wwPDB EM Validation Summary Report

Nov 19, 2022 – 09:21 PM EST

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

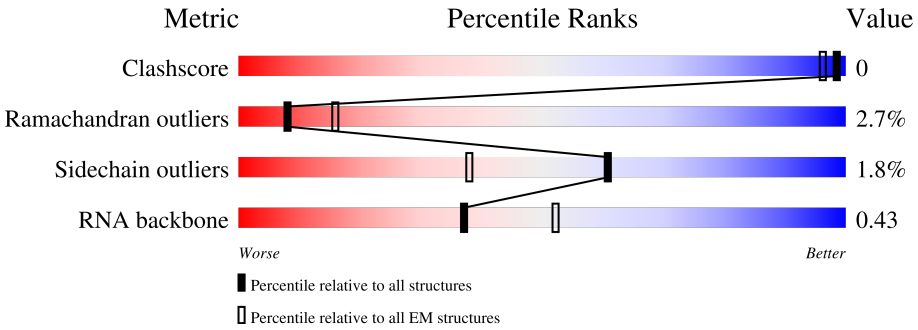
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 <=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	54% 91% 9%
2	AC	208	50% 90% 9%
3	AD	206	52% 89% 10%
4	AE	152	42% 91% 9%
5	AF	101	18% 87% 13%
6	AG	152	25% 86% 14%
7	AH	130	39% 91% 8%

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Mol	Chain	Length	Quality of chain
8	AI	128	27% 90% 9%
9	AJ	100	46% 85% 13%
10	AK	118	29% 89% 9%
11	AL	124	24% 81% 16%
12	AM	115	36% 82% 17%
13	AN	101	38% 82% 17%
14	AO	89	35% 82% 17%
15	AP	81	46% 86% 14%
16	AQ	82	39% 90% 10%
17	AR	57	37% 86% 14%
18	AS	81	26% 85% 15%
19	AT	86	23% 92% 8%
20	AU	53	42% 79% 19%
21	AA	1533	18% 26% 50% 20%
22	A1	76	37% 26% 55% 14%
23	A2	15	47% 13% 47% 27% 13%
24	A3	77	47% 16% 56% 26%
25	BC	273	51% 86% 14%
26	BD	209	47% 91% 8%
27	BE	201	21% 91% 9%
28	BF	179	27% 89% 9%
29	BG	177	33% 93% 6%
30	BH	149	66% 94% 6%
31	BI	142	83% 95%
32	BJ	142	42% 90% 9%

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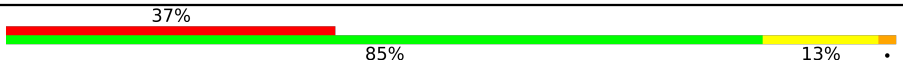
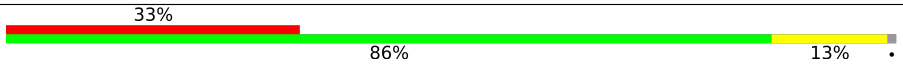
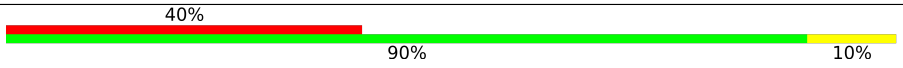
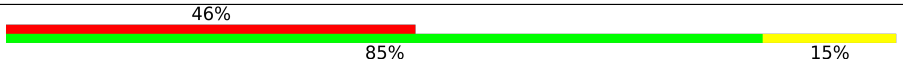
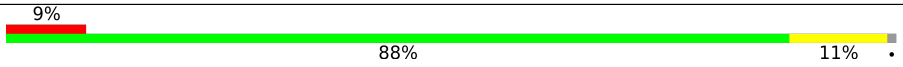
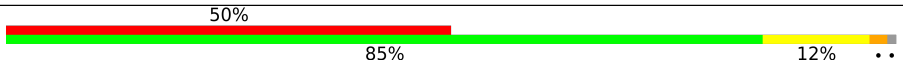
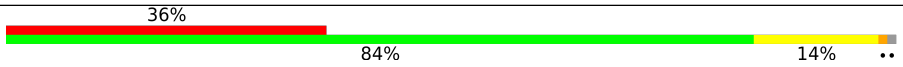
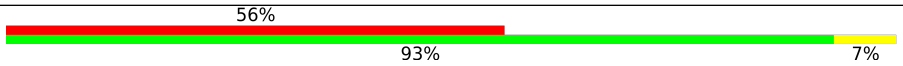
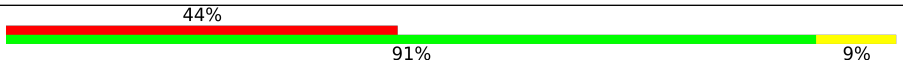
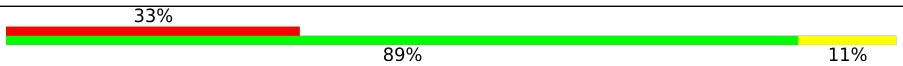
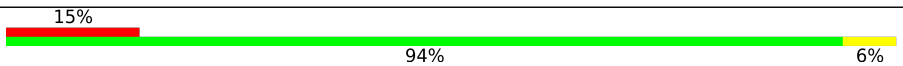
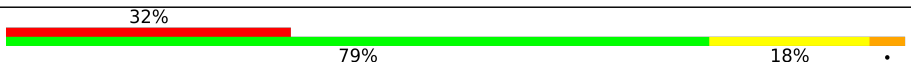
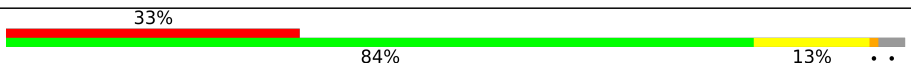
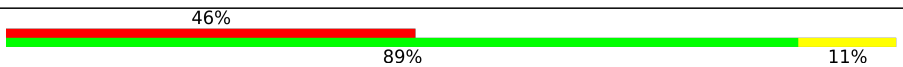
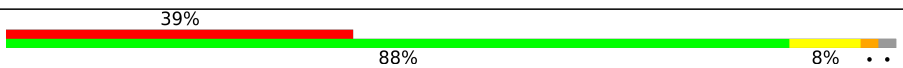
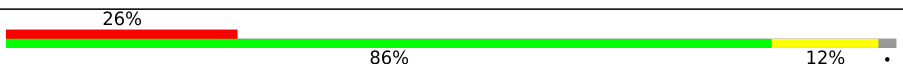
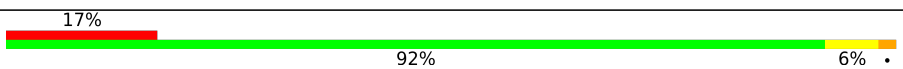
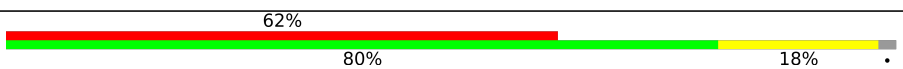
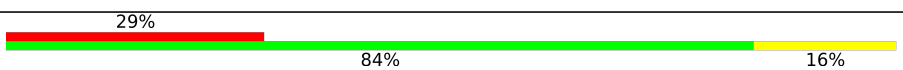
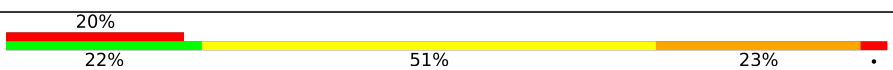
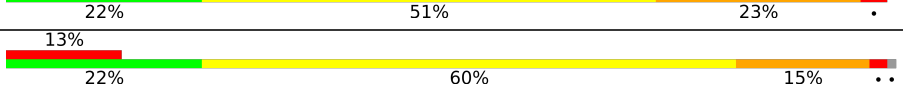
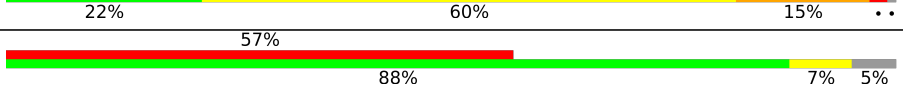
Mol	Chain	Length	Quality of chain
33	BK	123	
34	BL	144	
35	BM	136	
36	BN	121	
37	BO	117	
38	BP	115	
39	BQ	118	
40	BR	103	
41	BS	110	
42	BT	94	
43	BU	104	
44	BV	94	
45	BW	80	
46	BX	79	
47	BY	63	
48	BZ	59	
49	B0	57	
50	B1	52	
51	B2	46	
52	B3	65	
53	B4	38	
54	BA	2903	
55	BB	118	
56	B5	234	

2 Entry composition (i)

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

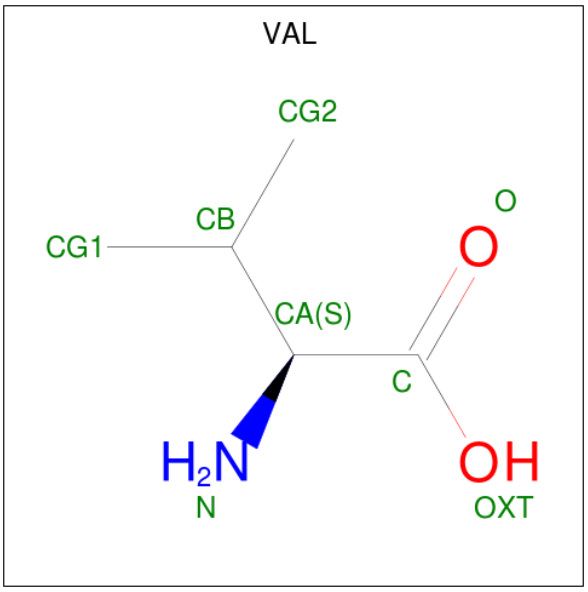
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

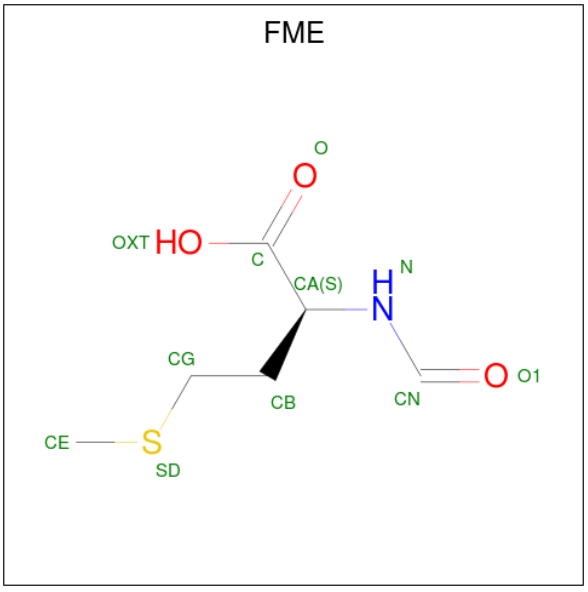
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



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: $C_6H_{11}NO_3S$).



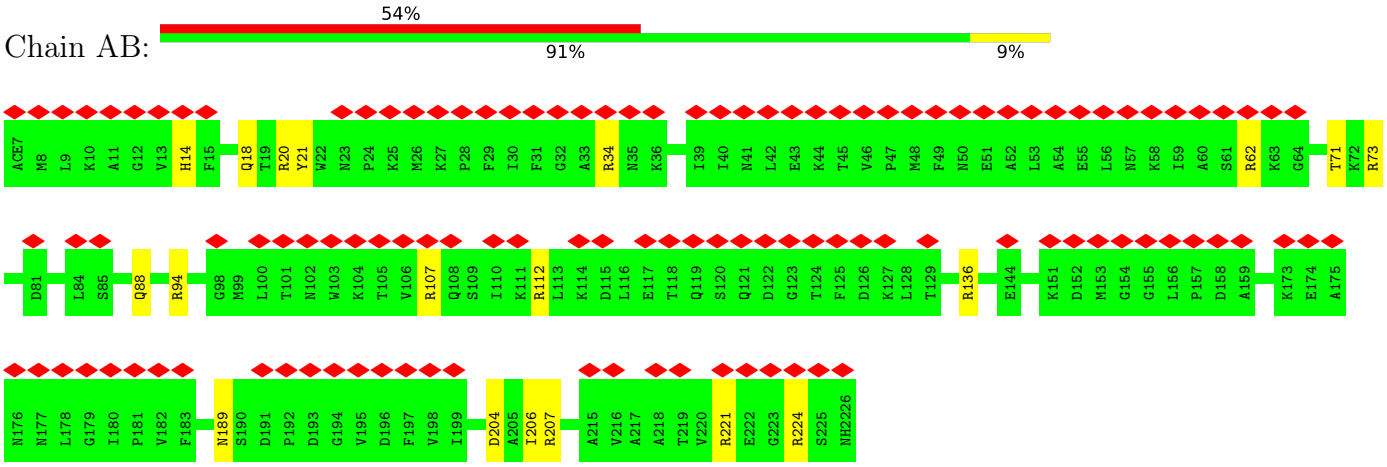
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	BA	1	10	6	1	2	1	0

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.

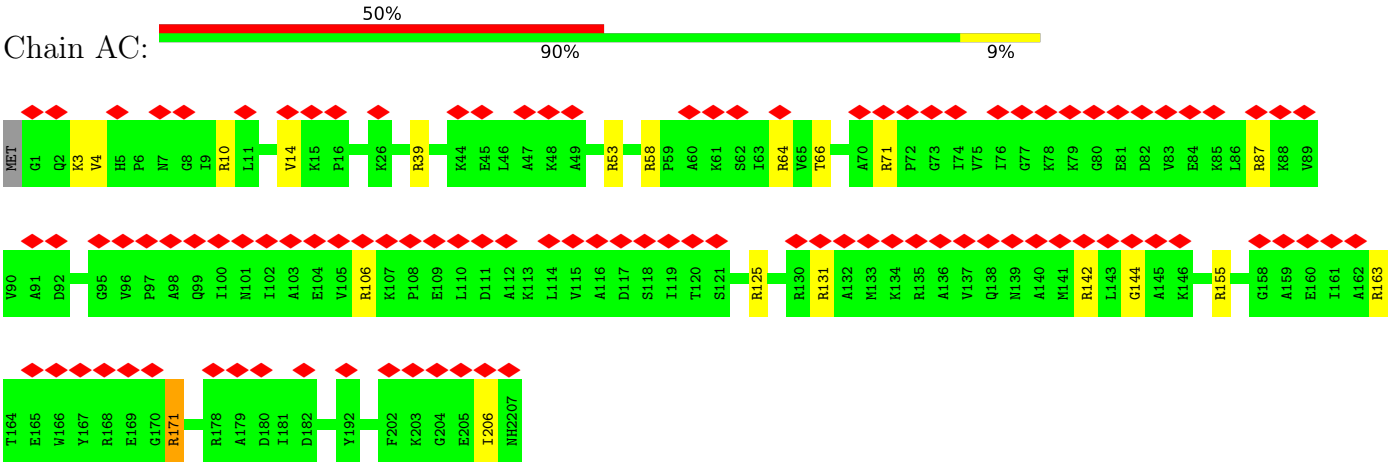
• Molecule 1: 30S ribosomal protein S2

Chain AB:



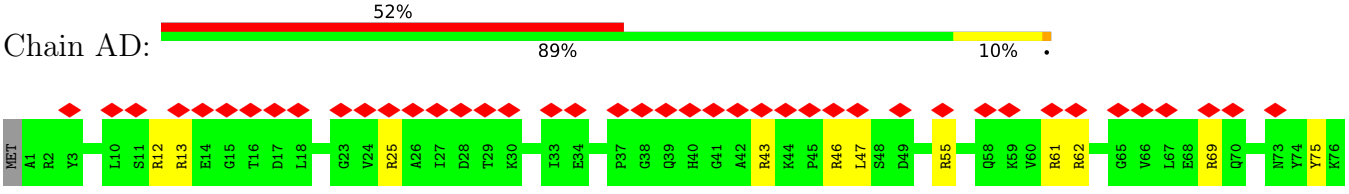
• Molecule 2: 30S ribosomal protein S3

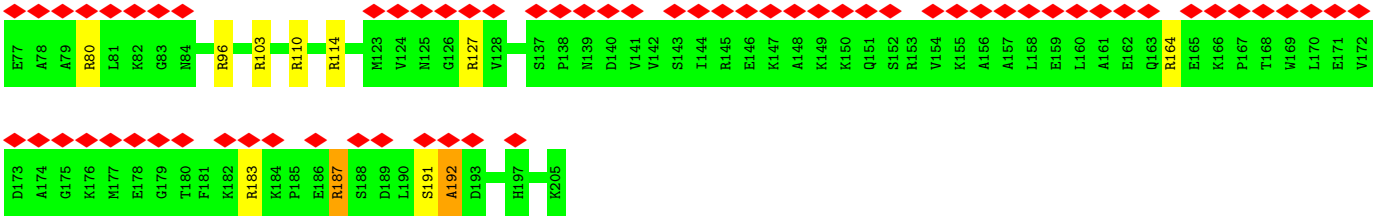
Chain AC:



