wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 11:54 PM EST

PDB ID	:	4V78
EMDB ID	:	EMD-2475
Title	:	E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post3a)
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	:	20.00 Å(reported)
Based on initial models	:	2K4C, 2HGP, 2WRI, 3I1O

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:

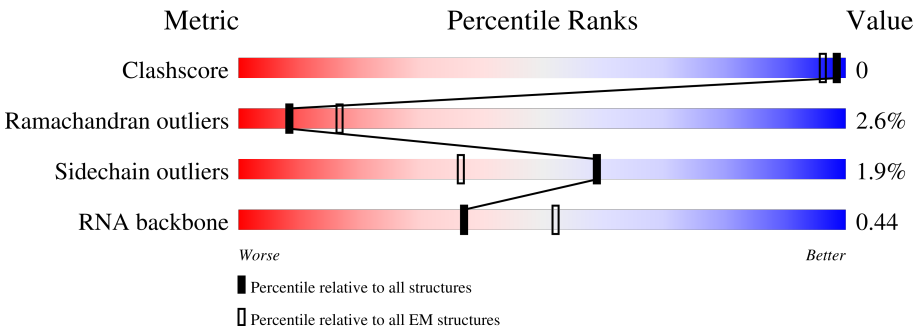
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 20.00 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	35%, 94%, 5% •
2	AC	208	37%, 87%, 12%
3	AD	206	22%, 86%, 12% •
4	AE	152	23%, 94%, 6%
5	AF	101	49%, 87%, 13%
6	AG	152	14%, 88%, 11% •
7	AH	130	8%, 92%, 8% •

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Mol	Chain	Length	Quality of chain
8	AI	128	5% 84% 16%
9	AJ	100	39% 86% 13%
10	AK	118	20% 92% 7%
11	AL	124	26% 85% 15%
12	AM	115	30% 90% 10%
13	AN	101	25% 87% 10%
14	AO	89	18% 88% 11%
15	AP	81	25% 78% 22%
16	AQ	82	37% 90% 9%
17	AR	57	42% 84% 16%
18	AS	81	56% 90% 9%
19	AT	86	20% 86% 13%
20	AU	53	8% 75% 25%
21	AA	1533	6% 23% 50% 22%
22	A1	76	33% 20% 46% 34%
23	A2	15	60% 27% 13%
24	A3	77	48% 23% 48% 23% 5%
25	BC	273	38% 89% 9%
26	BD	209	26% 90% 9%
27	BE	201	28% 89% 10%
28	BF	179	19% 89% 10%
29	BG	177	15% 89% 10%
30	BH	149	74% 95% 5%
31	BI	142	69% 95%
32	BJ	142	26% 90% 10%

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Mol	Chain	Length	Quality of chain
33	BK	123	40% 89% 11%
34	BL	144	40% 86% 12%
35	BM	136	22% 90% 9%
36	BN	121	25% 88% 11%
37	BO	117	21% 87% 11%
38	BP	115	25% 84% 15%
39	BQ	118	30% 85% 14%
40	BR	103	29% 92% 8%
41	BS	110	25% 92% 7%
42	BT	94	13% 91% 7%
43	BU	104	43% 88% 12%
44	BV	94	14% 95% 5%
45	BW	80	28% 89% 10%
46	BX	79	14% 86% 11%
47	BY	63	59% 92% 8%
48	BZ	59	31% 85% 12%
49	B0	57	28% 77% 21%
50	B1	52	27% 87% 13%
51	B2	46	59% 78% 22%
52	B3	65	37% 85% 14%
53	B4	38	16% 87% 13%
54	BA	2903	8% 22% 52% 22%
55	BB	118	17% 59% 19%
56	B5	234	63% 88% 7% 5%

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
			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
			Total	C	N	O	S		
27	BE	201	1552	974	283	290	5	0	0

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

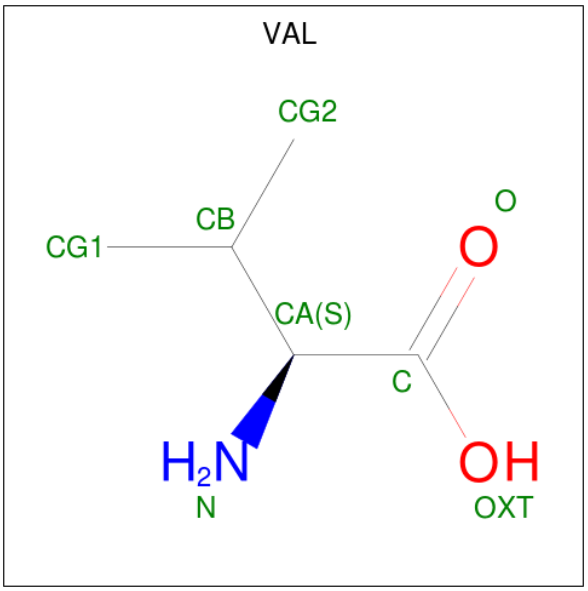
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

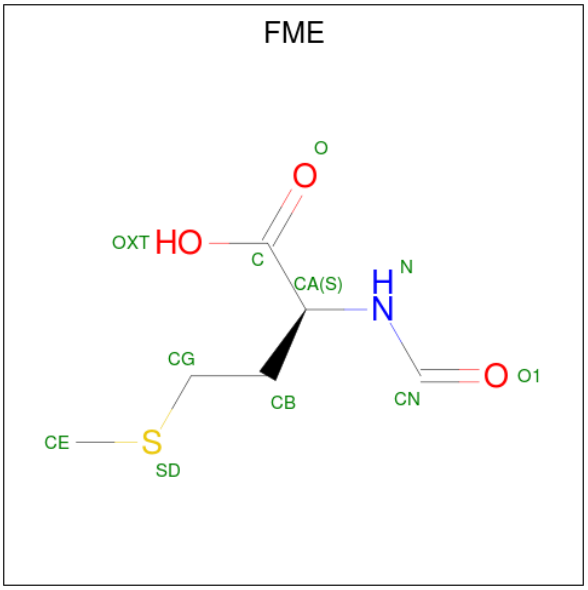
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	B5	223	1658	1038	302	312	6	0	0

- 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: $C_6H_{11}NO_3S$).



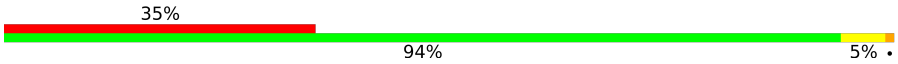
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	BA	1	10	6	1	2	1	0

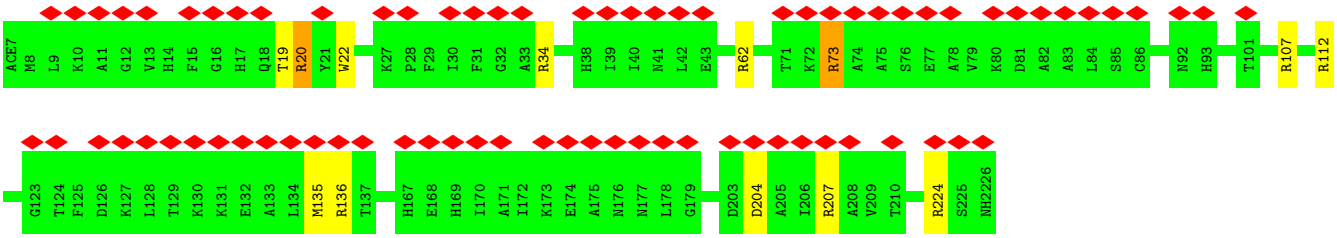
3 Residue-property plots (i)

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

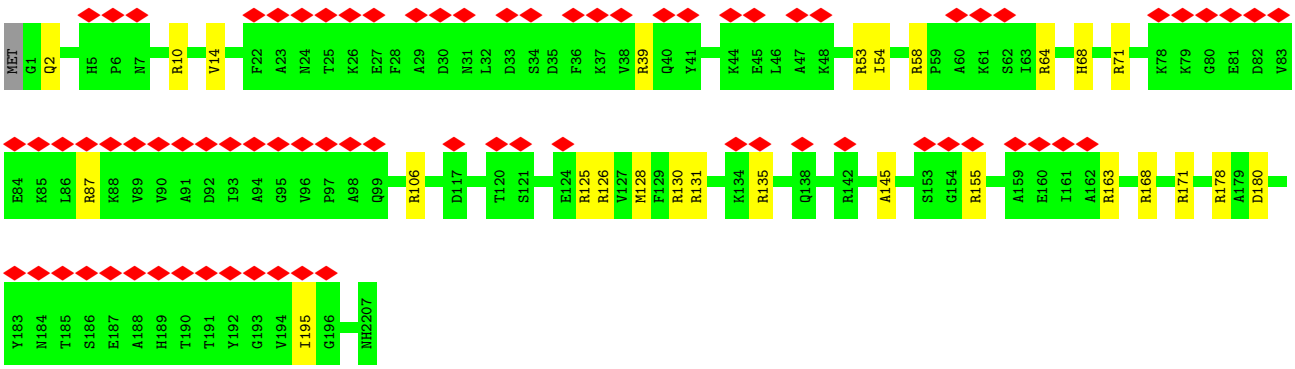
Chain AB:





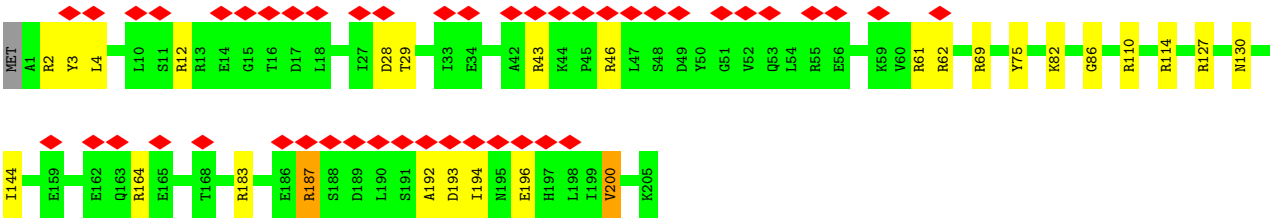
- Molecule 2: 30S ribosomal protein S3

Chain AC:



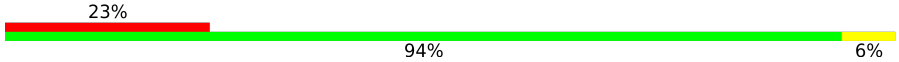
- Molecule 3: 30S ribosomal protein S4

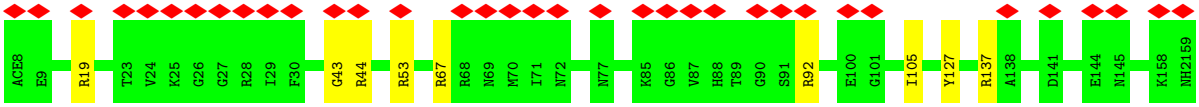
Chain AD:



- Molecule 4: 30S ribosomal protein S5

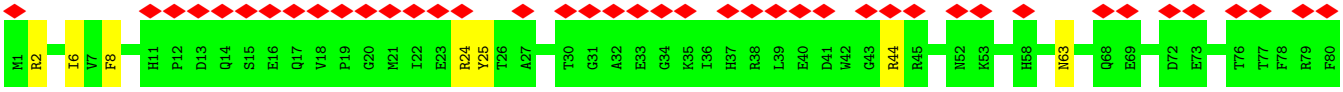
Chain AE:

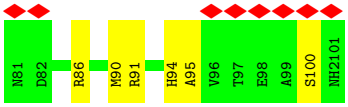




- Molecule 5: 30S ribosomal protein S6

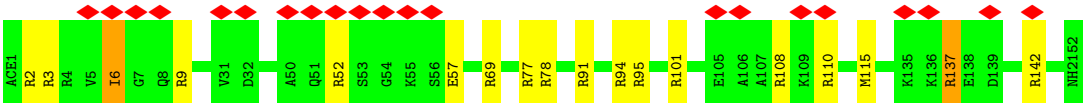
Chain AF:





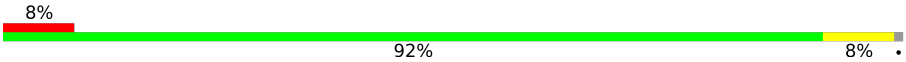
- Molecule 6: 30S ribosomal protein S7

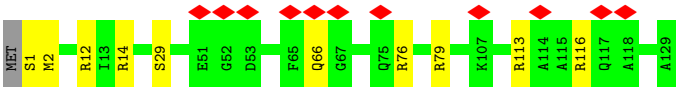
Chain AG:



- Molecule 7: 30S ribosomal protein S8

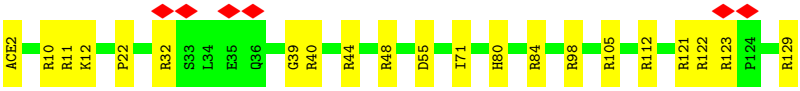
Chain AH:





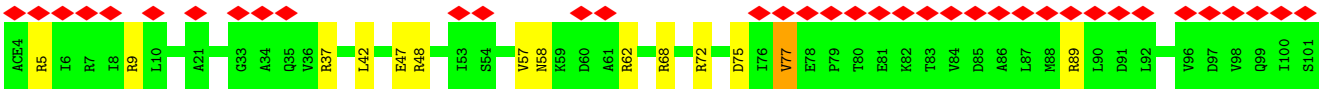
- Molecule 8: 30S ribosomal protein S9

Chain AI:



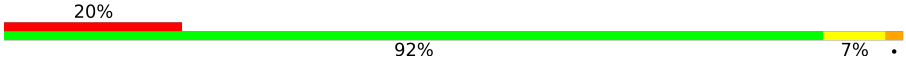
- Molecule 9: 30S ribosomal protein S10

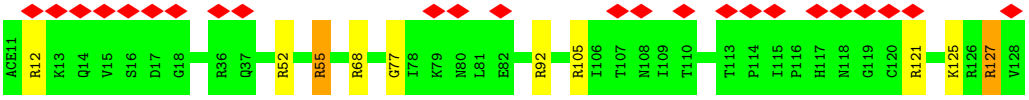
Chain AJ:



• Molecule 10: 30S ribosomal protein S11

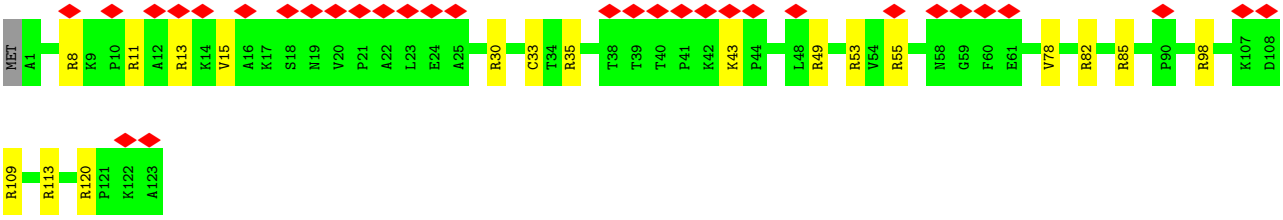
Chain AK:





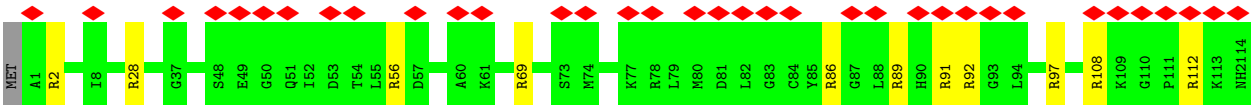
• Molecule 11: 30S ribosomal protein S12

Chain AL:



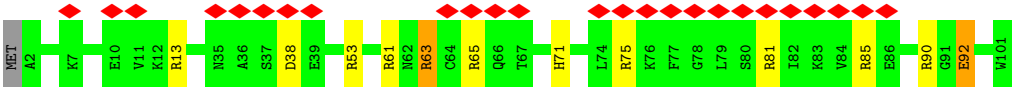
• Molecule 12: 30S ribosomal protein S13

Chain AM:



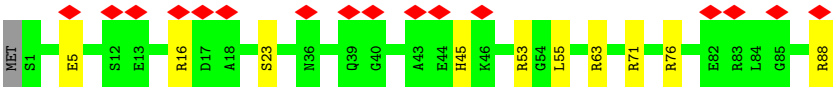
• Molecule 13: 30S ribosomal protein S14

Chain AN:



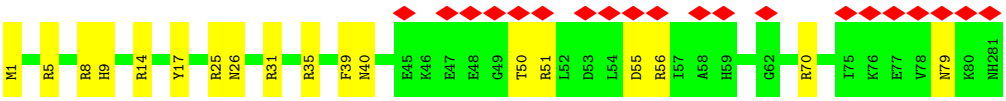
• Molecule 14: 30S ribosomal protein S15

Chain AO:



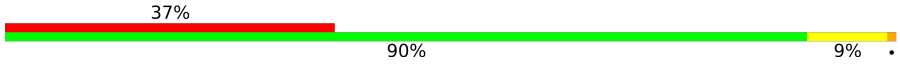
• Molecule 15: 30S ribosomal protein S16

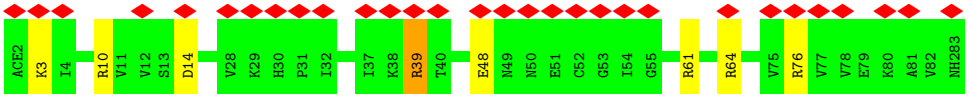
Chain AP:



• Molecule 16: 30S ribosomal protein S17

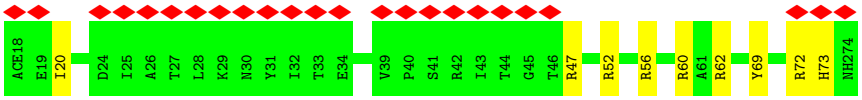
Chain AQ:





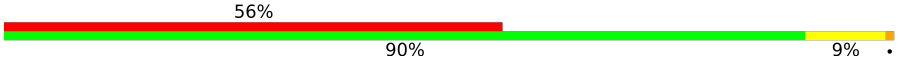
• Molecule 17: 30S ribosomal protein S18

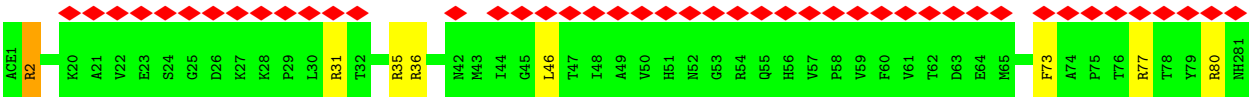
Chain AR:



• Molecule 18: 30S ribosomal protein S19

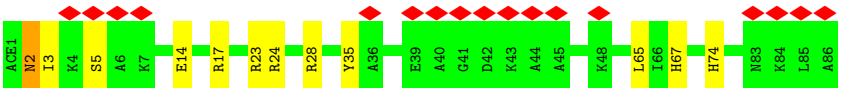
Chain AS:





• Molecule 19: 30S ribosomal protein S20

Chain AT:

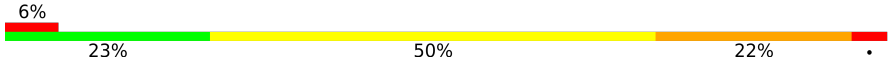


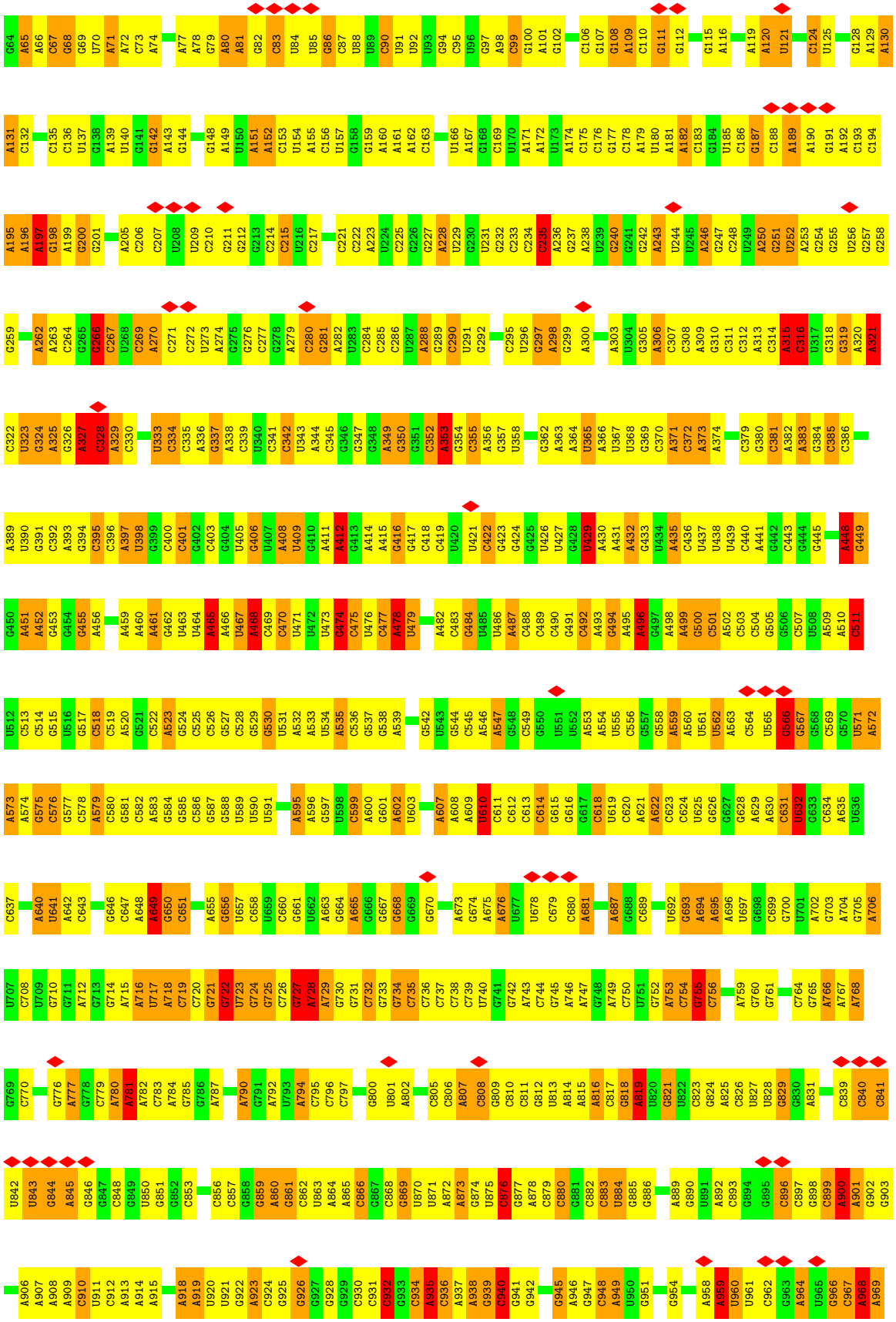
• Molecule 20: 30S ribosomal protein S21

Chain AU:

• Molecule 21: 16S ribosomal RNA

Chain AA:

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A131 C132 C135 C136 U137 G138 A139 U140 G141 G142 A143 G144 G148 A149 U150 A151 A152 C153 U154 A155 C156 U157 G158 G159 A160 A161 A162 C163 U166 A167 G168 C169 U170 A171 A172 U173 A174 C175 C176 G177 C178 A179 U180 A181 A182 C183 G184 U185 C186 G187 C188 A189 A190 G191 A192 C193 C194
A195 A196 A197 G198 A199 G200 G201 A205 C206 C207 U208 U209 C210 G211 G212 G213 C214 C215 U216 C217 C221 C222 A223 U224 C225 G226 G227 A228 U229 G230 U231 G232 C233 C234 C235 A236 G237 A238 U239 G240 G241 G242 A243 U244 U245 A246 G247 C248 U249 A250 G251 U252 A253 G254 G255 U256 G257 G258
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C322 U323 G324 A325 G326 A327 C328 A329 C330 U333 C334 C335 A336 G337 A338 C339 U340 C341 C342 U343 A344 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 G362 A363 A364 U365 A366 U367 U368 G369 C370 A371 C372 A373 A374 C379 G380 C381 A382 A383 G384 C385 C386
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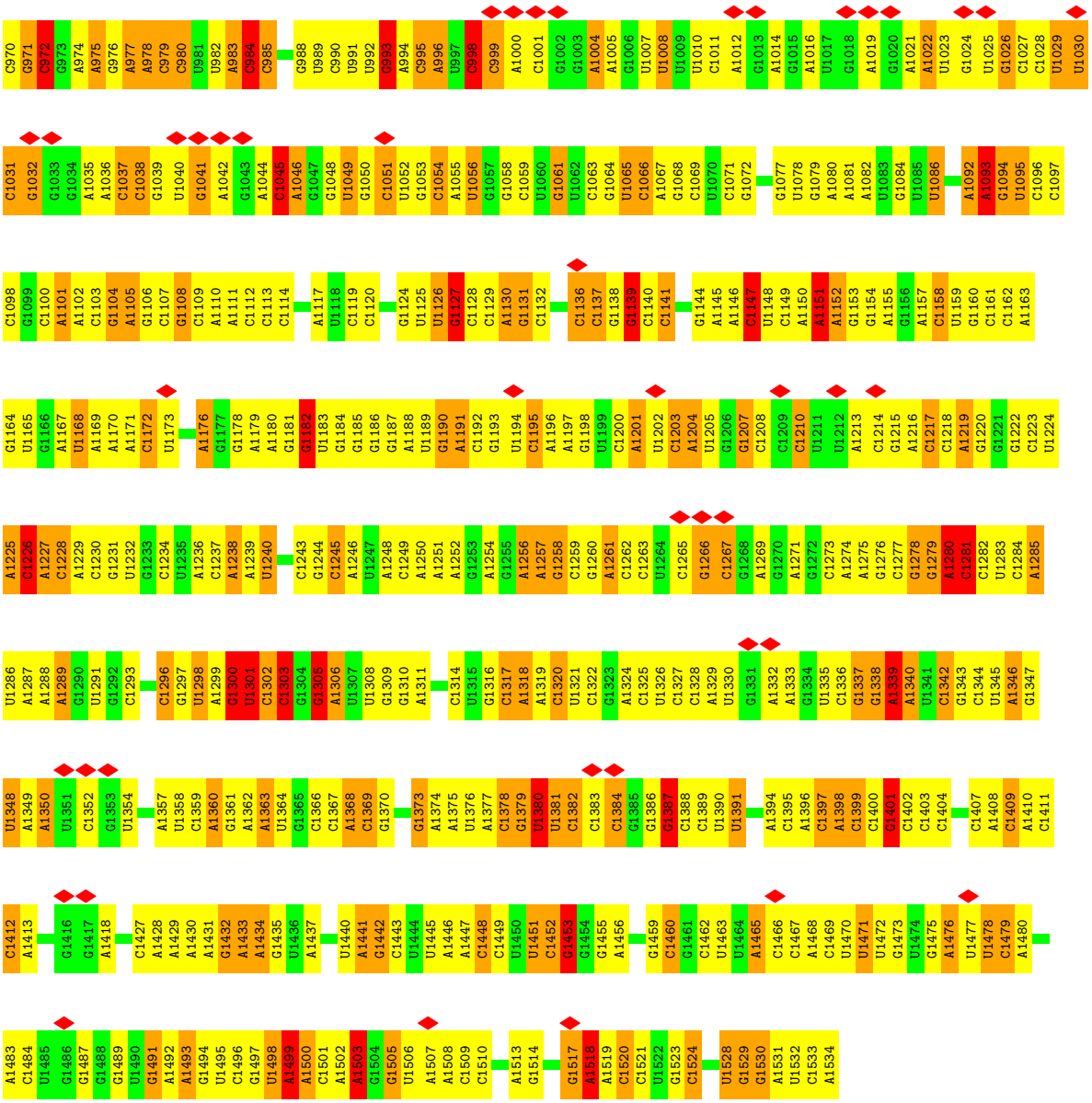


