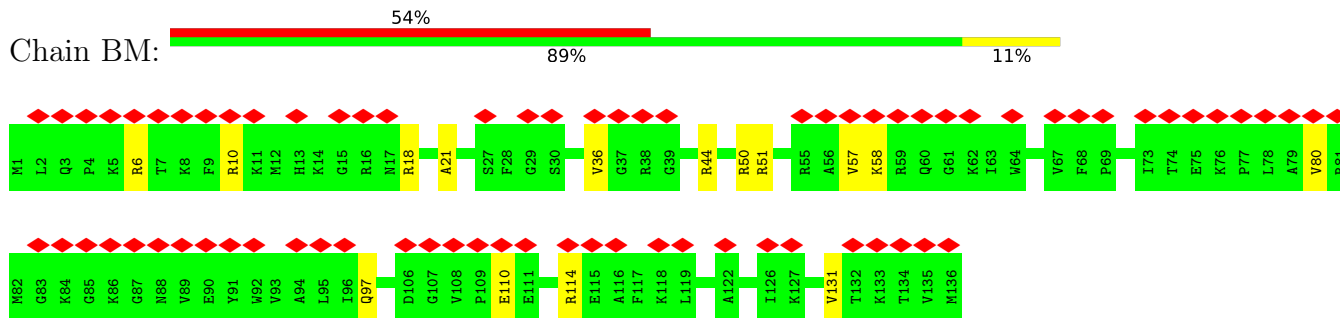
- Molecule 33: 50S ribosomal protein L14



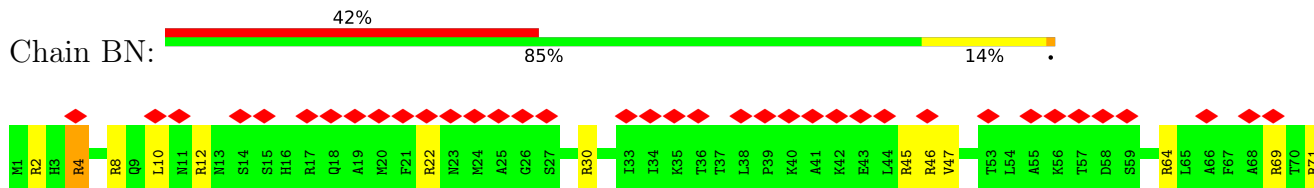
- Molecule 34: 50S ribosomal protein L15

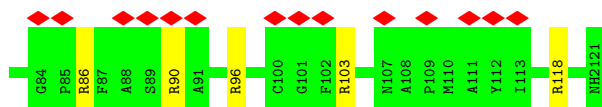


- Molecule 35: 50S ribosomal protein L16

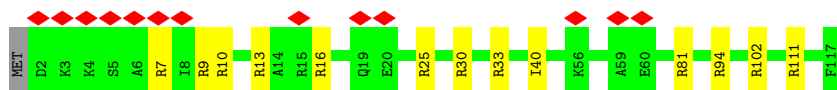
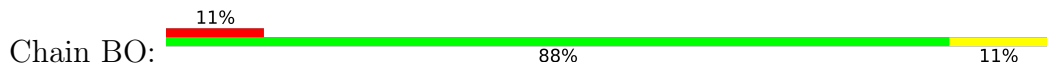


- Molecule 36: 50S ribosomal protein L17

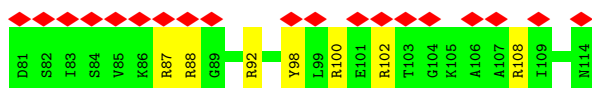
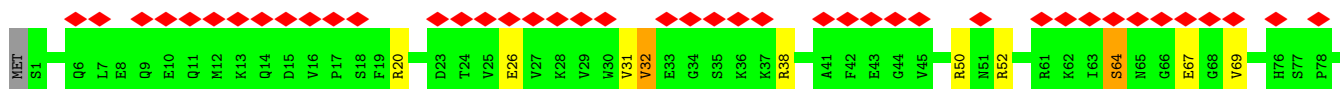
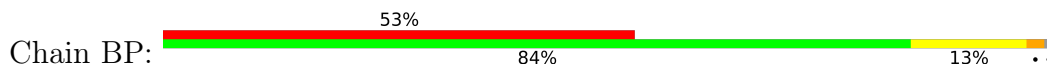




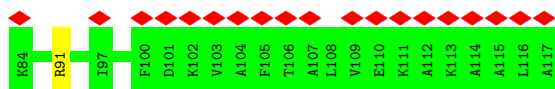
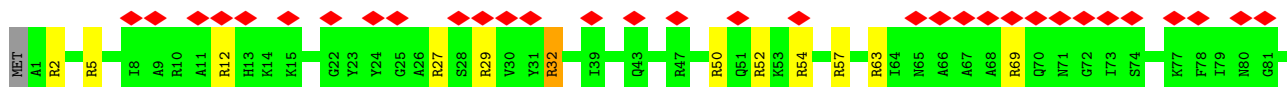
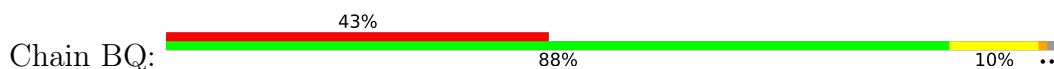
- Molecule 37: 50S ribosomal protein L18



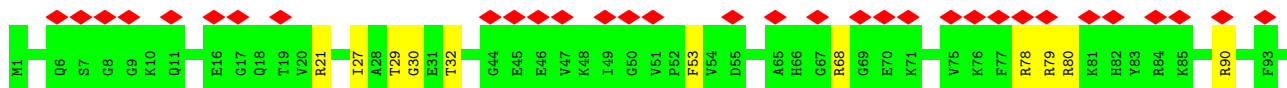
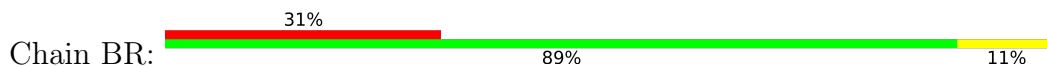
- Molecule 38: 50S ribosomal protein L19



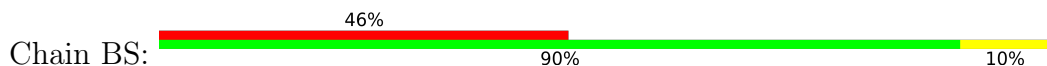
- Molecule 39: 50S ribosomal protein L20

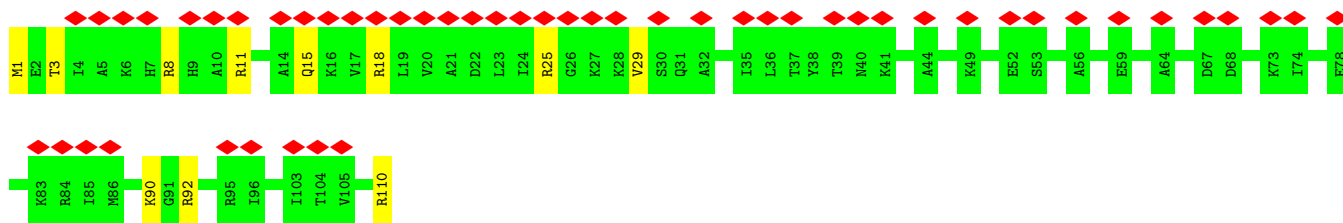


- Molecule 40: 50S ribosomal protein L21

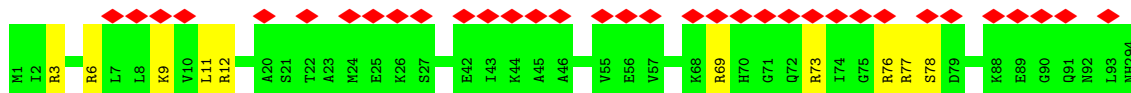
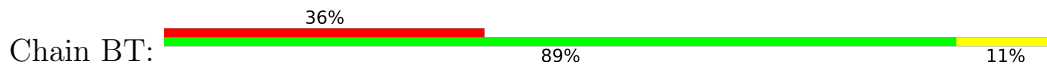


- Molecule 41: 50S ribosomal protein L22

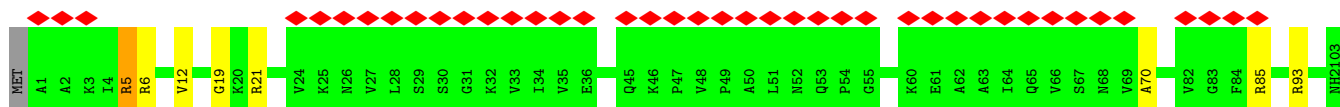
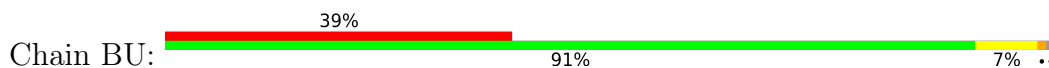




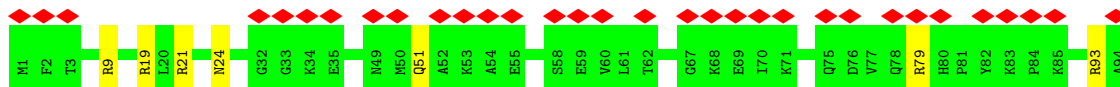
• Molecule 42: 50S ribosomal protein L23



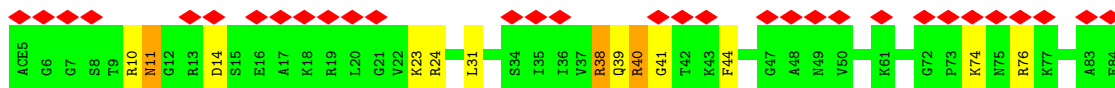
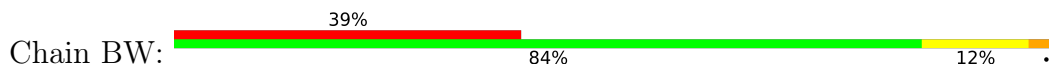
• Molecule 43: 50S ribosomal protein L24



