wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 06:40 PM EST

PDB ID	:	4V74
EMDB ID	:	EMD-1720
Title	:	70S-fMetVal-tRNAVal-tRNAfMet complex in hybrid pre-translocation state (pre5b)
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	:	3I1O, 2HGP, 2K4C, 2WRI

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:

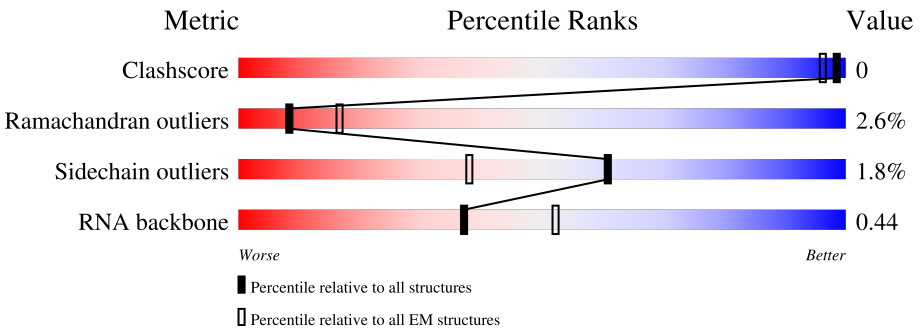
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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	42% 95% 5% •
2	AC	208	51% 89% 10%
3	AD	206	41% 88% 12%
4	AE	152	42% 89% 11% •
5	AF	101	13% 90% 9% •
6	AG	152	23% 87% 12% •
7	AH	130	27% 89% 10% •

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Mol	Chain	Length	Quality of chain
8	AI	128	35% 82% 16%
9	AJ	100	21% 84% 15%
10	AK	118	23% 92% 7%
11	AL	124	31% 83% 15%
12	AM	115	28% 85% 14%
13	AN	101	40% 86% 13%
14	AO	89	6% 85% 13%
15	AP	81	43% 84% 16%
16	AQ	82	34% 91% 9%
17	AR	57	33% 79% 21%
18	AS	81	25% 88% 11%
19	AT	86	24% 93% 7%
20	AU	53	42% 79% 21%
21	AA	1533	12% 25% 49% 22%
22	A1	76	24% 17% 55% 24%
23	A2	15	7% 7% 80% 13%
24	A3	77	19% 22% 52% 25%
25	BC	273	53% 87% 12%
26	BD	209	34% 90% 9%
27	BE	201	32% 91% 9%
28	BF	179	22% 89% 11%
29	BG	177	38% 89% 11%
30	BH	149	85% 95% 5%
31	BI	142	99% 94% 5%
32	BJ	142	28% 90% 10%

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Mol	Chain	Length	Quality of chain
33	BK	123	46% 88% 11%
34	BL	144	33% 85% 13%
35	BM	136	40% 85% 15%
36	BN	121	15% 87% 12%
37	BO	117	14% 87% 11%
38	BP	115	40% 87% 12%
39	BQ	118	36% 84% 15%
40	BR	103	25% 90% 10%
41	BS	110	33% 89% 11%
42	BT	94	21% 85% 15%
43	BU	104	32% 89% 10%
44	BV	94	29% 95% 5%
45	BW	80	44% 82% 14%
46	BX	79	30% 82% 14%
47	BY	63	44% 90% 10%
48	BZ	59	31% 83% 15%
49	B0	57	30% 86% 12%
50	B1	52	25% 94% 6%
51	B2	46	52% 78% 22%
52	B3	65	54% 85% 14%
53	B4	38	34% 87% 13%
54	BA	2903	12% 23% 51% 23%
55	BB	118	6% 25% 51% 21%
56	B5	234	40% 89% 6% 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

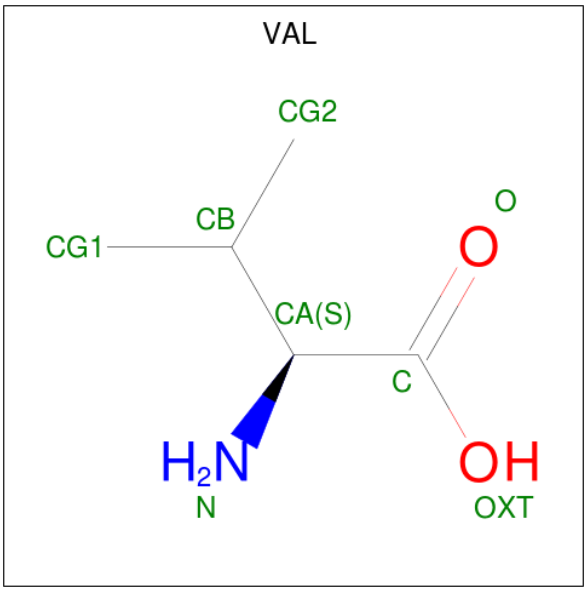
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

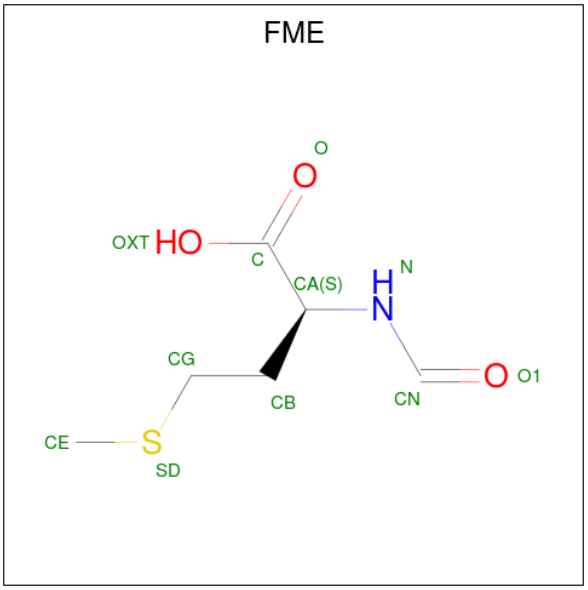
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	B5	223	1658	1038	302	312	6	0	0

- 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: $C_6H_{11}NO_3S$).



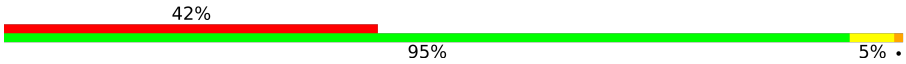
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	BA	1	10	6	1	2	1	0

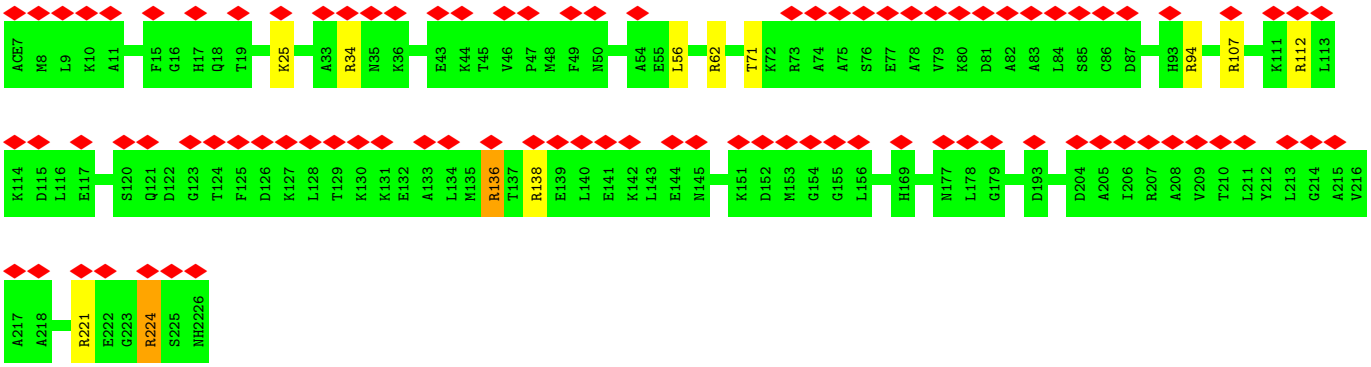
3 Residue-property plots (i)

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

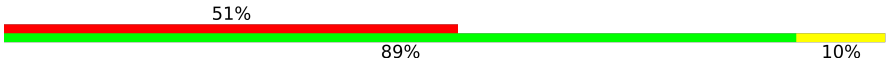
Chain AB:

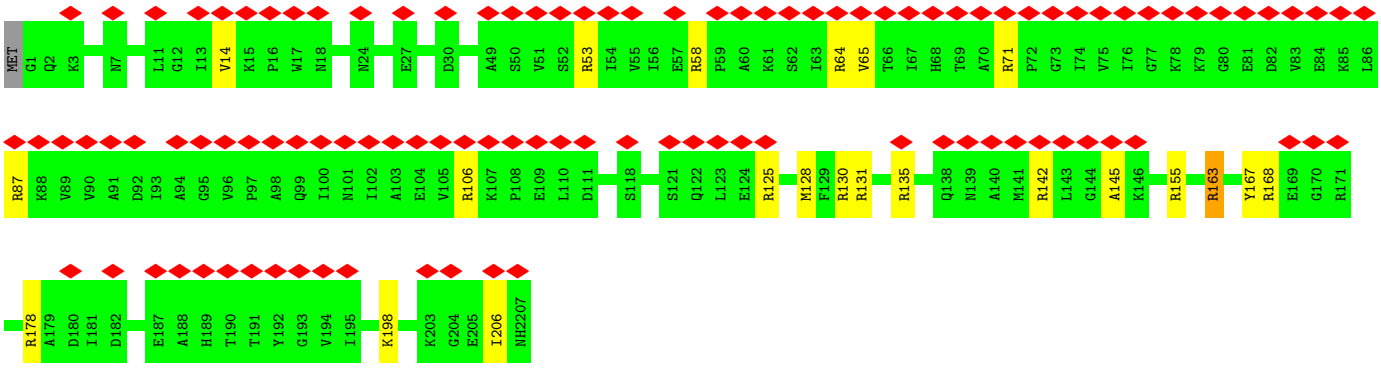




- Molecule 2: 30S ribosomal protein S3

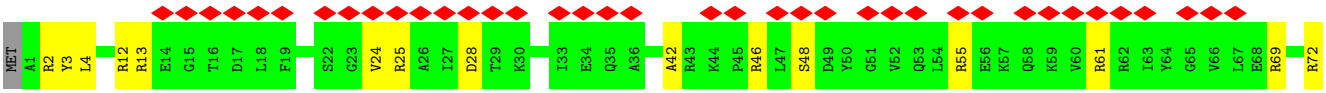
Chain AC:

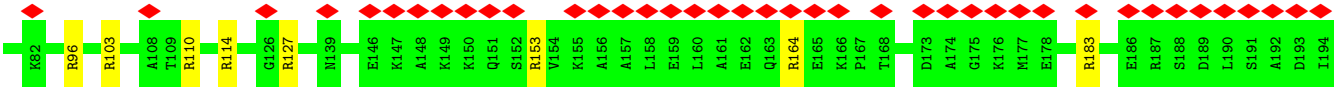


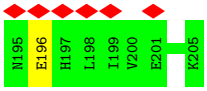


- Molecule 3: 30S ribosomal protein S4

Chain AD:

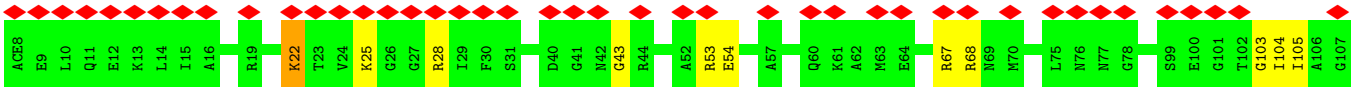


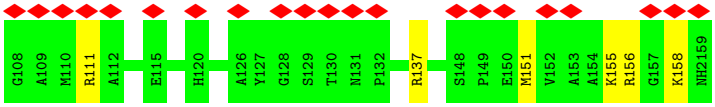




• Molecule 4: 30S ribosomal protein S5

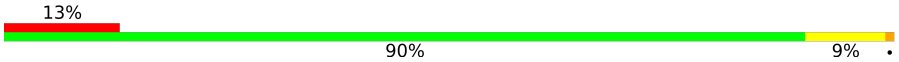
Chain AE:

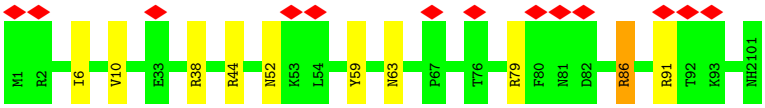




• Molecule 5: 30S ribosomal protein S6

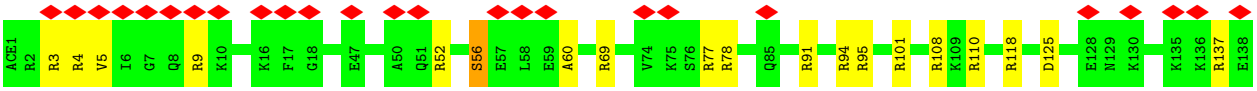
Chain AF:

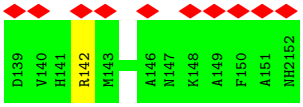




• Molecule 6: 30S ribosomal protein S7

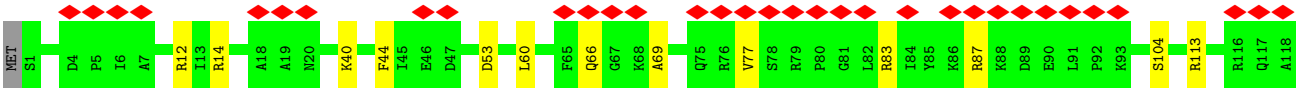
Chain AG:

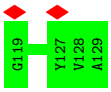




• Molecule 7: 30S ribosomal protein S8

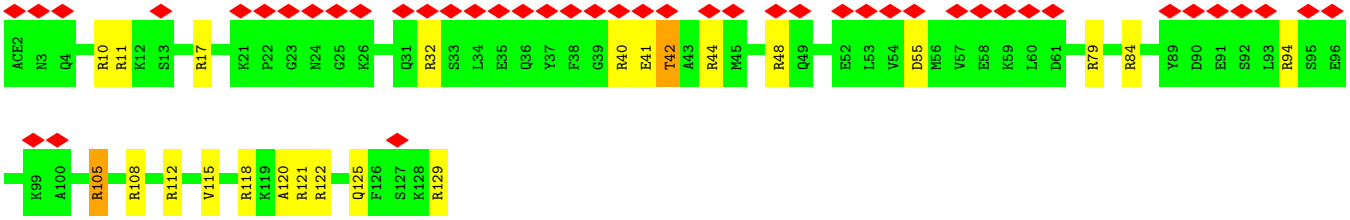
Chain AH:





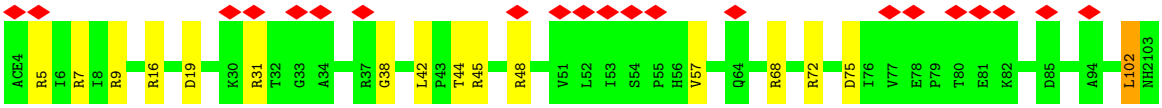
- Molecule 8: 30S ribosomal protein S9

Chain AI:



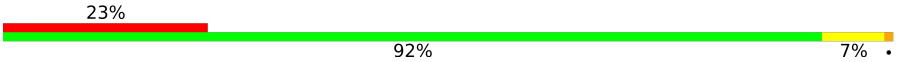
- Molecule 9: 30S ribosomal protein S10

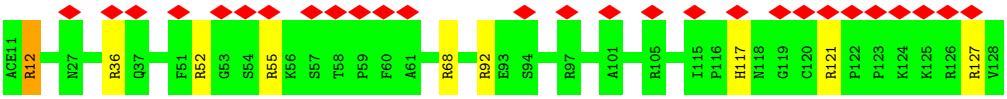
Chain AJ:



- Molecule 10: 30S ribosomal protein S11

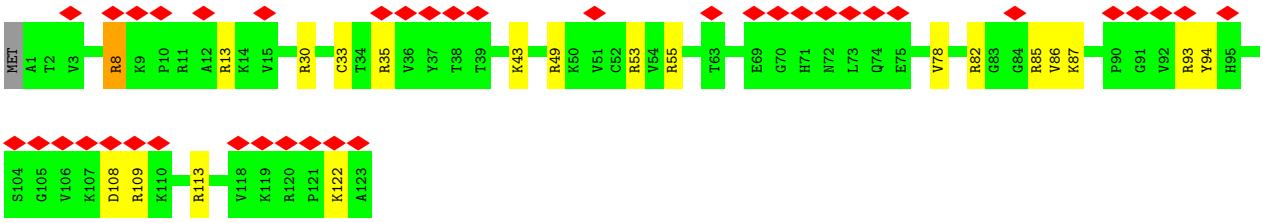
Chain AK:





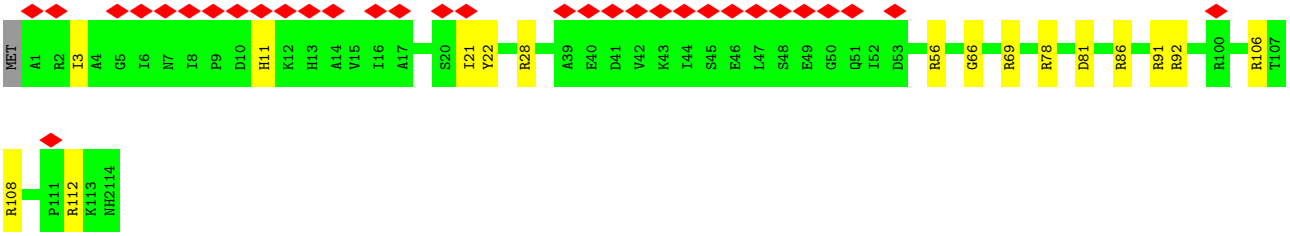
- Molecule 11: 30S ribosomal protein S12

Chain AL:



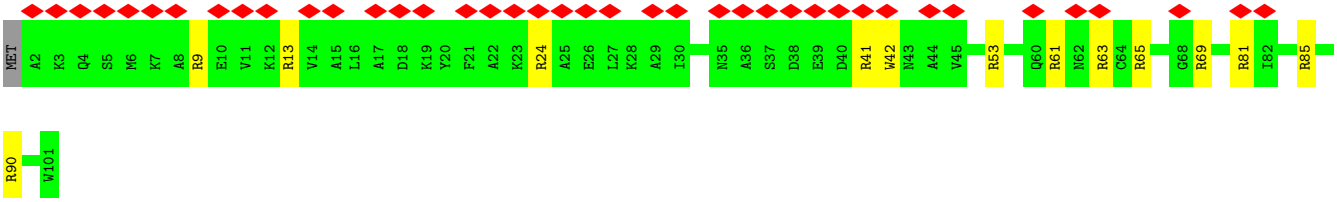
- Molecule 12: 30S ribosomal protein S13

Chain AM:



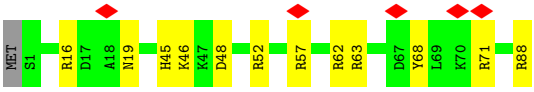
- Molecule 13: 30S ribosomal protein S14

Chain AN:



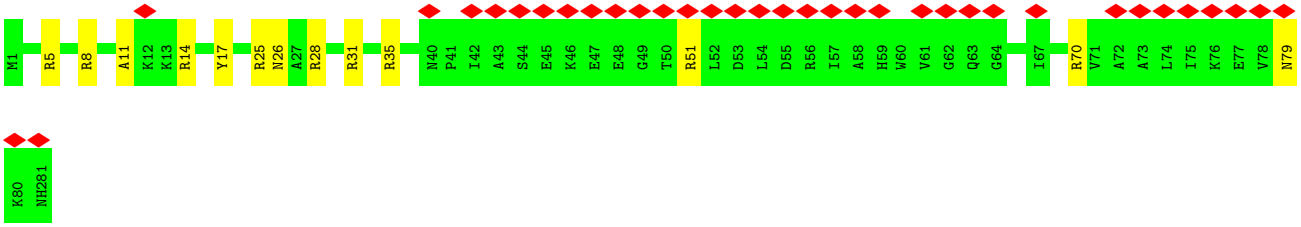
- Molecule 14: 30S ribosomal protein S15

Chain AO:



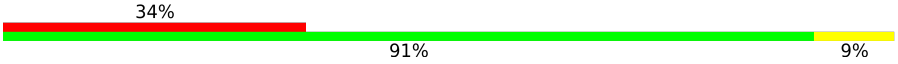
- Molecule 15: 30S ribosomal protein S16

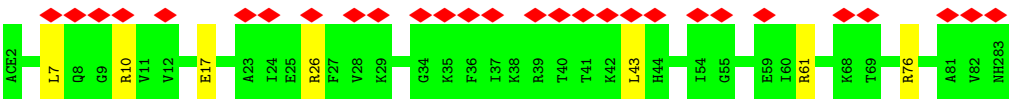
Chain AP:



- Molecule 16: 30S ribosomal protein S17

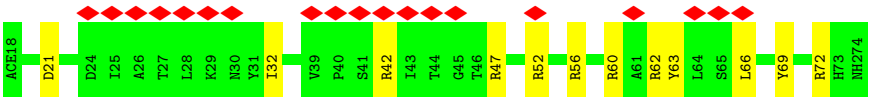
Chain AQ:





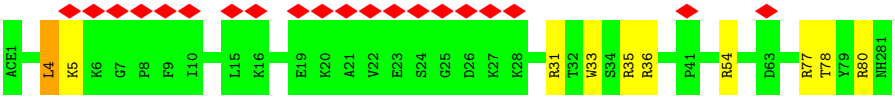
- Molecule 17: 30S ribosomal protein S18

Chain AR:



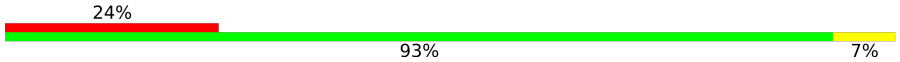
- Molecule 18: 30S ribosomal protein S19

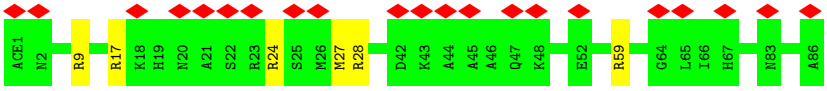
Chain AS:



• Molecule 19: 30S ribosomal protein S20

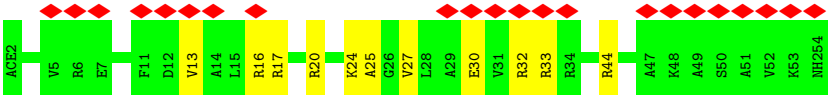
Chain AT:





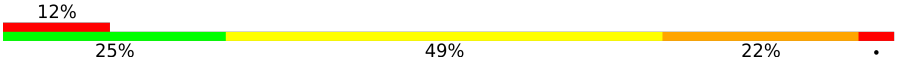
• Molecule 20: 30S ribosomal protein S21