• Molecule 22: fMet-Val-tRNA-Val

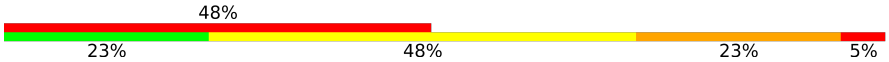
Chain A1: 33% 20% 46% 34%

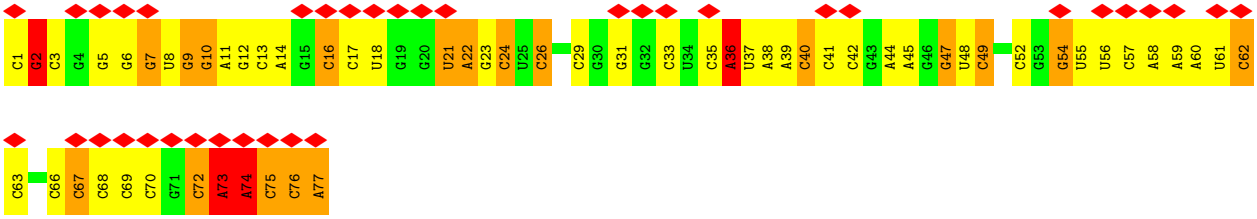
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2: 60% 27% 13%

• Molecule 24: tRNA-fMet

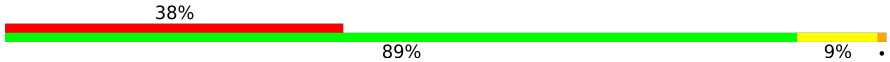
Chain A3:

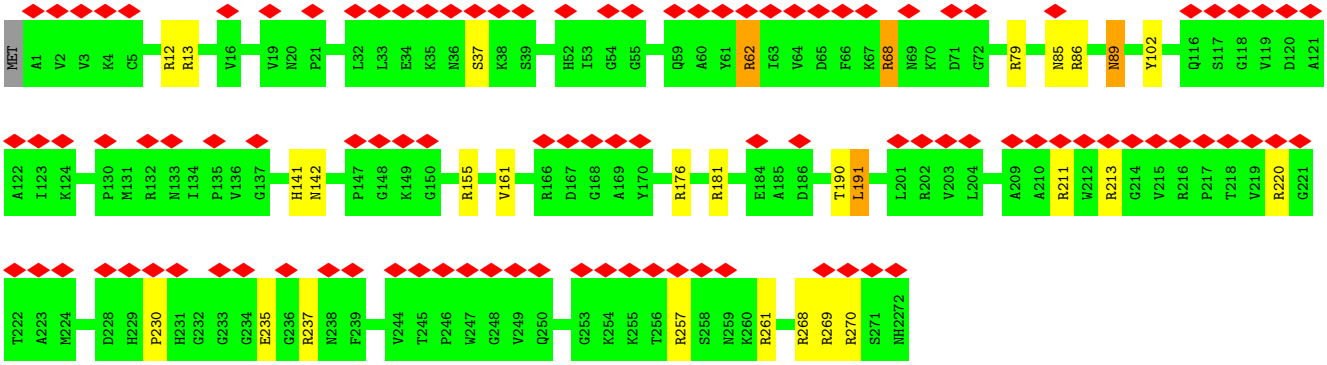




• Molecule 25: 50S ribosomal protein L2

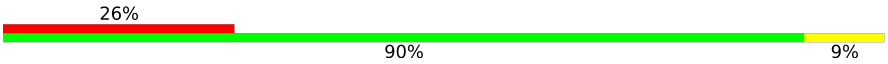
Chain BC:

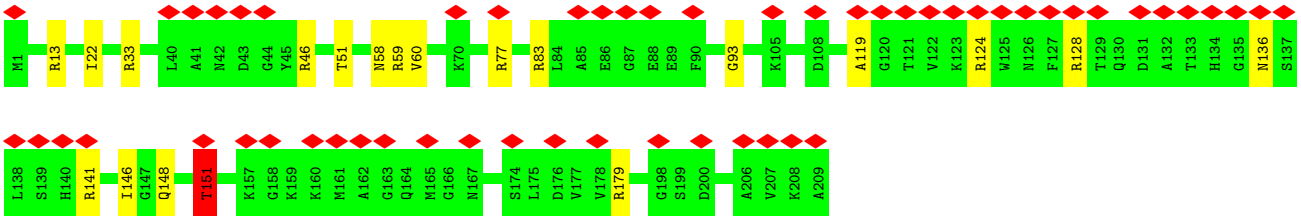




• Molecule 26: 50S ribosomal protein L3

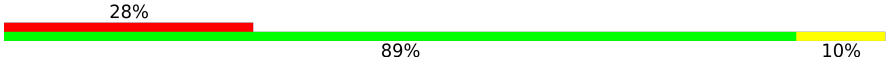
Chain BD:

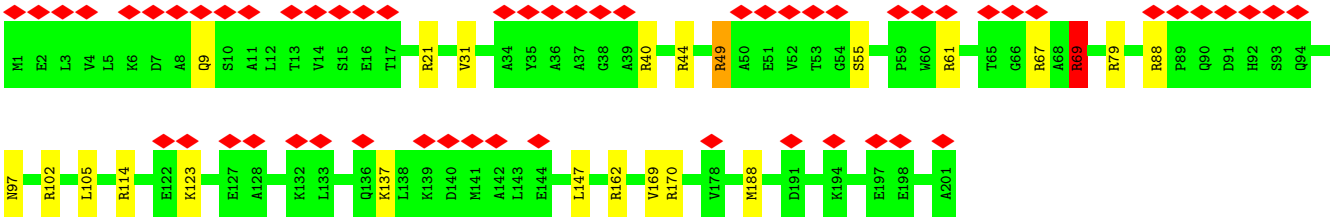




• Molecule 27: 50S ribosomal protein L4

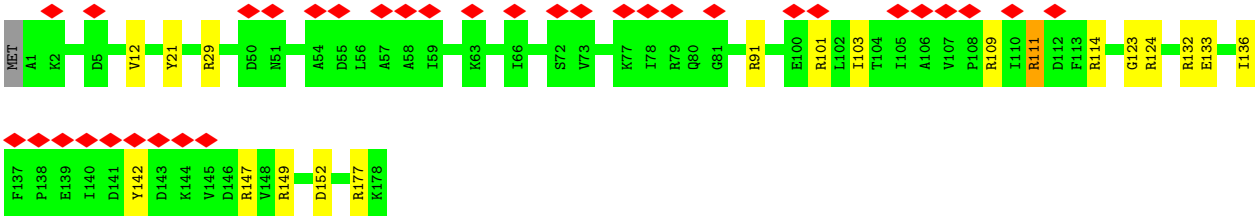
Chain BE:





• Molecule 28: 50S ribosomal protein L5

Chain BF:

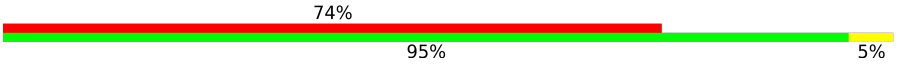


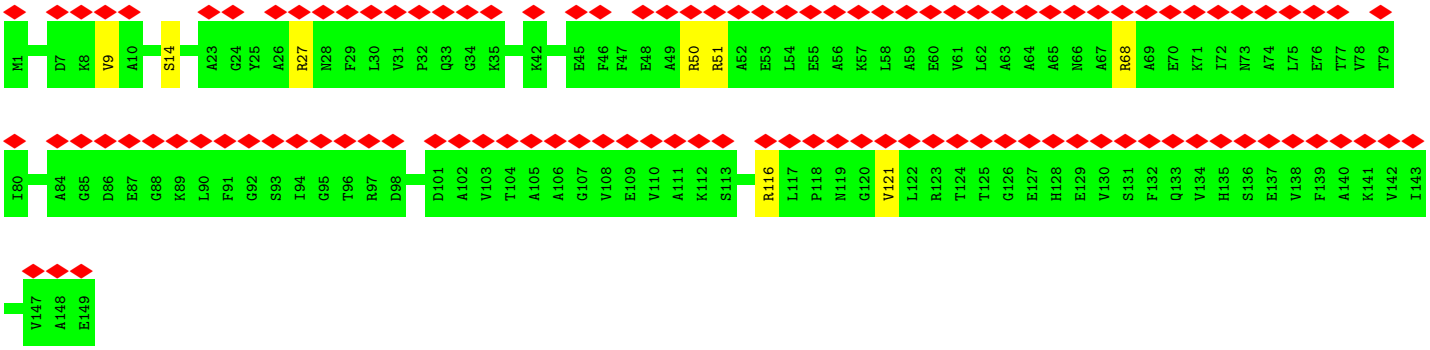
• Molecule 29: 50S ribosomal protein L6

Chain BG:

• Molecule 30: 50S ribosomal protein L9

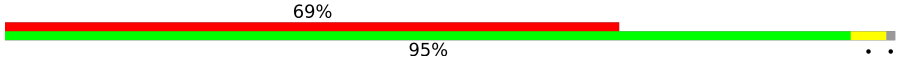
Chain BH:

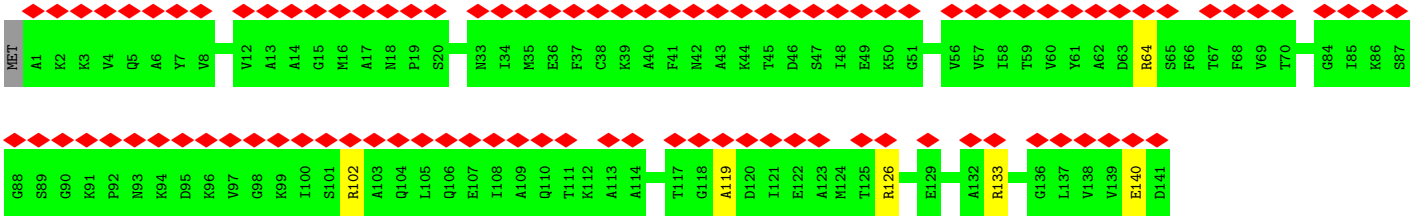




• Molecule 31: 50S ribosomal protein L11

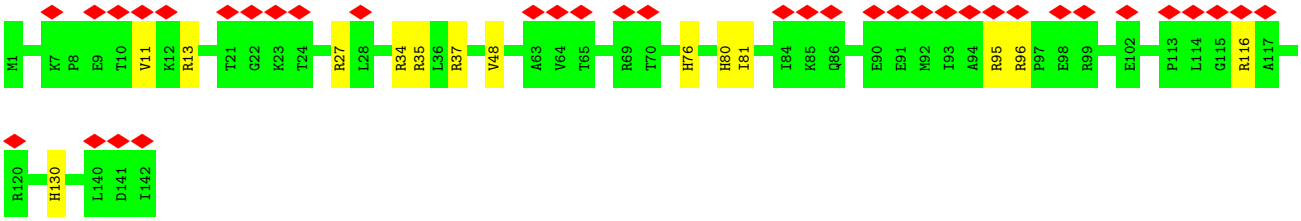
Chain BI:





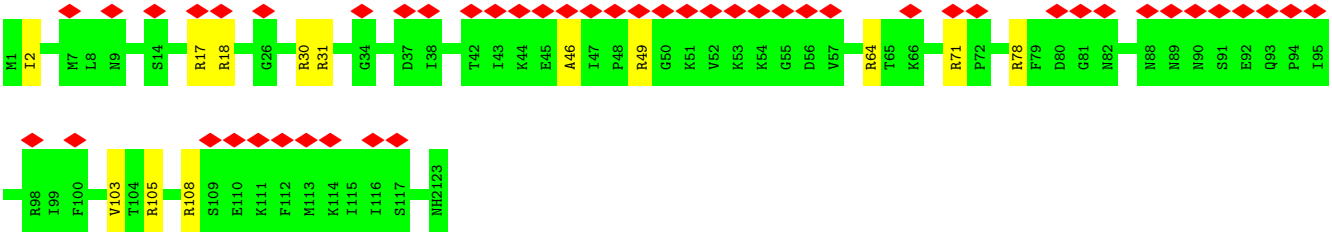
• Molecule 32: 50S ribosomal protein L13

Chain BJ: 26% 90% 10%



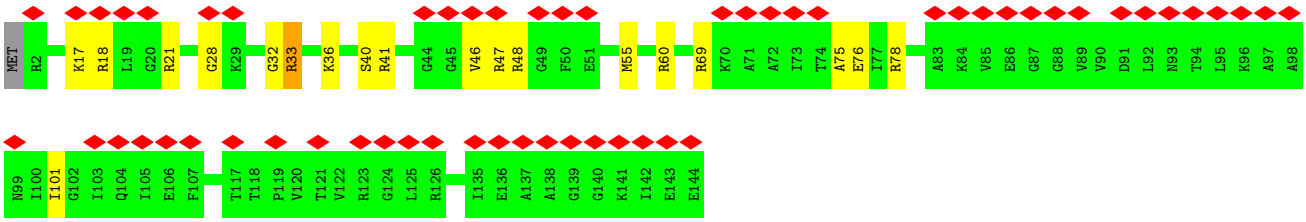
- Molecule 33: 50S ribosomal protein L14

Chain BK: 40% 89% 11%



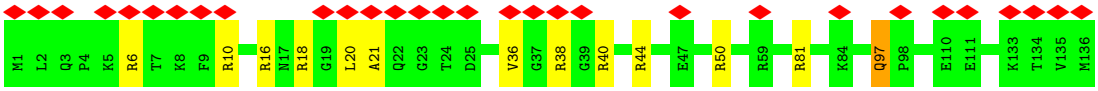
- Molecule 34: 50S ribosomal protein L15

Chain BL: 40% 86% 12%



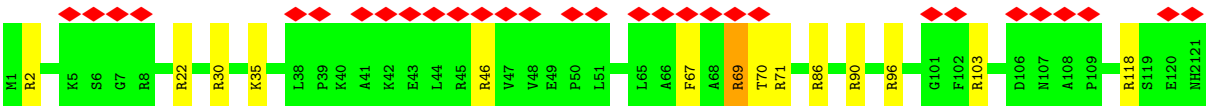
- Molecule 35: 50S ribosomal protein L16