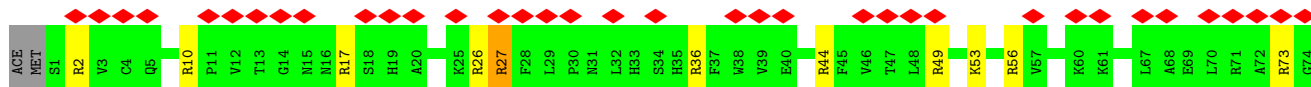
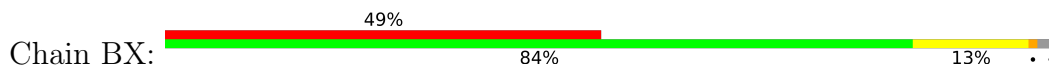
• Molecule 44: 50S ribosomal protein L25



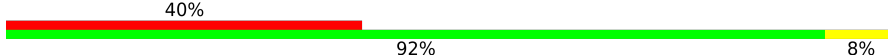
• Molecule 45: 50S ribosomal protein L27

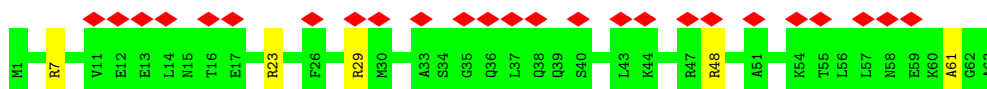


• Molecule 46: 50S ribosomal protein L28




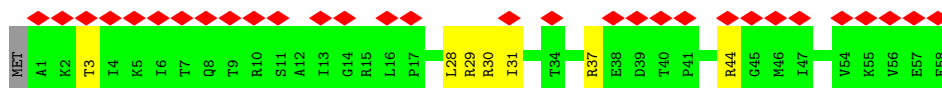
• Molecule 47: 50S ribosomal protein L29

Chain BY: 




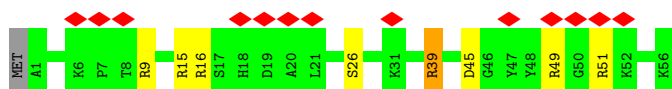
- Molecule 48: 50S ribosomal protein L30

Chain BZ: 




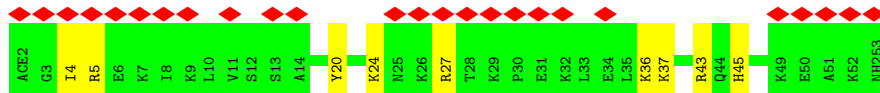
- Molecule 49: 50S ribosomal protein L32

Chain B0: 




- Molecule 50: 50S ribosomal protein L33

Chain B1: 

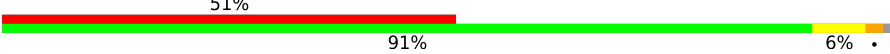


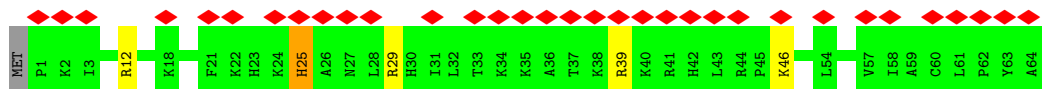
- Molecule 51: 50S ribosomal protein L34

Chain B2: 




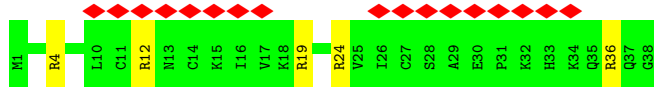
- Molecule 52: 50S ribosomal protein L35

Chain B3: 

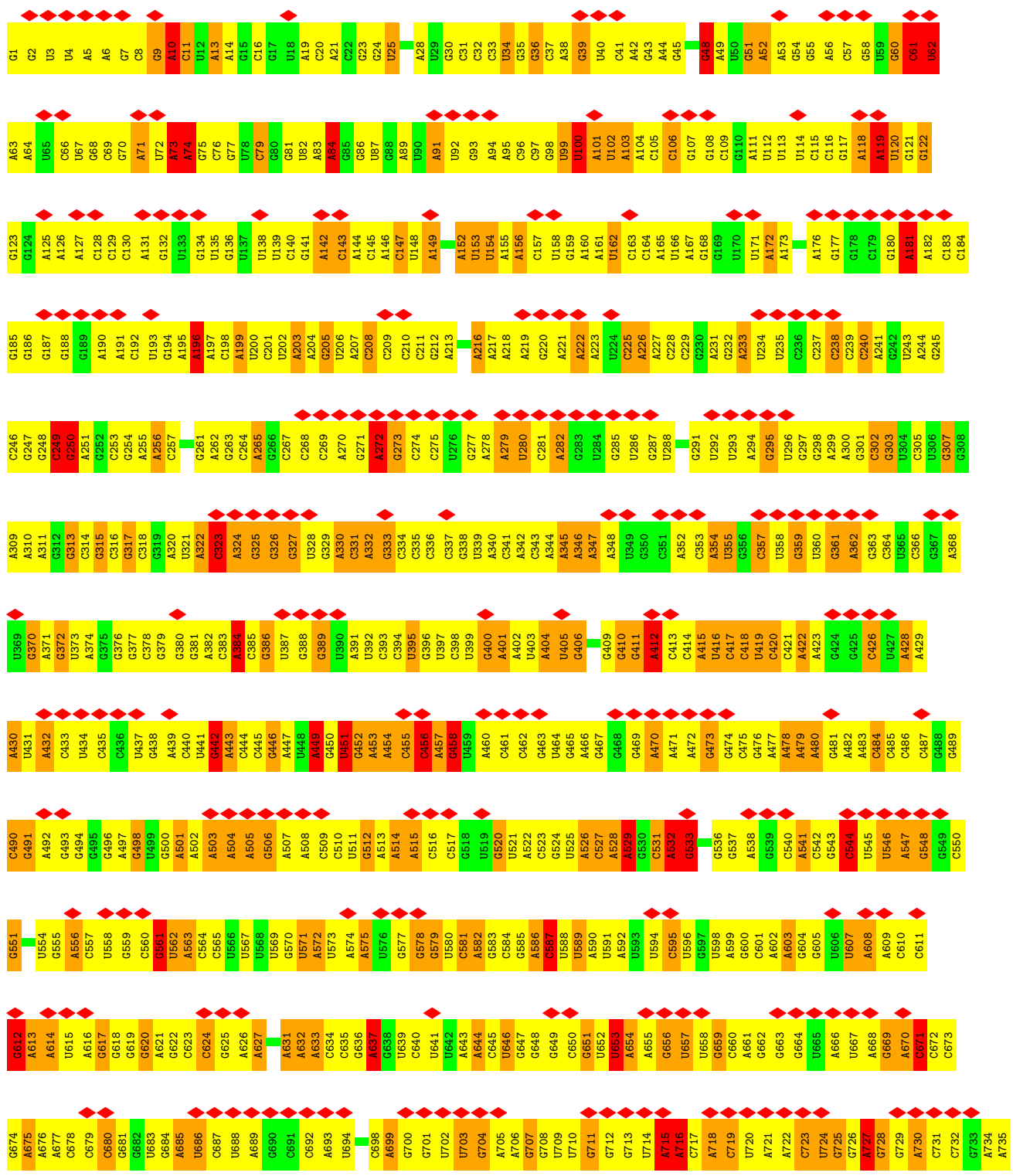
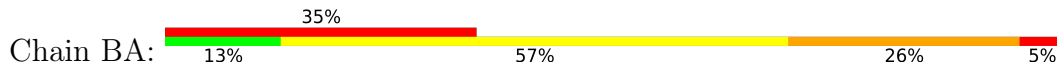


- Molecule 53: 50S ribosomal protein L36

Chain B4: 