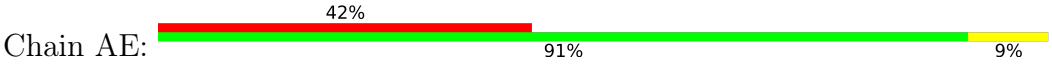
• Molecule 3: 30S ribosomal protein S4

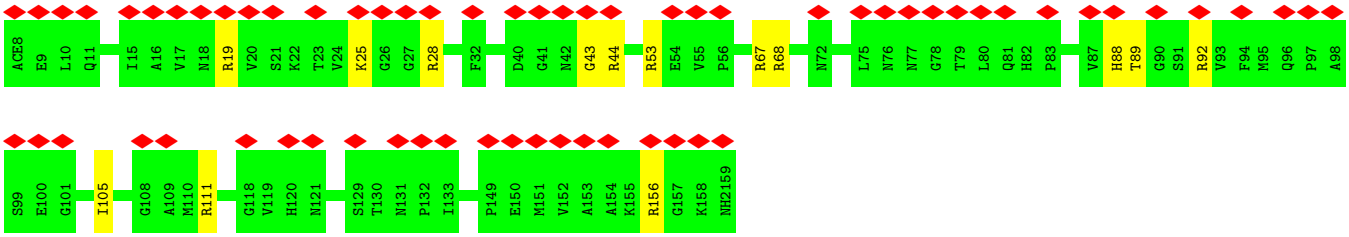
Chain AD:



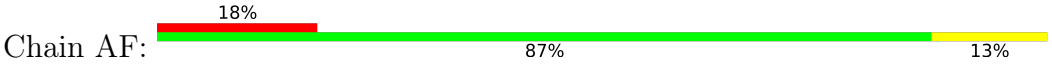


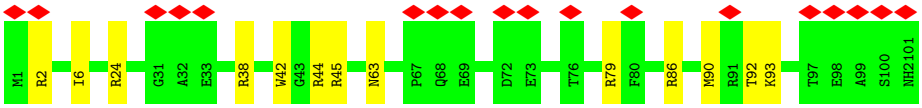
• Molecule 4: 30S ribosomal protein S5



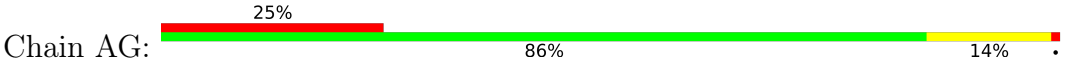


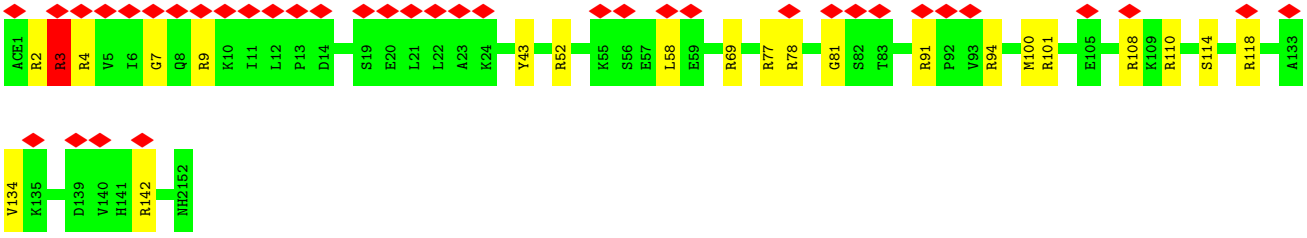
• Molecule 5: 30S ribosomal protein S6



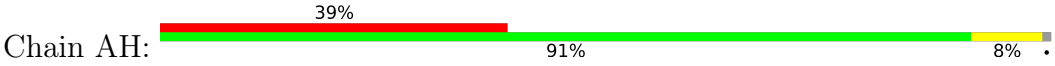


• Molecule 6: 30S ribosomal protein S7



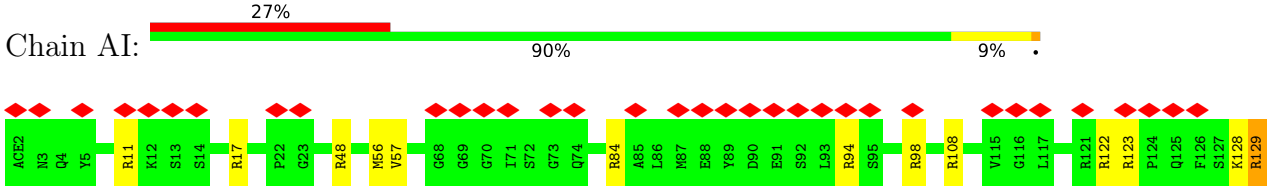


• Molecule 7: 30S ribosomal protein S8



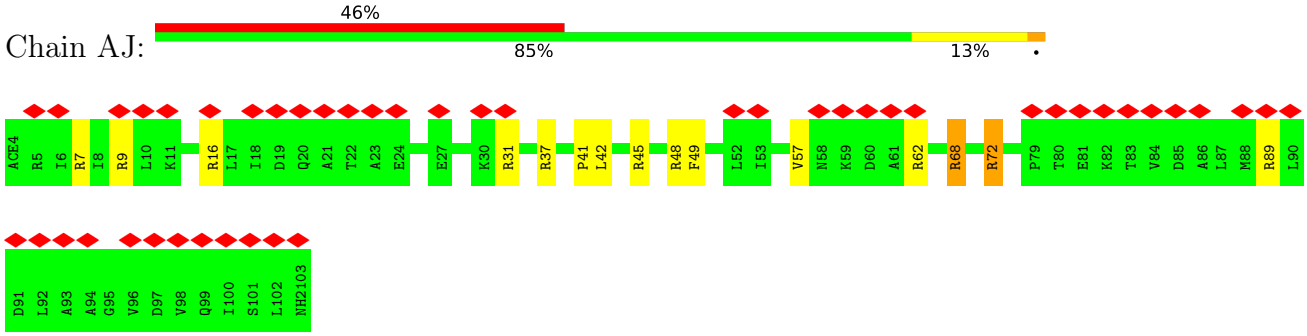
• Molecule 8: 30S ribosomal protein S9

Chain AI:



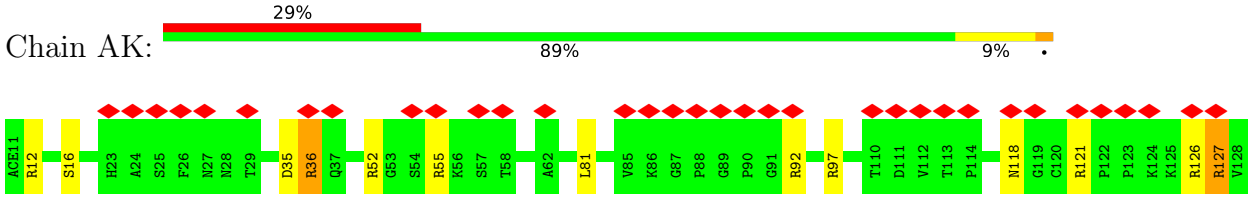
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



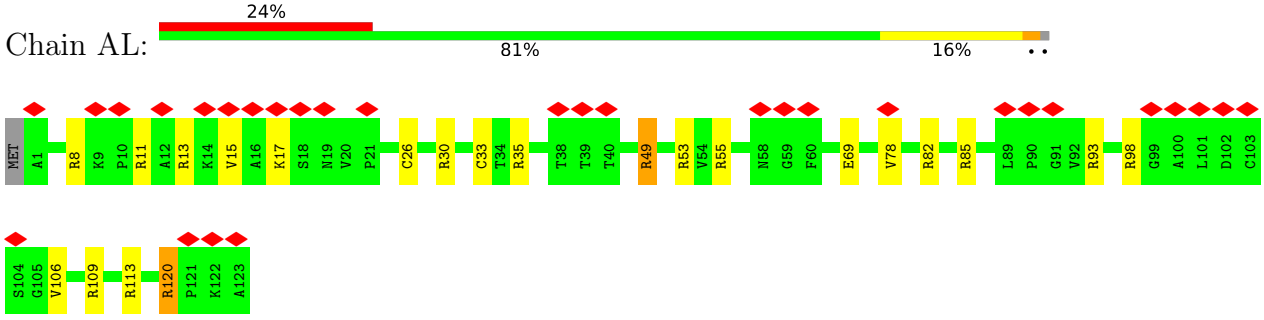
• Molecule 10: 30S ribosomal protein S11

Chain AK:



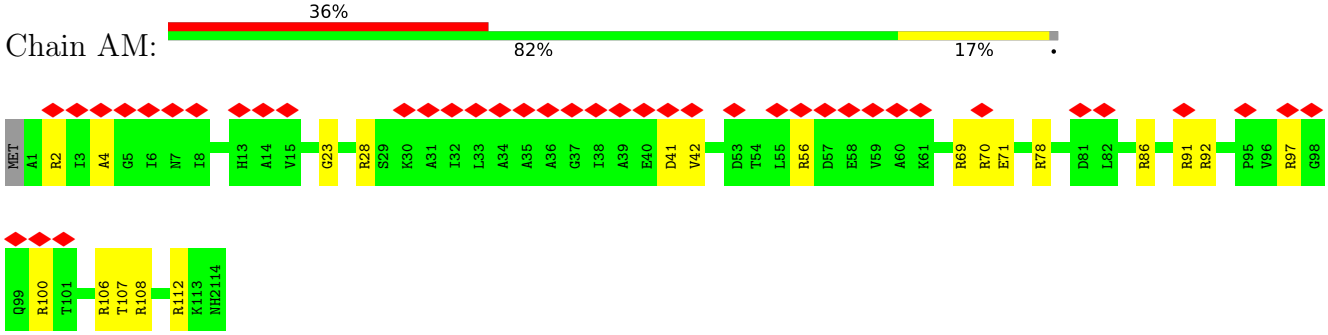
• Molecule 11: 30S ribosomal protein S12

Chain AL:



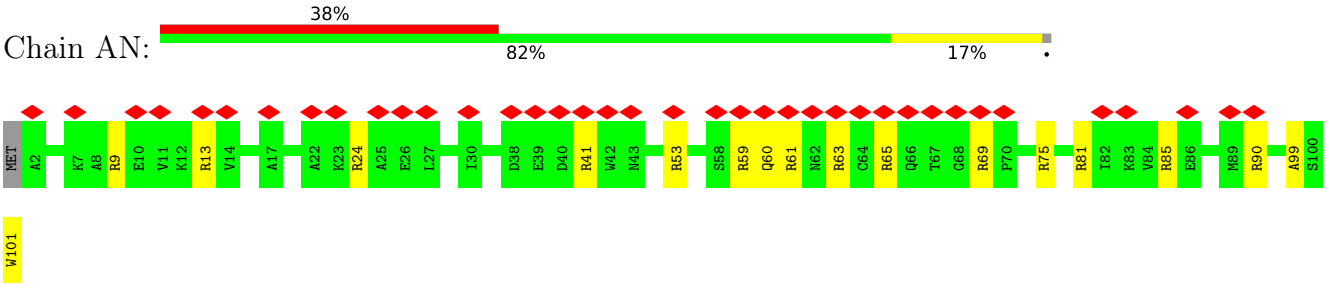
• Molecule 12: 30S ribosomal protein S13

Chain AM:



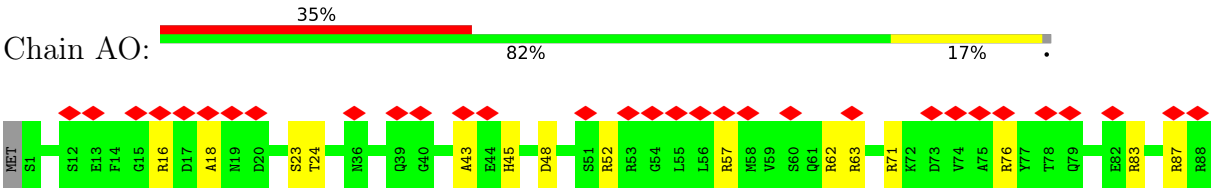
• Molecule 13: 30S ribosomal protein S14

Chain AN:



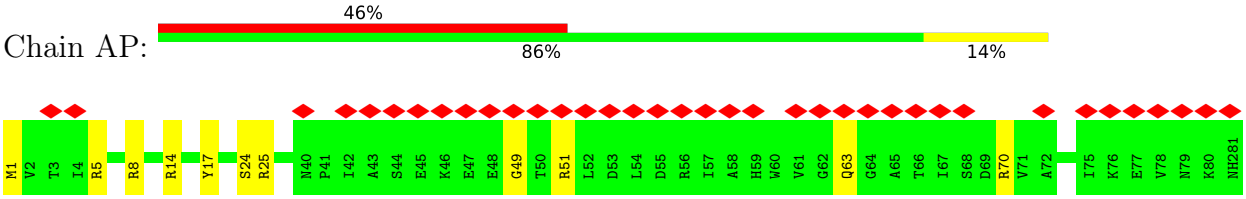
• Molecule 14: 30S ribosomal protein S15

Chain AO:



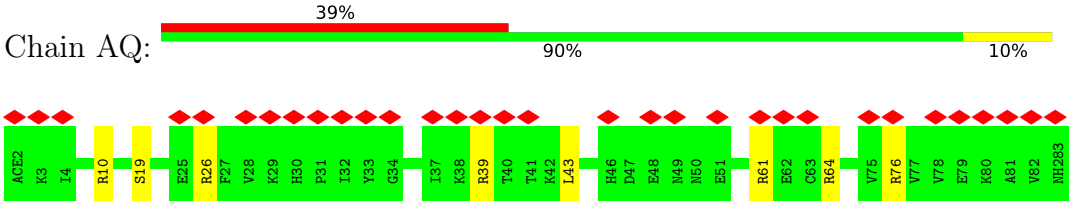
• Molecule 15: 30S ribosomal protein S16

Chain AP:



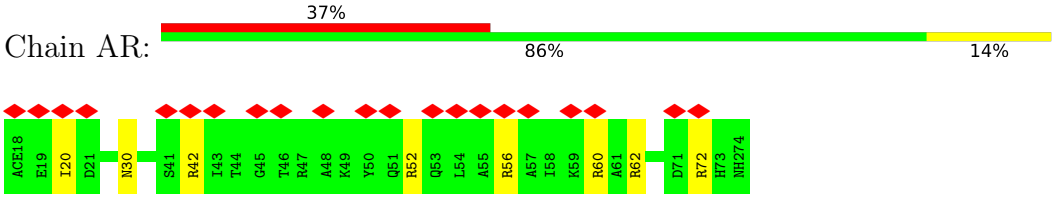
• Molecule 16: 30S ribosomal protein S17

Chain AQ:



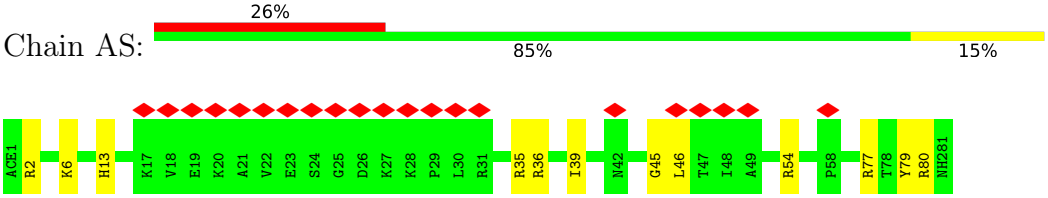
• Molecule 17: 30S ribosomal protein S18

Chain AR:



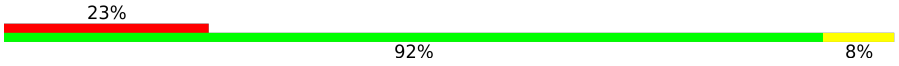
• Molecule 18: 30S ribosomal protein S19

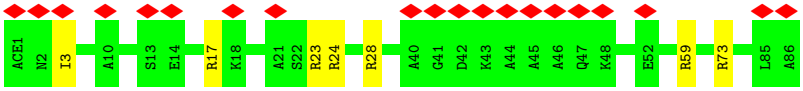
Chain AS:



• Molecule 19: 30S ribosomal protein S20

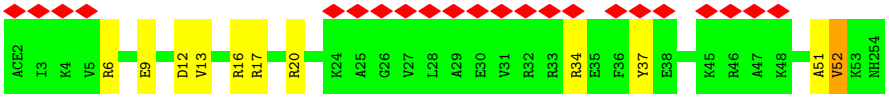
Chain AT:





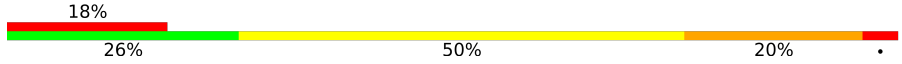
• Molecule 20: 30S ribosomal protein S21

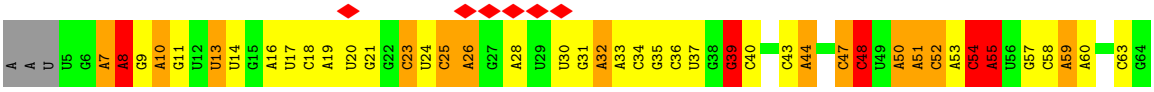
Chain AU:

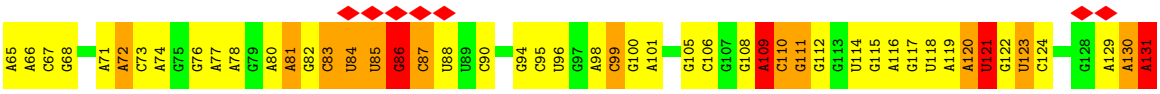


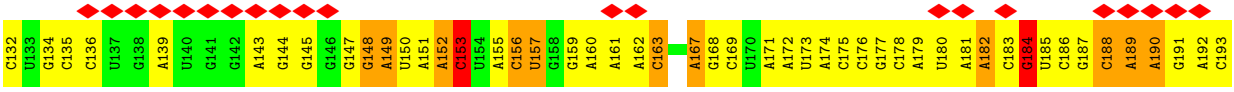
• Molecule 21: 16S ribosomal RNA

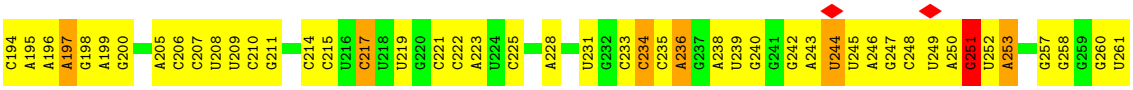
Chain AA:

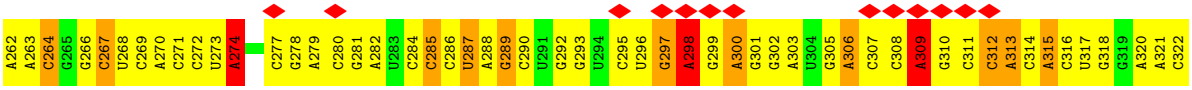


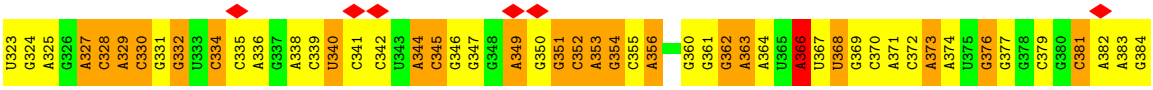


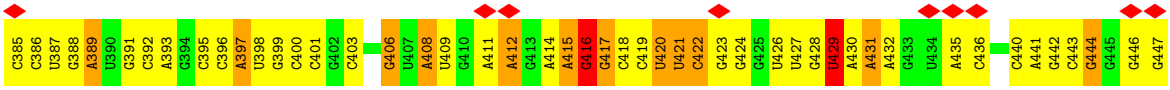


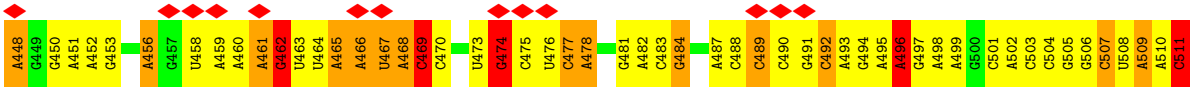


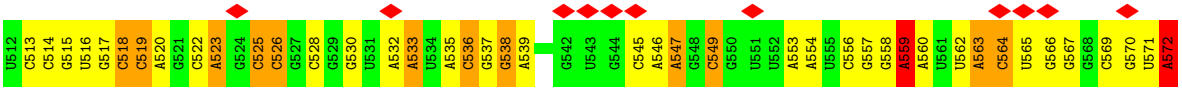


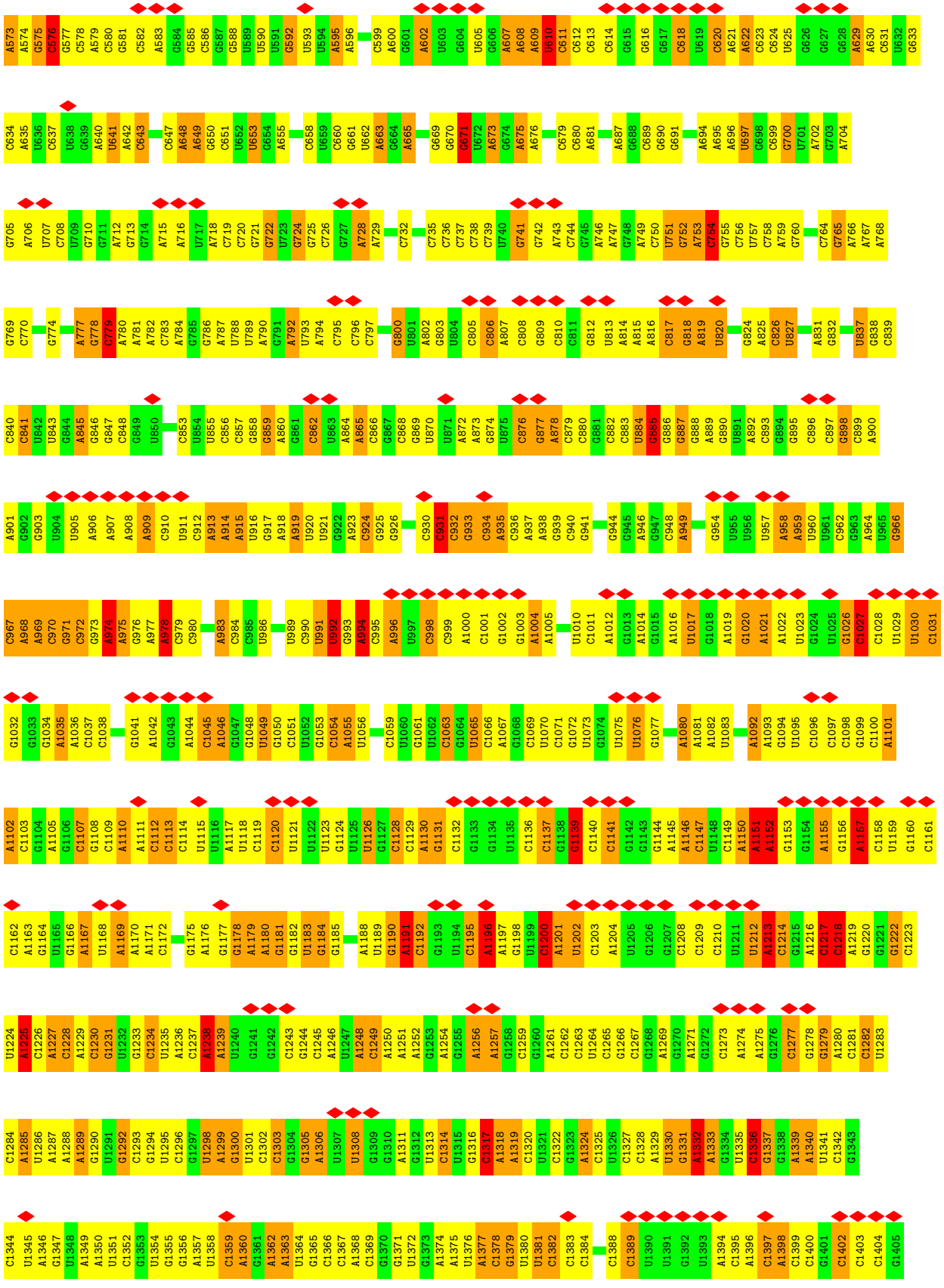








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C634 A635 U636 C637 U638 G639 A640 U641 A642 C643
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G824 A825 C826 U827
A831 G832
U837 G838 C839
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G1041 A1042 G1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056
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A1188 U1189 G1190 A1191 C1192 G1193 U1194 C1195 A1196 A1197 G1198 U1199 G1200 A1201 U1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 A1216 C1217 C1218 A1219 G1220 G1221 G1222 C1223
U1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 C1245 A1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 C1262 C1263 U1264 C1265 C1266 C1267 G1268 A1269 G1270 A1271 G1272 C1273 A1274 A1275 G1276 C1277 G1278 G1279 A1280 C1281 C1282 U1283
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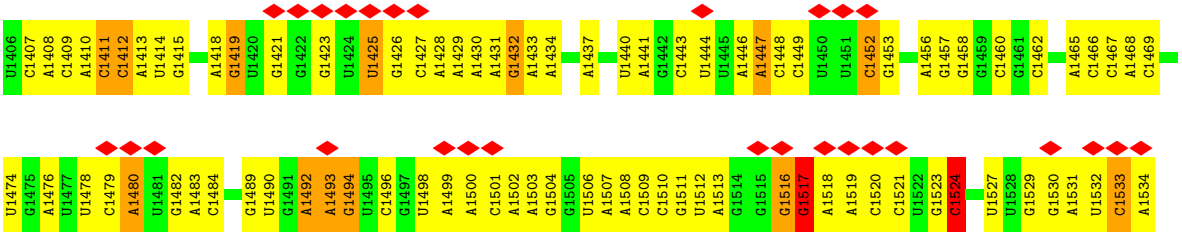
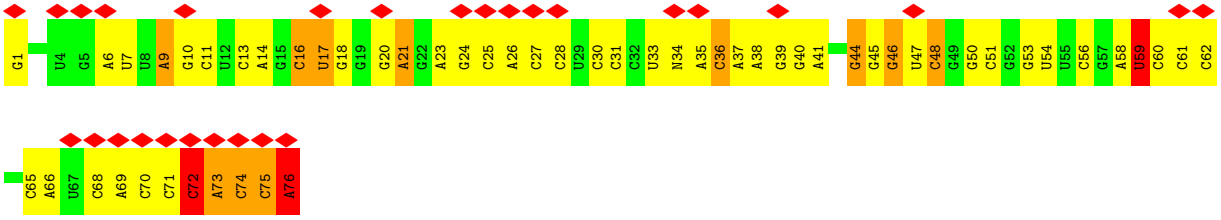
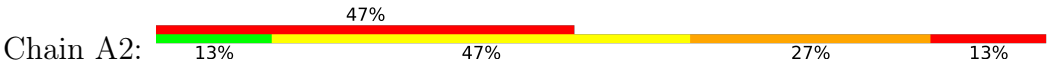
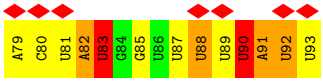


• Molecule 22: fMet-Val-tRNA-Val

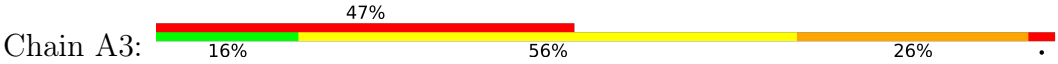


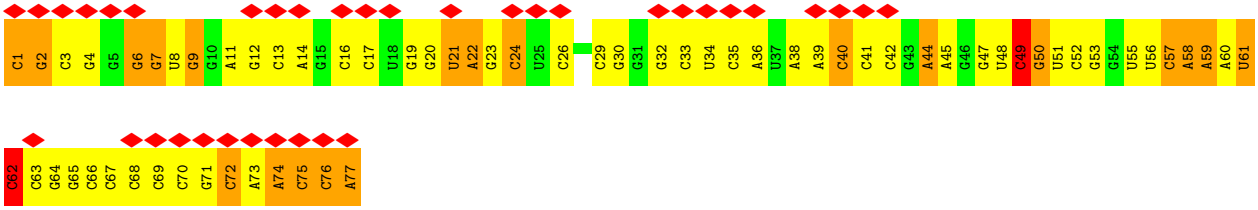
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'



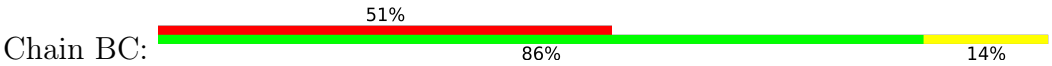


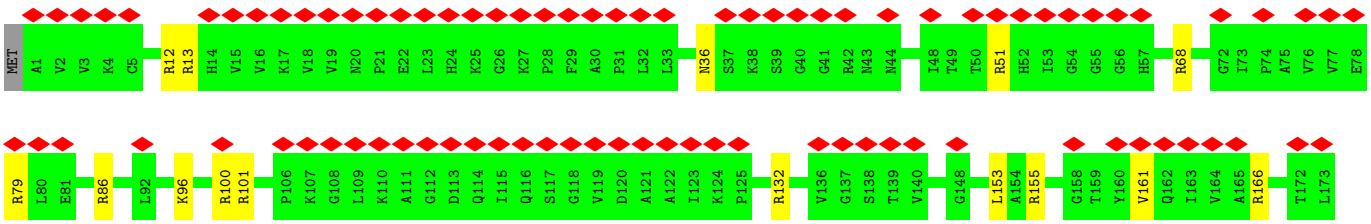
• Molecule 24: tRNA-fMet

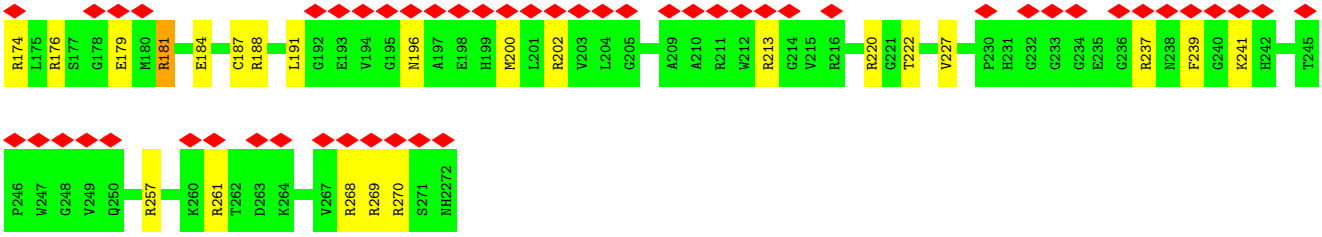




• Molecule 25: 50S ribosomal protein L2

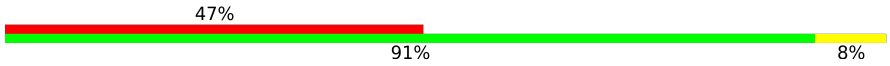


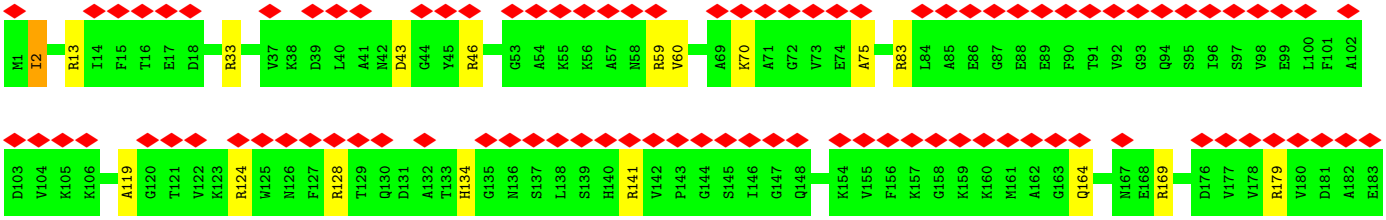




• Molecule 26: 50S ribosomal protein L3

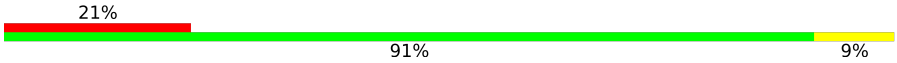
Chain BD:

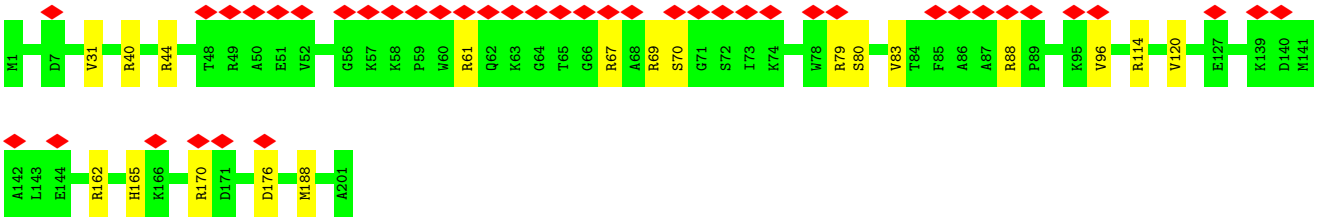




• Molecule 27: 50S ribosomal protein L4

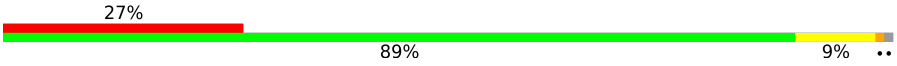
Chain BE:

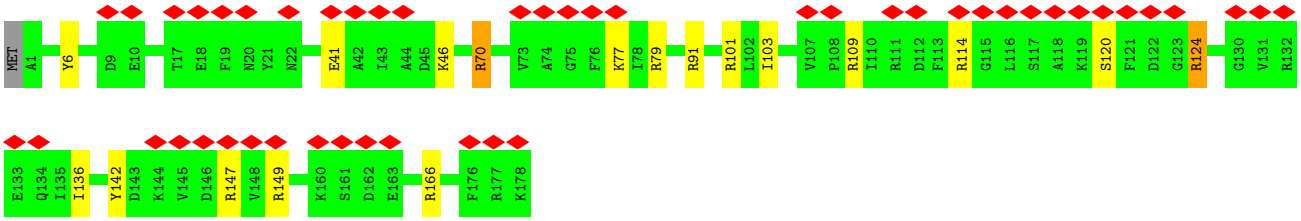




• Molecule 28: 50S ribosomal protein L5

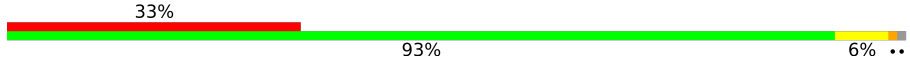
Chain BF:

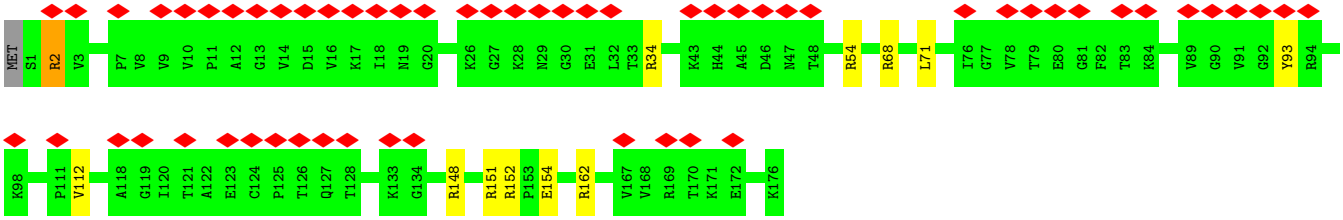




• Molecule 29: 50S ribosomal protein L6

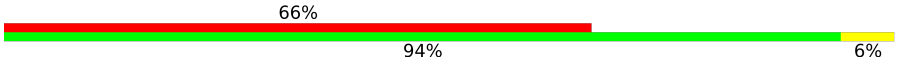
Chain BG:

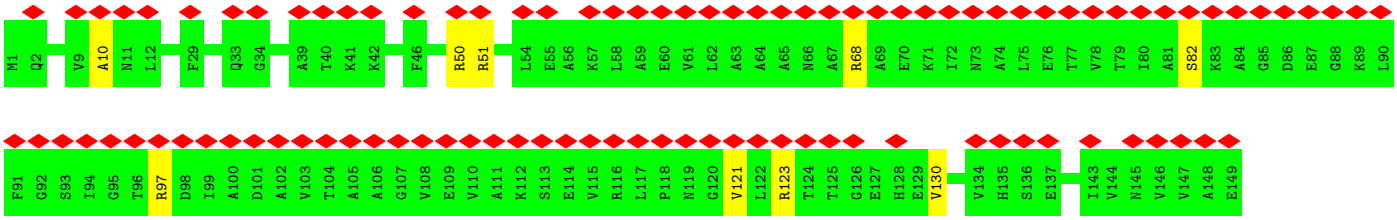




• Molecule 30: 50S ribosomal protein L9

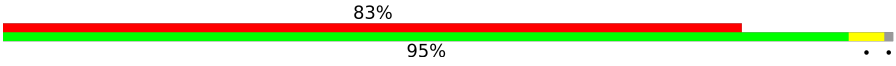
Chain BH:

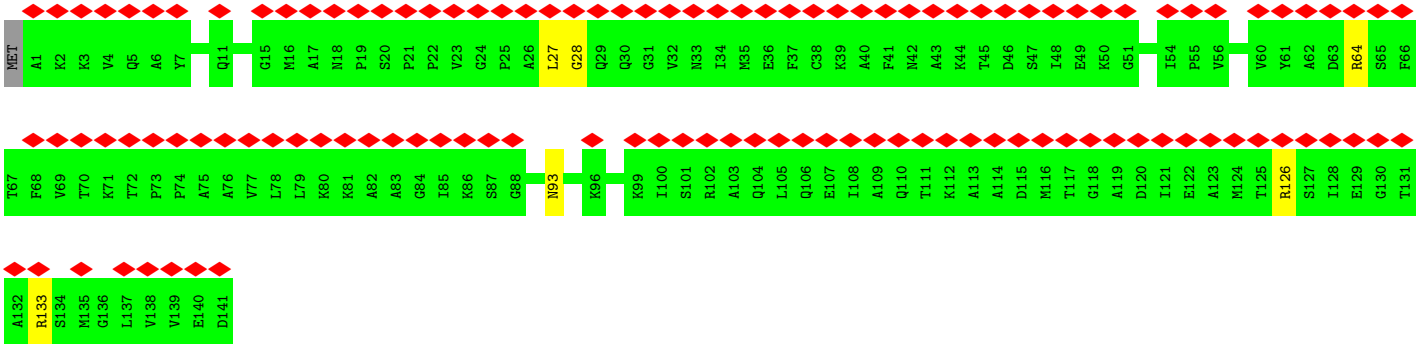




• Molecule 31: 50S ribosomal protein L11

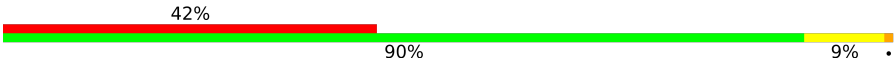
Chain BI:

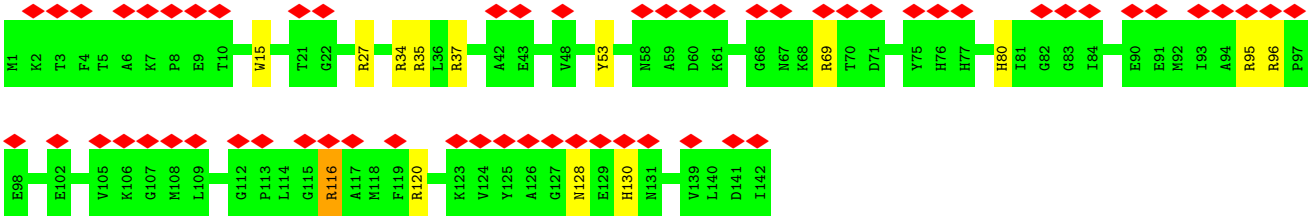




• Molecule 32: 50S ribosomal protein L13

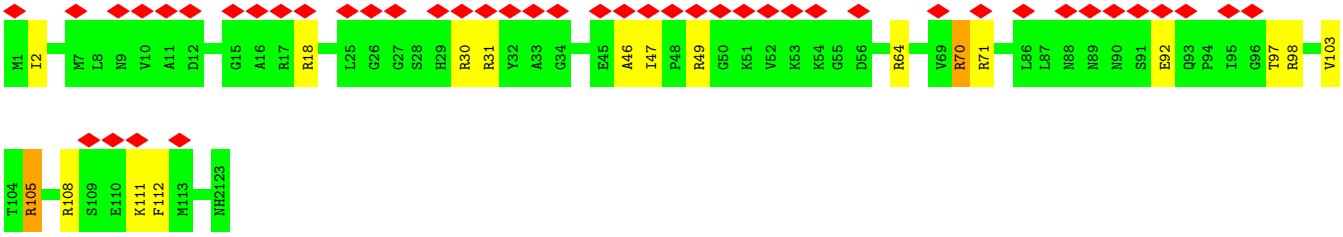
Chain BJ:



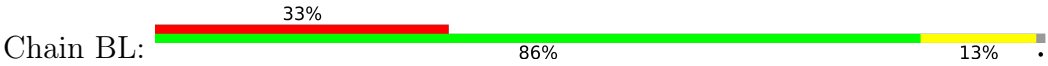


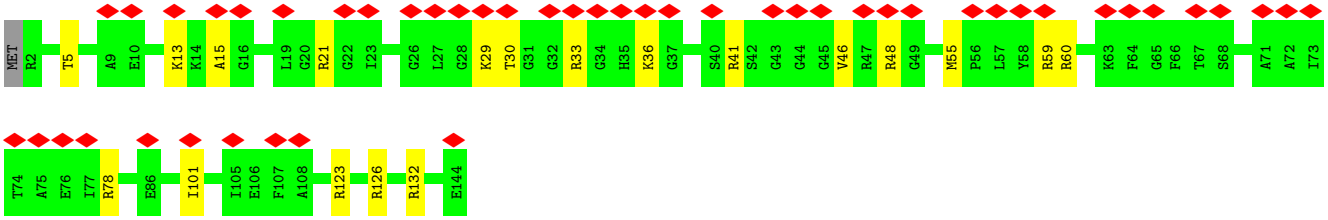
• Molecule 33: 50S ribosomal protein L14

Chain BK:

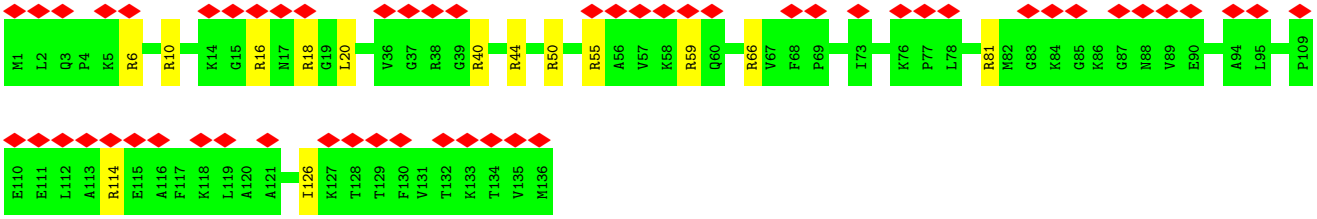


• Molecule 34: 50S ribosomal protein L15

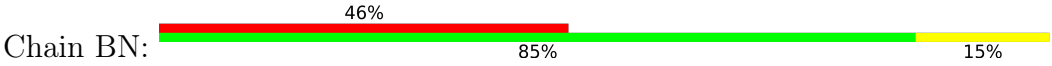


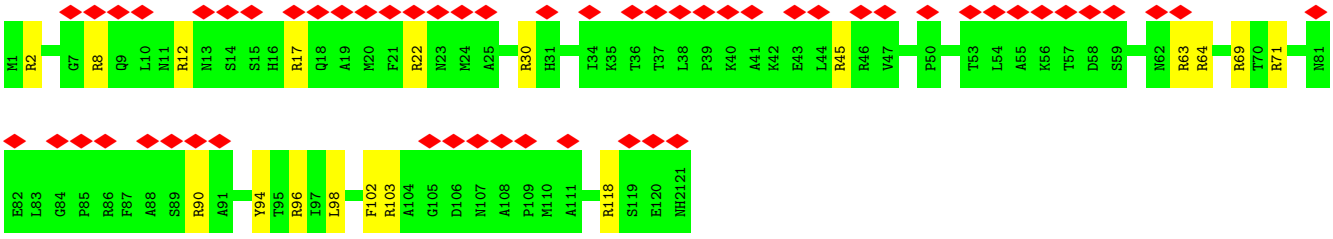


• Molecule 35: 50S ribosomal protein L16

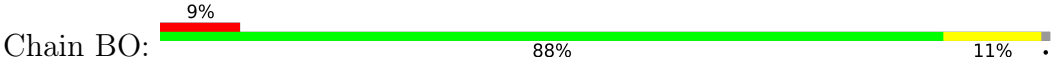


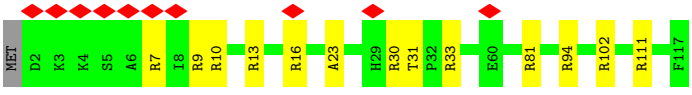
• Molecule 36: 50S ribosomal protein L17





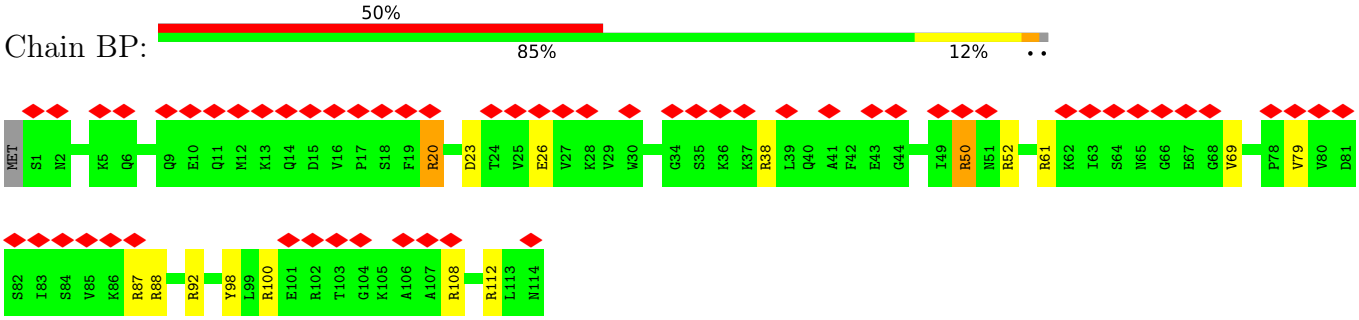
• Molecule 37: 50S ribosomal protein L18





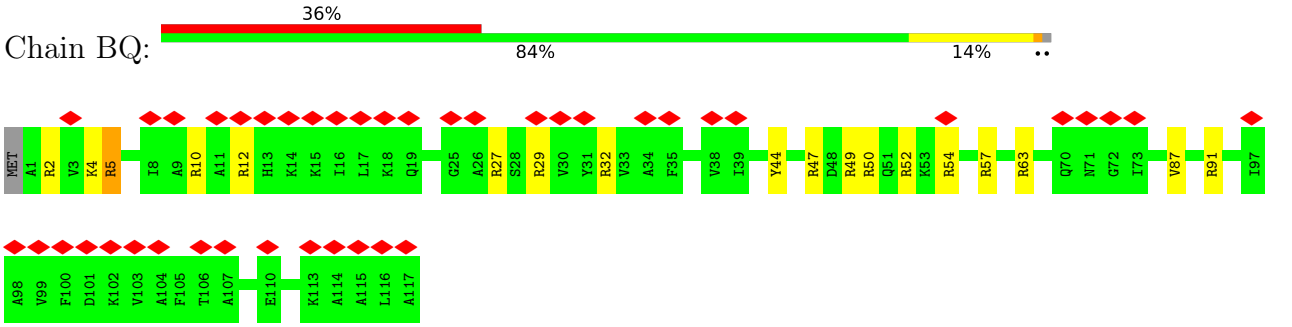
• Molecule 38: 50S ribosomal protein L19

Chain BP:



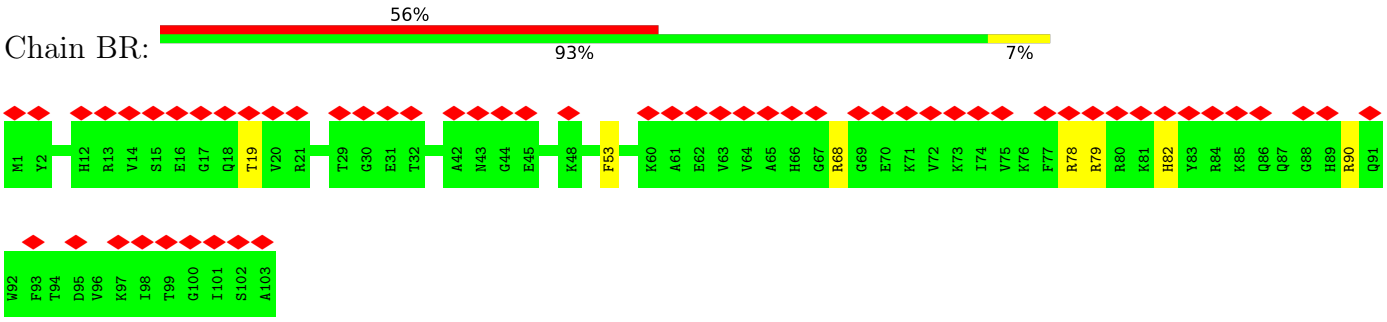
• Molecule 39: 50S ribosomal protein L20