Chain BM: 22% 90% 9%



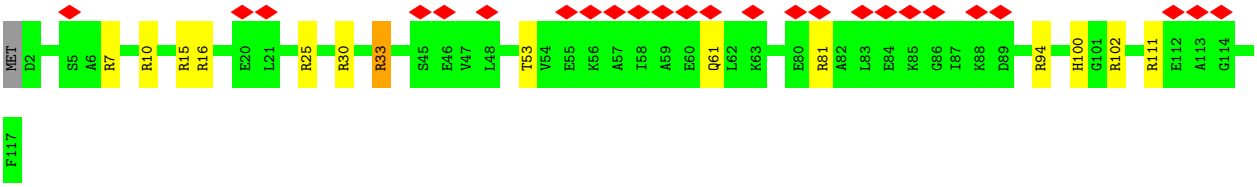
- Molecule 36: 50S ribosomal protein L17

Chain BN: 25% 88% 11%



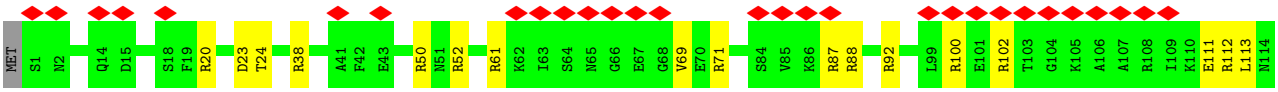
- Molecule 37: 50S ribosomal protein L18

Chain BO:



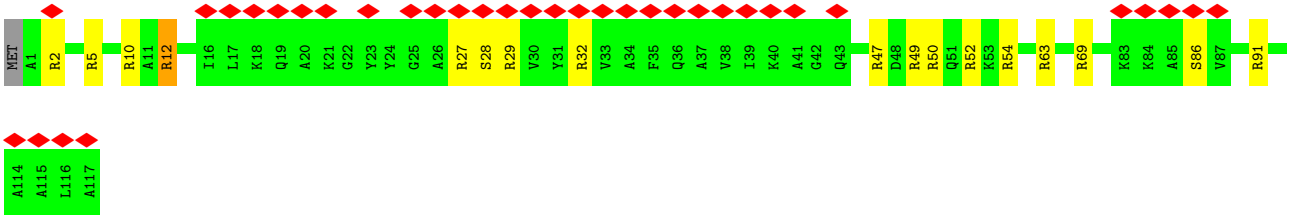
- Molecule 38: 50S ribosomal protein L19

Chain BP:



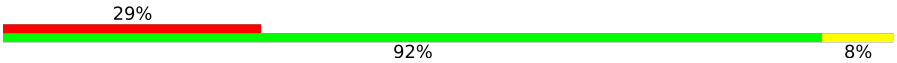
- Molecule 39: 50S ribosomal protein L20

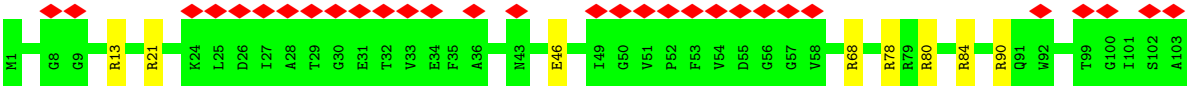
Chain BQ:



- Molecule 40: 50S ribosomal protein L21

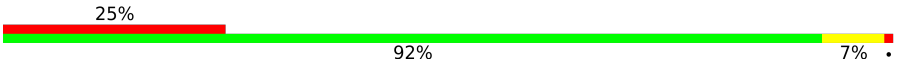
Chain BR:

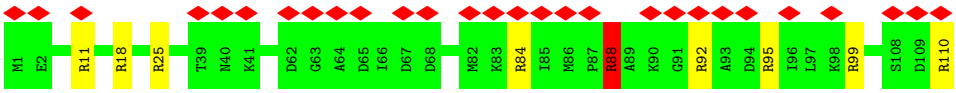




- Molecule 41: 50S ribosomal protein L22

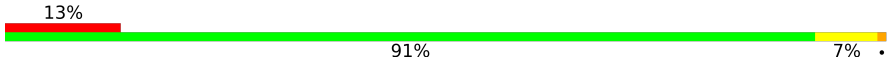
Chain BS:

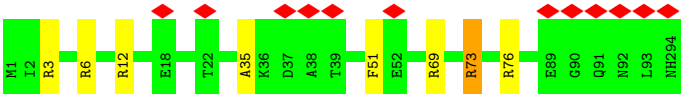




- Molecule 42: 50S ribosomal protein L23

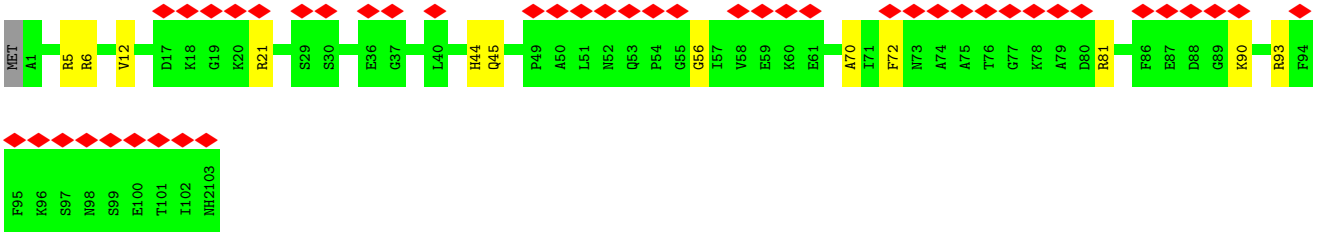
Chain BT:





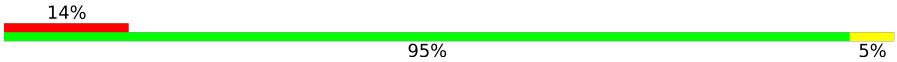
- Molecule 43: 50S ribosomal protein L24

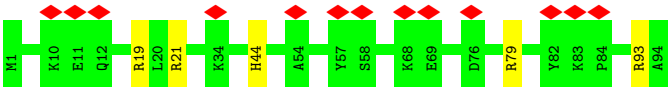
Chain BU:



- Molecule 44: 50S ribosomal protein L25

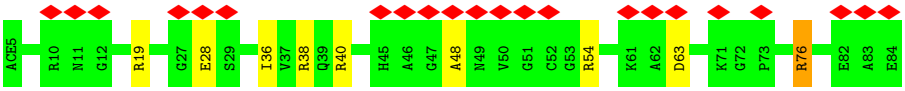
Chain BV:





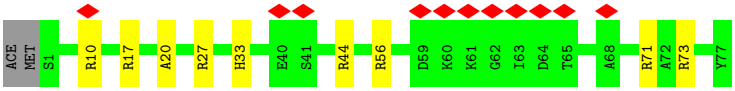
- Molecule 45: 50S ribosomal protein L27

Chain BW:



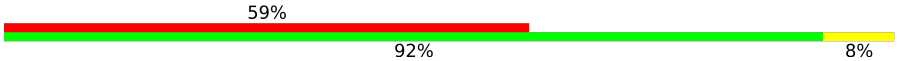
- Molecule 46: 50S ribosomal protein L28

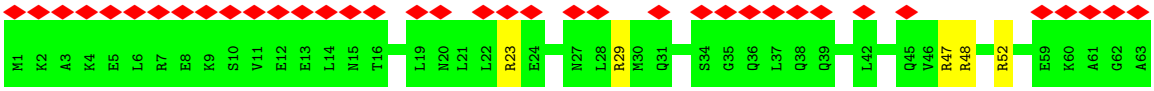
Chain BX:



- Molecule 47: 50S ribosomal protein L29

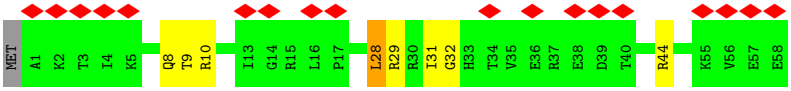
Chain BY:





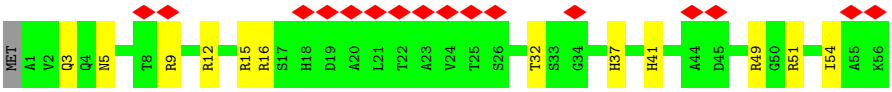
- Molecule 48: 50S ribosomal protein L30

Chain BZ:



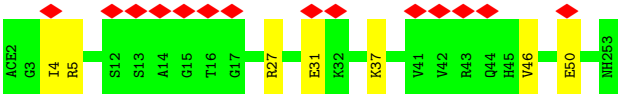
- Molecule 49: 50S ribosomal protein L32

Chain B0:



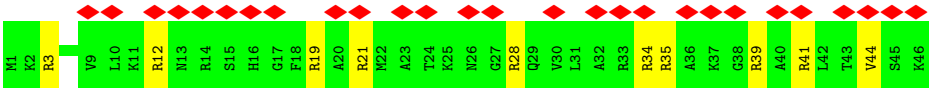
• Molecule 50: 50S ribosomal protein L33

Chain B1:



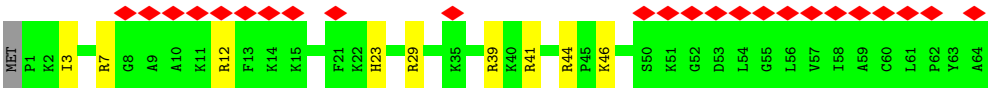
• Molecule 51: 50S ribosomal protein L34

Chain B2:



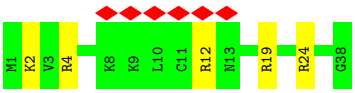
• Molecule 52: 50S ribosomal protein L35

Chain B3:



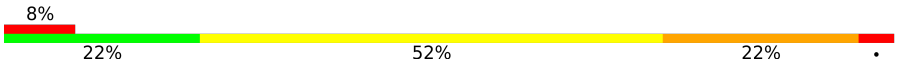
• Molecule 53: 50S ribosomal protein L36

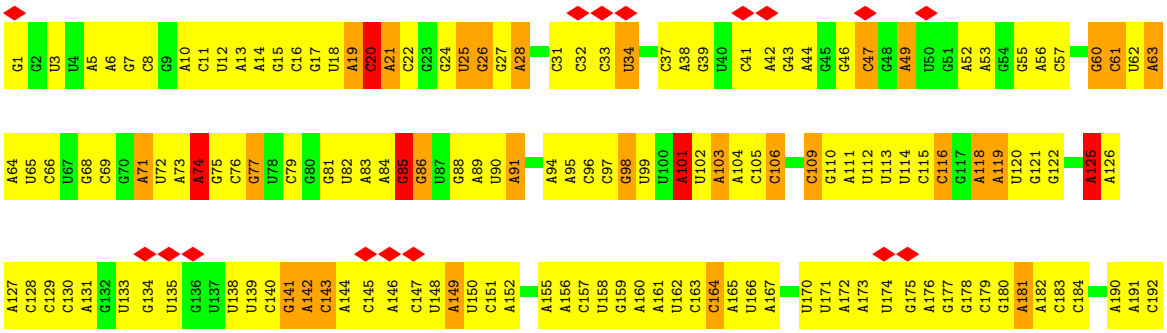
Chain B4:

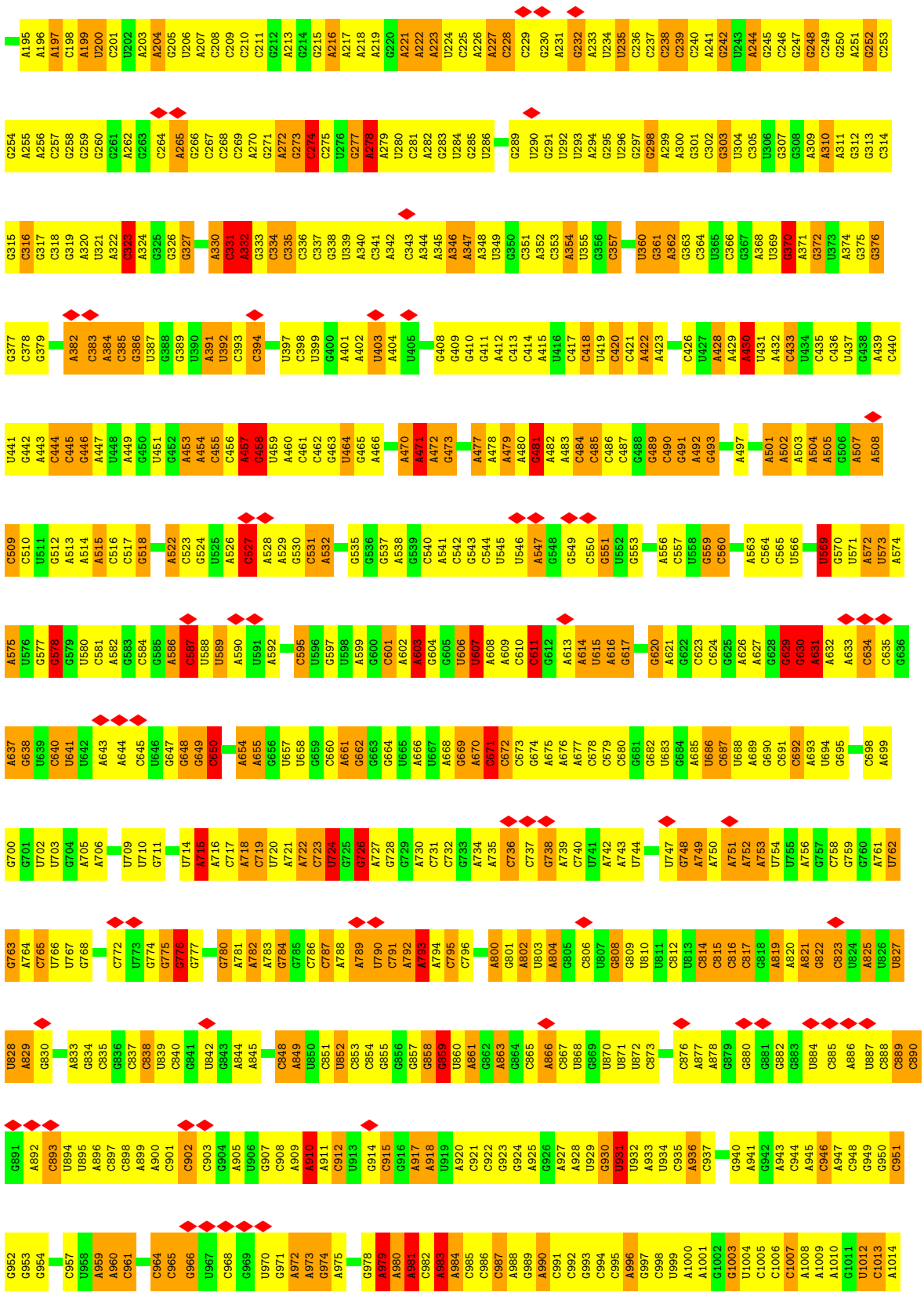


• Molecule 54: 23S ribosomal RNA

Chain BA:



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G254 A255 A256 C257 C258 G259 G260 G261 A262 G263 C264 A265 C266 C267 C268 C269 A270 C271 A272 G273 C274 C275 U276 G277 A278 A279 U280 C281 A282 C283 U284 G285 U286 G289 U290 C291 U292 U293 A294 G295 U296 G297 G298 A299 A300 G301 C302 G303 U304 C305 U306 G307 G308 A309 A310 A311 G312 G313 C314
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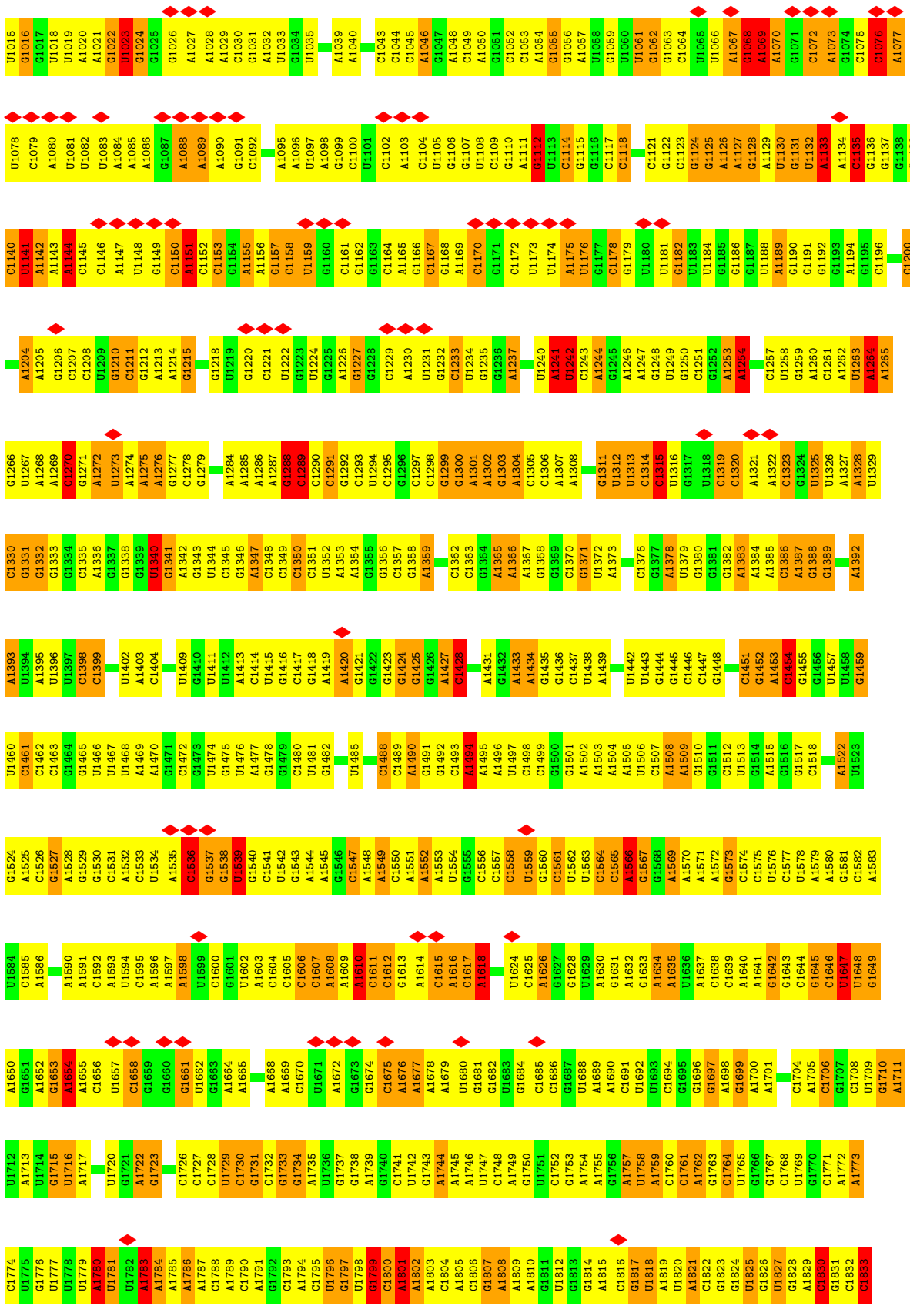
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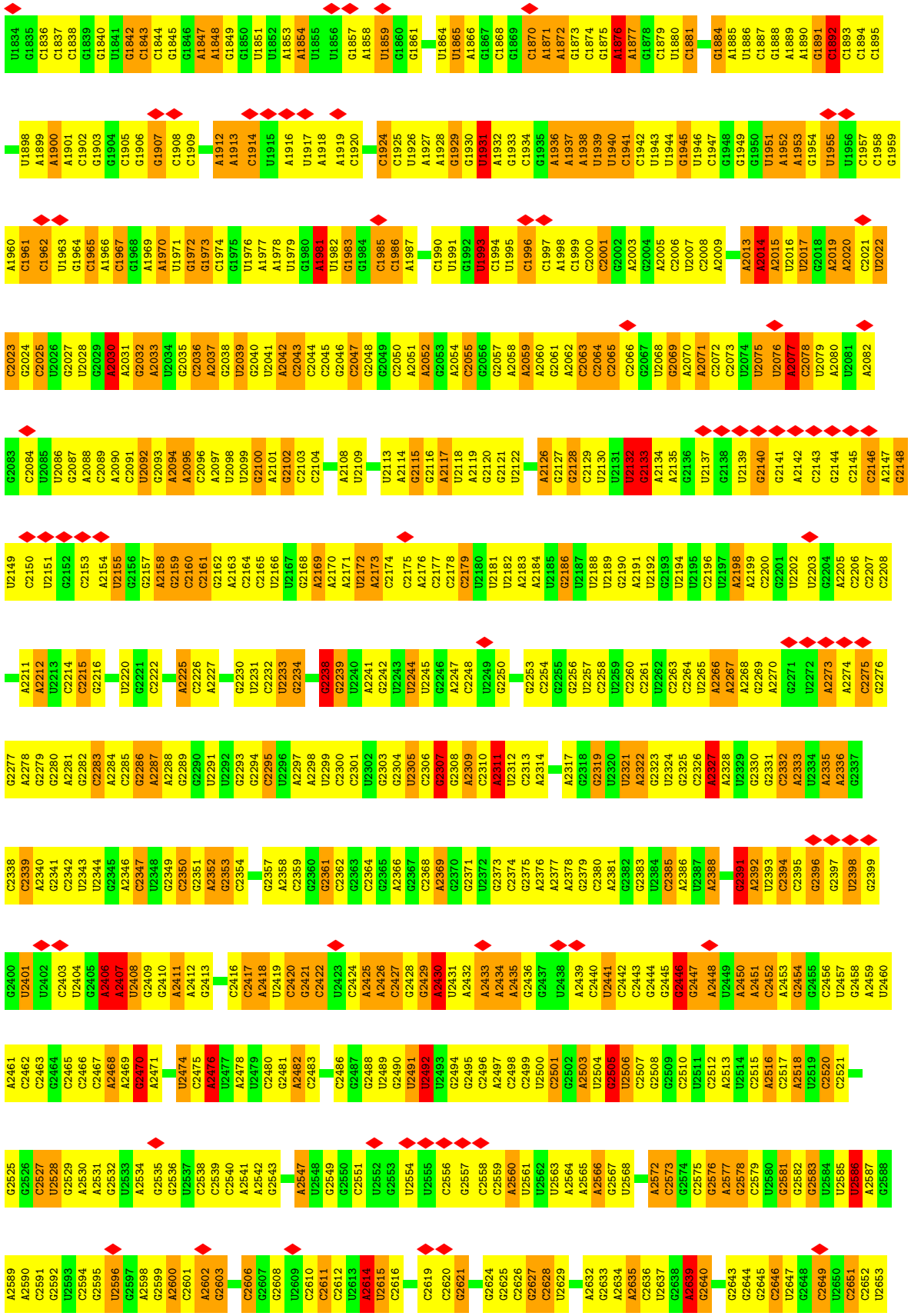
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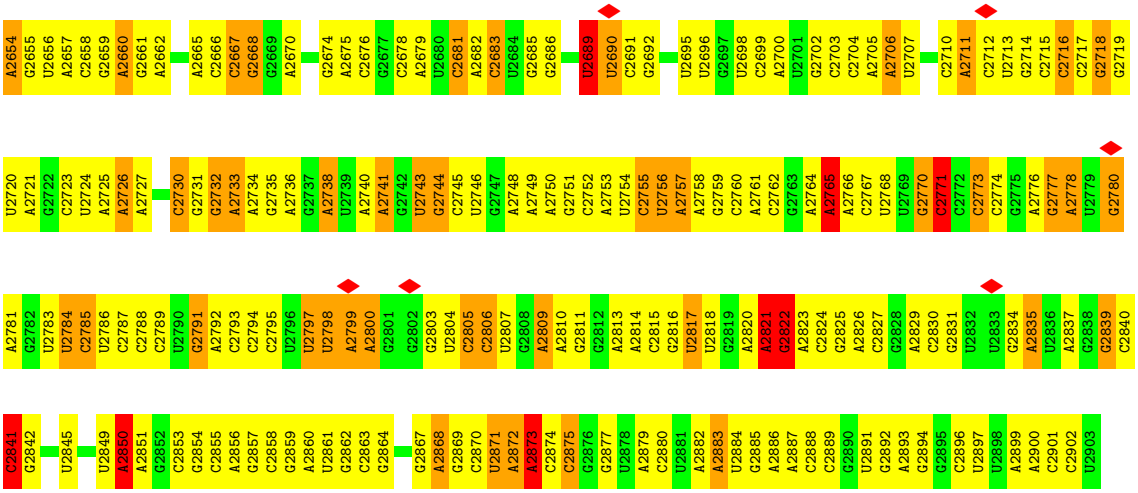
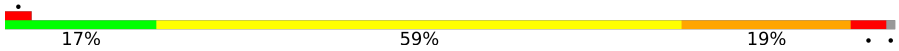
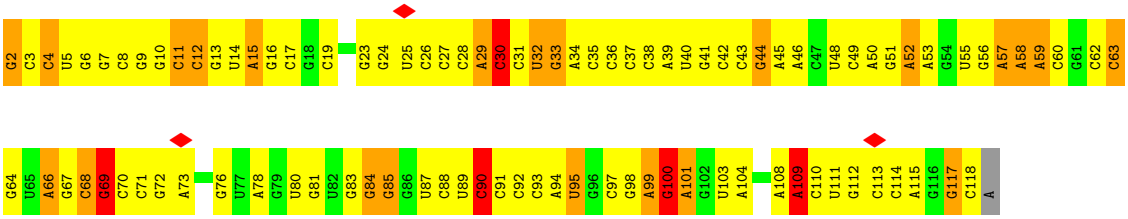


- Molecule 55: 5S ribosomal RNA

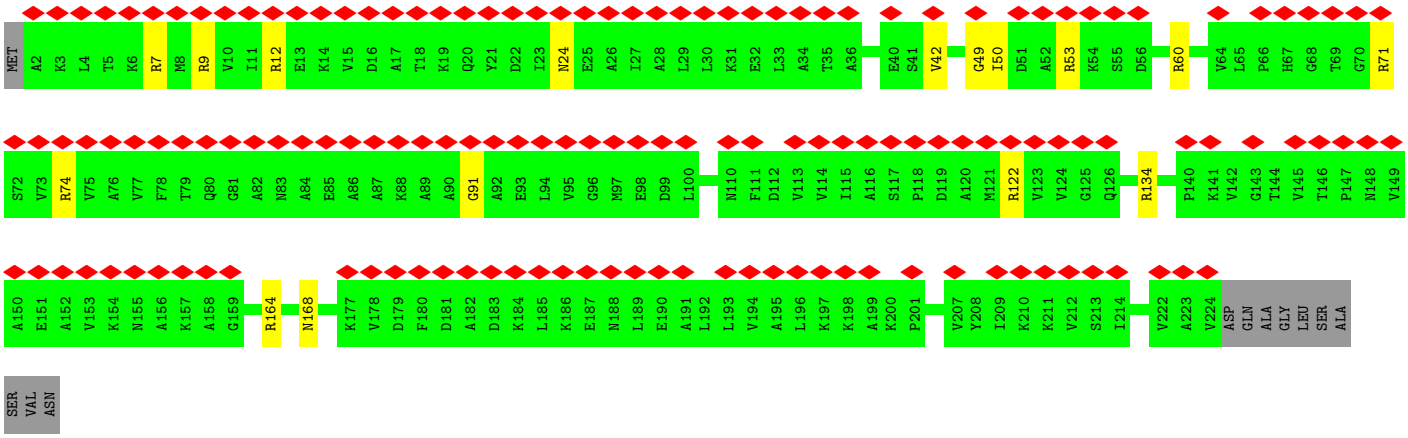
Chain BB:





- 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	5371	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 ($e^-/Å^2$)	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	222.167	Depositor
Minimum map value	-162.027	Depositor
Average map value	0.002	Depositor
Map value standard deviation	24.233	Depositor
Recommended contour level	25.0	Depositor
Map size (Å)	359.04, 359.04, 359.04	wwPDB
Map dimensions	96, 96, 96	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.74, 3.74, 3.74	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: ACE, 6MZ, FME, CM0, H2U, 5MU, PSU, 4SU, NH2, 7MG, OMC

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	0.67	0/1736	1.06	12/2340 (0.5%)
2	AC	0.70	0/1651	1.18	18/2225 (0.8%)
3	AD	0.74	0/1665	1.20	17/2227 (0.8%)
4	AE	0.66	0/1119	1.03	7/1506 (0.5%)
5	AF	0.71	0/835	1.12	7/1128 (0.6%)
6	AG	0.72	0/1188	1.27	17/1593 (1.1%)
7	AH	0.69	0/989	1.07	8/1326 (0.6%)
8	AI	0.77	0/1035	1.21	13/1377 (0.9%)
9	AJ	0.71	0/797	1.16	9/1079 (0.8%)
10	AK	0.73	0/894	1.10	8/1207 (0.7%)
11	AL	0.73	0/969	1.29	17/1300 (1.3%)
12	AM	0.72	0/884	1.36	14/1181 (1.2%)
13	AN	0.75	0/817	1.18	10/1088 (0.9%)
14	AO	0.70	0/722	1.18	7/964 (0.7%)
15	AP	0.74	0/648	1.27	11/870 (1.3%)
16	AQ	0.66	0/658	1.17	7/883 (0.8%)
17	AR	0.76	0/463	1.17	6/623 (1.0%)
18	AS	0.72	0/653	1.19	7/879 (0.8%)
19	AT	0.67	0/672	1.13	6/890 (0.7%)
20	AU	0.83	0/431	1.48	7/572 (1.2%)
21	AA	1.61	27/36759 (0.1%)	2.23	2065/57346 (3.6%)
22	A1	1.63	0/1668	2.16	80/2595 (3.1%)
23	A2	1.49	0/343	2.31	18/531 (3.4%)
24	A3	1.64	0/1722	2.26	102/2685 (3.8%)
25	BC	0.73	0/2121	1.28	21/2852 (0.7%)
26	BD	0.65	0/1586	1.19	14/2134 (0.7%)
27	BE	0.66	0/1571	1.22	14/2113 (0.7%)
28	BF	0.72	0/1444	1.18	12/1937 (0.6%)
29	BG	0.65	0/1343	1.14	9/1816 (0.5%)
30	BH	0.62	0/1122	1.08	5/1515 (0.3%)
31	BI	0.63	0/1046	1.03	4/1410 (0.3%)
32	BJ	0.71	0/1152	1.22	10/1551 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BK	0.70	0/947	1.23	10/1268 (0.8%)
34	BL	0.72	0/1054	1.29	10/1403 (0.7%)
35	BM	0.71	0/1093	1.19	9/1460 (0.6%)
36	BN	0.75	0/973	1.34	12/1301 (0.9%)
37	BO	0.71	0/902	1.27	13/1209 (1.1%)
38	BP	0.70	0/929	1.22	11/1242 (0.9%)
39	BQ	0.76	0/960	1.30	16/1278 (1.3%)
40	BR	0.68	0/829	1.18	8/1107 (0.7%)
41	BS	0.63	0/864	1.22	10/1156 (0.9%)
42	BT	0.62	0/744	1.19	7/994 (0.7%)
43	BU	0.65	0/787	1.21	6/1051 (0.6%)
44	BV	0.66	0/766	1.06	4/1025 (0.4%)
45	BW	0.71	0/604	1.26	7/799 (0.9%)
46	BX	0.72	0/635	1.28	7/848 (0.8%)
47	BY	0.65	0/510	1.24	5/677 (0.7%)
48	BZ	0.67	0/453	1.23	5/605 (0.8%)
49	B0	0.72	0/450	1.30	7/599 (1.2%)
50	B1	0.68	0/417	1.10	2/556 (0.4%)
51	B2	0.79	0/380	1.49	9/498 (1.8%)
52	B3	0.70	0/513	1.23	6/676 (0.9%)
53	B4	0.69	0/303	1.35	5/397 (1.3%)
54	BA	1.48	61/69796 (0.1%)	2.23	4183/108888 (3.8%)
55	BB	1.48	1/2800 (0.0%)	2.19	150/4367 (3.4%)
56	B5	0.62	0/1673	1.09	11/2255 (0.5%)
All	All	1.34	89/160085 (0.1%)	2.01	7075/239402 (3.0%)

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	1
10	AK	0	1
21	AA	0	374
22	A1	0	20
23	A2	0	5
24	A3	0	13
25	BC	0	1
26	BD	0	1
31	BI	0	1
35	BM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	BN	0	1
54	BA	0	623
55	BB	0	30
All	All	0	1072

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2507	C	C4-N4	-5.63	1.28	1.33
21	AA	742	G	C2-N2	-5.58	1.28	1.34
21	AA	756	C	C4-N4	-5.57	1.28	1.33
54	BA	2164	C	C4-N4	-5.44	1.29	1.33
21	AA	984	C	C4-N4	-5.43	1.29	1.33

The worst 5 of 7075 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1617	C	N3-C2-O2	-16.02	110.69	121.90
54	BA	640	C	N3-C2-O2	-15.80	110.84	121.90
24	A3	73	A	N1-C6-N6	-13.57	110.46	118.60
54	BA	1847	A	N1-C6-N6	-13.18	110.69	118.60
54	BA	323	C	O4'-C1'-N1	12.86	118.49	108.20

There are no chirality outliers.

5 of 1072 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	25	C	Sidechain
21	AA	26	A	Sidechain
21	AA	5	U	Sidechain
3	AD	75	TYR	Sidechain
10	AK	127	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	1	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	1	0
9	AJ	790	0	832	0	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	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16457	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	839	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	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	31205	8	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	99454	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)
54:BA:1068:G:H1'	54:BA:1069:A:C6	2.45	0.51
54:BA:1131:G:C5	54:BA:2025:C:H4'	2.50	0.46
22:A1:53:G:C8	22:A1:54:5MU:H72	2.50	0.46
18:AS:46:LEU:H	18:AS:46:LEU:HD23	1.81	0.46
3:AD:86:GLY:H	3:AD:200:VAL:HG23	1.81	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%)	200 (92%)	15 (7%)	3 (1%)	11	46
2	AC	205/208 (99%)	188 (92%)	12 (6%)	5 (2%)	6	33
3	AD	203/206 (98%)	190 (94%)	7 (3%)	6 (3%)	4	28
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	7	38
5	AF	99/101 (98%)	83 (84%)	12 (12%)	4 (4%)	3	23
6	AG	150/152 (99%)	133 (89%)	14 (9%)	3 (2%)	7	38
7	AH	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
8	AI	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	6	33
9	AJ	98/100 (98%)	87 (89%)	6 (6%)	5 (5%)	2	19
10	AK	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	42
11	AL	121/124 (98%)	109 (90%)	8 (7%)	4 (3%)	4	26
12	AM	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
13	AN	98/101 (97%)	86 (88%)	9 (9%)	3 (3%)	4	27
14	AO	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6	34
15	AP	79/81 (98%)	64 (81%)	9 (11%)	6 (8%)	1	13
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	12	48
17	AR	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	8	40
18	AS	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	12	48
19	AT	84/86 (98%)	75 (89%)	5 (6%)	4 (5%)	2	21
20	AU	51/53 (96%)	34 (67%)	13 (26%)	4 (8%)	1	13
25	BC	270/273 (99%)	241 (89%)	21 (8%)	8 (3%)	4	28
26	BD	207/209 (99%)	181 (87%)	18 (9%)	8 (4%)	3	23
27	BE	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	2	22
28	BF	176/179 (98%)	151 (86%)	20 (11%)	5 (3%)	5	30
29	BG	174/177 (98%)	151 (87%)	16 (9%)	7 (4%)	3	23
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	11	46
31	BI	139/142 (98%)	128 (92%)	10 (7%)	1 (1%)	22	63
32	BJ	140/142 (99%)	123 (88%)	14 (10%)	3 (2%)	7	36
33	BK	121/123 (98%)	104 (86%)	13 (11%)	4 (3%)	4	26
34	BL	141/144 (98%)	110 (78%)	23 (16%)	8 (6%)	1	18
35	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	6	35
36	BN	119/121 (98%)	102 (86%)	16 (13%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
38	BP	112/115 (97%)	96 (86%)	12 (11%)	4 (4%)	3	25
39	BQ	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	17	57
40	BR	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
41	BS	108/110 (98%)	95 (88%)	12 (11%)	1 (1%)	17	57
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	6	35
43	BU	101/104 (97%)	83 (82%)	13 (13%)	5 (5%)	2	20
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	63 (81%)	11 (14%)	4 (5%)	2	19
46	BX	75/79 (95%)	68 (91%)	5 (7%)	2 (3%)	5	31
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	50 (89%)	3 (5%)	3 (5%)	2	19
49	B0	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	3	24
50	B1	50/52 (96%)	42 (84%)	4 (8%)	4 (8%)	1	12
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6	34
52	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	26
53	B4	36/38 (95%)	27 (75%)	8 (22%)	1 (3%)	5	30
56	B5	221/234 (94%)	207 (94%)	11 (5%)	3 (1%)	11	46
All	All	5876/6008 (98%)	5232 (89%)	490 (8%)	154 (3%)	8	31

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	73	ARG
2	AC	14	VAL
3	AD	82	LYS
9	AJ	77	VAL
15	AP	79	ASN

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%)	178 (99%)	2 (1%)	73	84
2	AC	170/171 (99%)	169 (99%)	1 (1%)	86	92
3	AD	172/173 (99%)	167 (97%)	5 (3%)	42	64
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%)	121 (98%)	2 (2%)	62	79
7	AH	104/105 (99%)	101 (97%)	3 (3%)	42	64
8	AI	105/105 (100%)	101 (96%)	4 (4%)	33	57
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	50	70
10	AK	90/90 (100%)	89 (99%)	1 (1%)	73	84
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	49	69
14	AO	76/77 (99%)	74 (97%)	2 (3%)	46	66
15	AP	65/65 (100%)	62 (95%)	3 (5%)	27	52
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	44	65
17	AR	48/48 (100%)	46 (96%)	2 (4%)	30	54
18	AS	70/70 (100%)	69 (99%)	1 (1%)	67	80
19	AT	65/65 (100%)	62 (95%)	3 (5%)	27	52
20	AU	44/44 (100%)	42 (96%)	2 (4%)	27	52
25	BC	216/217 (100%)	211 (98%)	5 (2%)	50	70
26	BD	164/164 (100%)	162 (99%)	2 (1%)	71	83
27	BE	165/165 (100%)	160 (97%)	5 (3%)	41	63
28	BF	149/150 (99%)	146 (98%)	3 (2%)	55	74
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%)	113 (97%)	3 (3%)	46	66
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	55	74
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%)	97 (97%)	3 (3%)	41	63
37	BO	86/87 (99%)	82 (95%)	4 (5%)	26	51
38	BP	99/100 (99%)	95 (96%)	4 (4%)	31	55
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	52	71
40	BR	84/84 (100%)	83 (99%)	1 (1%)	71	83
41	BS	93/93 (100%)	92 (99%)	1 (1%)	73	84
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	49	69
44	BV	78/78 (100%)	77 (99%)	1 (1%)	69	81
45	BW	59/59 (100%)	58 (98%)	1 (2%)	60	78
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%)	46 (96%)	2 (4%)	30	54
49	B0	47/48 (98%)	43 (92%)	4 (8%)	10	33
50	B1	45/45 (100%)	44 (98%)	1 (2%)	52	71
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	50 (98%)	1 (2%)	55	74
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	71	83
All	All	4842/4870 (99%)	4750 (98%)	92 (2%)	59	75

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	BJ	76	HIS
38	BP	50	ARG
32	BJ	130	HIS
36	BN	69	ARG
39	BQ	28	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	AC	184	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	254 (16%)	77 (5%)
22	A1	73/76 (96%)	10 (13%)	3 (4%)
23	A2	14/15 (93%)	8 (57%)	5 (35%)
24	A3	76/77 (98%)	15 (19%)	5 (6%)
54	BA	2902/2903 (99%)	474 (16%)	117 (4%)
55	BB	116/118 (98%)	18 (15%)	2 (1%)
All	All	4710/4722 (99%)	779 (16%)	209 (4%)

5 of 779 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	15	G
21	AA	16	A
21	AA	22	G

5 of 209 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	670	A
54	BA	1288	G
54	BA	2602	A
54	BA	804	A
54	BA	1076	C

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	0.70	0	28,32,35	1.28	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	5MU	A1	54	22	19,22,23	0.79	0	28,32,35	1.34	4 (14%)
22	4SU	A1	7	22	18,21,22	1.34	1 (5%)	26,30,33	0.88	1 (3%)
22	CM0	A1	34	22	22,26,27	1.29	1 (4%)	28,37,40	1.35	2 (7%)
24	OMC	A3	33	24	19,22,23	0.79	0	26,31,34	0.96	1 (3%)
22	6MZ	A1	37	22	18,25,26	1.06	1 (5%)	16,36,39	1.43	2 (12%)
22	PSU	A1	55	22	18,21,22	0.79	0	22,30,33	1.13	2 (9%)
24	4SU	A3	8	24	18,21,22	1.42	1 (5%)	26,30,33	0.75	1 (3%)
24	PSU	A3	56	24	18,21,22	0.93	0	22,30,33	1.27	3 (13%)
22	7MG	A1	46	22	22,26,27	5.04	1 (4%)	29,39,42	1.41	1 (3%)
24	H2U	A3	21	24	18,21,22	1.31	2 (11%)	21,30,33	1.14	3 (14%)

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	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	CM0	A1	34	22	-	2/12/30/31	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	PSU	A1	55	22	-	1/7/25/26	0/2/2/2
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	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-23.38	1.32	1.46
24	A3	8	4SU	C5-C4	-5.03	1.36	1.42
22	A1	7	4SU	C5-C4	-4.63	1.36	1.42
22	A1	34	CM0	O5-C5	-4.41	1.26	1.36
24	A3	21	H2U	C2-N3	-3.45	1.31	1.38

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	5.84	111.74	103.38
22	A1	34	CM0	C7-O5-C5	4.99	124.11	117.58
22	A1	37	6MZ	C9-N6-C6	4.37	126.64	122.87
22	A1	54	5MU	C5M-C5-C6	-3.34	118.39	122.85
24	A3	55	5MU	C5M-C5-C6	-3.19	118.59	122.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	54	5MU	1	0

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	0.61	0	7,9,11	1.36	1 (14%)
57	VAL	A1	101	58,22	4,6,7	0.61	0	6,7,9	1.39	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	-	2/7/9/11	-
57	VAL	A1	101	58,22	-	0/5/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	A1	101	VAL	O-C-CA	-3.32	116.07	124.78
58	BA	3001	FME	C-CA-N	2.58	114.38	109.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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.