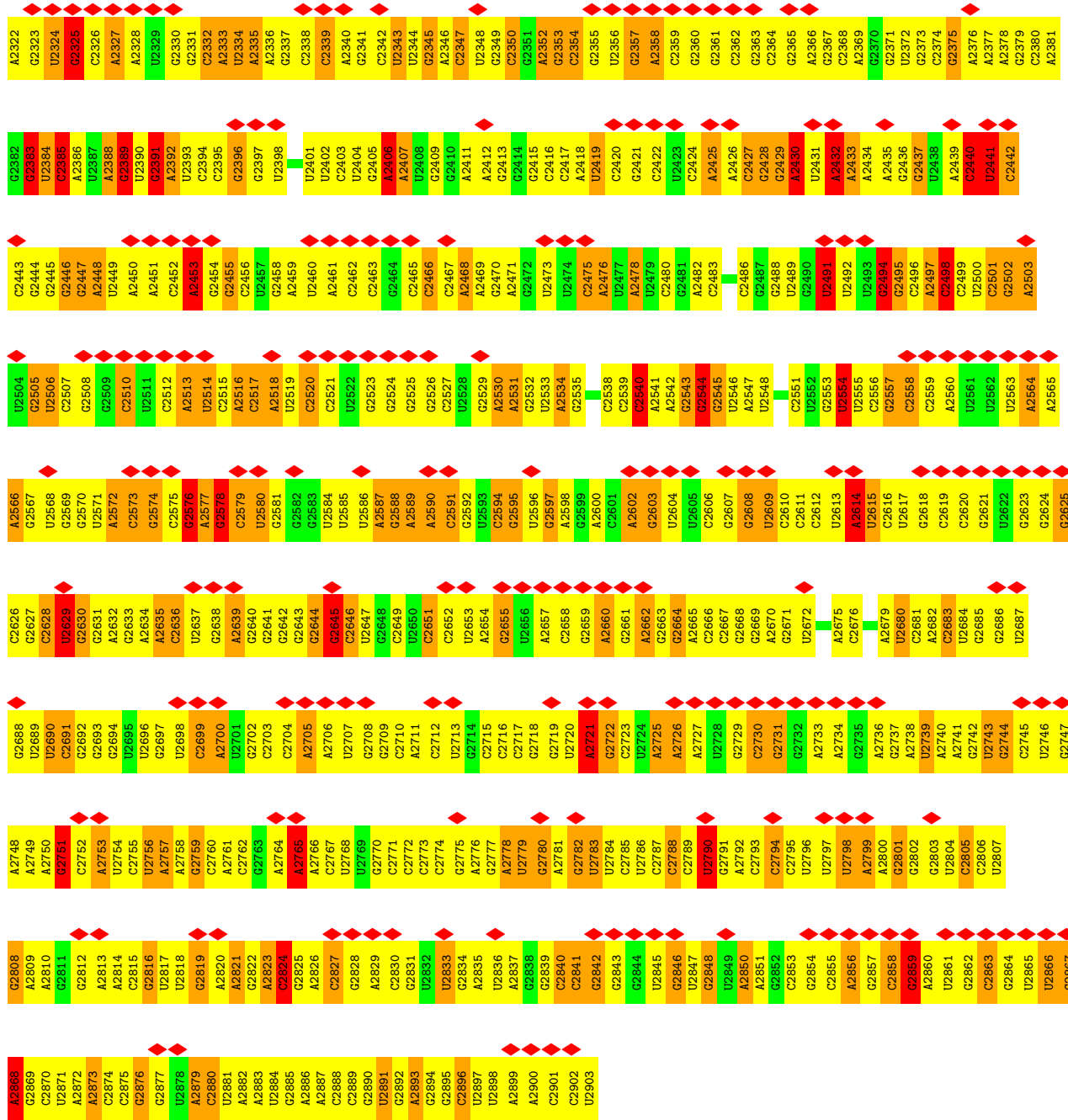


• Molecule 54: 23S ribosomal RNA

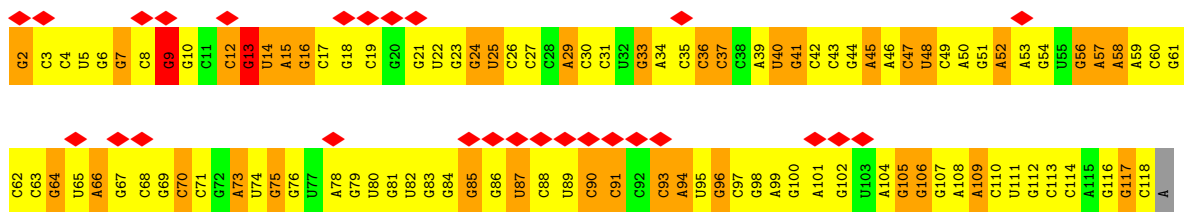
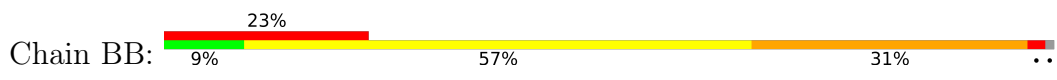


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U1409	G1410	U1411	U1412	A1413	C1414	U1415	G1416	G1417	G1418	A1419	A1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	C1428	G1429	G1430	A1431	G1432	A1433	A1434	G1435	G1436	C1437	U1438	A1439	A1440	G1441	U1442	U1443	G1444	C1445	C1446	G1447	G1448	G1449	G1450	C1451	G1452	A1453	A1454	G1455	G1456	U1457	U1458	G1459	U1460	C1461	C1462	C1463	G1464	G1465	U1466	A1528				
C1349	C1350	C1351	U1352	A1353	A1354	G1355	G1356	C1357	G1358	G1359	G1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	U1372	A1373	G1374	U1375	C1376	G1377	A1378	U1379	G1380	G1381	G1382	A1383	A1384	A1385	C1386	A1387	G1388	G1389	U1390	U1391	A1392	A1393	U1394	A1395	A1396	U1397	C1398	C1399	G1400	G1401	U1402	A1403	C1404	U1405	G1406	G1407	G1408			
C1289	C1290	U1291	U1292	C1293	U1294	C1295	G1296	U1297	C1298	G1299	A1301	A1302	G1303	A1304	C1305	A1306	A1307	A1308	G1309	G1310	G1311	U1312	U1313	C1314	C1315	U1316	G1317	U1318	C1319	A1320	A1321	A1322	C1323	G1324	U1325	A1326	A1327	A1328	U1329	G1330	G1331	G1332	G1333	G1334	A1335	A1336	U1337	G1338	G1339	U1340	G1341	A1342	G1343	U1344	G1345	U1346	A1347	C1348				
G1228	C1229	U1230	U1231	C1232	U1234	G1235	G1236	A1237	G1238	U1239	U1240	A1241	U1242	A1244	G1245	A1246	A1247	G1248	U1249	U1250	C1251	A1252	A1254	U1255	G1256	C1257	U1258	G1259	A1260	C1261	A1262	U1263	A1264	A1265	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1274	A1275	A1276	C1277	C1278	G1281	U1282	G1283	A1284	A1285	A1286	A1287	G1288							
U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	C1114	U1115	G1116	C1117	U1118	U1119	C1120	C1121	G1122	C1123	U1124	G1125	A1126	A1127	G1128	A1129	U1130	G1131	U1132	A1133	A1134	U1135	G1136	U1137	G1138	G1139	C1140	U1141	A1142	A1143	A1144	C1145	U1146	U1147	U1148	U1149	C1150	A1151	C1152	C1153	G1154	A1155	A1156	U1157	U1158	U1159	C1160	C1161	C1164	A1165				
C1045	A1046	G1047	A1048	C1049	U1050	G1051	C1052	C1053	A1054	U1055	G1056	A1057	U1058	U1059	U1060	G1061	G1062	C1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	C1076	A1077	U1078	G1079	A1080	U1081	U1082	A1083	A1084	A1085	U1086	G1087	U1088	A1089	A1090	C1091	C1092	U1093	U1094	A1095	A1096	A1098	G1099	C1100	U1101	C1102	A1103	C1104				
C985	C986	C987	A988	G989	A990	C991	G992	G993	C994	C995	A996	G997	G998	U999	A1000	A1001	G1002	U1003	C1005	C1006	C1007	A1008	A1009	A1010	G1011	U1012	C1013	A1014	U1015	G1016	U1017	U1018	U1019	A1020	A1021	C1022	U1023	G1024	G1025	A1026	A1027	A1028	A1029	C1030	G1031	A1032	U1033	G1034	U1035	G1036	G1037	G1038	A1039	A1040	U1041	C1042	C1043	C1044				
G824	A825	G826	A827	A828	U829	G830	U831	U832	A833	U834	C835	A836	C837	G838	G839	G840	A841	A842	A843	A844	C845	C846	A847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	U870	A871	A872	A873	A874	A875	G876	G877	A878	A879	A880	A881	C882	C883	A884		
G797	G798	U799	A800	G801	U802	A803	A804	G805	C806	U807	G808	G809	U810	U811	C812	U813	C814	C815	C816	C817	G818	A819	A820	A821	G822	C823	U824	A825	U826	U827	U828	A829	A830	G831	U832	A833	G836	C837	C838	U839	C840	G841	A844	A845	U846	U847	C848	A849	U850	C851	U852	A853	A854	A855	G856	G858						
G859	U860	A861	G862	A863	G864	C865	A866	C867	U868	U872	C873	A877	A878	G879	G880	G881	G882	G883	U884	C885	A886	A887	C888	C889	C890	A891	A892	C893	U894	U895	C896	U897	C898	C899	A900	C901	G904	A905	U906	C907	C908	A909	A910	A911	C912	U913	G914	C915	G916	A917	A918	U919	U920	A921	A922	A923	A924	C925	G926	G927	G928	G929
C736	C737	A738	C740	U741	A742	U743	U744	G745	U746	U747	G748	A749	U750	A751	A752	U754	U755	A756	U757	C758	G759	A761	U762	C763	A764	C765	U766	U767	G768	U769	G770	G771	U772	G773	G774	G775	G776	U779	G780	A781	A782	G783	G784	G785	C786	C787	A788	A789	U790	A791	A792	A793	A794	C795	C796							