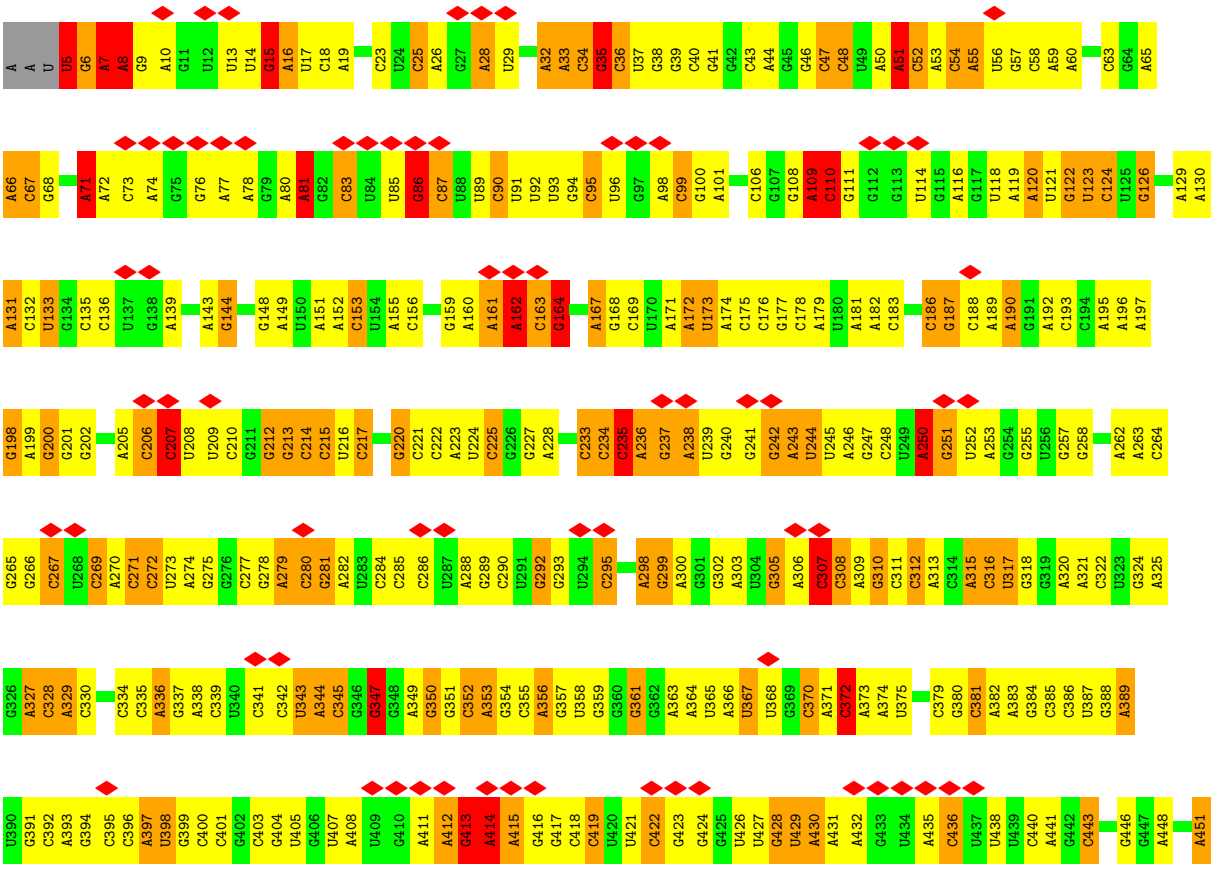
Chain AU:

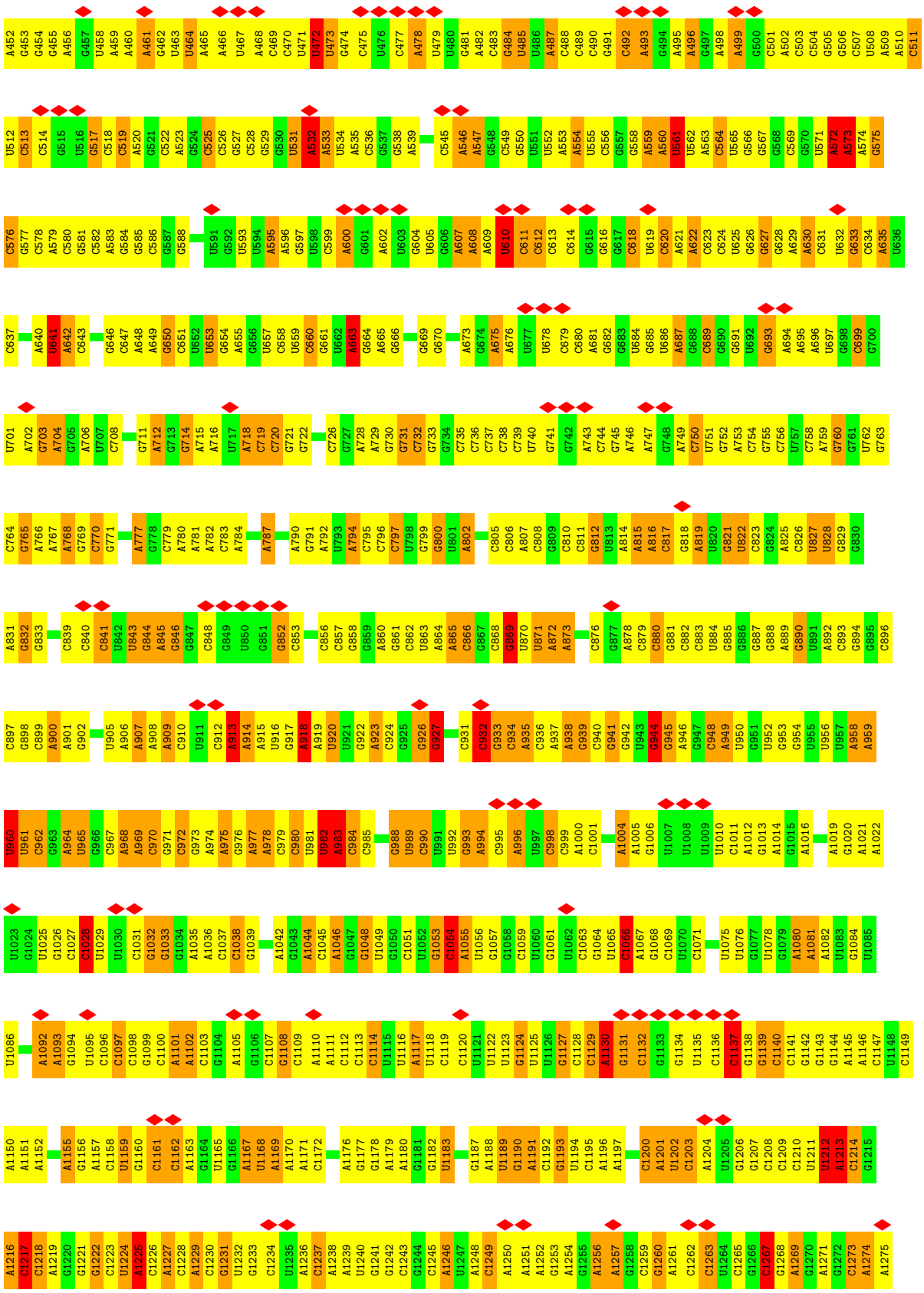


• Molecule 21: 16S ribosomal RNA

Chain AA:



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U512 C513 C514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G524 C525 C526 C527 C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 C545 A546 A547 G548 C549 G550 U551 U552 A553 A554 U555 C556 G557 G558 A559 A560 U561 U562 A563 C564 U565 C566 G567 G568 C569 G570 U571 A572 A573 A574 G575
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C764 G765 A766 A767 A768 G769 C770 G771 A777 G778 C779 A780 A781 A782 C783 A784 A787 A790 G791 A792 U793 A794 C795 C796 C797 U798 G799 G800 U801 A802 C805 C806 A807 C808 G809 C810 C811 G812 U813 A814 A815 A816 C817 G818 A819 U820 G821 U822 C823 G824 A825 C826 U827 U828 G829 G830
A831 G832 G833 C839 C840 C841 U842 U843 G844 A845 G846 G847 C848 G849 U850 G851 G852 C853 C856 C857 G858 G859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 C876 G877 A878 C879 C880 C881 C882 C883 U884 G885 G886 C887 G888 A889 G890 U891 A892 C893 G894 G895 C896
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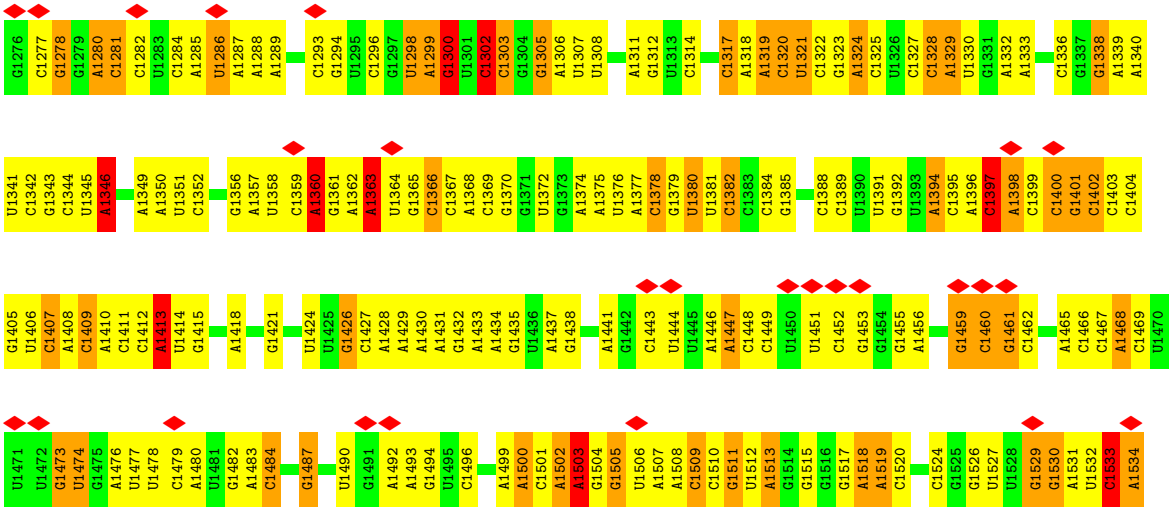
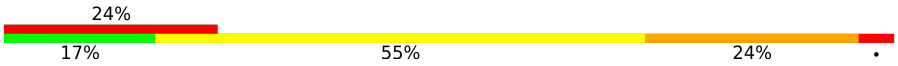
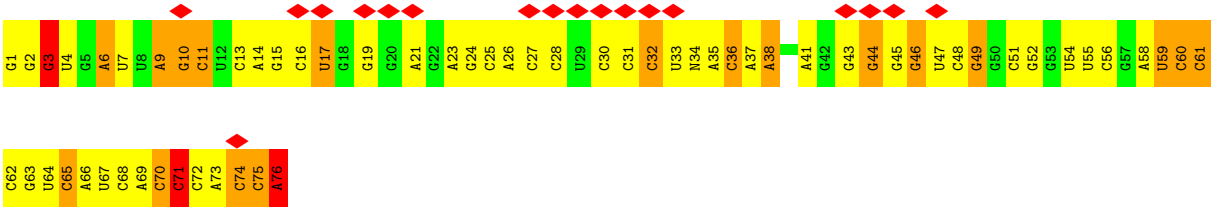
A1216 G1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 G1242 C1243 G1244 C1245 A1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 C1262 C1263 U1264 C1265 G1266 C1267 G1268 A1269 G1270 A1271 G1272 C1273 A1274 A1275



- Molecule 22: fMet-Val-tRNA-Val

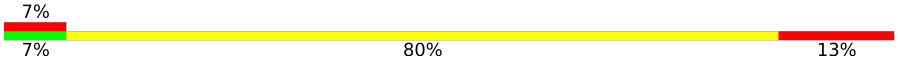
Chain A1:





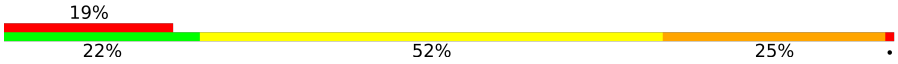
- Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

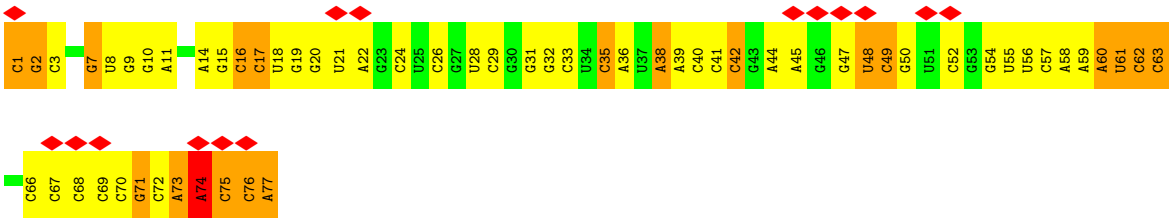
Chain A2:



- Molecule 24: tRNA-fMet

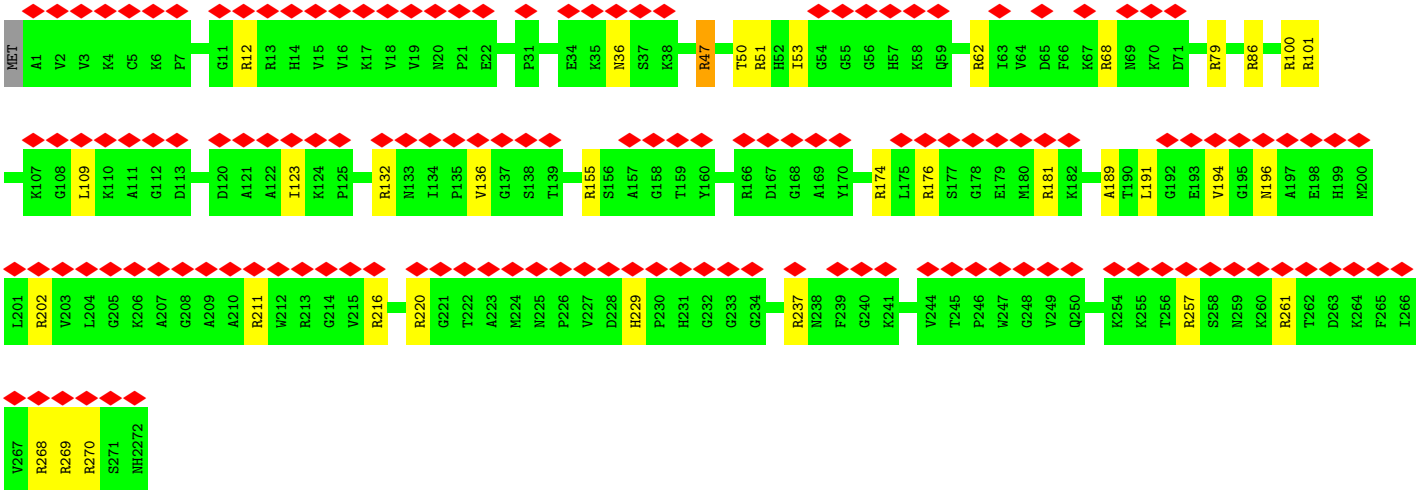
Chain A3:





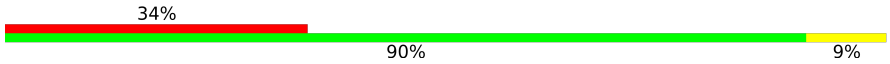
- Molecule 25: 50S ribosomal protein L2

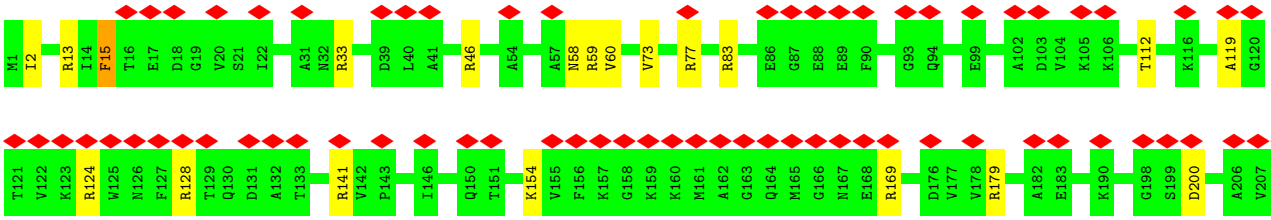
Chain BC:



- Molecule 26: 50S ribosomal protein L3

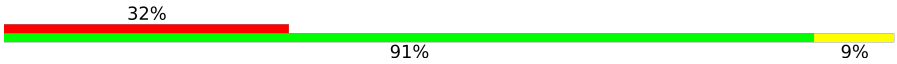
Chain BD:

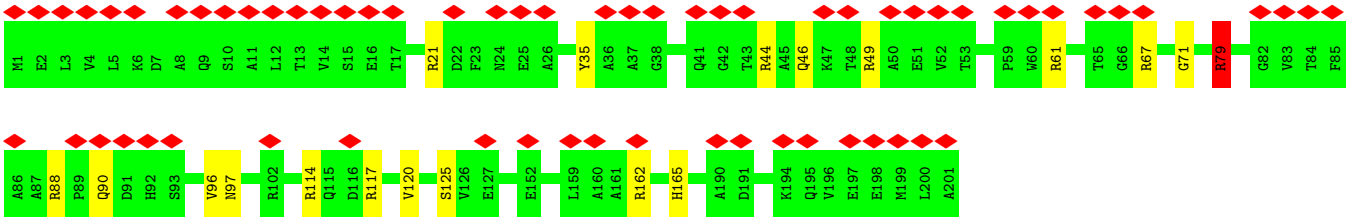




- Molecule 27: 50S ribosomal protein L4

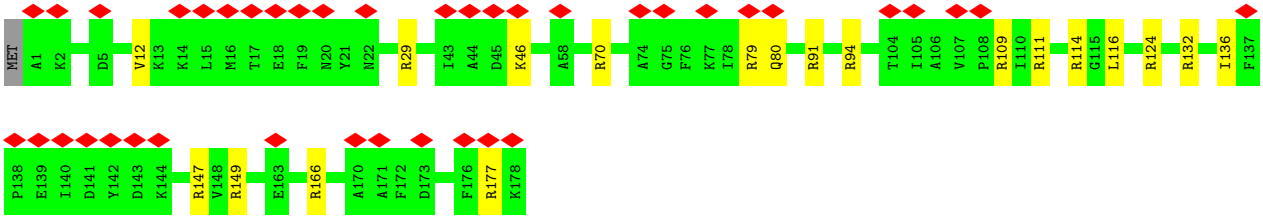
Chain BE:





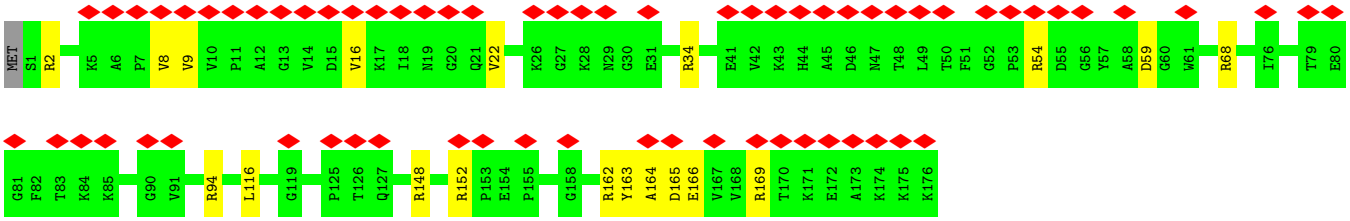
- Molecule 28: 50S ribosomal protein L5

Chain BF:



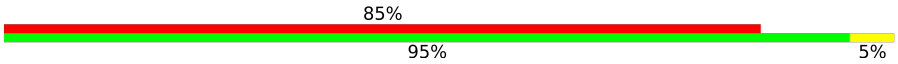
- Molecule 29: 50S ribosomal protein L6

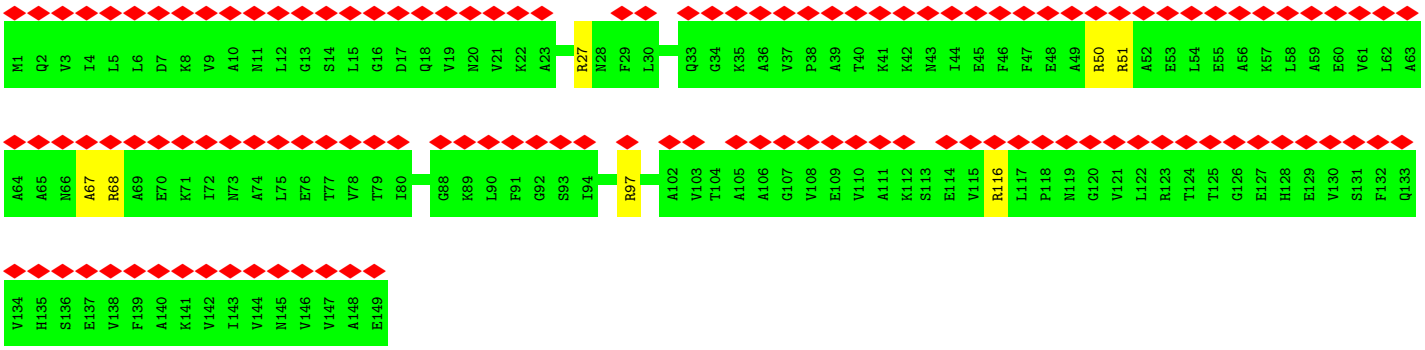
Chain BG:



- Molecule 30: 50S ribosomal protein L9

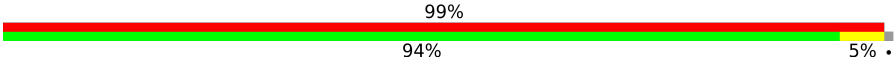
Chain BH:

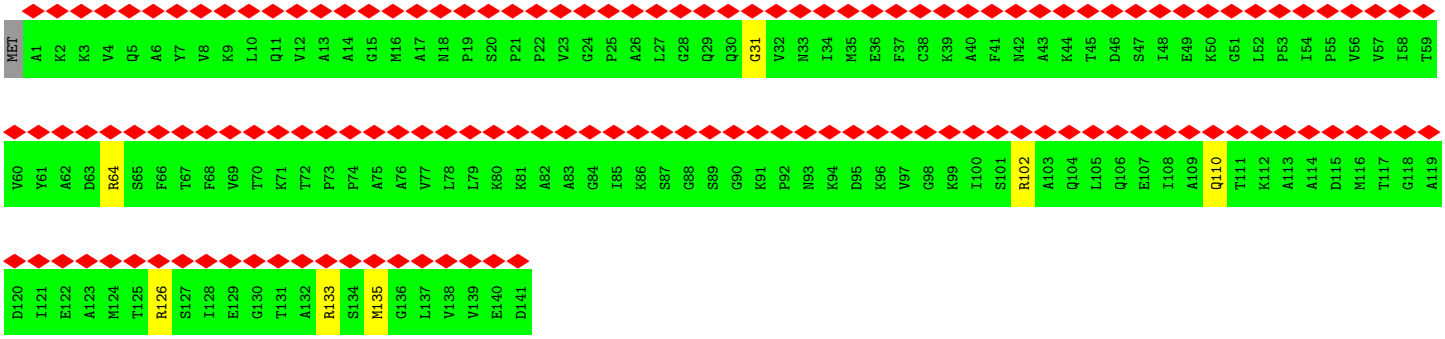




- Molecule 31: 50S ribosomal protein L11

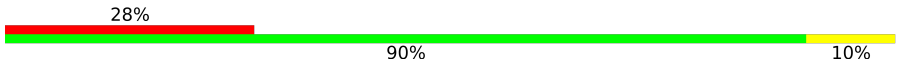
Chain BI:

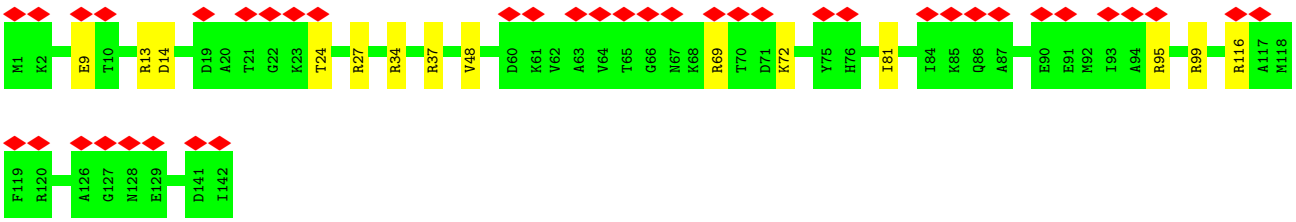




- Molecule 32: 50S ribosomal protein L13

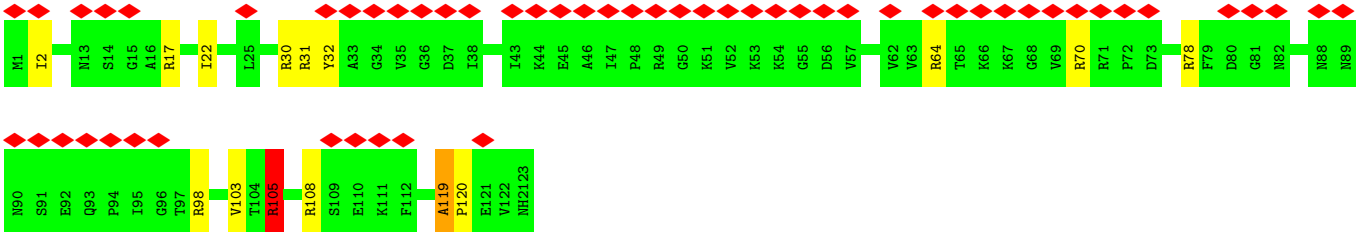
Chain BJ:





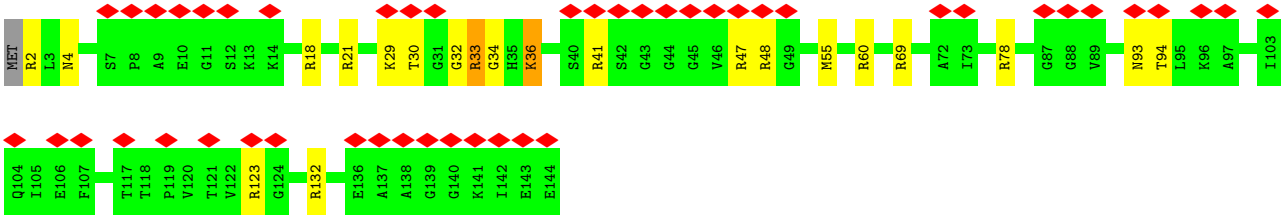
• Molecule 33: 50S ribosomal protein L14

Chain BK:



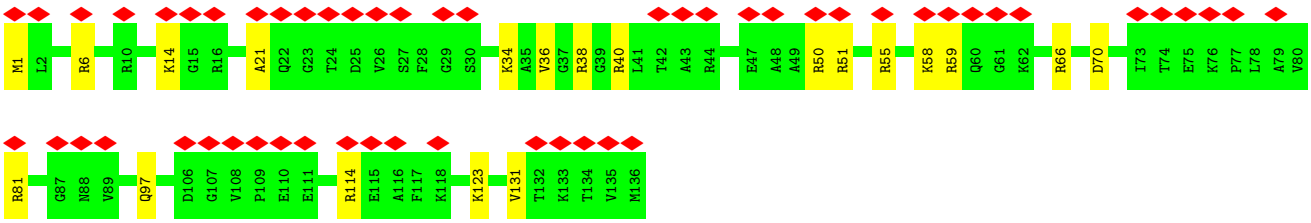
• Molecule 34: 50S ribosomal protein L15

Chain BL:



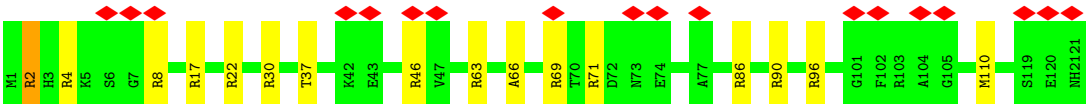
• Molecule 35: 50S ribosomal protein L16

Chain BM:



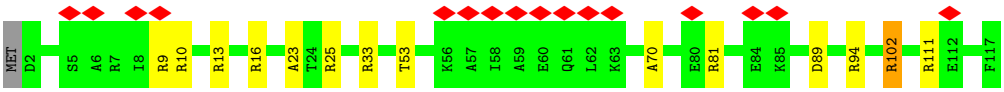
• Molecule 36: 50S ribosomal protein L17

Chain BN:



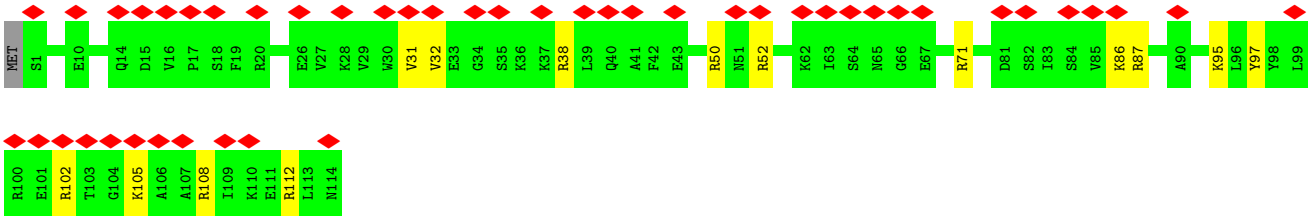
• Molecule 37: 50S ribosomal protein L18

Chain BO:



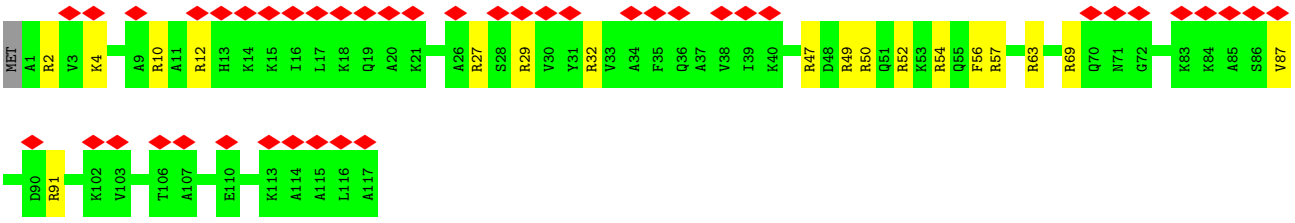
• Molecule 38: 50S ribosomal protein L19

Chain BP: 40% 87% 12%



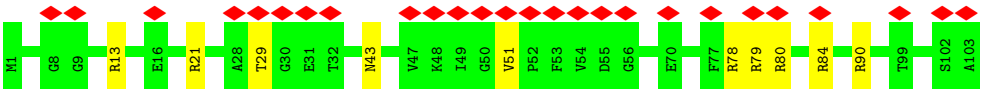
- Molecule 39: 50S ribosomal protein L20

Chain BQ: 36% 84% 15%



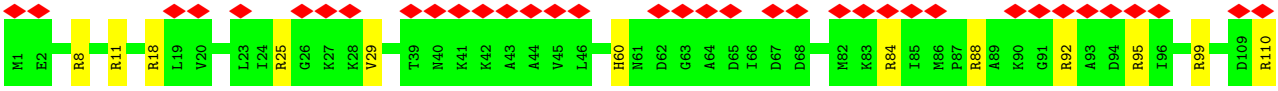
- Molecule 40: 50S ribosomal protein L21

Chain BR: 25% 90% 10%



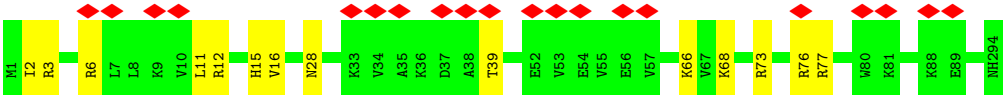
- Molecule 41: 50S ribosomal protein L22

Chain BS: 33% 89% 11%



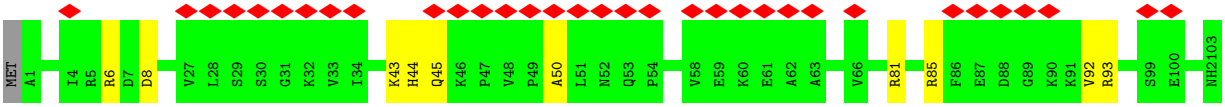
- Molecule 42: 50S ribosomal protein L23

Chain BT: 21% 85% 15%



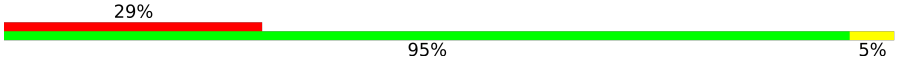
- Molecule 43: 50S ribosomal protein L24

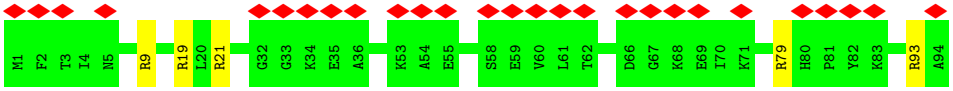
Chain BU: 32% 89% 10%



• Molecule 44: 50S ribosomal protein L25

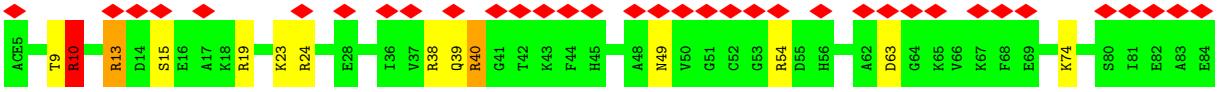
Chain BV:





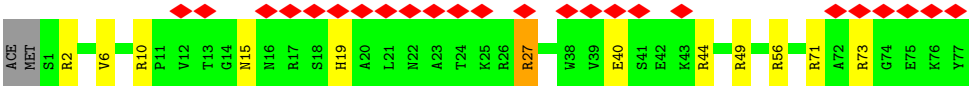
• Molecule 45: 50S ribosomal protein L27

Chain BW:



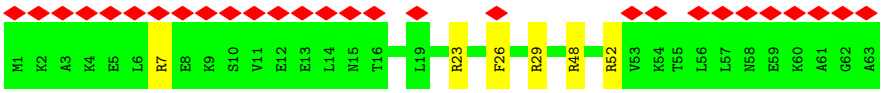
• Molecule 46: 50S ribosomal protein L28

Chain BX:



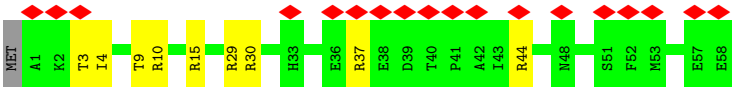
• Molecule 47: 50S ribosomal protein L29

Chain BY:



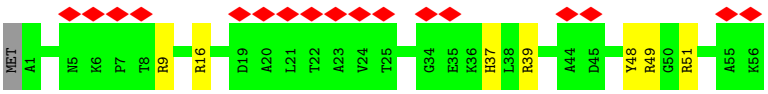
• Molecule 48: 50S ribosomal protein L30

Chain BZ:



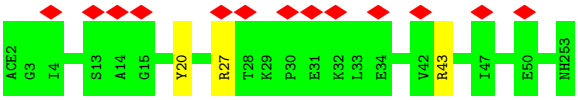
• Molecule 49: 50S ribosomal protein L32

Chain B0:



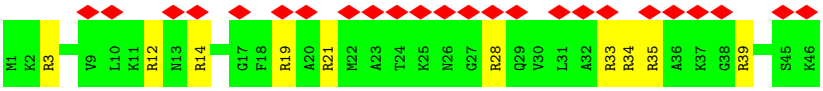
• Molecule 50: 50S ribosomal protein L33

Chain B1: 25% 94% 6%



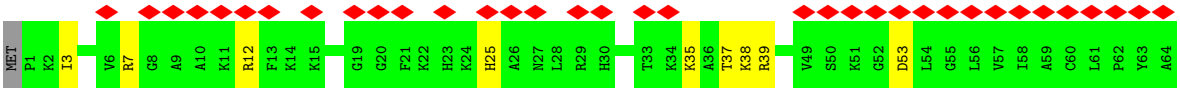
• Molecule 51: 50S ribosomal protein L34

Chain B2: 52% 78% 22%



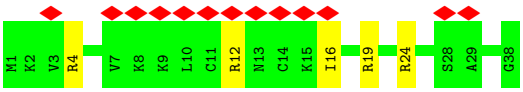
• Molecule 52: 50S ribosomal protein L35