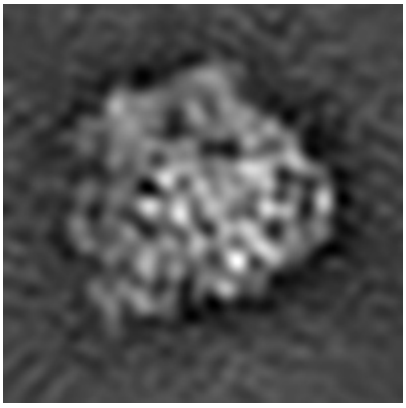
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2475. These allow visual inspection of the internal detail of the map and identification of artifacts.

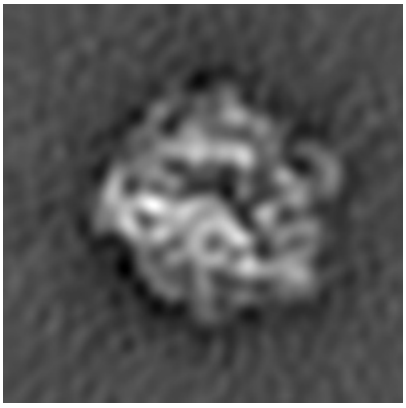
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

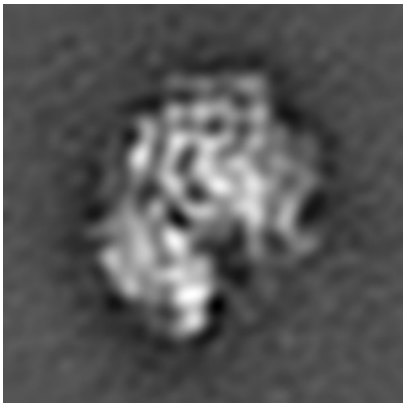
6.1.1 Primary map



X



Y



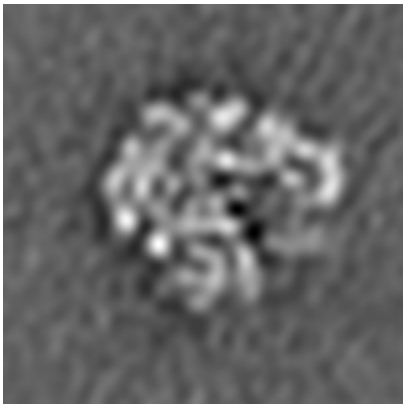
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 48



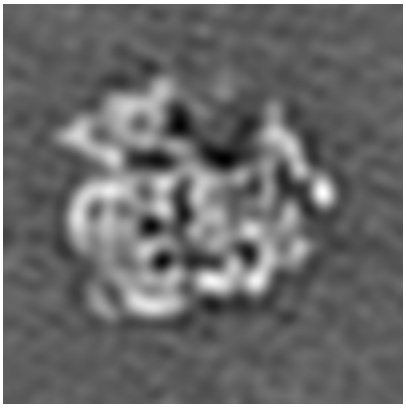
Y Index: 48

Z Index: 48

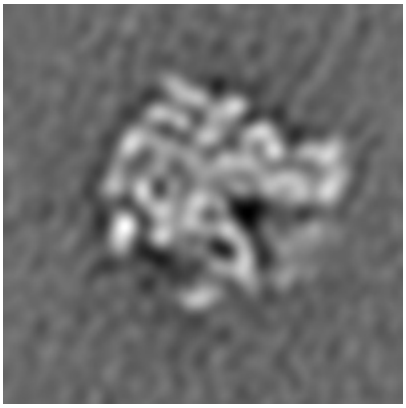
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 43



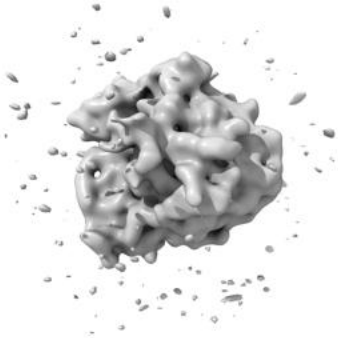
Y Index: 51

Z Index: 46

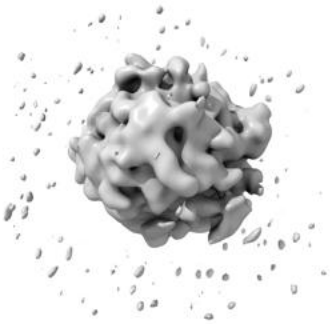
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

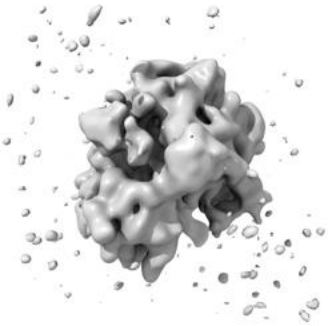
6.4.1 Primary map



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.

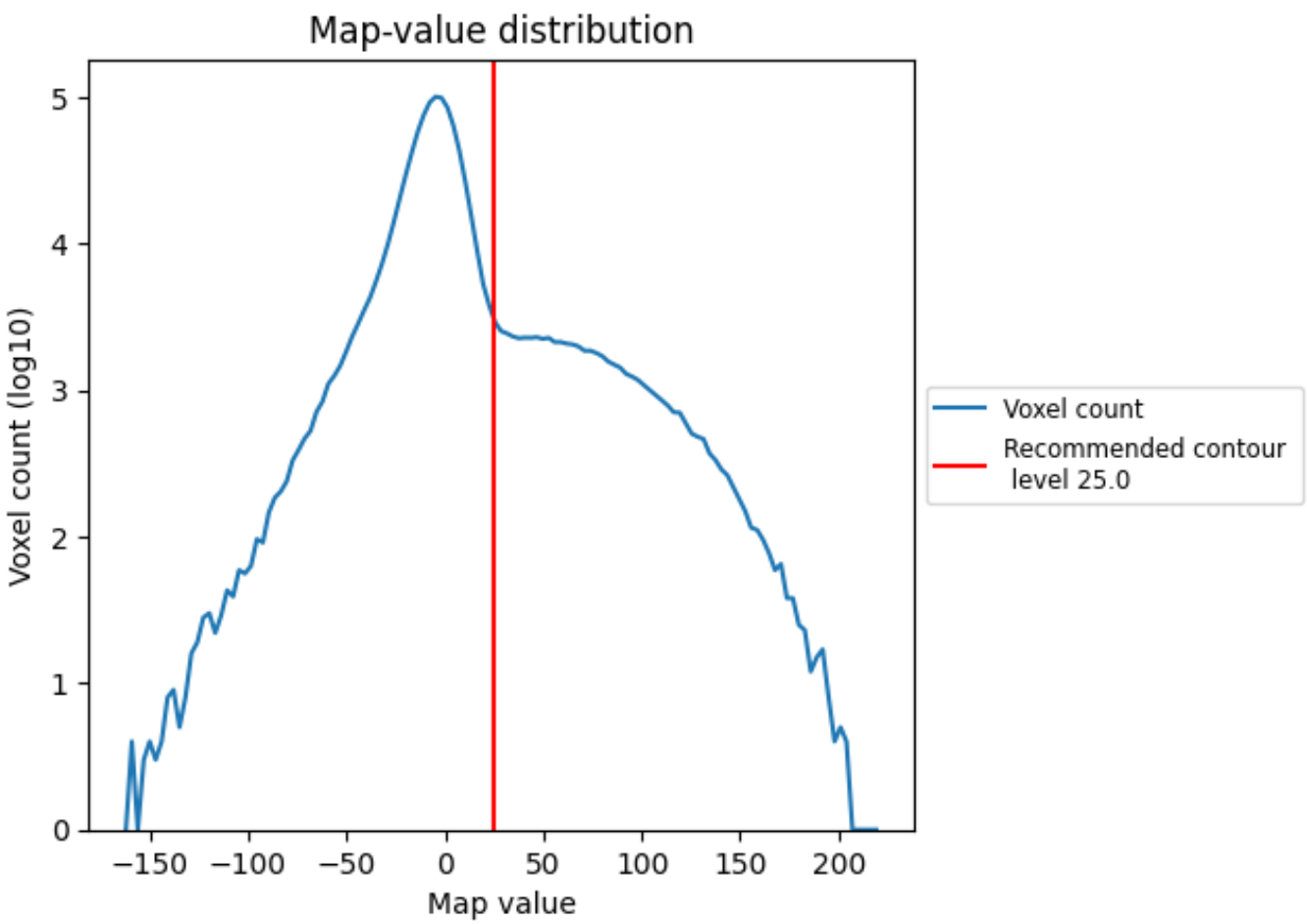
6.5 Mask visualisation (i)

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

7 Map analysis (i)

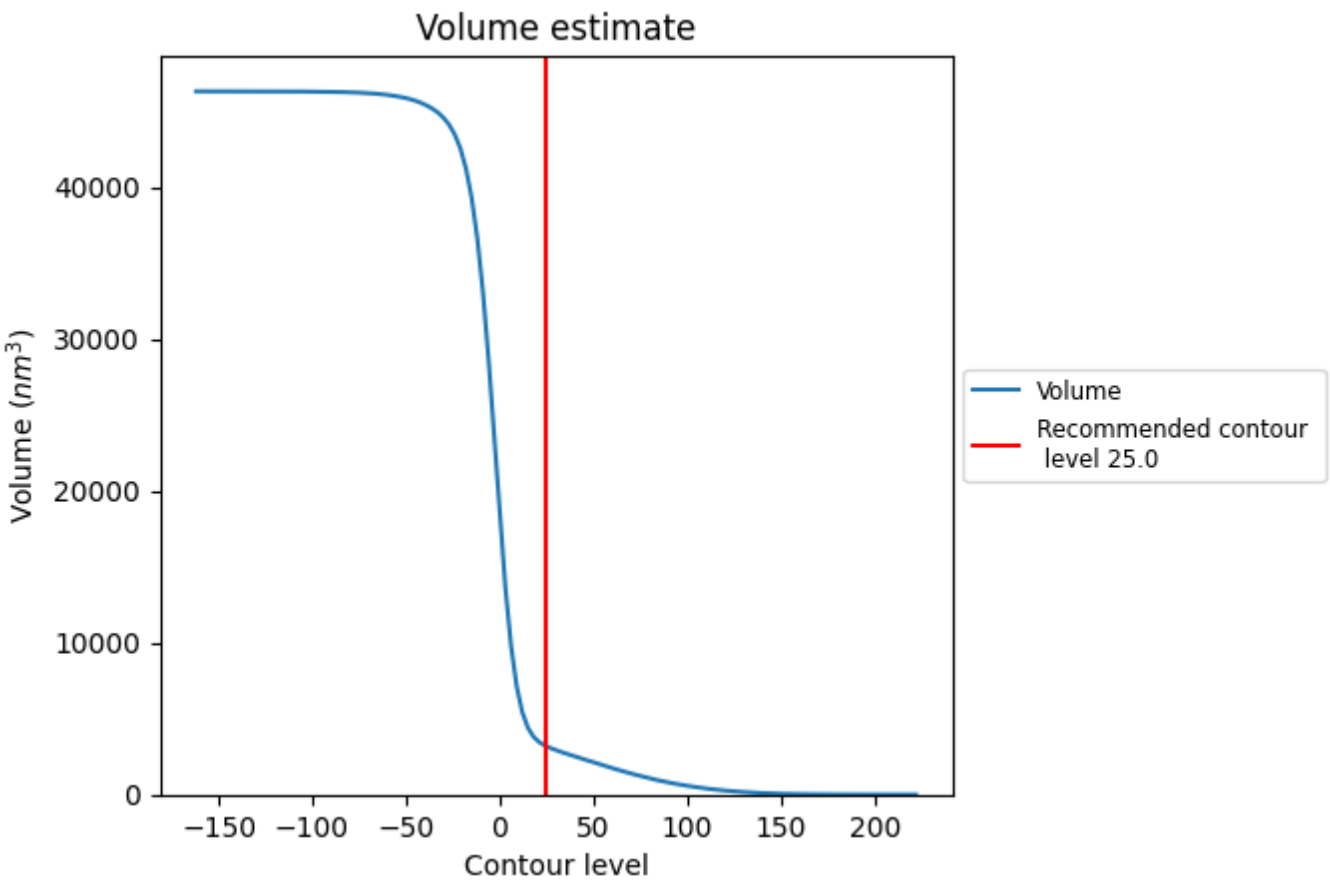
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