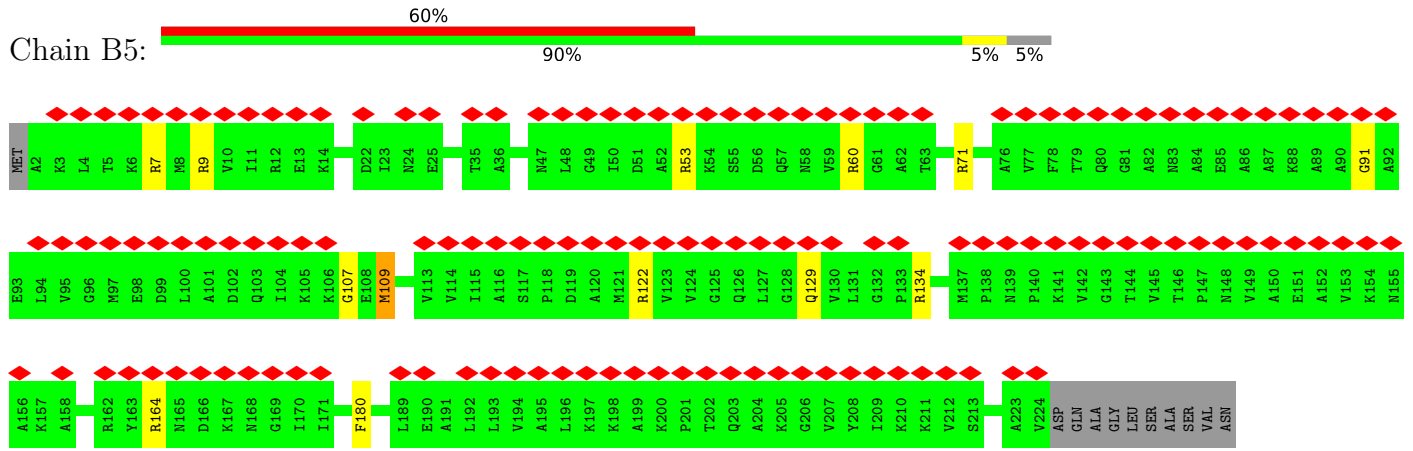
G1830	G1831	A1590	A1591	A1592	A1593	A1594	A1595	C1836	G1837	A1598	A1599	C1600	G1601	U1542	G1543	A1544	A1545	G1546	C1547	A1548	A1549	C1550	A1551	A1552	A1553	U1554	G1555	C1556	C1557	C1558	U1559	G1560	C1561	U1562	U1563	C1564	C1565	C1566	G1567	A1568	A1569	A1570	A1571	A1572	G1573	C1574	C1575	U1576	C1577	U1578	A1579	A1580	G1581	C1582	A1583	C1584	C1585	A1586	G1587	G1588	U1589	A1590	A1591	C1592	A1593	A1594	C1595	A1596	A1597	U1598	U1599	G1600	G1601	U1602	A1603	A1604	C1605	C1606	C1607	A1608	A1609	A1610	C1611	G1612	G1613	C1614	A1615	A1616	C1617	A1618	G1619	G1620	U1621	U1622	C1623	G1624	C1625	G1626	A1627	G1628	A1629	A1630	G1631	A1632	G1633	A1634	A1635	U1636	U1637	C1638	C1639	A1640	A1641	U1642	G1643	A1644	G1645	C1646	U1647	U1648	U1649	A1650	G1651	A1652	G1653	A1654	A1655	A1656	U1657	C1658	U1662	G1663	A1664	A1665	G1666	G1667	A1668	C1670	A1671	A1672	G1673	G1674	C1675	A1676	A1677	A1678	A1679	U1680	G1681	A1682	U1683	C1684	G1685	C1686	G1687	A1688	A1689	A1690	C1691	U1692	U1693	C1694	G1695	G1696	A1697	A1698	U1699	A1700	C1699	G1701	A1702	G1703	C1704	A1705	C1706	G1707	C1708	U1709	G1710	A1711	U1712	A1713	U1714	G1715	U1716	A1717	G1718	U1719	U1720	G1721	A1722	G1723	U1724	A1725	C1726	G1727	A1728	U1729	C1730	G1731	C1732	A1735	U1736	G1737	G1738	A1739	G1740	C1741	U1742	G1743	A1744	A1745	A1746	U1747	C1748	U1749	A1750	U1751	C1752	G1753	A1754	A1755	G1756	A1757	U1758	A1759	G1760	U1761	A1762	G1763	C1764	A1765	G1766	C1767	G1768	U1769	G1770	A1771	A1772	A1773	C1774	U1775	G1776	U1777	U1778	U1779	A1780	U1781	U1782	A1783	A1784	U1785	A1786	A1787	C1788	A1789	C1790	A1791	G1792	C1793	A1794	C1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	A1803	C1804	A1805	C1806	G1807	A1808	A1809	A1810	G1813	G1814	A1815	C1816	G1817	U1818	A1819	U1820	A1821	C1822	A1823	G1824	A1825	U1826	U1827	G1828	A1829	C1830	C1831	C1832	C1833	U1834	G1835	C1836	U1837	G1839	C1843	C1844	G1845	G1846	A1847	A1848	G1849	G1850	U1851	U1852	A1853	A1854	G1857	A1858	U1859	G1860	G1861	G1862	G1863	U1864	U1865	A1866	G1867	C1868	G1869	U1870	A1871	U1872	G1873	C1874	G1875	A1876	A1877	G1878	C1879	U1880	C1881	U1882	U1883	G1884	U1886	C1887	G1888	A1889	A1890	G1891	U1892	G1893	C1894	A1895	U1896	U1897	U1898	C1900	U1901	A1902	C1903	G1904	C1905	G1906	G1907	C1908	U1909	A1910	U1911	A1912	A1913	C1914	U1915	U1916	A1917	A1918	A1919	C1920	U1923	C1924	C1925	U1926	A1927	A1928	G1929	C1930	U1931	A1932	U1933	C1934	U1935	A1936	A1937	A1938	U1939	C1940	U1941	U1943	U1944	U1945	U1946	C1947	G1948	G1949	U1950	U1951	A1952	C1953	A1954	U1955	U1956	C1957	G1959	U1898	A1899	C1961	C1962	U1963	G1964	C1965	A1966	U1967	U1968	A1969	A1970	U1971	G1972	U1973	C1974	U1975	U1976	A1977	A1978	U1979	G1980	A1981	U1982	G1983	G1984	C1985	U1986	A1987	G1988	G1989	C1990	U1991	U1992	U1993	A1994	U1995	C1996	G1997	A1998	C1999	C2000	C2001	G2002	C2003	G2004	C2005	C2006	U2007	C2008	A2009	U2010	G2011	G2012	A2013	A2014	A2015	A2016	U2017	A2018	A2019	A2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	A2029	A2030	A2031	G2032	A2033	U2034	C2035	C2036	A2037	G2038	U2039	G2040	U2041	A2042	C2043	C2044	C2045	U2046	C2047	G2048	C2049	C2050	A2051	A2052	C2053	A2054	C2055	C2056	U2057	A2058	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2067	U2068	G2069	A2070	A2071	C2072	A2073	A2074	A2075	U2076	A2077	C2078	U2079	U2080	U2081	A2082	G2083	C2084	U2085	U2086	A2088	C2089	A2090	C2091	U2092	G2093	G2094	A2095	C2096	A2097	U2098	U2099	G2100	A2101	G2102	C2103	U2105	U2106	U2107	A2108	U2109	G2110	U2111	G2112	U2113	A2114	G2115	G2116	A2117	A2119	U2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	U2136	U2137	G2138	U2139	G2140	A2141	A2142	C2143	G2144	C2145	C2146	A2147	C2150	U2151	G2152	C2153	A2154	U2155	A2156	G2157	A2158	G2159	C2160	C2161	G2162	A2163	A2225	A2226	A2227	G2228	U2229	G2230	U2231	G2232	G2233	G2234	G2235	U2236	G2237	G2238	U2240	A2241	G2242	U2243	U2244	U2245	G2246	A2247	C2248	U2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	A2257	C2258	U2259	G2260	U2261	U2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	G2271	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2279	G2280	G2281	A2282	G2283	C2284	C2285	G2286	A2287	A2288	G2289	G2290	U2291	G2292	G2293	G2294	C2295	C2296	A2297	U2298	U2299	C2300	C2301	U2302	C2303	G2304	U2305	C2306	G2307	C2308	A2309	C2310	A2311	U2312	C2313	A2314	G2315	G2316	G2317	A2318	U2319	U2320	U2321
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• 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	13091	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	191.487	Depositor
Minimum map value	-133.057	Depositor
Average map value	-0.914	Depositor
Map value standard deviation	20.362	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: 6MZ, ACE, FME, NH2, OMC, PSU, 5MU, 4SU, 7MG, CM0, H2U

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	0.76	0/1736	1.10	10/2340 (0.4%)
2	AC	0.81	0/1651	1.19	17/2225 (0.8%)
3	AD	0.83	0/1665	1.27	20/2227 (0.9%)
4	AE	0.79	0/1119	1.16	9/1506 (0.6%)
5	AF	0.79	0/835	1.15	7/1128 (0.6%)
6	AG	0.81	0/1188	1.19	11/1593 (0.7%)
7	AH	0.80	0/989	1.09	8/1326 (0.6%)
8	AI	0.88	0/1035	1.34	14/1377 (1.0%)
9	AJ	0.81	0/797	1.22	11/1079 (1.0%)
10	AK	0.85	0/894	1.20	10/1207 (0.8%)
11	AL	0.85	0/969	1.25	13/1300 (1.0%)
12	AM	0.84	0/884	1.30	14/1181 (1.2%)
13	AN	0.88	1/817 (0.1%)	1.43	16/1088 (1.5%)
14	AO	0.86	0/722	1.26	12/964 (1.2%)
15	AP	0.88	0/648	1.25	6/870 (0.7%)
16	AQ	0.78	0/658	1.13	5/883 (0.6%)
17	AR	0.85	0/463	1.25	8/623 (1.3%)
18	AS	0.84	0/653	1.26	8/879 (0.9%)
19	AT	0.79	0/672	1.24	8/890 (0.9%)
20	AU	0.96	0/431	1.57	12/572 (2.1%)
21	AA	2.03	752/36759 (2.0%)	2.33	2571/57346 (4.5%)
22	A1	2.04	28/1668 (1.7%)	2.30	106/2595 (4.1%)
23	A2	1.81	3/343 (0.9%)	2.39	25/531 (4.7%)
24	A3	2.06	38/1722 (2.2%)	2.29	111/2685 (4.1%)
25	BC	0.85	0/2121	1.31	31/2852 (1.1%)
26	BD	0.77	0/1586	1.22	10/2134 (0.5%)
27	BE	0.75	0/1571	1.20	13/2113 (0.6%)
28	BF	0.79	0/1444	1.21	11/1937 (0.6%)
29	BG	0.76	0/1343	1.18	10/1816 (0.6%)
30	BH	0.72	0/1122	1.10	7/1515 (0.5%)
31	BI	0.71	0/1046	1.07	3/1410 (0.2%)
32	BJ	0.77	0/1152	1.24	12/1551 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BK	0.79	0/947	1.30	11/1268 (0.9%)
34	BL	0.82	0/1054	1.36	14/1403 (1.0%)
35	BM	0.84	0/1093	1.24	9/1460 (0.6%)
36	BN	0.89	0/973	1.43	19/1301 (1.5%)
37	BO	0.85	0/902	1.32	11/1209 (0.9%)
38	BP	0.85	0/929	1.42	13/1242 (1.0%)
39	BQ	0.86	0/960	1.33	14/1278 (1.1%)
40	BR	0.79	0/829	1.18	6/1107 (0.5%)
41	BS	0.76	0/864	1.20	8/1156 (0.7%)
42	BT	0.77	0/744	1.27	8/994 (0.8%)
43	BU	0.78	0/787	1.20	5/1051 (0.5%)
44	BV	0.75	0/766	1.17	6/1025 (0.6%)
45	BW	0.84	0/604	1.29	5/799 (0.6%)
46	BX	0.87	0/635	1.39	11/848 (1.3%)
47	BY	0.77	0/510	1.26	4/677 (0.6%)
48	BZ	0.84	0/453	1.29	5/605 (0.8%)
49	B0	0.85	0/450	1.33	7/599 (1.2%)
50	B1	0.77	0/417	1.21	4/556 (0.7%)
51	B2	0.98	0/380	1.49	10/498 (2.0%)
52	B3	0.76	0/513	1.16	4/676 (0.6%)
53	B4	0.86	0/303	1.39	5/397 (1.3%)
54	BA	1.91	1309/69796 (1.9%)	2.32	5106/108888 (4.7%)
55	BB	2.03	85/2800 (3.0%)	2.33	222/4367 (5.1%)
56	B5	0.71	0/1673	1.10	10/2255 (0.4%)
All	All	1.71	2216/160085 (1.4%)	2.09	8646/239402 (3.6%)

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	2
8	AI	0	1
10	AK	0	1
21	AA	0	365
22	A1	0	10
23	A2	0	1
24	A3	0	14
25	BC	0	2
33	BK	0	1
34	BL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	BA	0	666
55	BB	0	30
All	All	0	1094

The worst 5 of 2216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1044	C	C4-N4	-7.34	1.27	1.33
54	BA	2752	C	C4-N4	-7.31	1.27	1.33
24	A3	3	C	C4-N4	-7.23	1.27	1.33
21	AA	6	G	C6-N1	-7.22	1.34	1.39
21	AA	1479	C	C4-N4	-7.20	1.27	1.33

The worst 5 of 8646 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2510	C	N3-C2-O2	-15.56	111.01	121.90
54	BA	975	A	N1-C6-N6	-13.84	110.30	118.60
54	BA	479	A	N1-C6-N6	-13.45	110.53	118.60
21	AA	412	A	N1-C6-N6	-12.78	110.93	118.60
54	BA	900	A	N1-C6-N6	-12.71	110.97	118.60

There are no chirality outliers.