Chain BQ:



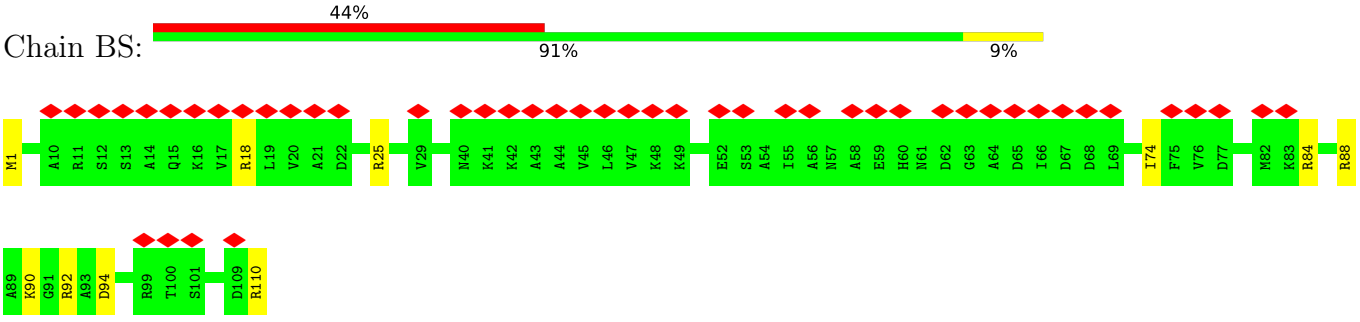
• Molecule 40: 50S ribosomal protein L21

Chain BR:



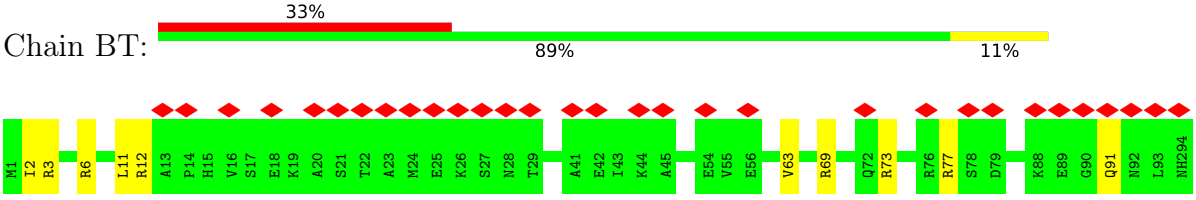
• Molecule 41: 50S ribosomal protein L22

Chain BS:



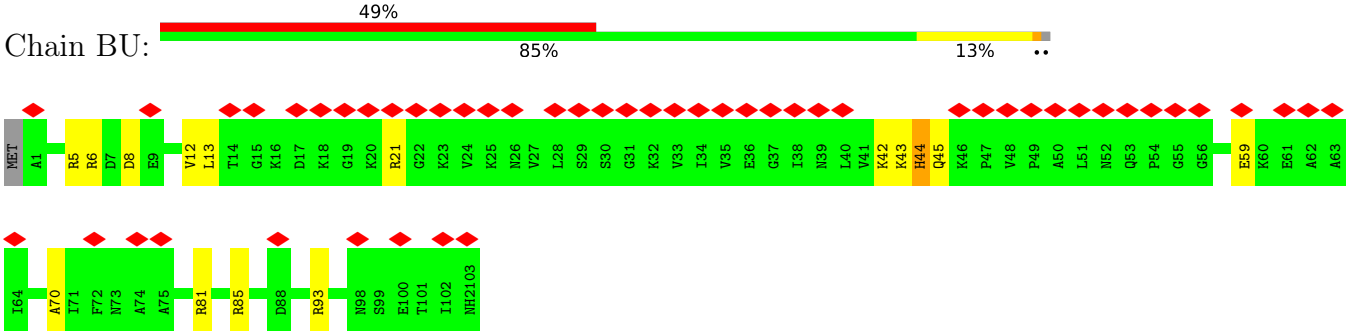
• Molecule 42: 50S ribosomal protein L23

Chain BT:



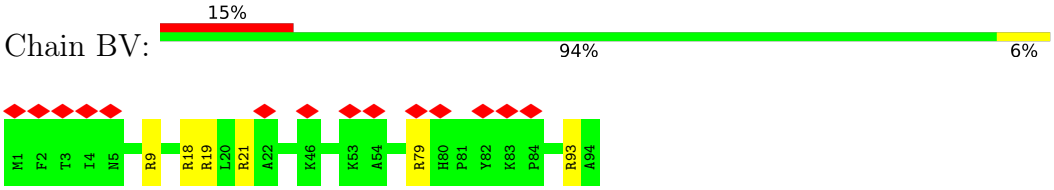
• Molecule 43: 50S ribosomal protein L24

Chain BU:



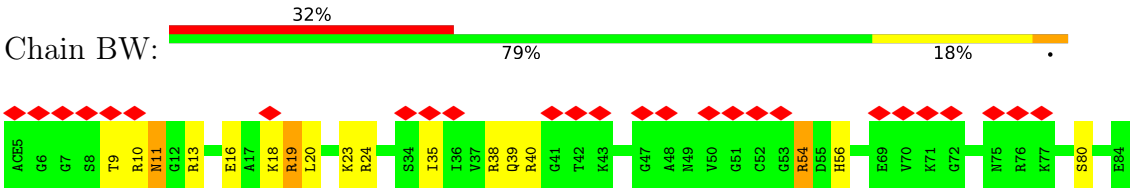
• Molecule 44: 50S ribosomal protein L25

Chain BV:



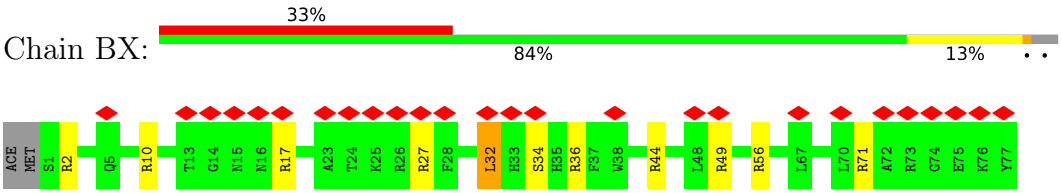
• Molecule 45: 50S ribosomal protein L27

Chain BW:



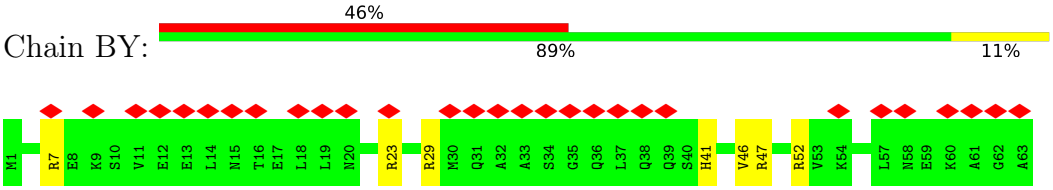
• Molecule 46: 50S ribosomal protein L28

Chain BX:



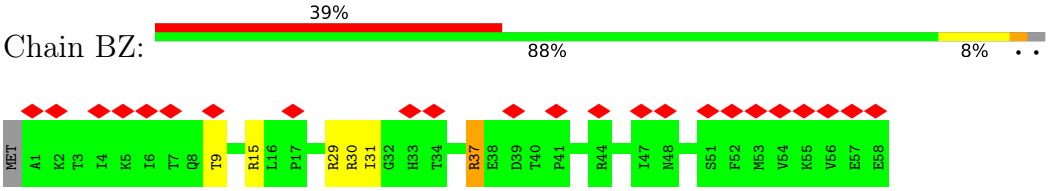
• Molecule 47: 50S ribosomal protein L29

Chain BY:



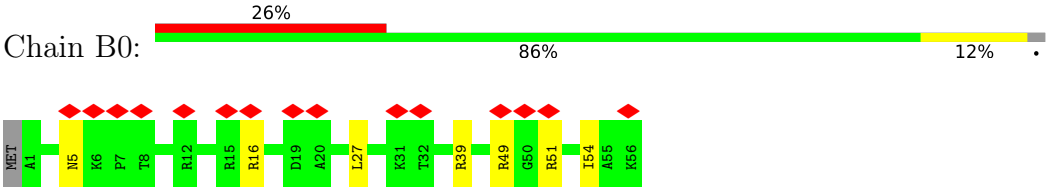
• Molecule 48: 50S ribosomal protein L30

Chain BZ:



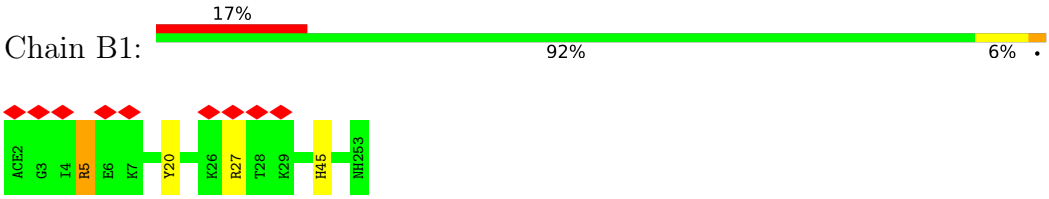
• Molecule 49: 50S ribosomal protein L32

Chain B0:



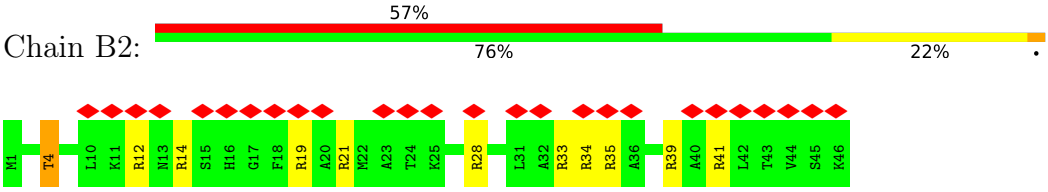
• Molecule 50: 50S ribosomal protein L33

Chain B1:



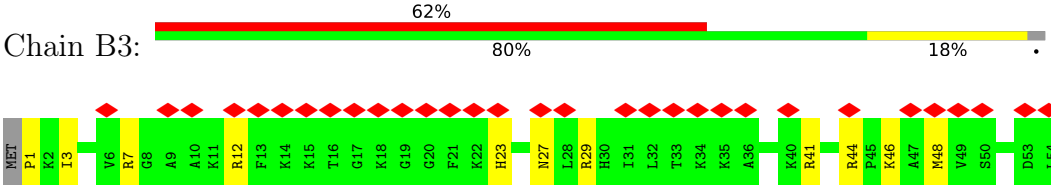
• Molecule 51: 50S ribosomal protein L34

Chain B2:



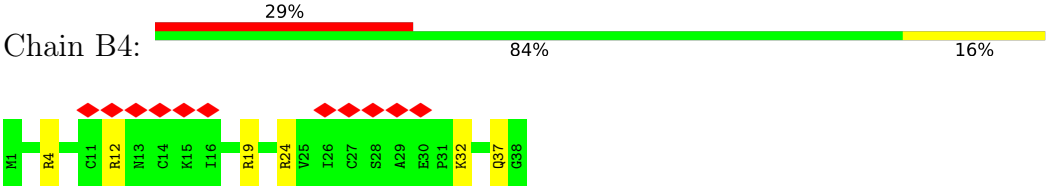
• Molecule 52: 50S ribosomal protein L35

Chain B3:



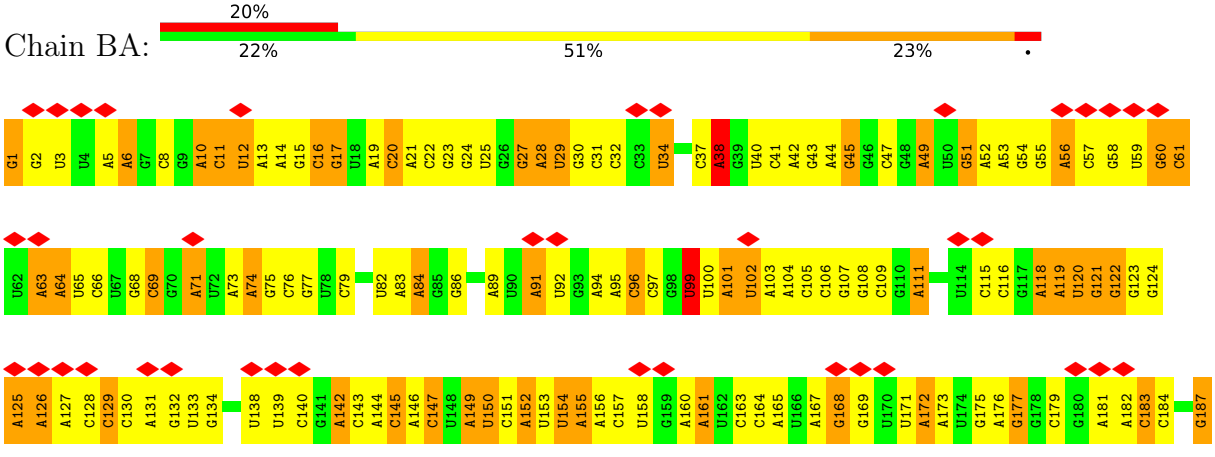
• Molecule 53: 50S ribosomal protein L36

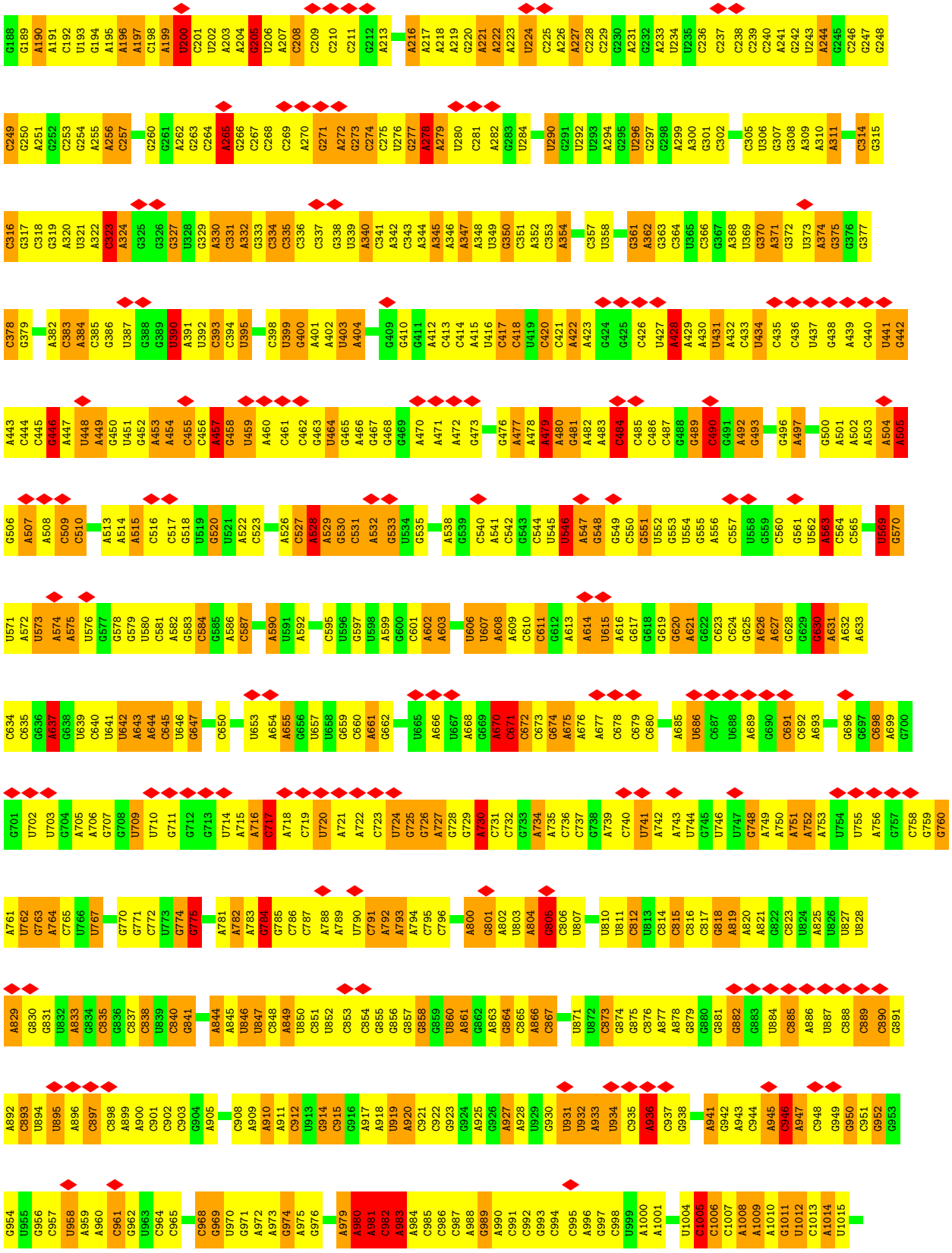
Chain B4:

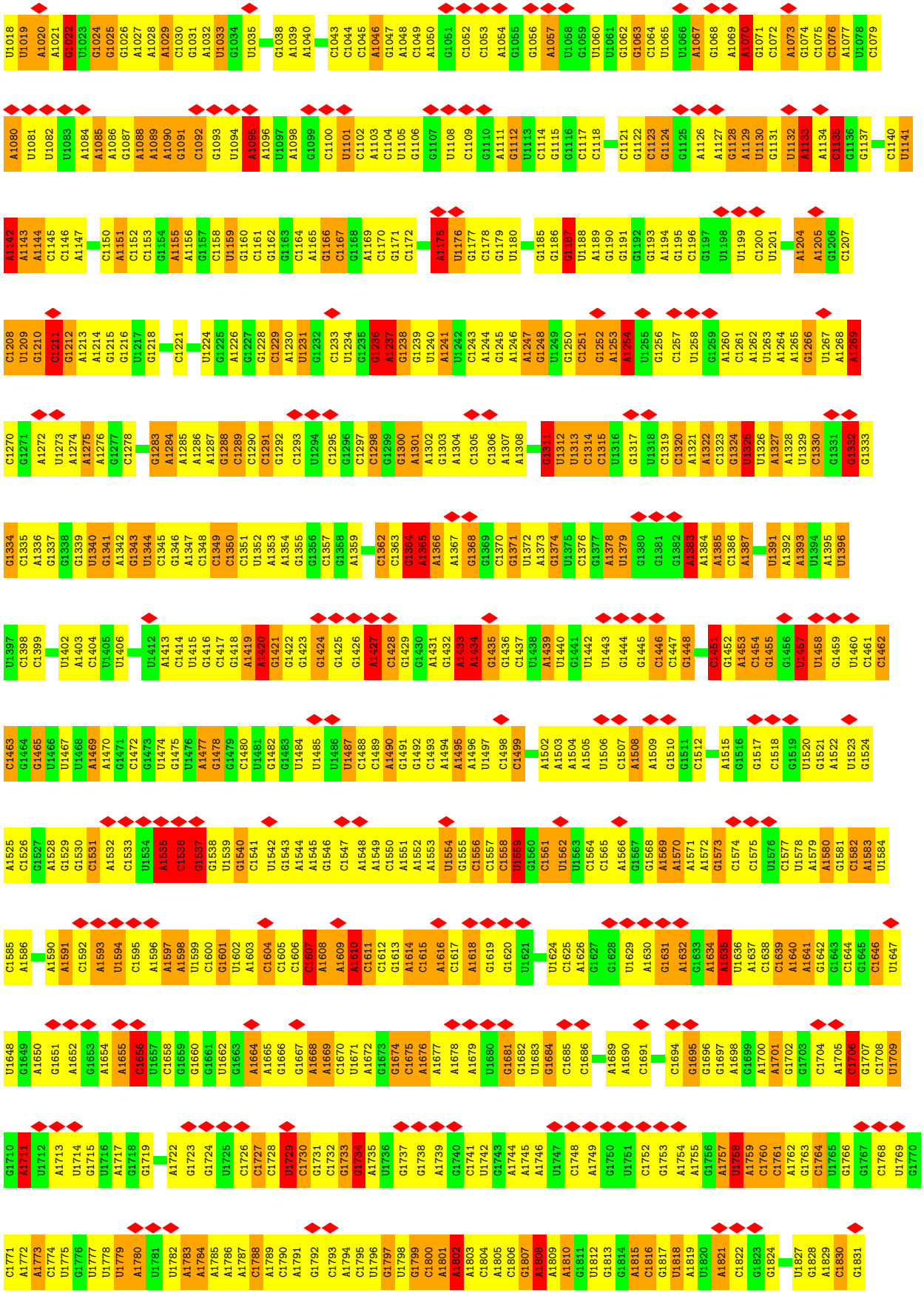


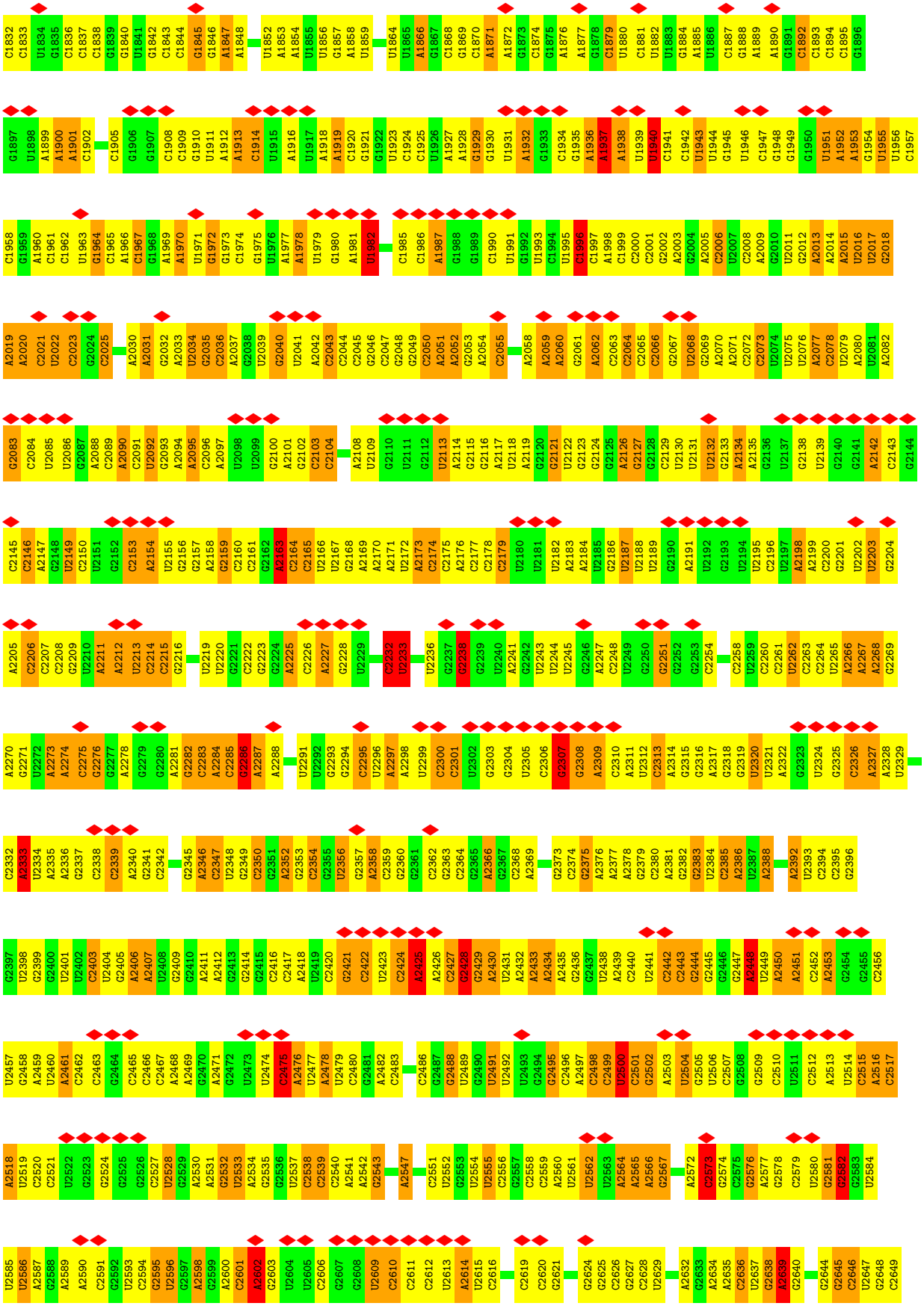
• Molecule 54: 23S ribosomal RNA

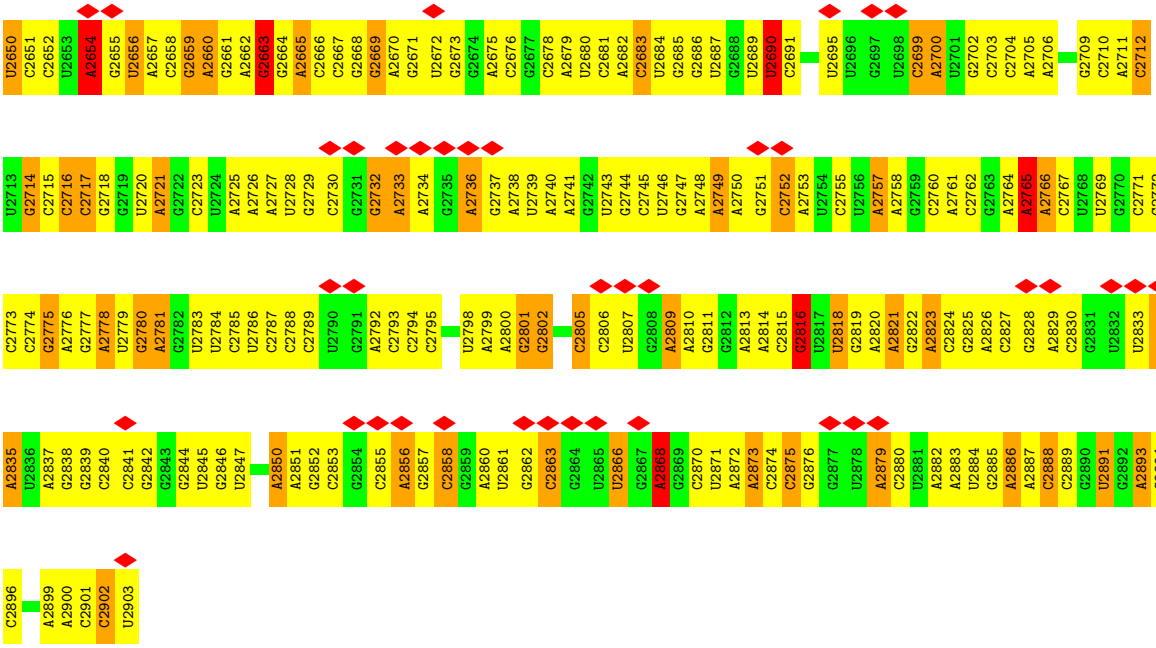
Chain BA:





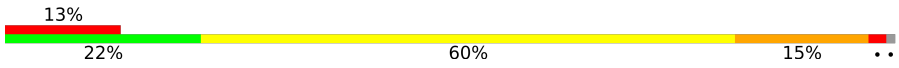


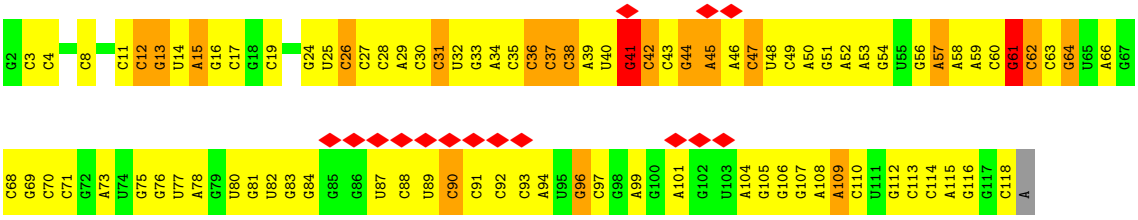




• Molecule 55: 5S ribosomal RNA

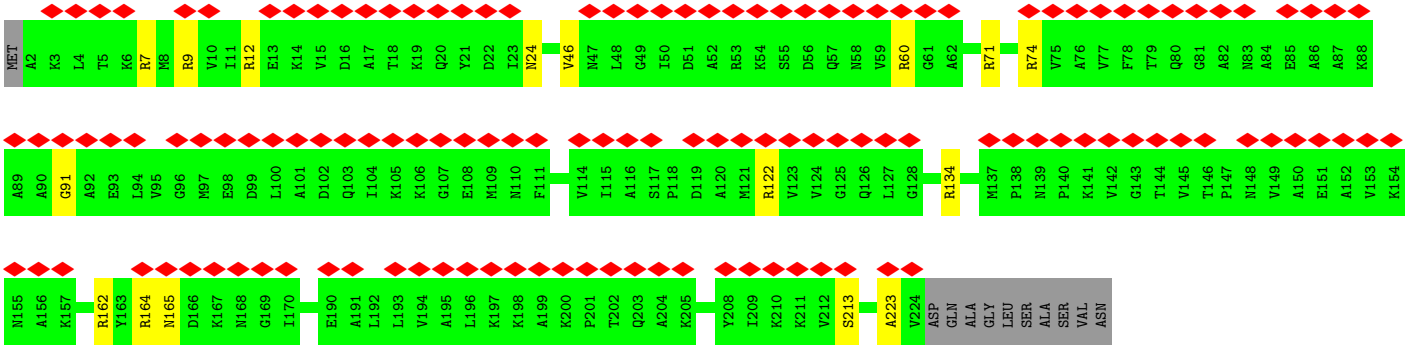
Chain BB:





• Molecule 56: 50S ribosomal protein L1

Chain B5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5656	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	172.869	Depositor
Minimum map value	-108.132	Depositor
Average map value	-1.067	Depositor
Map value standard deviation	18.681	Depositor
Recommended contour level	22.0	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	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: FME, 4SU, OMC, 7MG, 5MU, ACE, PSU, CM0, H2U, 6MZ, NH2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

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

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

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

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

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

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

There are no chirality outliers.