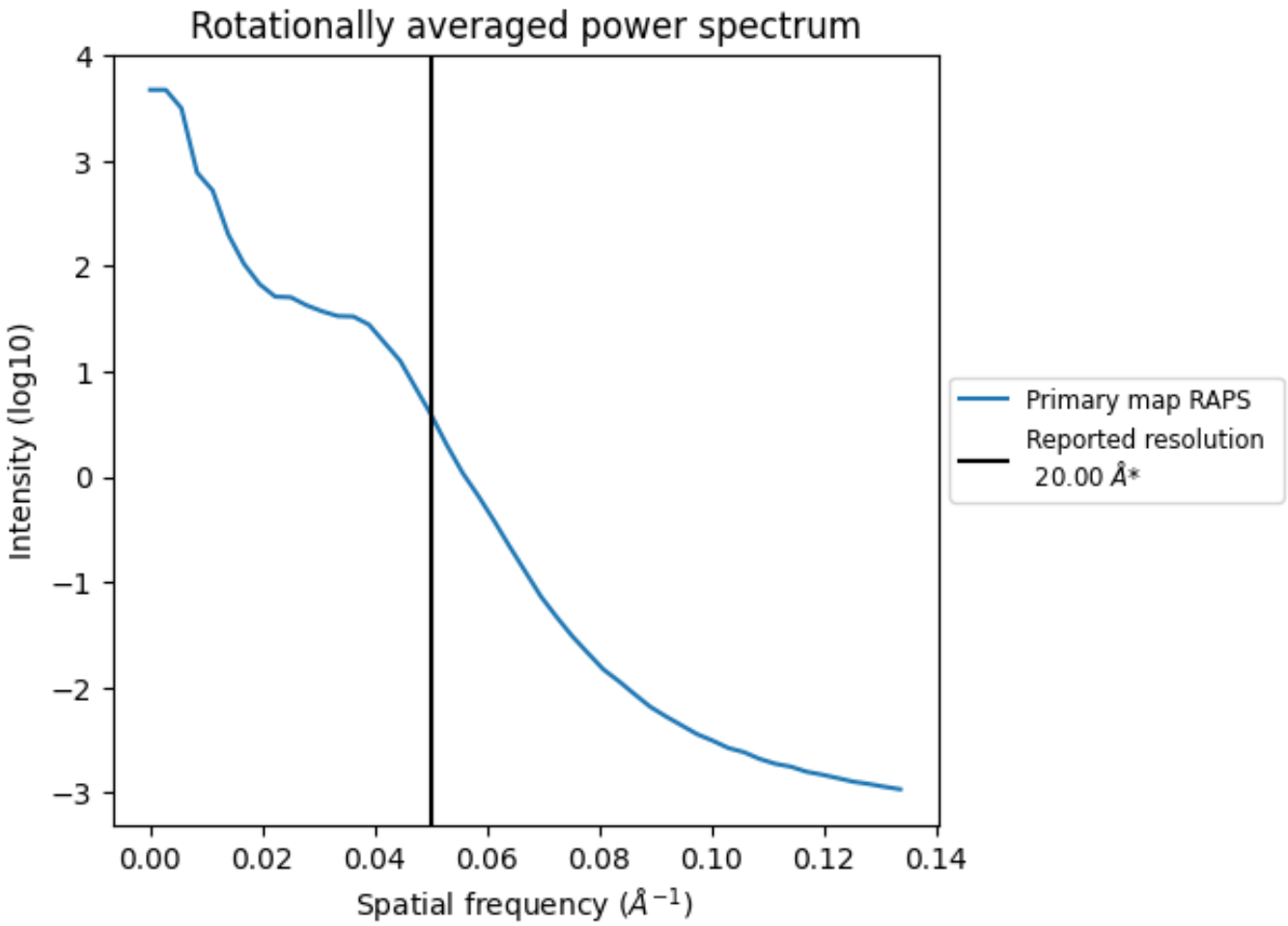
7.2 Volume estimate (i)



The volume at the recommended contour level is 3179 nm^3; this corresponds to an approximate mass of 2872 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 0.050 Å^{-1}

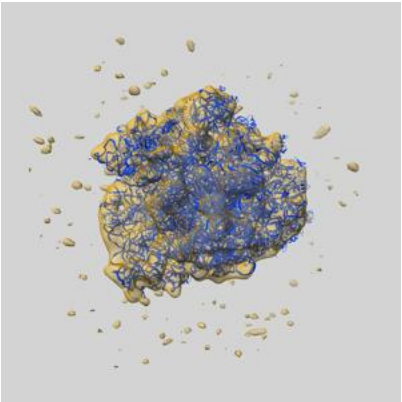
8 Fourier-Shell correlation (i)

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

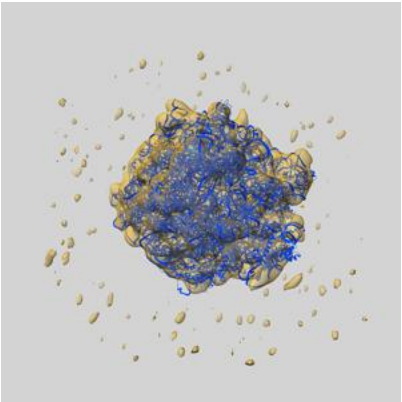
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2475 and PDB model 4V78. Per-residue inclusion information can be found in section 3 on page 17.

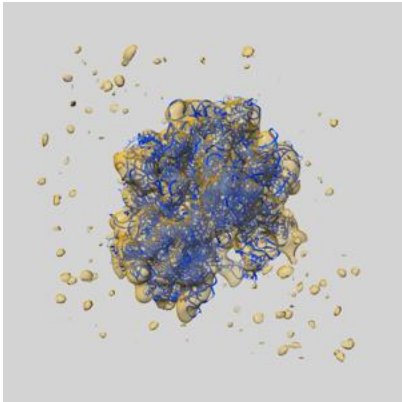
9.1 Map-model overlay (i)



X



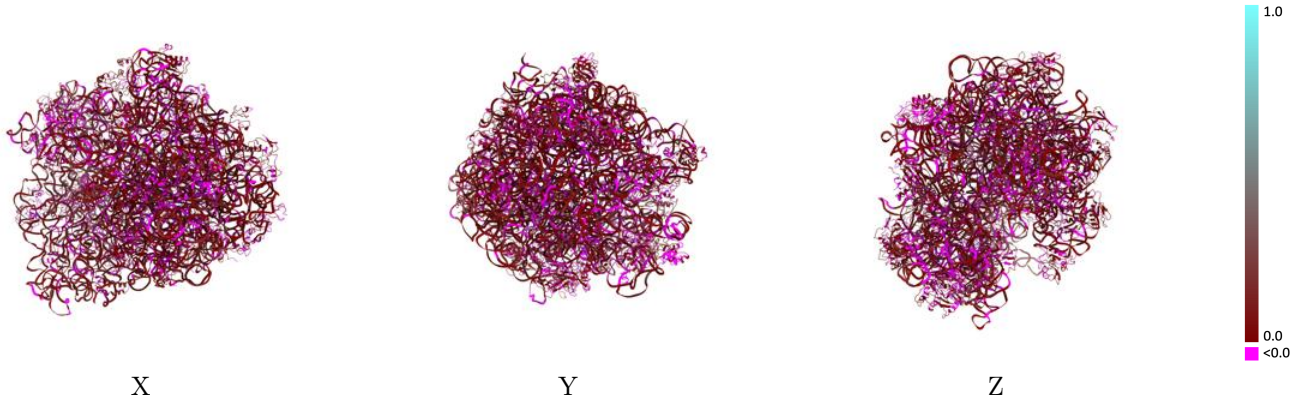
Y



Z

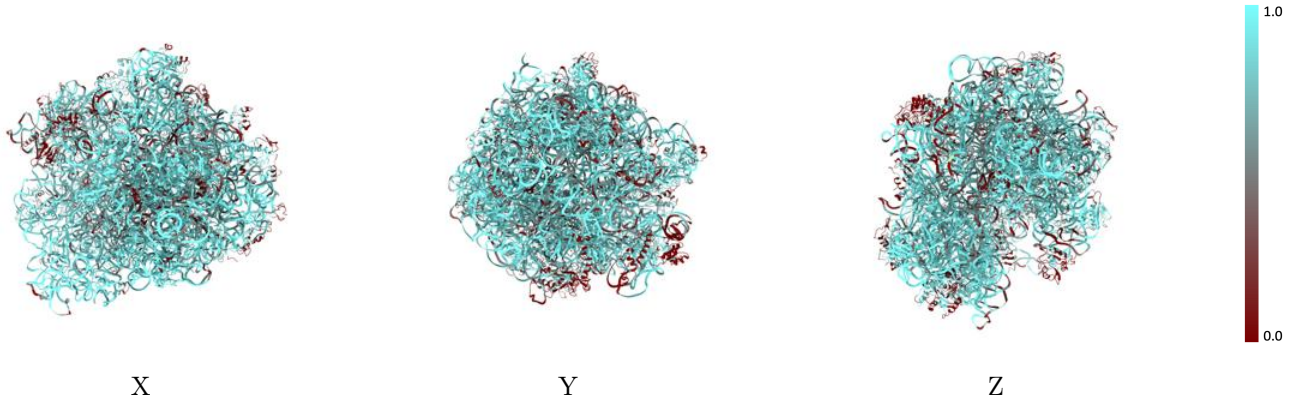
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



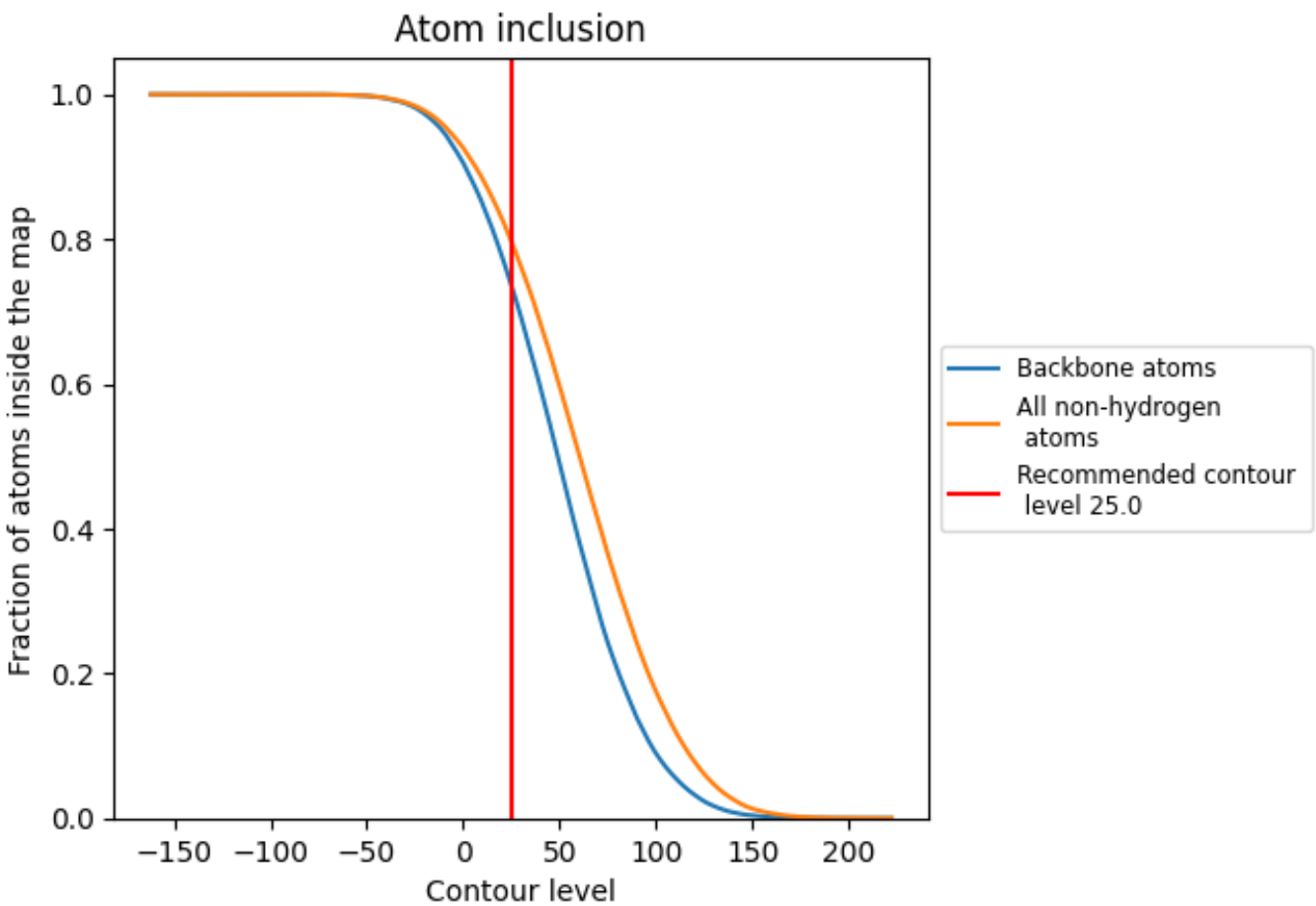
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.7965	0.0510
A1	0.5153	0.0490
A2	0.9191	0.0520
A3	0.4756	0.0280
AA	0.8875	0.0630
AB	0.6055	0.0440
AC	0.6048	0.0260
AD	0.7233	0.0170
AE	0.7394	0.0430
AF	0.4906	0.0440
AG	0.8316	0.0380
AH	0.8604	0.0550
AI	0.9174	0.0200
AJ	0.6257	-0.0080
AK	0.7708	0.0520
AL	0.6992	0.0160
AM	0.6722	0.0430
AN	0.7455	0.0050
AO	0.7928	0.0410
AP	0.7391	0.0280
AQ	0.5732	0.0190
AR	0.5604	0.0150
AS	0.4375	0.0090
AT	0.8021	0.0310
AU	0.8875	0.0510
B0	0.6729	0.0180
B1	0.6733	0.0320
B2	0.3915	-0.0410
B3	0.6151	-0.0450
B4	0.7979	-0.0020
B5	0.3092	0.0100
BA	0.8619	0.0640
BB	0.8974	0.0650
BC	0.5721	-0.0060
BD	0.6983	0.0200

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Chain	Atom inclusion	Q-score
BE	0.6717	0.0260
BF	0.7650	0.0330
BG	0.7911	0.0360
BH	0.2172	0.0310
BI	0.2720	0.0380
BJ	0.6927	0.0220
BK	0.5481	0.0350
BL	0.5630	0.0080
BM	0.7380	0.0230
BN	0.7270	-0.0020
BO	0.7509	0.0270
BP	0.7466	0.0400
BQ	0.6883	-0.0030
BR	0.6826	0.0520
BS	0.6758	0.0060
BT	0.8506	0.0140
BU	0.5417	0.0130
BV	0.8293	0.0630
BW	0.7113	0.0170
BX	0.8003	0.0480
BY	0.3843	-0.0030
BZ	0.6178	0.0340