5 of 1094 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	6	G	Sidechain
2	AC	168	ARG	Sidechain
2	AC	172	VAL	Peptide
8	AI	124	PRO	Peptide
10	AK	115	ILE	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	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AC	1625	0	1699	0	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	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	2	0
20	AU	429	0	453	0	0
21	AA	32828	0	15886	9	0
22	A1	1627	0	798	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	801	1	0
25	BC	2083	0	2157	2	0
26	BD	1565	0	1616	3	0
27	BE	1552	0	1619	1	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	2	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	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	0	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	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	1	0
51	B2	377	0	418	1	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	30186	21	0
55	BB	2504	0	1181	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	97702	45	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 45 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)
19:AT:40:ALA:HB1	19:AT:41:GLY:HA2	1.81	0.62
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
26:BD:154:LYS:HE3	26:BD:156:PHE:CE1	2.46	0.51
54:BA:931:U:C5	54:BA:1167:C:H1'	2.46	0.50
21:AA:5:U:H4'	21:AA:6:G:C6	2.46	0.50

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%)	195 (89%)	22 (10%)	1 (0%)	29	69
2	AC	205/208 (99%)	191 (93%)	12 (6%)	2 (1%)	15	55
3	AD	203/206 (98%)	185 (91%)	15 (7%)	3 (2%)	10	46
4	AE	150/152 (99%)	134 (89%)	9 (6%)	7 (5%)	2	21
5	AF	99/101 (98%)	86 (87%)	6 (6%)	7 (7%)	1	14
6	AG	150/152 (99%)	143 (95%)	7 (5%)	0	100	100
7	AH	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
8	AI	126/128 (98%)	110 (87%)	12 (10%)	4 (3%)	4	26
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	19
10	AK	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	57
11	AL	121/124 (98%)	111 (92%)	10 (8%)	0	100	100
12	AM	112/115 (97%)	98 (88%)	12 (11%)	2 (2%)	8	40
13	AN	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	15	55
14	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	13	50
15	AP	79/81 (98%)	68 (86%)	7 (9%)	4 (5%)	2	19
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	5	32
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	8	40
18	AS	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
19	AT	84/86 (98%)	74 (88%)	8 (10%)	2 (2%)	6	33
20	AU	51/53 (96%)	27 (53%)	14 (28%)	10 (20%)	0	2
25	BC	270/273 (99%)	238 (88%)	21 (8%)	11 (4%)	3	23
26	BD	207/209 (99%)	178 (86%)	18 (9%)	11 (5%)	2	19
27	BE	199/201 (99%)	177 (89%)	17 (8%)	5 (2%)	5	32
28	BF	176/179 (98%)	151 (86%)	21 (12%)	4 (2%)	6	34
29	BG	174/177 (98%)	152 (87%)	13 (8%)	9 (5%)	2	19
30	BH	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	11	46
31	BI	139/142 (98%)	125 (90%)	10 (7%)	4 (3%)	4	29
32	BJ	140/142 (99%)	125 (89%)	8 (6%)	7 (5%)	2	20
33	BK	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	5	32
34	BL	141/144 (98%)	117 (83%)	12 (8%)	12 (8%)	1	12
35	BM	134/136 (98%)	117 (87%)	12 (9%)	5 (4%)	3	24
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
38	BP	112/115 (97%)	91 (81%)	15 (13%)	6 (5%)	2	19
39	BQ	115/118 (98%)	100 (87%)	15 (13%)	0	100	100
40	BR	101/103 (98%)	94 (93%)	3 (3%)	4 (4%)	3	23
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	8	38
42	BT	92/94 (98%)	78 (85%)	11 (12%)	3 (3%)	4	26
43	BU	101/104 (97%)	85 (84%)	12 (12%)	4 (4%)	3	23
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	65 (83%)	6 (8%)	7 (9%)	1	11
46	BX	75/79 (95%)	70 (93%)	3 (4%)	2 (3%)	5	31
47	BY	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	9	44
48	BZ	56/59 (95%)	50 (89%)	4 (7%)	2 (4%)	3	25
49	B0	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	8	38
50	B1	50/52 (96%)	43 (86%)	3 (6%)	4 (8%)	1	12
51	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
52	B3	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	4	26
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	11	46
All	All	5876/6008 (98%)	5249 (89%)	458 (8%)	169 (3%)	7	29

5 of 169 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	149	PRO
8	AI	44	ARG
16	AQ	80	LYS
20	AU	6	ARG
20	AU	9	GLU

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%)	177 (98%)	3 (2%)	60	78
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%)	110 (97%)	3 (3%)	44	65
5	AF	87/87 (100%)	86 (99%)	1 (1%)	73	84
6	AG	123/123 (100%)	123 (100%)	0	100	100
7	AH	104/105 (99%)	102 (98%)	2 (2%)	57	75
8	AI	105/105 (100%)	105 (100%)	0	100	100
9	AJ	86/86 (100%)	82 (95%)	4 (5%)	26	51
10	AK	90/90 (100%)	88 (98%)	2 (2%)	52	71
11	AL	103/104 (99%)	102 (99%)	1 (1%)	76	86
12	AM	91/92 (99%)	88 (97%)	3 (3%)	38	61
13	AN	83/84 (99%)	81 (98%)	2 (2%)	49	69
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	47 (98%)	1 (2%)	53	72
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	62 (95%)	3 (5%)	27	52
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	43	65
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%)	148 (99%)	1 (1%)	84	90
29	BG	137/138 (99%)	134 (98%)	3 (2%)	52	71
30	BH	114/114 (100%)	113 (99%)	1 (1%)	78	87
31	BI	109/110 (99%)	106 (97%)	3 (3%)	43	65
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	60	78
33	BK	103/103 (100%)	99 (96%)	4 (4%)	32	56
34	BL	102/103 (99%)	101 (99%)	1 (1%)	76	86
35	BM	109/109 (100%)	106 (97%)	3 (3%)	43	65

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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%)	95 (96%)	4 (4%)	31	55
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	73	84
40	BR	84/84 (100%)	83 (99%)	1 (1%)	71	83
41	BS	93/93 (100%)	90 (97%)	3 (3%)	39	61
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	83 (100%)	0	100	100
44	BV	78/78 (100%)	76 (97%)	2 (3%)	46	66
45	BW	59/59 (100%)	55 (93%)	4 (7%)	16	41
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%)	37 (97%)	1 (3%)	46	66
52	B3	51/52 (98%)	50 (98%)	1 (2%)	55	74
53	B4	34/34 (100%)	33 (97%)	1 (3%)	42	64
56	B5	173/181 (96%)	170 (98%)	3 (2%)	60	78
All	All	4842/4870 (99%)	4756 (98%)	86 (2%)	61	77

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	BL	46	VAL
41	BS	15	GLN
35	BM	97	GLN
38	BP	67	GLU
45	BW	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
18	AS	56	HIS

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Mol	Chain	Res	Type
26	BD	134	HIS
32	BJ	77	HIS
13	AN	62	ASN
1	AB	145	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	250 (16%)	72 (4%)
22	A1	73/76 (96%)	8 (10%)	6 (8%)
23	A2	14/15 (93%)	3 (21%)	1 (7%)
24	A3	76/77 (98%)	9 (11%)	6 (7%)
54	BA	2902/2903 (99%)	460 (15%)	132 (4%)
55	BB	116/118 (98%)	17 (14%)	3 (2%)
All	All	4710/4722 (99%)	747 (15%)	220 (4%)

5 of 747 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U

5 of 220 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	651	G
54	BA	1300	G
55	BB	57	A
54	BA	2494	G
54	BA	675	A

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
24	H2U	A3	21	24	18,21,22	1.40	2 (11%)	21,30,33	1.11	3 (14%)
24	5MU	A3	55	24	19,22,23	0.97	1 (5%)	28,32,35	1.52	4 (14%)
22	5MU	A1	54	22	19,22,23	0.85	0	28,32,35	1.59	6 (21%)
22	4SU	A1	7	22	18,21,22	1.51	2 (11%)	26,30,33	1.11	2 (7%)
22	6MZ	A1	37	22	18,25,26	0.94	1 (5%)	16,36,39	1.74	2 (12%)
24	4SU	A3	8	24	18,21,22	1.61	3 (16%)	26,30,33	0.83	1 (3%)
24	PSU	A3	56	24	18,21,22	1.08	1 (5%)	22,30,33	1.58	4 (18%)
22	PSU	A1	55	22	18,21,22	1.03	1 (5%)	22,30,33	1.33	2 (9%)
24	OMC	A3	33	24	19,22,23	0.96	0	26,31,34	1.14	2 (7%)
22	CM0	A1	34	23,22	22,26,27	1.50	3 (13%)	28,37,40	1.30	3 (10%)
22	7MG	A1	46	22	22,26,27	4.94	2 (9%)	29,39,42	1.50	2 (6%)

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
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	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
24	PSU	A3	56	24	-	2/7/25/26	0/2/2/2
22	PSU	A1	55	22	-	2/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
22	CM0	A1	34	23,22	-	2/12/30/31	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-22.83	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	8	4SU	C5-C4	-5.34	1.35	1.42
22	A1	34	CM0	O5-C5	-5.14	1.24	1.36
22	A1	7	4SU	C5-C4	-4.77	1.36	1.42
24	A3	21	H2U	C2-N3	-3.58	1.31	1.38

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	6.33	112.43	103.38
22	A1	37	6MZ	C9-N6-C6	5.36	127.49	122.87
22	A1	54	5MU	C5M-C5-C6	-4.17	117.27	122.85
24	A3	55	5MU	C5M-C5-C6	-4.13	117.34	122.85
22	A1	55	PSU	C6-C5-C4	3.99	120.99	118.20

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	55	PSU	C2'-C1'-C5-C6
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
58	FME	BA	3001	57	8,9,10	0.82	0	7,9,11	1.10	0
57	VAL	A1	101	22,58	4,6,7	0.77	0	6,7,9	1.08	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	22,58	-	0/5/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-2.62	117.91	124.78

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.