5 of 1051 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	75	TYR	Sidechain
3	AD	96	ARG	Sidechain
4	AE	53	ARG	Sidechain
8	AI	129	ARG	Sidechain
9	AJ	72	ARG	Sidechain

5.2 Too-close contacts (i)

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

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

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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	1	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31298	6	0
55	BB	2504	0	1269	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99612	17	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 17 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AL:69:GLU:H	11:AL:106:VAL:HG13	1.75	0.52
54:BA:1349:C:N4	54:BA:1383:A:H61	2.11	0.49
54:BA:1324:G:H3'	54:BA:1325:U:H5"	1.97	0.46
4:AE:88:HIS:CG	4:AE:89:THR:H	2.32	0.45
33:BK:111:LYS:HE3	33:BK:112:PHE:CZ	2.52	0.45

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	201 (92%)	15 (7%)	2 (1%)	17	57
2	AC	205/208 (99%)	190 (93%)	9 (4%)	6 (3%)	4	29
3	AD	203/206 (98%)	191 (94%)	9 (4%)	3 (2%)	10	46
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	7	38
5	AF	99/101 (98%)	87 (88%)	7 (7%)	5 (5%)	2	19
6	AG	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	3	23
7	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	19	60
8	AI	126/128 (98%)	110 (87%)	15 (12%)	1 (1%)	19	60
9	AJ	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	3	23
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	17	57
11	AL	121/124 (98%)	110 (91%)	9 (7%)	2 (2%)	9	42
12	AM	112/115 (97%)	92 (82%)	16 (14%)	4 (4%)	3	25
13	AN	98/101 (97%)	92 (94%)	4 (4%)	2 (2%)	7	38
14	AO	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	1	18
15	AP	79/81 (98%)	69 (87%)	6 (8%)	4 (5%)	2	19
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	8	40
18	AS	79/81 (98%)	69 (87%)	7 (9%)	3 (4%)	3	24
19	AT	84/86 (98%)	80 (95%)	3 (4%)	1 (1%)	13	50
20	AU	51/53 (96%)	38 (74%)	9 (18%)	4 (8%)	1	13
25	BC	270/273 (99%)	235 (87%)	27 (10%)	8 (3%)	4	28
26	BD	207/209 (99%)	185 (89%)	16 (8%)	6 (3%)	4	29
27	BE	199/201 (99%)	180 (90%)	11 (6%)	8 (4%)	3	23
28	BF	176/179 (98%)	157 (89%)	13 (7%)	6 (3%)	3	26
29	BG	174/177 (98%)	155 (89%)	18 (10%)	1 (1%)	25	66
30	BH	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	7	38
31	BI	139/142 (98%)	129 (93%)	9 (6%)	1 (1%)	22	63
32	BJ	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	4	29
33	BK	121/123 (98%)	103 (85%)	13 (11%)	5 (4%)	3	23
34	BL	141/144 (98%)	109 (77%)	24 (17%)	8 (6%)	1	18
35	BM	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10	46
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%)	107 (93%)	5 (4%)	3 (3%)	5 31
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	7 38
41	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	8 38
42	BT	92/94 (98%)	79 (86%)	9 (10%)	4 (4%)	2 22
43	BU	101/104 (97%)	87 (86%)	9 (9%)	5 (5%)	2 20
44	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100 100
45	BW	78/80 (98%)	54 (69%)	15 (19%)	9 (12%)	0 6
46	BX	75/79 (95%)	64 (85%)	8 (11%)	3 (4%)	3 23
47	BY	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	9 44
48	BZ	56/59 (95%)	52 (93%)	1 (2%)	3 (5%)	2 19
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2 19
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100 100
51	B2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	6 34
52	B3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4 26
53	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5 30
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	11 46
All	All	5876/6008 (98%)	5259 (90%)	459 (8%)	158 (3%)	8 31

5 of 158 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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%)	175 (97%)	5 (3%)	43 65
2	AC	170/171 (99%)	169 (99%)	1 (1%)	86 92
3	AD	172/173 (99%)	172 (100%)	0	100 100
4	AE	113/113 (100%)	113 (100%)	0	100 100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	73 84
6	AG	123/123 (100%)	119 (97%)	4 (3%)	38 61
7	AH	104/105 (99%)	103 (99%)	1 (1%)	76 86
8	AI	105/105 (100%)	103 (98%)	2 (2%)	57 75
9	AJ	86/86 (100%)	85 (99%)	1 (1%)	71 83
10	AK	90/90 (100%)	85 (94%)	5 (6%)	21 46
11	AL	103/104 (99%)	102 (99%)	1 (1%)	76 86
12	AM	91/92 (99%)	89 (98%)	2 (2%)	52 71
13	AN	83/84 (99%)	82 (99%)	1 (1%)	71 83
14	AO	76/77 (99%)	75 (99%)	1 (1%)	69 81
15	AP	65/65 (100%)	64 (98%)	1 (2%)	65 80
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	44 65
17	AR	48/48 (100%)	47 (98%)	1 (2%)	53 72
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%)	41 (93%)	3 (7%)	16 41
25	BC	216/217 (100%)	211 (98%)	5 (2%)	50 70
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%)	145 (97%)	4 (3%)	44 65
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%)	109 (100%)	0	100 100
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	60 78
33	BK	103/103 (100%)	100 (97%)	3 (3%)	42 64
34	BL	102/103 (99%)	102 (100%)	0	100 100
35	BM	109/109 (100%)	108 (99%)	1 (1%)	78 87

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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%)	84 (98%)	2 (2%)	50 70
38	BP	99/100 (99%)	97 (98%)	2 (2%)	55 74
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%)	91 (98%)	2 (2%)	52 71
42	BT	80/80 (100%)	80 (100%)	0	100 100
43	BU	83/84 (99%)	80 (96%)	3 (4%)	35 59
44	BV	78/78 (100%)	78 (100%)	0	100 100
45	BW	59/59 (100%)	54 (92%)	5 (8%)	10 33
46	BX	67/68 (98%)	66 (98%)	1 (2%)	65 80
47	BY	55/55 (100%)	55 (100%)	0	100 100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	53 72
49	B0	47/48 (98%)	47 (100%)	0	100 100
50	B1	45/45 (100%)	43 (96%)	2 (4%)	28 53
51	B2	38/38 (100%)	37 (97%)	1 (3%)	46 66
52	B3	51/52 (98%)	47 (92%)	4 (8%)	12 36
53	B4	34/34 (100%)	33 (97%)	1 (3%)	42 64
56	B5	173/181 (96%)	171 (99%)	2 (1%)	71 83
All	All	4842/4870 (99%)	4755 (98%)	87 (2%)	61 77

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

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

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

Mol	Chain	Res	Type
26	BD	173	GLN

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

5.3.3 RNA (i)

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

5 of 764 RNA backbone outliers are listed below:

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

5 of 238 RNA pucker outliers are listed below:

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

5.4 Non-standard residues in protein, DNA, RNA chains (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	5MU	A3	55	24	19,22,23	0.69	0	28,32,35	1.32	4 (14%)
22	4SU	A1	7	22	18,21,22	1.35	1 (5%)	26,30,33	0.99	2 (7%)
22	6MZ	A1	37	22	18,25,26	0.93	0	16,36,39	1.44	2 (12%)
24	PSU	A3	56	24	18,21,22	0.96	0	22,30,33	1.20	2 (9%)
22	PSU	A1	55	22	18,21,22	0.82	0	22,30,33	1.00	0
22	5MU	A1	54	22	19,22,23	0.75	0	28,32,35	1.36	3 (10%)
24	4SU	A3	8	24	18,21,22	1.36	1 (5%)	26,30,33	0.86	1 (3%)
24	H2U	A3	21	24	18,21,22	1.35	2 (11%)	21,30,33	1.22	4 (19%)
24	OMC	A3	33	24	19,22,23	0.75	0	26,31,34	0.95	1 (3%)
22	7MG	A1	46	22	22,26,27	4.76	2 (9%)	29,39,42	1.40	1 (3%)
22	CM0	A1	34	22,23	22,26,27	1.41	3 (13%)	28,37,40	1.50	3 (10%)

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-22.10	1.33	1.46
24	A3	8	4SU	C5-C4	-4.86	1.36	1.42
22	A1	34	CM0	O5-C5	-4.86	1.25	1.36
22	A1	7	4SU	C5-C4	-4.74	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C4-N3	-3.22	1.32	1.37

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	46	7MG	N9-C8-N7	5.67	111.49	103.38
22	A1	34	CM0	C7-O5-C5	5.40	124.65	117.58
22	A1	37	6MZ	C9-N6-C6	4.14	126.44	122.87
22	A1	54	5MU	C5M-C5-C6	-3.78	117.80	122.85
24	A3	55	5MU	C5M-C5-C6	-3.67	117.94	122.85

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	37	6MZ	N1-C6-N6-C9
22	A1	46	7MG	C4'-C5'-O5'-P
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	55	PSU	O4'-C1'-C5-C4

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	0.63	0	6,7,9	0.89	0
58	FME	BA	3001	57	8,9,10	0.79	0	7,9,11	1.89	2 (28%)

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	-	0/5/6/8	-
58	FME	BA	3001	57	-	1/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	BA	3001	FME	CA-N-CN	3.33	127.95	122.82
58	BA	3001	FME	C-CA-N	2.69	114.59	109.73

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.

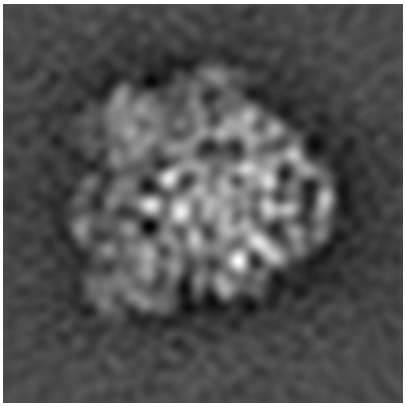
6 Map visualisation

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

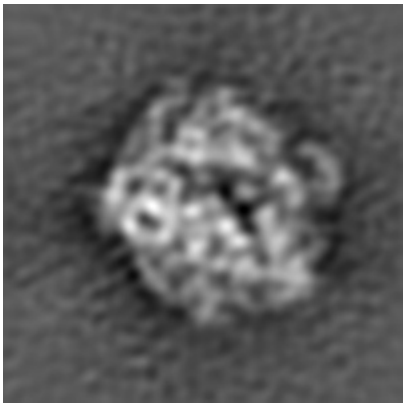
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

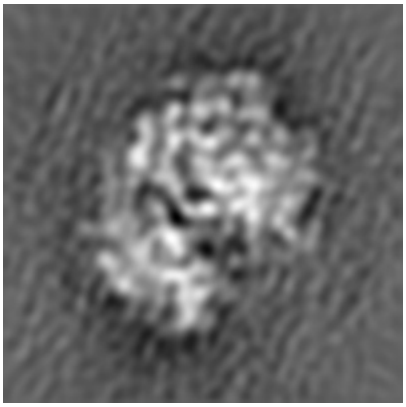
6.1.1 Primary map



X



Y

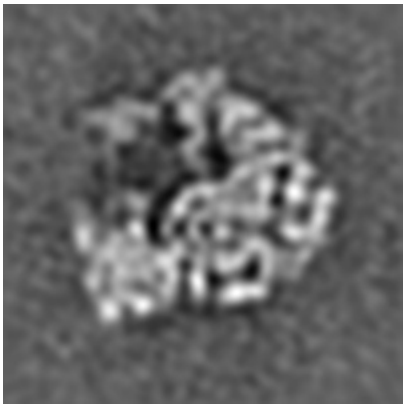


Z

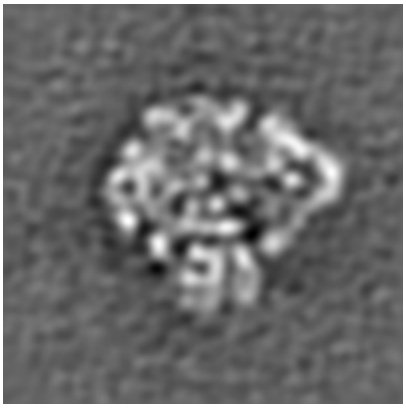
The images above show the map projected in three orthogonal directions.

6.2 Central slices

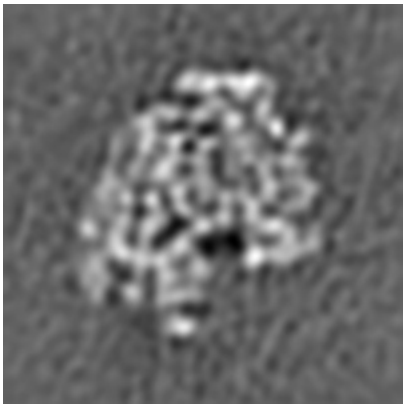
6.2.1 Primary map



X Index: 64



Y Index: 64

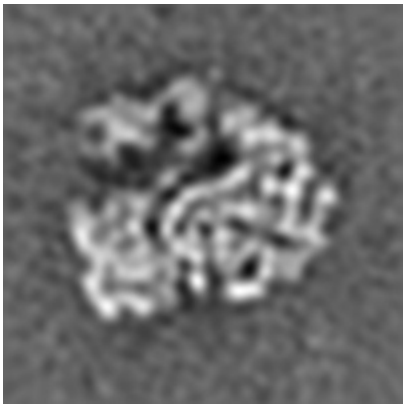


Z Index: 64

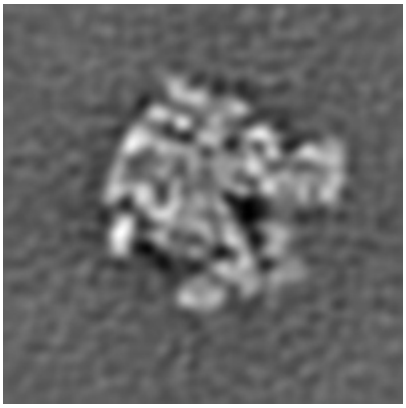
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

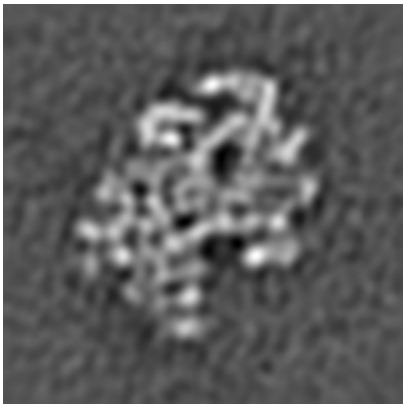
6.3.1 Primary map



X Index: 62



Y Index: 69

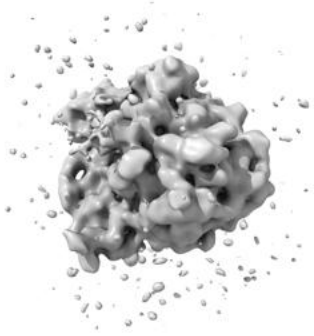


Z Index: 61

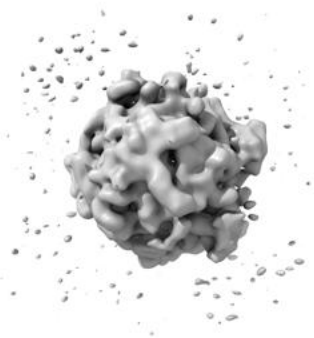
The images above show the largest variance slices of the map in three orthogonal directions.

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

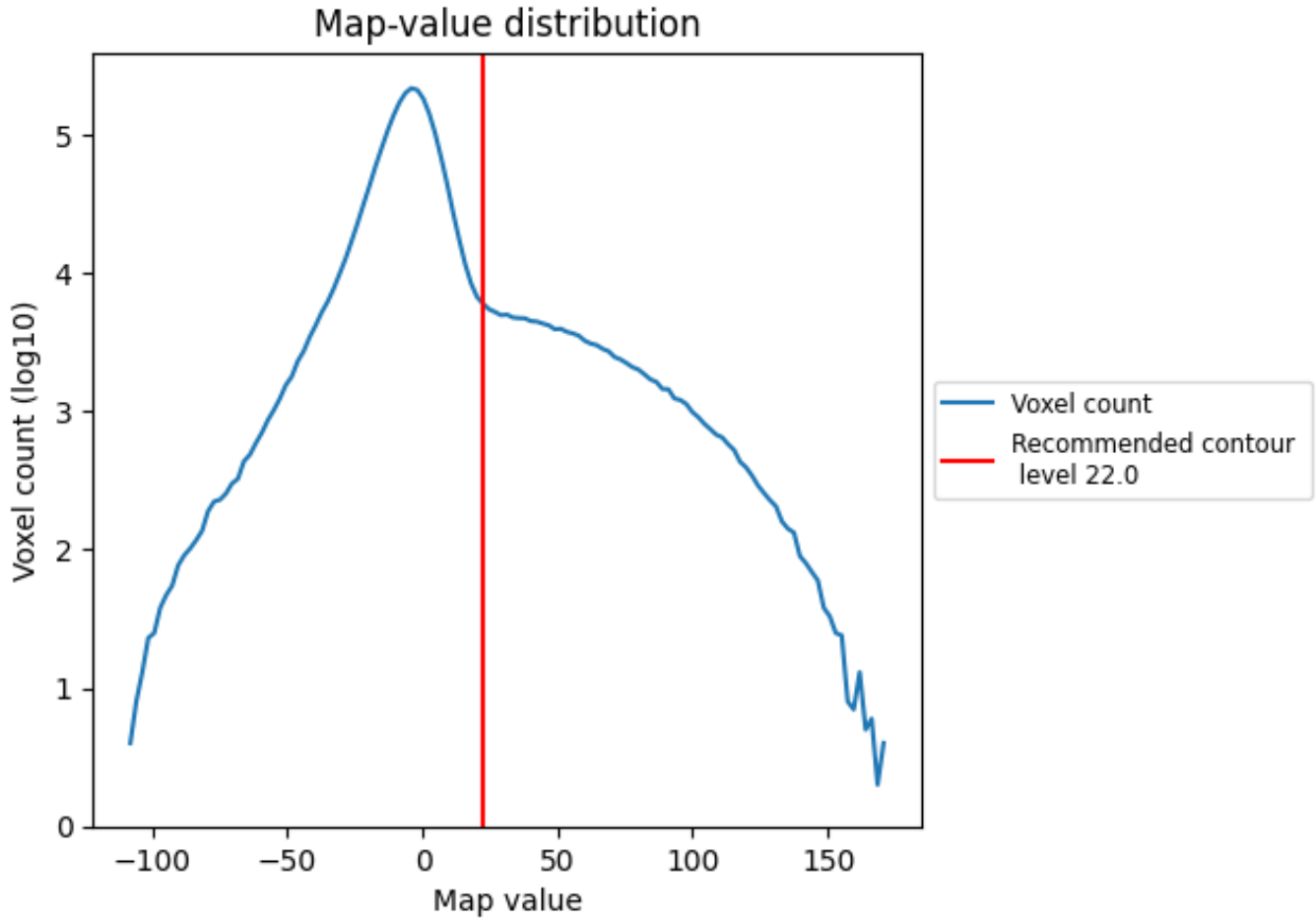
6.5 Mask visualisation (i)