Chain B3: 54% 85% 14%



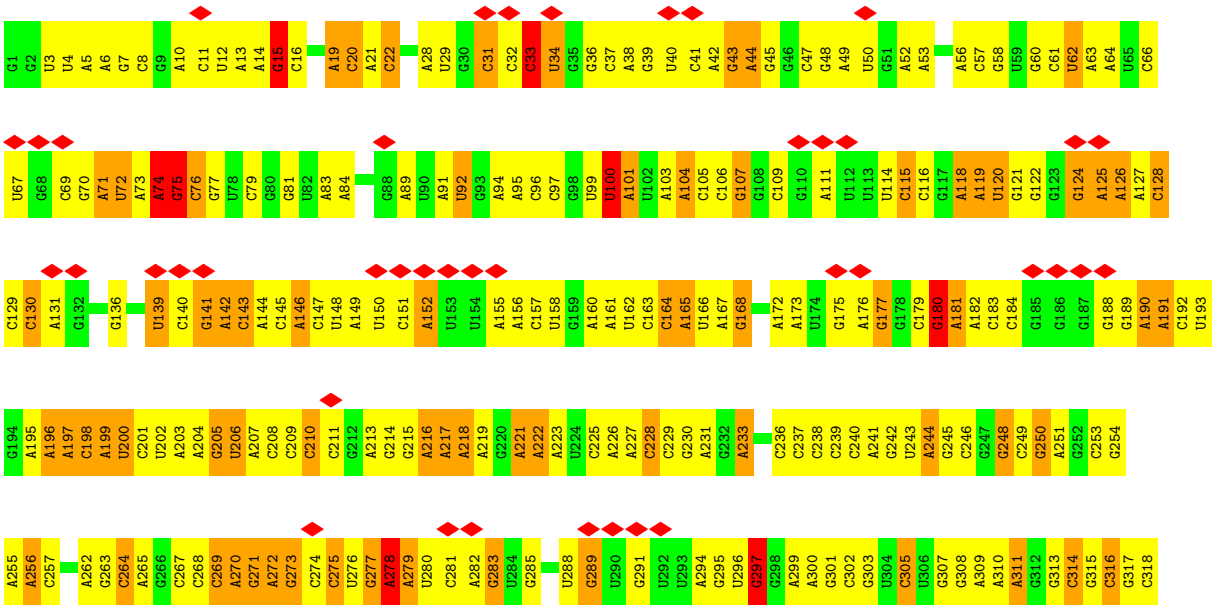
• Molecule 53: 50S ribosomal protein L36

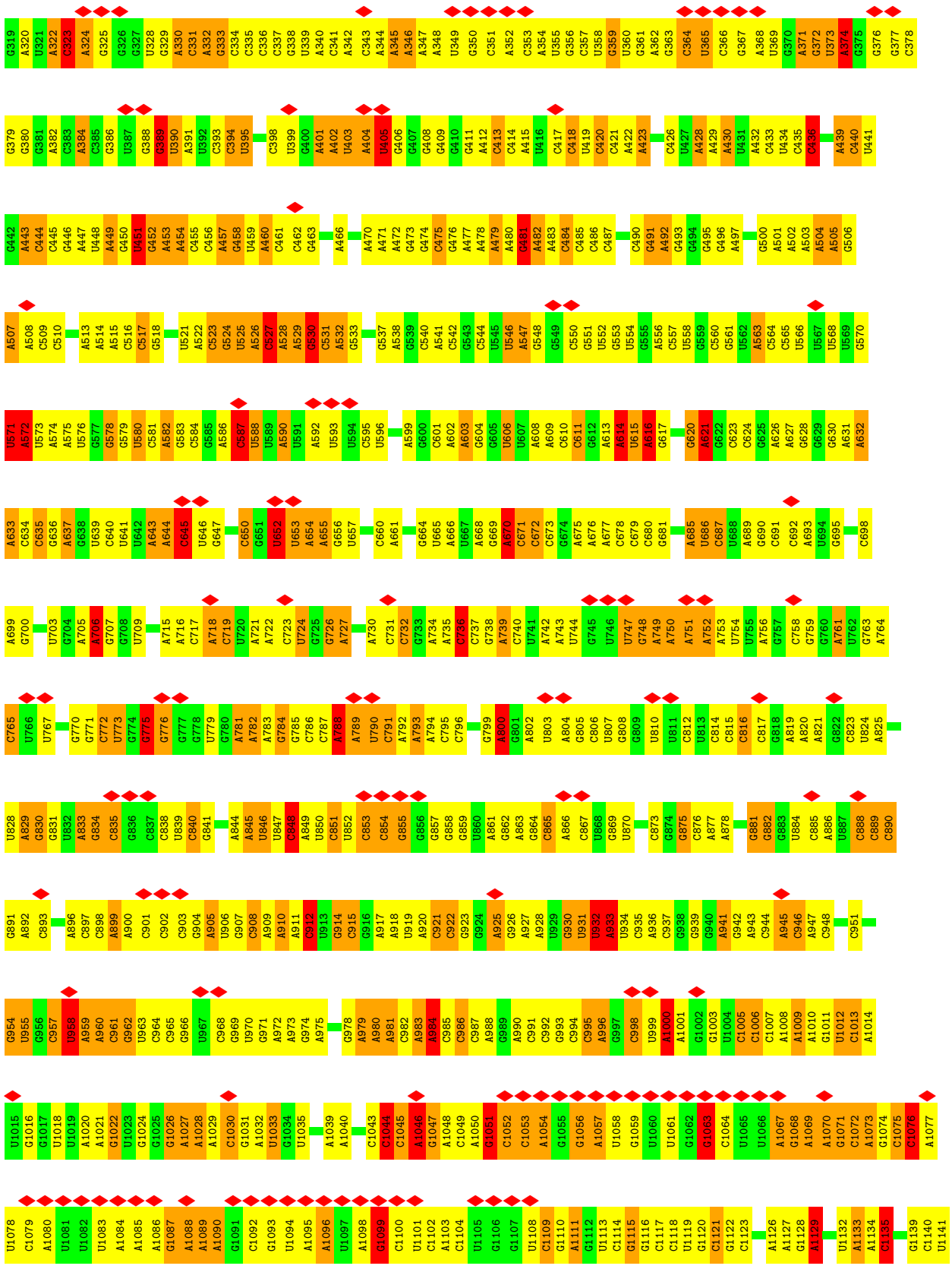
Chain B4: 34% 87% 13%



• Molecule 54: 23S ribosomal RNA

Chain BA: 12% 23% 51% 23%

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G379 G380 G381 A382 C383 A384 C385 G386 U387 G388 G389 U390 A391 U392 C393 C394 U395 C398 U399 G400 A401 A402 U403 A404 U405 C406 G407 G408 G409 G410 G411 A412 C413 C414 A415 U416 C417 C418 U419 G420 C421 A422 A423 C426 U427 A428 A429 A430 U431 A432 C433 U434 C435 C436 A439 C440 U441
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U571 A572 U573 A574 A575 U576 G577 G578 G579 U580 C581 A582 G583 C584 G585 A586 C587 U588 U589 A590 U591 A592 U593 U594 C595 U596 A599 G600 C601 A602 A603 G604 G605 U606 U607 A608 A609 C610 C611 G612 A613 A614 U615 A616 G617 G620 A621 G622 C623 C624 G625 A626 A627 G628 G629 G630 A631 A632
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U828 A829 G830 G831 U832 A833 G834 C835 G836 C837 C838 U839 C840 G841 A844 A845 U846 U847 C848 A849 U850 C851 U852 C853 C854 G855 G856 G857 G858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 U870 C873 G874 G875 C876 A877 A878 G881 G882 G883 U884 C885 A886 U887 C888 C889 C890
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G954 U955 G956 C957 U958 A959 A960 C961 G962 U963 C964 C965 G966 U967 C968 G969 U970 G971 A972 A973 G974 A975 G978 A979 A980 A981 C982 A983 A984 C985 C986 C987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 U1004 C1005 C1006 C1007 A1008 A1009 A1010 G1011 U1012 C1013 A1014
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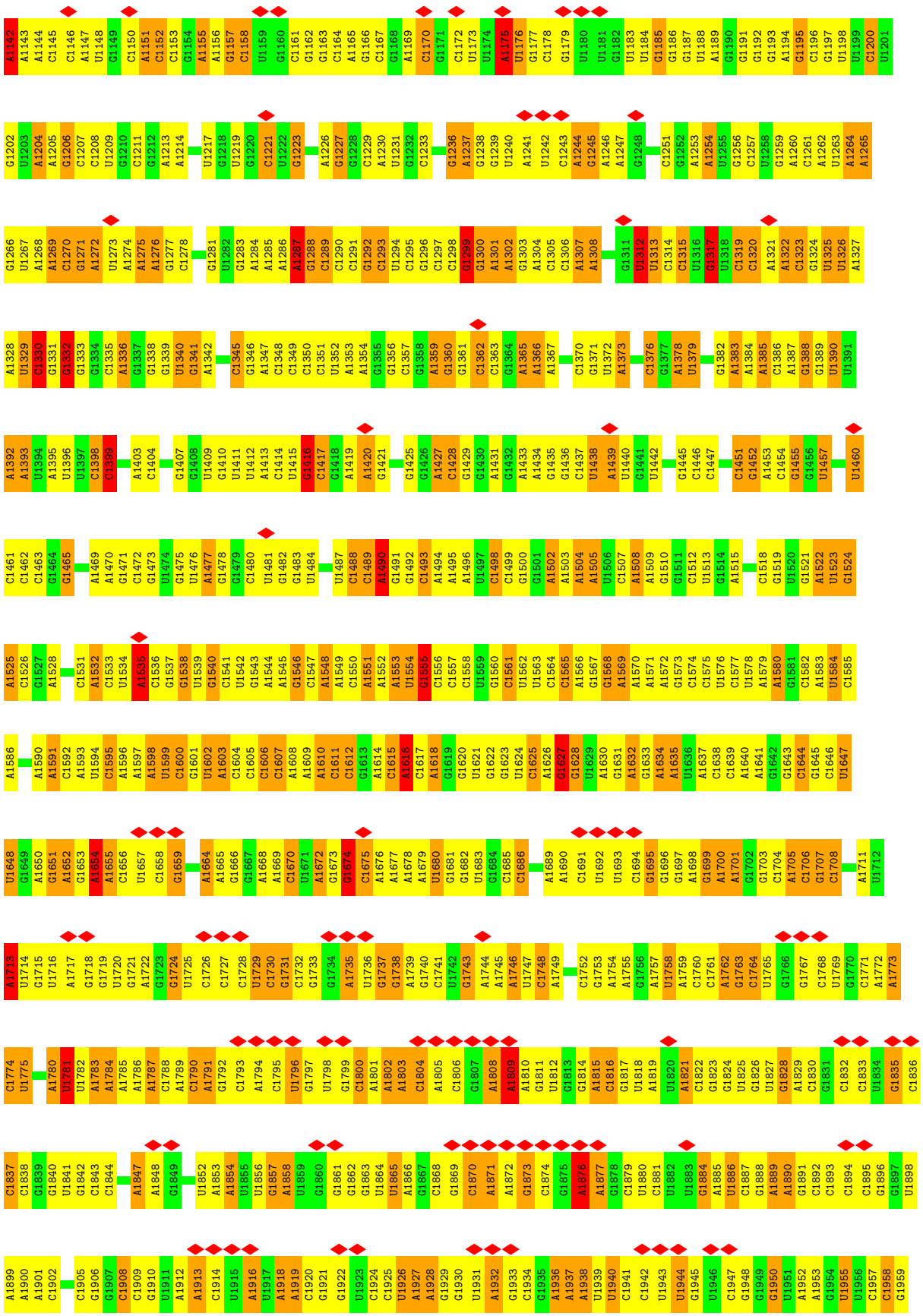
U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 G1116 C1117 C1118 U1119 G1120 C1121 G1122 C1123 A1126 A1127 G1128 A1129 U1132 A1133 A1134 C1135 G1139 C1140 U1141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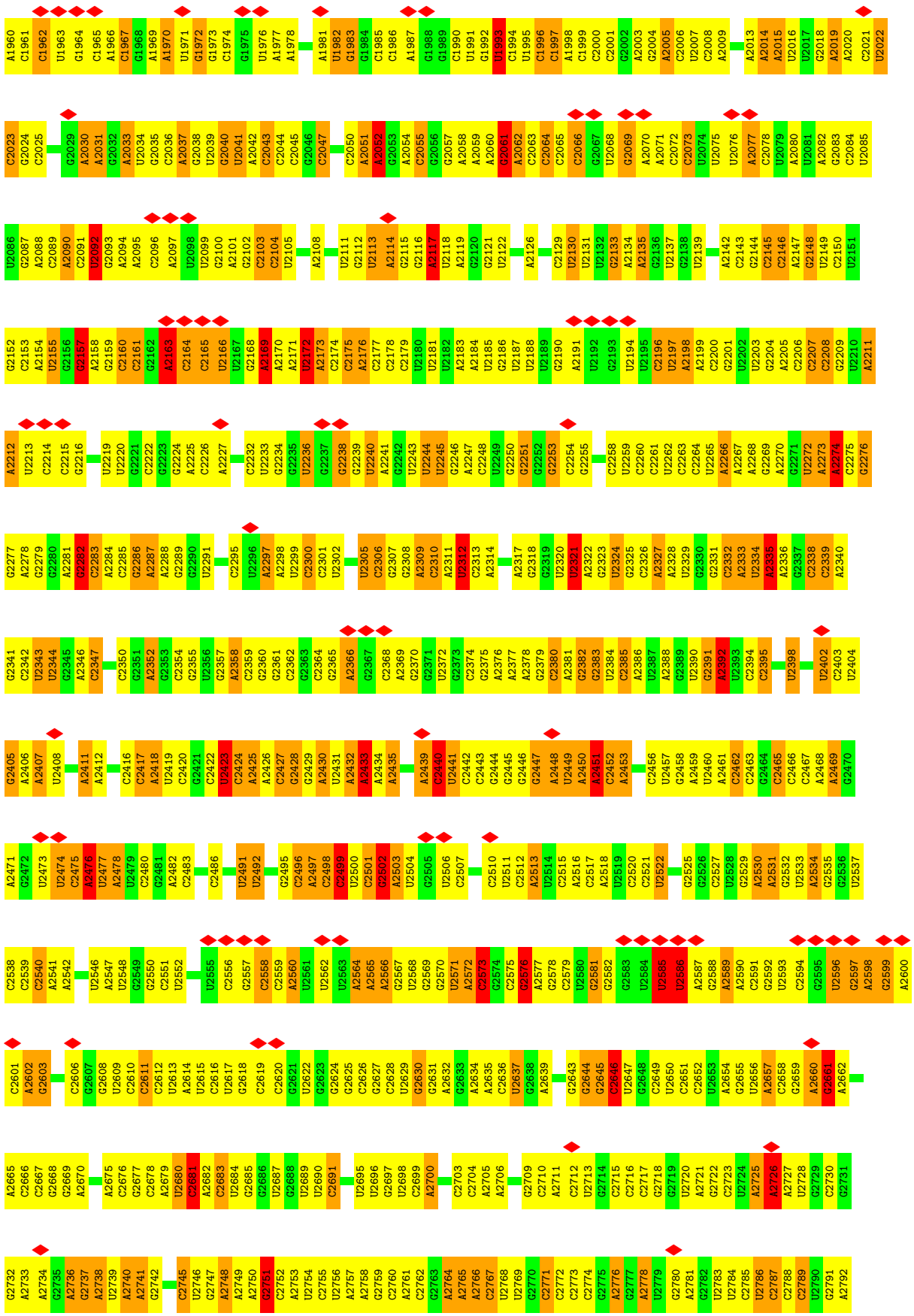
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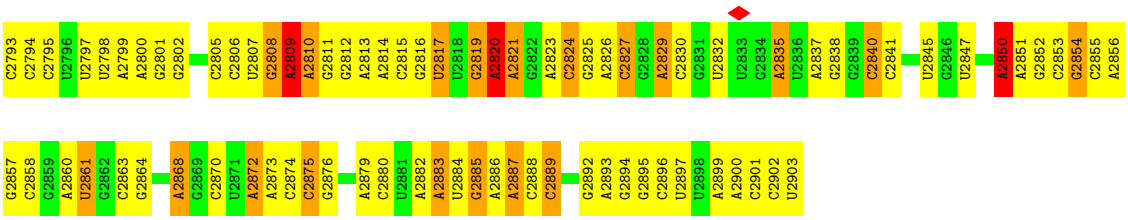
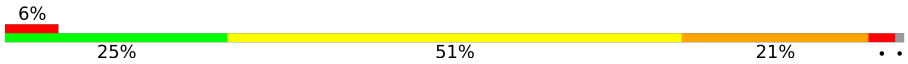
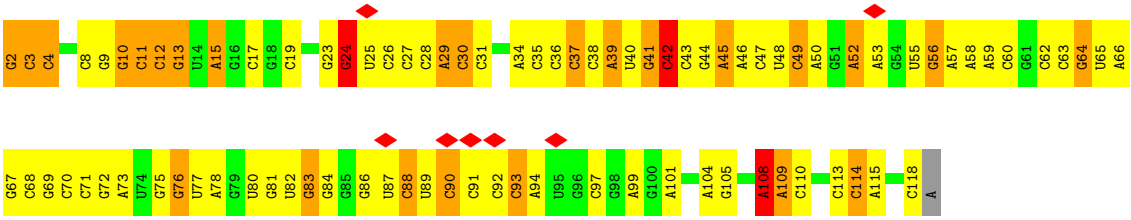