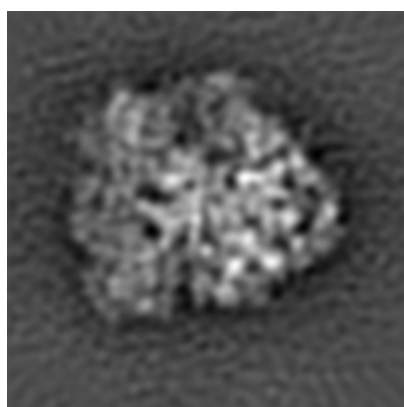
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2472. These allow visual inspection of the internal detail of the map and identification of artifacts.

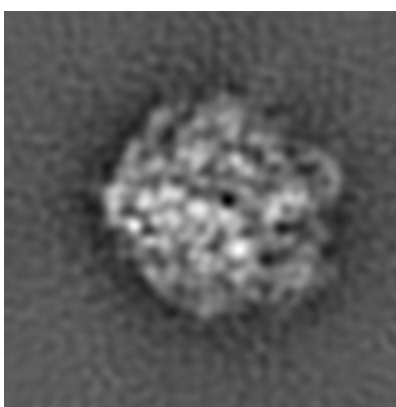
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

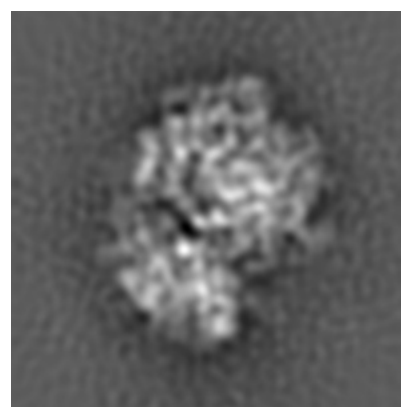
6.1.1 Primary map



X



Y

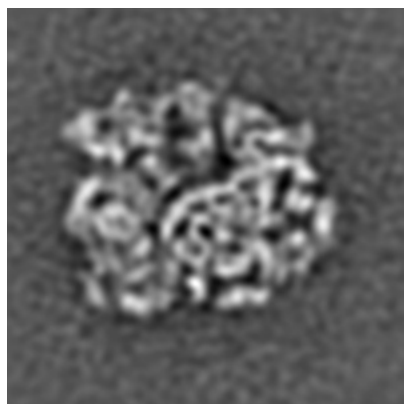


Z

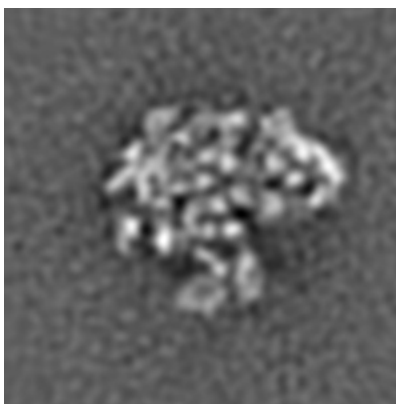
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

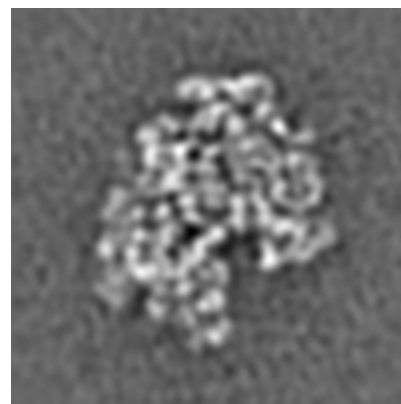
6.2.1 Primary map



X Index: 64



Y Index: 64

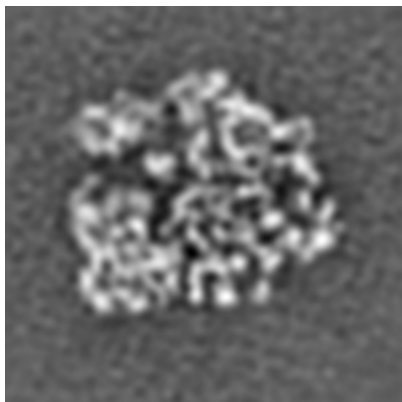


Z Index: 64

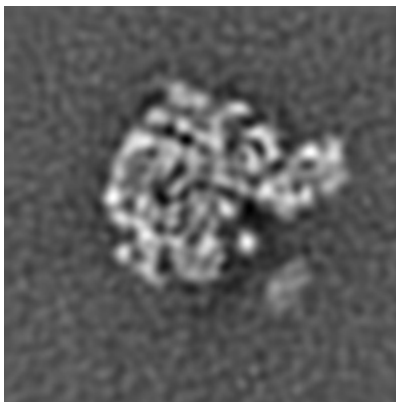
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

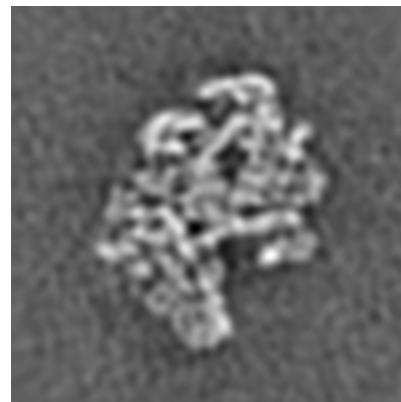
6.3.1 Primary map



X Index: 67



Y Index: 71

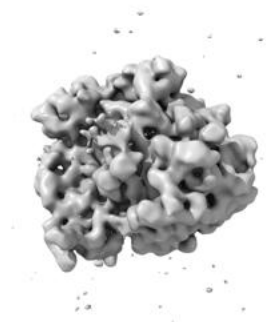


Z Index: 61

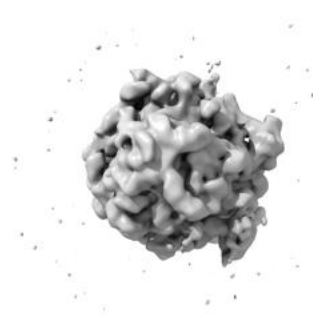
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

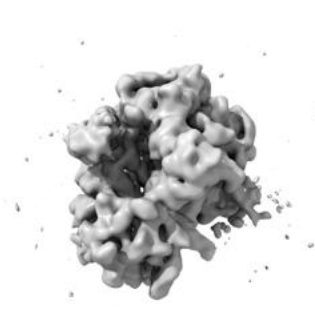
6.4.1 Primary map



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.