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

7 Map analysis

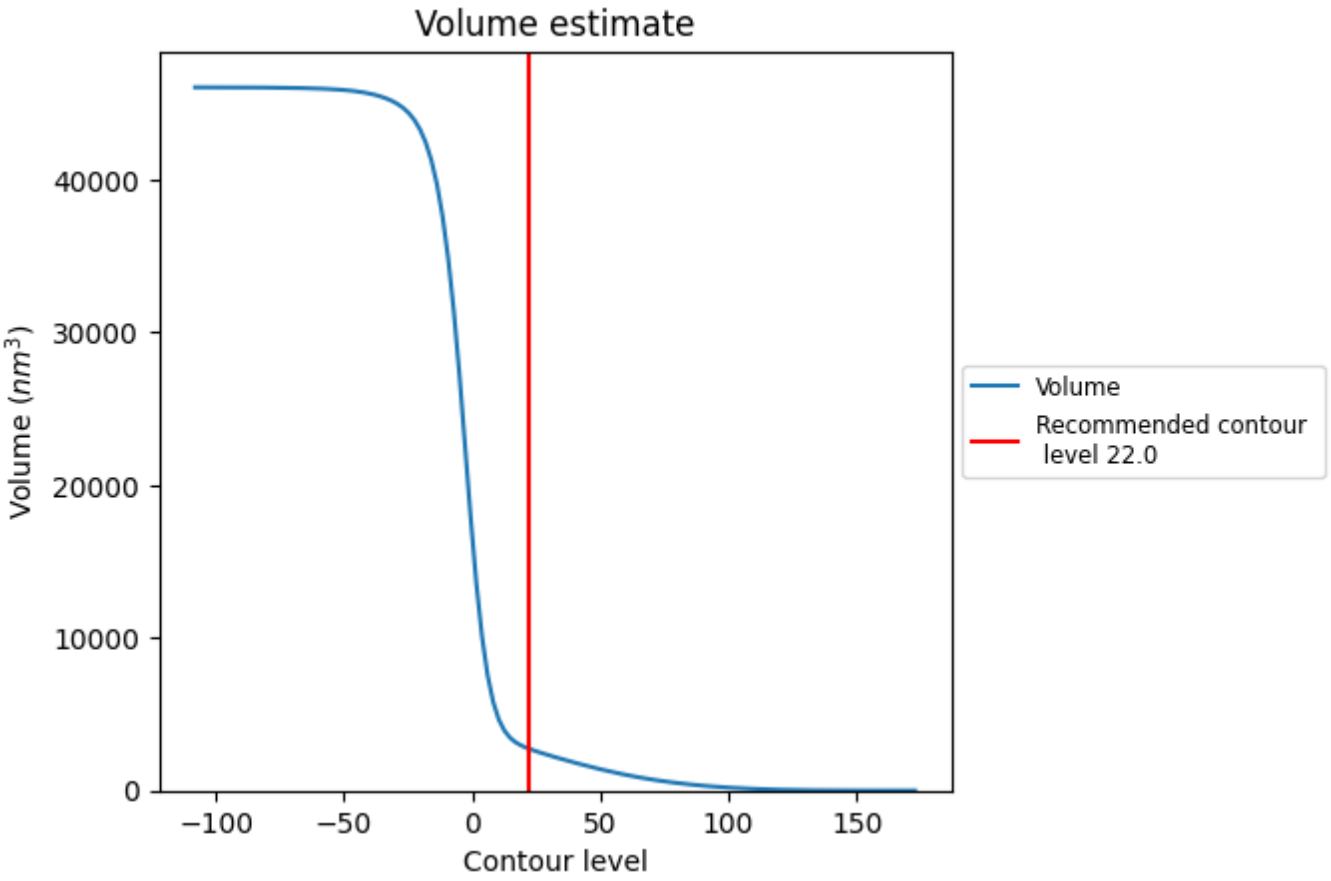
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

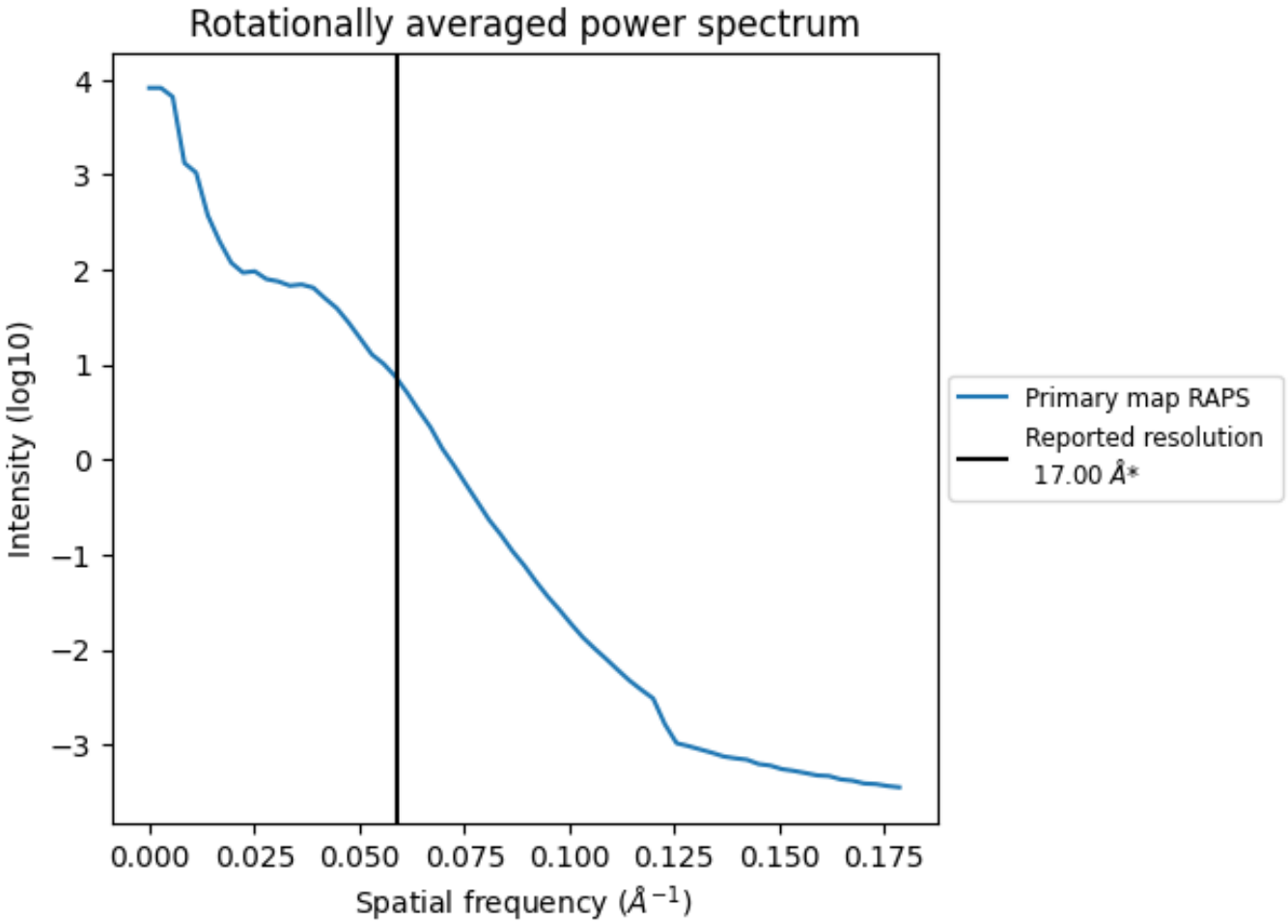
7.2 Volume estimate (i)



The volume at the recommended contour level is 2749 nm^3; this corresponds to an approximate mass of 2483 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.059 $Å^{-1}$

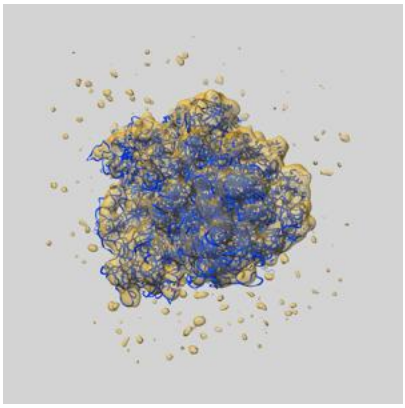
8 Fourier-Shell correlation (i)

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

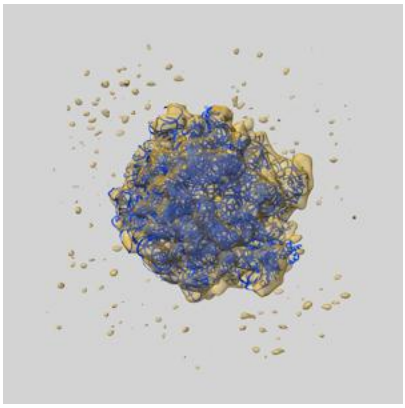
9 Map-model fit

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

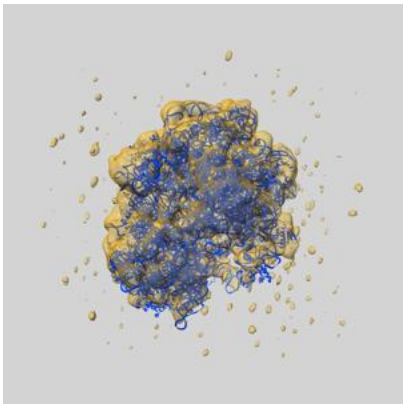
9.1 Map-model overlay



X



Y



Z

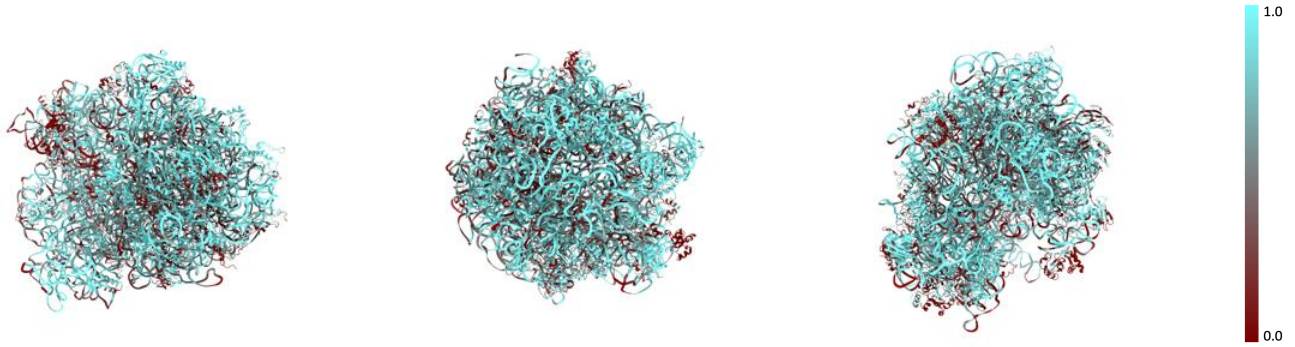
The images above show the 3D surface view of the map at the recommended contour level 22.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

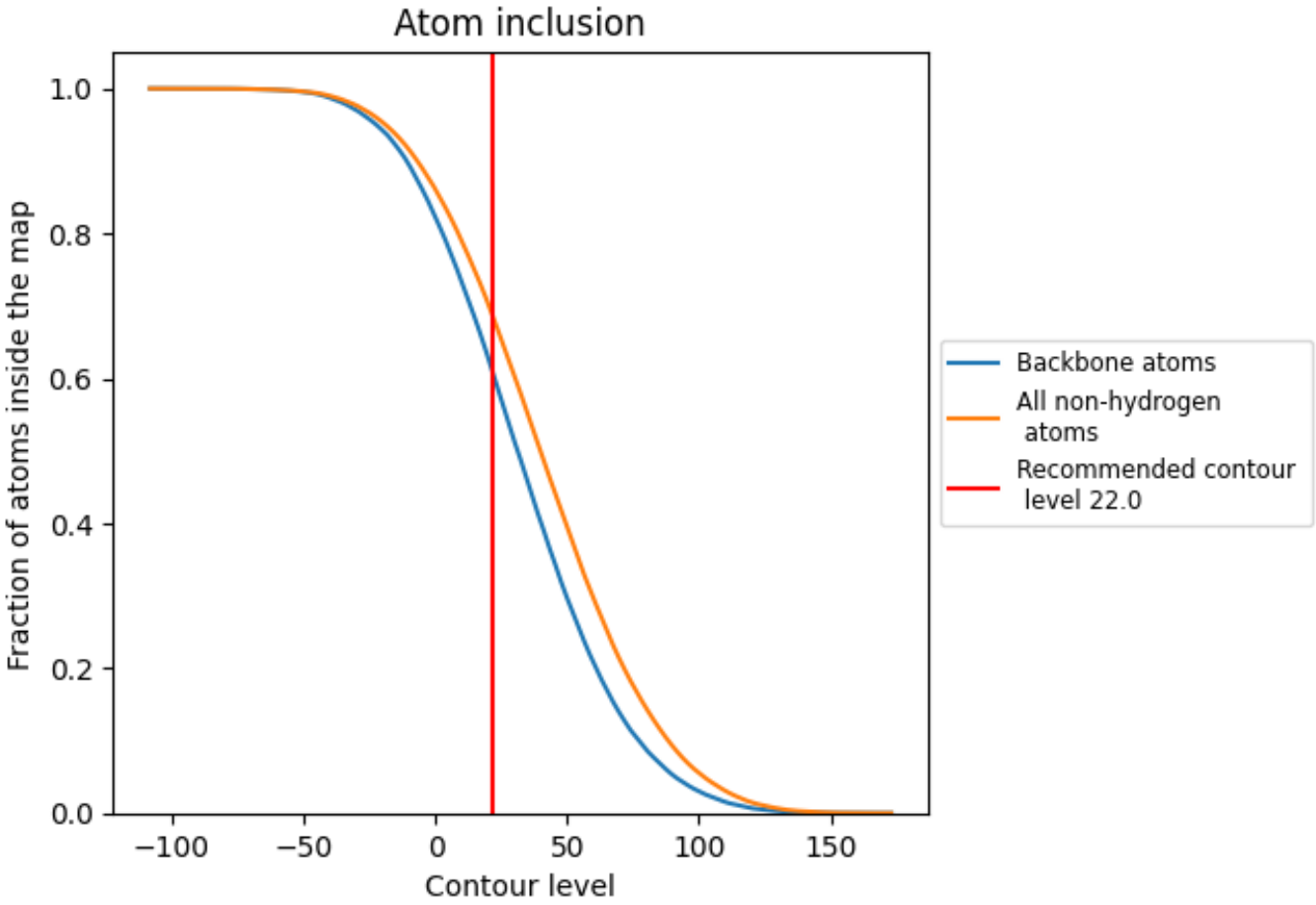
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (22.0).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (22.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6841	0.0370
A1	0.5759	0.0450
A2	0.4822	-0.0220
A3	0.5152	0.0290
AA	0.7516	0.0460
AB	0.4446	0.0190
AC	0.4725	0.0350
AD	0.4491	0.0100
AE	0.5506	0.0400
AF	0.8168	0.0540
AG	0.7096	0.0210
AH	0.5708	0.0210
AI	0.7319	0.0200
AJ	0.5131	0.0170
AK	0.6702	0.0270
AL	0.7003	0.0340
AM	0.6071	0.0290
AN	0.5879	0.0120
AO	0.6319	0.0260
AP	0.5300	0.0040
AQ	0.5402	0.0080
AR	0.6059	-0.0260
AS	0.7404	0.0290
AT	0.7301	-0.0140
AU	0.5672	-0.0090
B0	0.7009	0.0580
B1	0.7723	0.0440
B2	0.3775	-0.0020
B3	0.3768	-0.0360
B4	0.6781	0.0220
B5	0.3784	0.0000
BA	0.7388	0.0460
BB	0.7891	0.0500
BC	0.4735	0.0120
BD	0.5072	0.0100

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Chain	Atom inclusion	Q-score
BE	0.7434	0.0260
BF	0.6978	0.0560
BG	0.6353	0.0470
BH	0.3303	0.0120
BI	0.1419	0.0320
BJ	0.5145	0.0170
BK	0.5766	0.0300
BL	0.6142	-0.0030
BM	0.5585	0.0190
BN	0.5222	-0.0100
BO	0.8644	0.0310
BP	0.4820	0.0120
BQ	0.6355	0.0180
BR	0.4178	-0.0060
BS	0.5275	-0.0100
BT	0.6196	0.0130
BU	0.5065	0.0190
BV	0.7520	0.0480
BW	0.6598	0.0160
BX	0.5940	0.0040
BY	0.5412	0.0370
BZ	0.5400	0.0060