• Molecule 55: 5S ribosomal RNA

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	3052	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	162.319	Depositor
Minimum map value	-108.564	Depositor
Average map value	-1.515	Depositor
Map value standard deviation	18.464	Depositor
Recommended contour level	20.0	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: PSU, OMC, NH2, FME, 6MZ, CM0, 7MG, ACE, H2U, 4SU, 5MU

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	0.70	0/1736	1.07	11/2340 (0.5%)
2	AC	0.72	0/1651	1.16	16/2225 (0.7%)
3	AD	0.77	0/1665	1.23	24/2227 (1.1%)
4	AE	0.70	0/1119	1.06	10/1506 (0.7%)
5	AF	0.74	0/835	1.17	6/1128 (0.5%)
6	AG	0.74	0/1188	1.21	19/1593 (1.2%)
7	AH	0.70	0/989	1.08	5/1326 (0.4%)
8	AI	0.81	0/1035	1.34	20/1377 (1.5%)
9	AJ	0.69	0/797	1.23	13/1079 (1.2%)
10	AK	0.74	0/894	1.15	10/1207 (0.8%)
11	AL	0.76	0/969	1.23	15/1300 (1.2%)
12	AM	0.75	0/884	1.32	11/1181 (0.9%)
13	AN	0.77	0/817	1.26	12/1088 (1.1%)
14	AO	0.74	0/722	1.16	8/964 (0.8%)
15	AP	0.76	0/648	1.27	11/870 (1.3%)
16	AQ	0.70	0/658	1.06	4/883 (0.5%)
17	AR	0.81	0/463	1.29	10/623 (1.6%)
18	AS	0.76	0/653	1.13	7/879 (0.8%)
19	AT	0.68	0/672	1.05	5/890 (0.6%)
20	AU	0.83	0/431	1.44	8/572 (1.4%)
21	AA	1.53	1/36759 (0.0%)	2.22	1991/57346 (3.5%)
22	A1	1.53	0/1668	2.20	85/2595 (3.3%)
23	A2	1.47	0/343	2.25	15/531 (2.8%)
24	A3	1.53	0/1722	2.18	81/2685 (3.0%)
25	BC	0.74	0/2121	1.30	26/2852 (0.9%)
26	BD	0.68	0/1586	1.20	14/2134 (0.7%)
27	BE	0.67	0/1571	1.15	11/2113 (0.5%)
28	BF	0.74	0/1444	1.18	14/1937 (0.7%)
29	BG	0.69	0/1343	1.12	8/1816 (0.4%)
30	BH	0.65	0/1122	1.10	6/1515 (0.4%)
31	BI	0.65	0/1046	1.06	4/1410 (0.3%)
32	BJ	0.73	0/1152	1.16	8/1551 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BK	0.70	0/947	1.21	10/1268 (0.8%)
34	BL	0.73	0/1054	1.36	17/1403 (1.2%)
35	BM	0.74	0/1093	1.21	11/1460 (0.8%)
36	BN	0.77	0/973	1.36	15/1301 (1.2%)
37	BO	0.72	0/902	1.25	11/1209 (0.9%)
38	BP	0.75	0/929	1.27	8/1242 (0.6%)
39	BQ	0.80	0/960	1.32	15/1278 (1.2%)
40	BR	0.70	0/829	1.22	7/1107 (0.6%)
41	BS	0.64	0/864	1.19	10/1156 (0.9%)
42	BT	0.65	0/744	1.19	7/994 (0.7%)
43	BU	0.68	0/787	1.10	4/1051 (0.4%)
44	BV	0.71	0/766	1.16	5/1025 (0.5%)
45	BW	0.77	0/604	1.36	9/799 (1.1%)
46	BX	0.75	0/635	1.28	10/848 (1.2%)
47	BY	0.65	0/510	1.17	5/677 (0.7%)
48	BZ	0.69	0/453	1.24	6/605 (1.0%)
49	B0	0.72	0/450	1.23	5/599 (0.8%)
50	B1	0.73	0/417	1.05	2/556 (0.4%)
51	B2	0.81	0/380	1.49	11/498 (2.2%)
52	B3	0.72	0/513	1.23	5/676 (0.7%)
53	B4	0.68	0/303	1.24	4/397 (1.0%)
54	BA	1.41	2/69796 (0.0%)	2.21	4018/108888 (3.7%)
55	BB	1.42	0/2800	2.17	151/4367 (3.5%)
56	B5	0.64	0/1673	1.08	9/2255 (0.4%)
All	All	1.28	3/160085 (0.0%)	2.00	6843/239402 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	1
4	AE	0	1
14	AO	0	2
21	AA	0	368
22	A1	0	21
23	A2	0	4
24	A3	0	16
43	BU	0	1
49	B0	0	1
54	BA	0	707

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	25
All	All	0	1147

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	6	G	C2-N2	-5.63	1.28	1.34
54	BA	1568	G	C2-N2	-5.08	1.29	1.34
54	BA	2627	G	C2-N2	-5.01	1.29	1.34

The worst 5 of 6843 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1301	A	O4'-C1'-N9	17.59	122.27	108.20
54	BA	2126	A	O4'-C1'-N9	13.48	118.98	108.20
21	AA	547	A	N1-C6-N6	-12.92	110.85	118.60
54	BA	323	C	O4'-C1'-N1	12.84	118.47	108.20
54	BA	2199	A	N1-C6-N6	-12.76	110.94	118.60

There are no chirality outliers.

5 of 1147 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	5	U	Sidechain
1	AB	224	ARG	Sidechain
4	AE	22	LYS	Peptide
14	AO	48	ASP	Peptide
14	AO	68	TYR	Sidechain

5.2 Too-close contacts (i)

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	3	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	1	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	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	3	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	2	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	1	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	1	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31341	4	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99659	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)
34:BL:30:THR:HG21	34:BL:36:LYS:H	1.72	0.54
54:BA:388:G:H2'	54:BA:389:G:H3'	1.91	0.52
42:BT:15:HIS:CG	42:BT:16:VAL:H	2.29	0.50
21:AA:1054:C:C6	23:A2:89:U:H1'	2.48	0.48
37:BO:53:THR:HG21	37:BO:70:ALA:HB1	1.98	0.46

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	200 (92%)	17 (8%)	1 (0%)	29	69
2	AC	205/208 (99%)	184 (90%)	15 (7%)	6 (3%)	4	29
3	AD	203/206 (98%)	185 (91%)	14 (7%)	4 (2%)	7	38
4	AE	150/152 (99%)	134 (89%)	10 (7%)	6 (4%)	3	23
5	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	1	17
6	AG	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	5	31
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	6	33
8	AI	126/128 (98%)	107 (85%)	15 (12%)	4 (3%)	4	26
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	19
10	AK	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	9	42
11	AL	121/124 (98%)	107 (88%)	8 (7%)	6 (5%)	2	20
12	AM	112/115 (97%)	94 (84%)	13 (12%)	5 (4%)	2	22
13	AN	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
14	AO	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	50
15	AP	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	3	24
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	8	40
18	AS	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	3	24
19	AT	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
20	AU	51/53 (96%)	32 (63%)	15 (29%)	4 (8%)	1	13
25	BC	270/273 (99%)	238 (88%)	25 (9%)	7 (3%)	5	31
26	BD	207/209 (99%)	185 (89%)	17 (8%)	5 (2%)	6	33
27	BE	199/201 (99%)	171 (86%)	20 (10%)	8 (4%)	3	23
28	BF	176/179 (98%)	155 (88%)	17 (10%)	4 (2%)	6	34
29	BG	174/177 (98%)	155 (89%)	12 (7%)	7 (4%)	3	23
30	BH	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	22	63
31	BI	139/142 (98%)	125 (90%)	12 (9%)	2 (1%)	11	46
32	BJ	140/142 (99%)	126 (90%)	11 (8%)	3 (2%)	7	36
33	BK	121/123 (98%)	107 (88%)	10 (8%)	4 (3%)	4	26
34	BL	141/144 (98%)	124 (88%)	11 (8%)	6 (4%)	2	22
35	BM	134/136 (98%)	115 (86%)	14 (10%)	5 (4%)	3	24
36	BN	119/121 (98%)	105 (88%)	11 (9%)	3 (2%)	5	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	108 (95%)	3 (3%)	3 (3%)	5	31
38	BP	112/115 (97%)	92 (82%)	17 (15%)	3 (3%)	5	31
39	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9	42
40	BR	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	4	28
41	BS	108/110 (98%)	105 (97%)	2 (2%)	1 (1%)	17	57
42	BT	92/94 (98%)	80 (87%)	6 (6%)	6 (6%)	1	16
43	BU	101/104 (97%)	83 (82%)	14 (14%)	4 (4%)	3	23
44	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
45	BW	78/80 (98%)	59 (76%)	17 (22%)	2 (3%)	5	31
46	BX	75/79 (95%)	68 (91%)	3 (4%)	4 (5%)	2	19
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	49 (88%)	4 (7%)	3 (5%)	2	19
49	B0	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
52	B3	62/65 (95%)	54 (87%)	5 (8%)	3 (5%)	2	21
53	B4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	30
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	29	69
All	All	5876/6008 (98%)	5245 (89%)	476 (8%)	155 (3%)	8	31