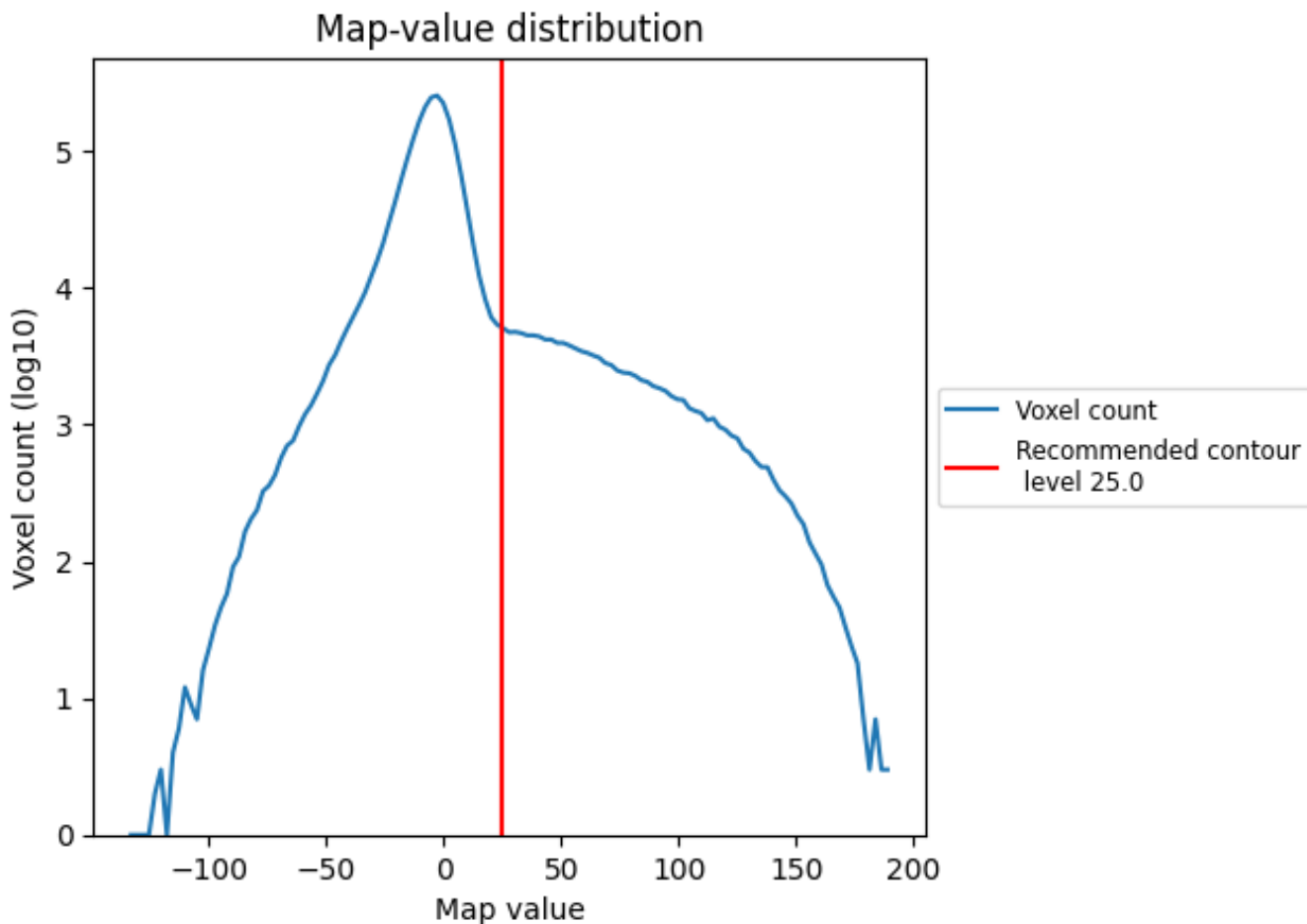
6.5 Mask visualisation

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

7 Map analysis [i](#)

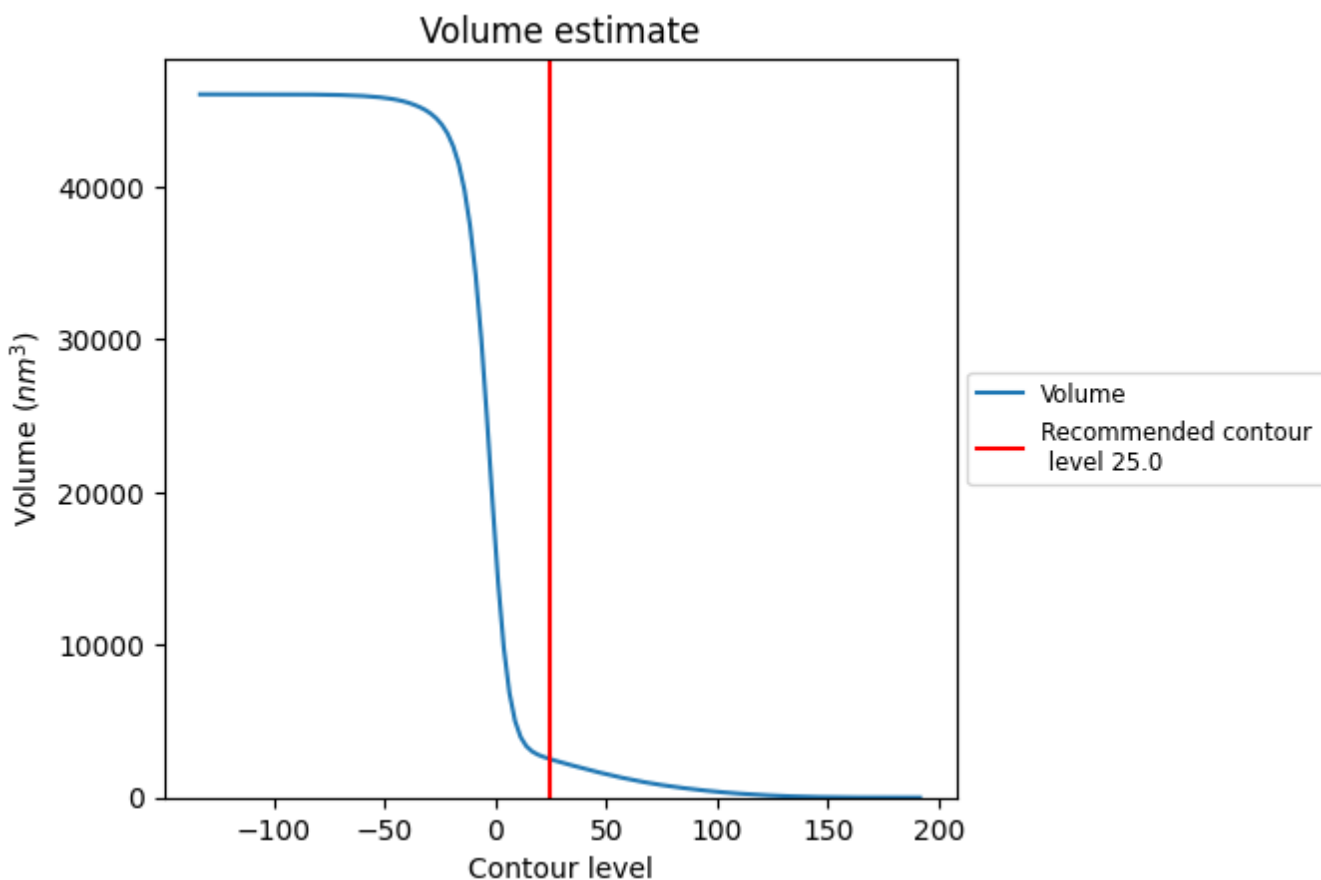
This section contains the results of statistical analysis of the map.

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.

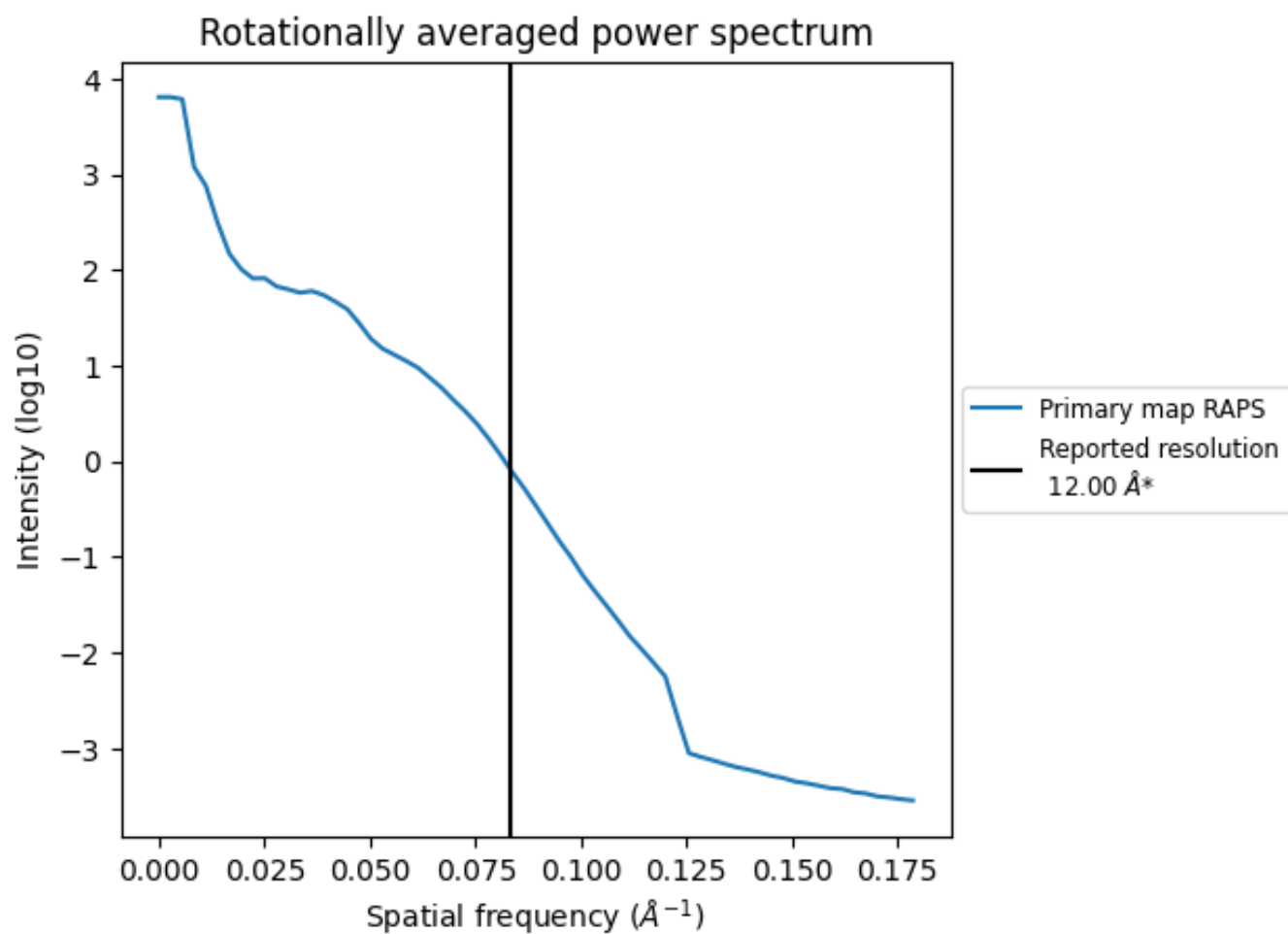
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2507 nm³; this corresponds to an approximate mass of 2264 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 0.083 Å⁻¹

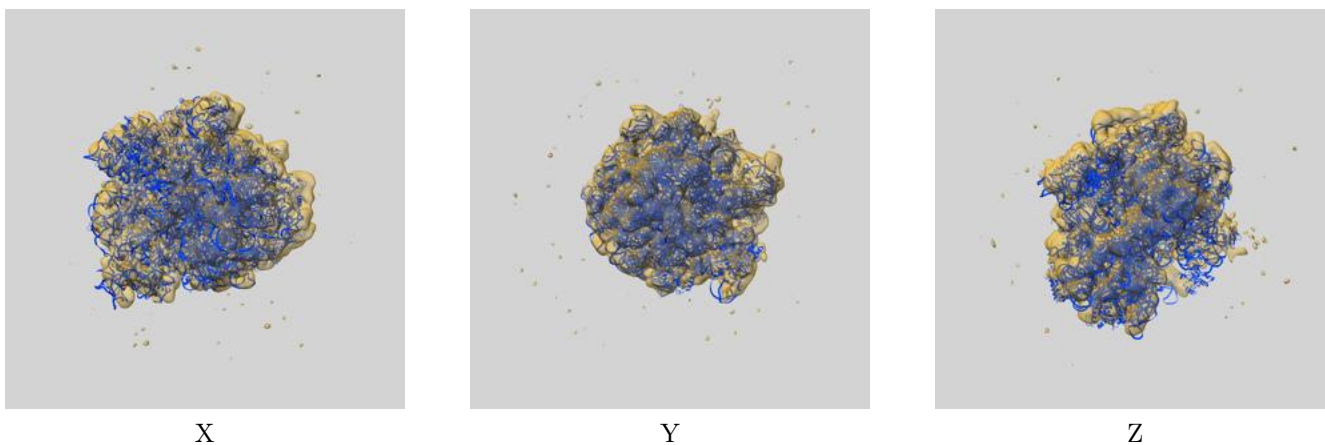
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

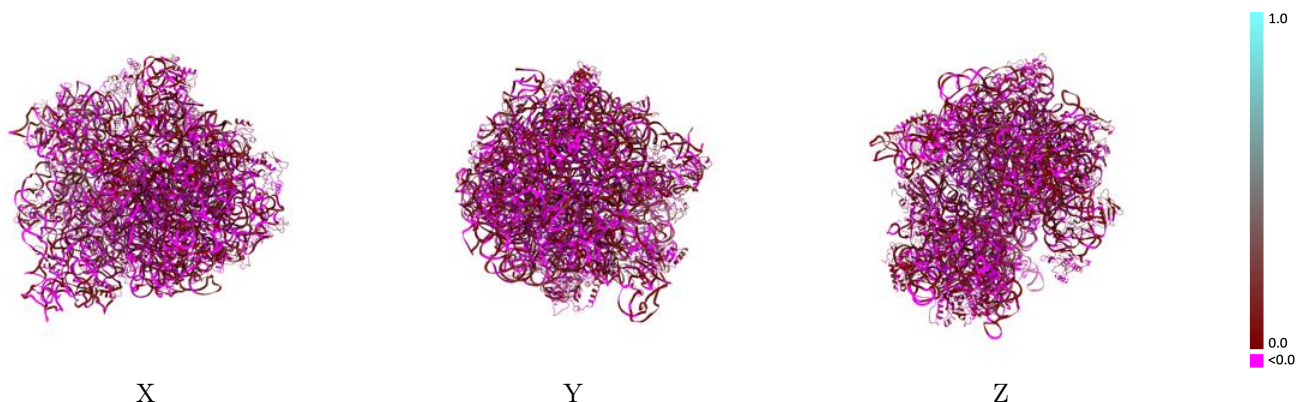
This section contains information regarding the fit between EMDB map EMD-2472 and PDB model 4V6Z. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



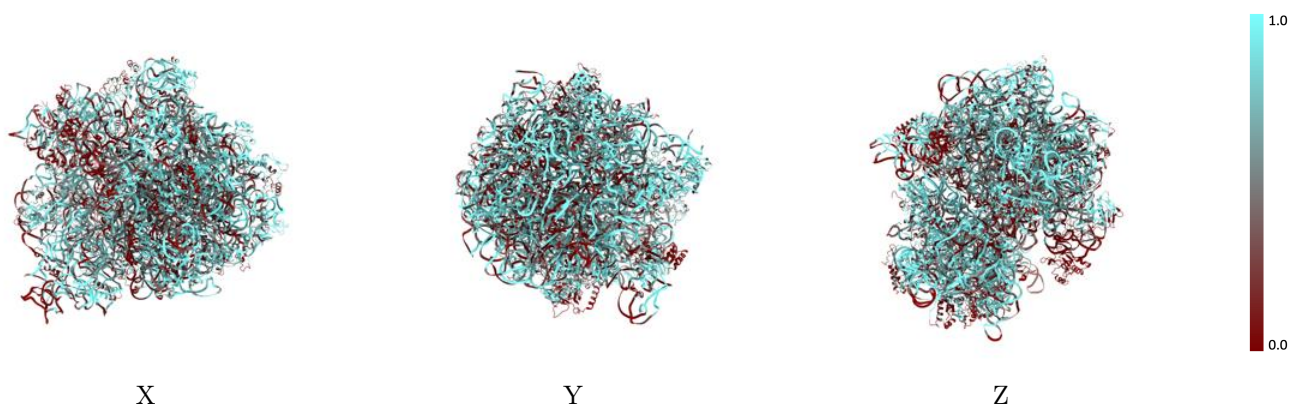
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



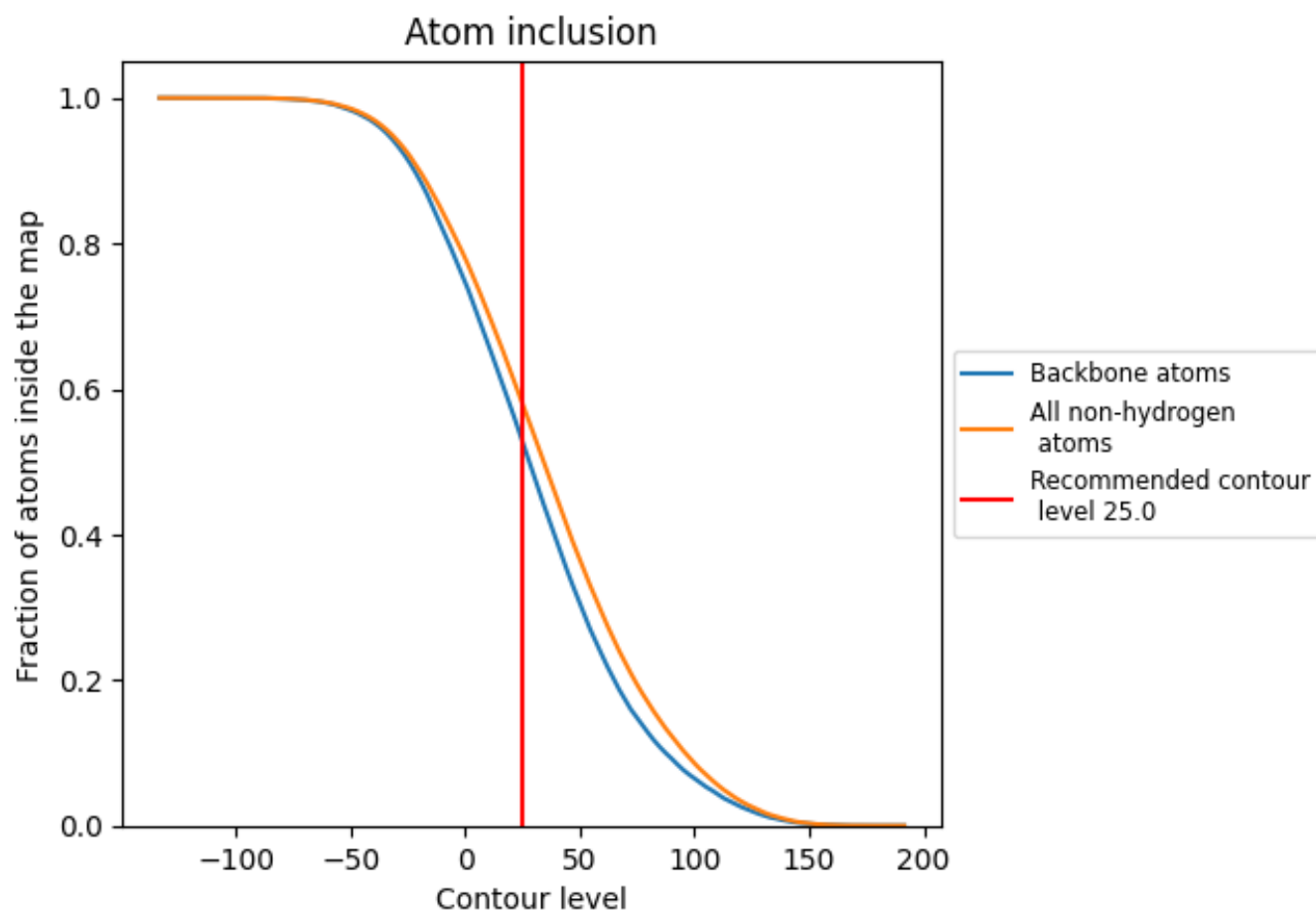
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 53% of all backbone atoms, 58% 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	0.5805	0.0150
A1	0.5165	0.0210
A2	0.4757	-0.0030
A3	0.3831	-0.0050
AA	0.6608	0.0230
AB	0.4762	0.0520
AC	0.5206	0.0090
AD	0.4340	0.0110
AE	0.5203	0.0300
AF	0.7139	0.0380
AG	0.5947	0.0120
AH	0.5115	0.0070
AI	0.7074	0.0030
AJ	0.4241	0.0030
AK	0.6725	0.0330
AL	0.6298	0.0140
AM	0.6533	0.0320
AN	0.3424	-0.0380
AO	0.7130	0.0190
AP	0.4344	0.0050
AQ	0.5449	0.0230
AR	0.5809	0.0020
AS	0.6651	0.0190
AT	0.7025	0.0010
AU	0.5819	0.0460
B0	0.7103	0.0380
B1	0.5124	0.0350
B2	0.4169	-0.0450
B3	0.4134	-0.0030
B4	0.5103	-0.0030
B5	0.3460	-0.0020
BA	0.5875	0.0150
BB	0.7177	0.0320
BC	0.4313	-0.0150
BD	0.4714	0.0100



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Chain	Atom inclusion	Q-score
BE	 0.5908	 -0.0060
BF	 0.5842	 0.0210
BG	 0.4588	 0.0220
BH	 0.2245	 0.0250
BI	 0.0000	 -0.0030
BJ	 0.4791	 -0.0040
BK	 0.4540	 0.0030
BL	 0.6083	 -0.0140
BM	 0.4261	 0.0170
BN	 0.5742	 -0.0180
BO	 0.8413	 0.0280
BP	 0.4291	 -0.0060
BQ	 0.5297	 -0.0060
BR	 0.6136	 -0.0070
BS	 0.4797	 0.0010
BT	 0.6279	 -0.0100
BU	 0.5690	 0.0050
BV	 0.6314	 0.0560
BW	 0.6220	 0.0220
BX	 0.4459	 -0.0480
BY	 0.5493	 0.0070
BZ	 0.4462	 0.0020