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	224	ARG
2	AC	14	VAL
5	AF	86	ARG
15	AP	11	ALA
15	AP	17	TYR

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	177 (98%)	3 (2%)	60	78
2	AC	170/171 (99%)	168 (99%)	2 (1%)	71	83
3	AD	172/173 (99%)	171 (99%)	1 (1%)	86	92
4	AE	113/113 (100%)	112 (99%)	1 (1%)	78	87
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	81	89
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%)	83 (96%)	3 (4%)	36	59
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	76	86
12	AM	91/92 (99%)	90 (99%)	1 (1%)	73	84
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%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	30	55
17	AR	48/48 (100%)	45 (94%)	3 (6%)	18	43
18	AS	70/70 (100%)	69 (99%)	1 (1%)	67	80
19	AT	65/65 (100%)	64 (98%)	1 (2%)	65	80
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	43	65
26	BD	164/164 (100%)	160 (98%)	4 (2%)	49	69
27	BE	165/165 (100%)	162 (98%)	3 (2%)	59	77
28	BF	149/150 (99%)	147 (99%)	2 (1%)	69	81
29	BG	137/138 (99%)	133 (97%)	4 (3%)	42	64
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	78	87
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	46	66
33	BK	103/103 (100%)	102 (99%)	1 (1%)	76	86
34	BL	102/103 (99%)	100 (98%)	2 (2%)	55	74
35	BM	109/109 (100%)	107 (98%)	2 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	76	86
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	55	74
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	52	71
40	BR	84/84 (100%)	84 (100%)	0	100	100
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%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	53 (90%)	6 (10%)	7	25
46	BX	67/68 (98%)	66 (98%)	1 (2%)	65	80
47	BY	55/55 (100%)	54 (98%)	1 (2%)	59	77
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	53	72
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%)	48 (94%)	3 (6%)	19	45
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	169 (98%)	4 (2%)	50	70
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	61	77

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

Mol	Chain	Res	Type
34	BL	93	ASN
45	BW	40	ARG
35	BM	97	GLN
41	BS	60	HIS
47	BY	26	PHE

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

Mol	Chain	Res	Type
12	AM	104	ASN

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Mol	Chain	Res	Type
44	BV	88	HIS
46	BX	15	ASN
49	B0	41	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	248 (16%)	86 (5%)
22	A1	73/76 (96%)	15 (20%)	7 (9%)
23	A2	14/15 (93%)	5 (35%)	3 (21%)
24	A3	76/77 (98%)	13 (17%)	5 (6%)
54	BA	2902/2903 (99%)	464 (15%)	110 (3%)
55	BB	117/118 (99%)	15 (12%)	4 (3%)
All	All	4712/4722 (99%)	760 (16%)	215 (4%)

5 of 760 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	16	A

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	389	G
54	BA	1087	G
54	BA	2430	A
54	BA	529	A
54	BA	670	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	$\#\|Z\| > 2$
22	PSU	A1	55	22	18,21,22	0.82	0	22,30,33	1.16	1 (4%)
22	4SU	A1	7	22	18,21,22	1.46	2 (11%)	26,30,33	1.07	2 (7%)
24	5MU	A3	55	24	19,22,23	0.73	0	28,32,35	1.46	4 (14%)
22	7MG	A1	46	22	22,26,27	4.75	1 (4%)	29,39,42	1.40	1 (3%)
22	CM0	A1	34	21,22	22,26,27	1.38	2 (9%)	28,37,40	1.04	0
22	5MU	A1	54	22	19,22,23	0.79	0	28,32,35	1.49	5 (17%)
24	4SU	A3	8	24	18,21,22	1.39	1 (5%)	26,30,33	0.79	1 (3%)
24	OMC	A3	33	24	19,22,23	0.80	0	26,31,34	1.14	2 (7%)
24	H2U	A3	21	24	18,21,22	1.38	2 (11%)	21,30,33	1.18	2 (9%)
22	6MZ	A1	37	22	18,25,26	1.04	1 (5%)	16,36,39	1.54	2 (12%)
24	PSU	A3	56	24	18,21,22	0.94	0	22,30,33	1.16	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
22	CM0	A1	34	21,22	-	4/12/30/31	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	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
24	PSU	A3	56	24	-	0/7/25/26	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	-22.05	1.33	1.46
22	A1	34	CM0	O5-C5	-5.02	1.25	1.36
22	A1	7	4SU	C5-C4	-5.00	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	8	4SU	C5-C4	-4.78	1.36	1.42
24	A3	21	H2U	C2-N3	-3.50	1.31	1.38

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	46	7MG	N9-C8-N7	5.85	111.75	103.38
22	A1	37	6MZ	C9-N6-C6	4.93	127.12	122.87
22	A1	54	5MU	C5M-C5-C6	-4.11	117.36	122.85
24	A3	55	5MU	C5M-C5-C6	-3.76	117.83	122.85
22	A1	54	5MU	C6-C5-C4	3.39	120.86	118.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	46	7MG	C4'-C5'-O5'-P
22	A1	34	CM0	C6-C5-O5-C7
22	A1	34	CM0	C4-C5-O5-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	VAL	A1	101	58,22	4,6,7	0.76	0	6,7,9	1.52	1 (16%)
58	FME	BA	3001	57	8,9,10	0.63	0	7,9,11	1.12	0

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	58,22	-	0/5/6/8	-
58	FME	BA	3001	57	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	A1	101	VAL	O-C-CA	-3.66	115.18	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

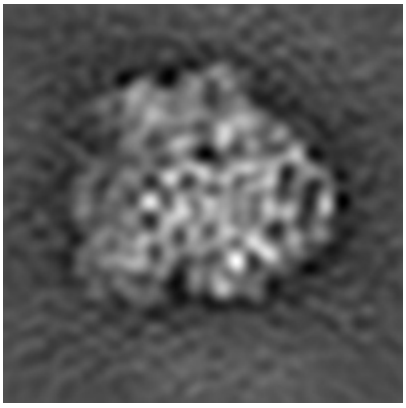
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1720. These allow visual inspection of the internal detail of the map and identification of artifacts.

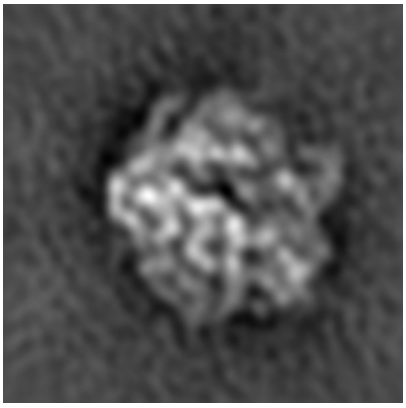
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

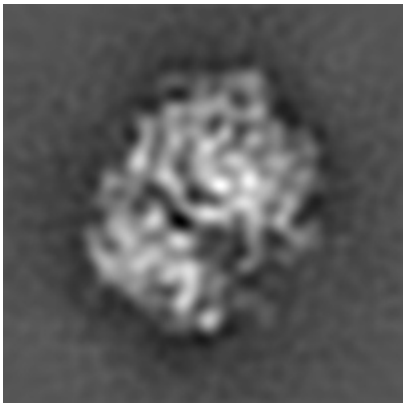
6.1.1 Primary map



X



Y



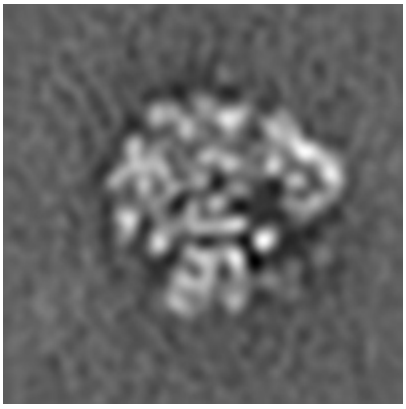
Z

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

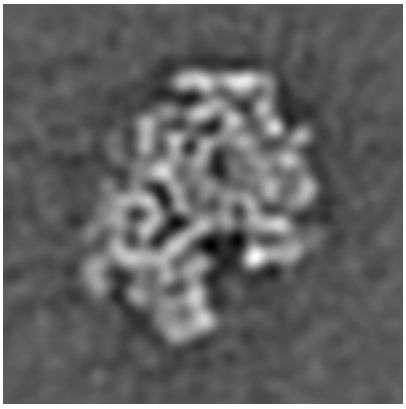
6.2 Central slices (i)

6.2.1 Primary map

X Index: 64



Y Index: 64

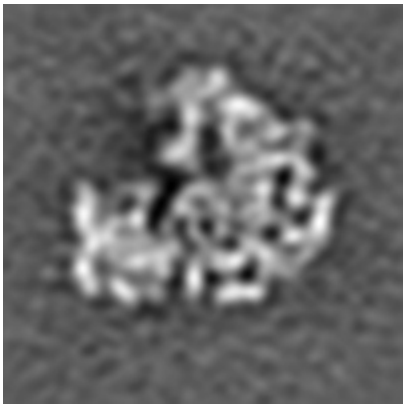


Z Index: 64

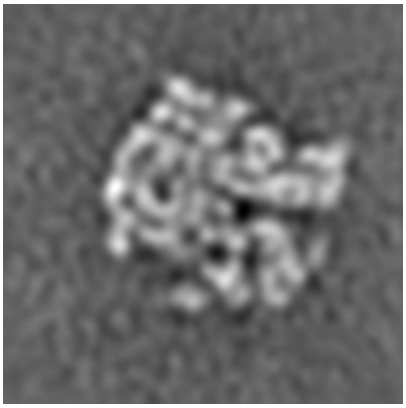
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

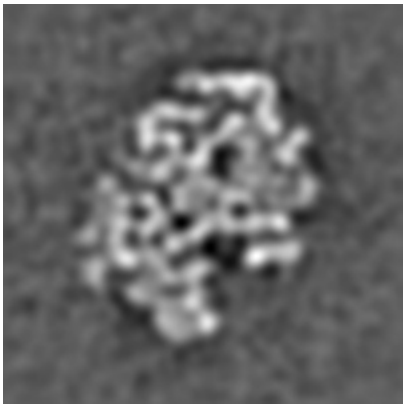
6.3.1 Primary map



X Index: 65



Y Index: 70

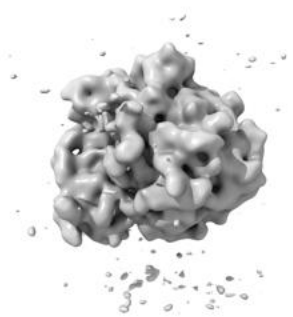


Z Index: 62

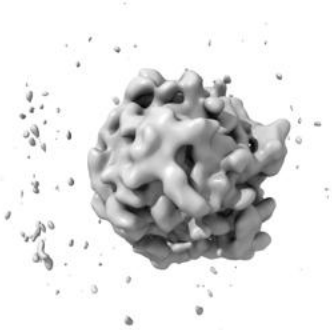
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

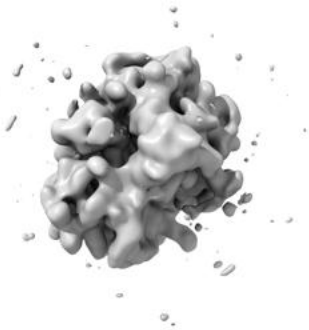
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 20.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

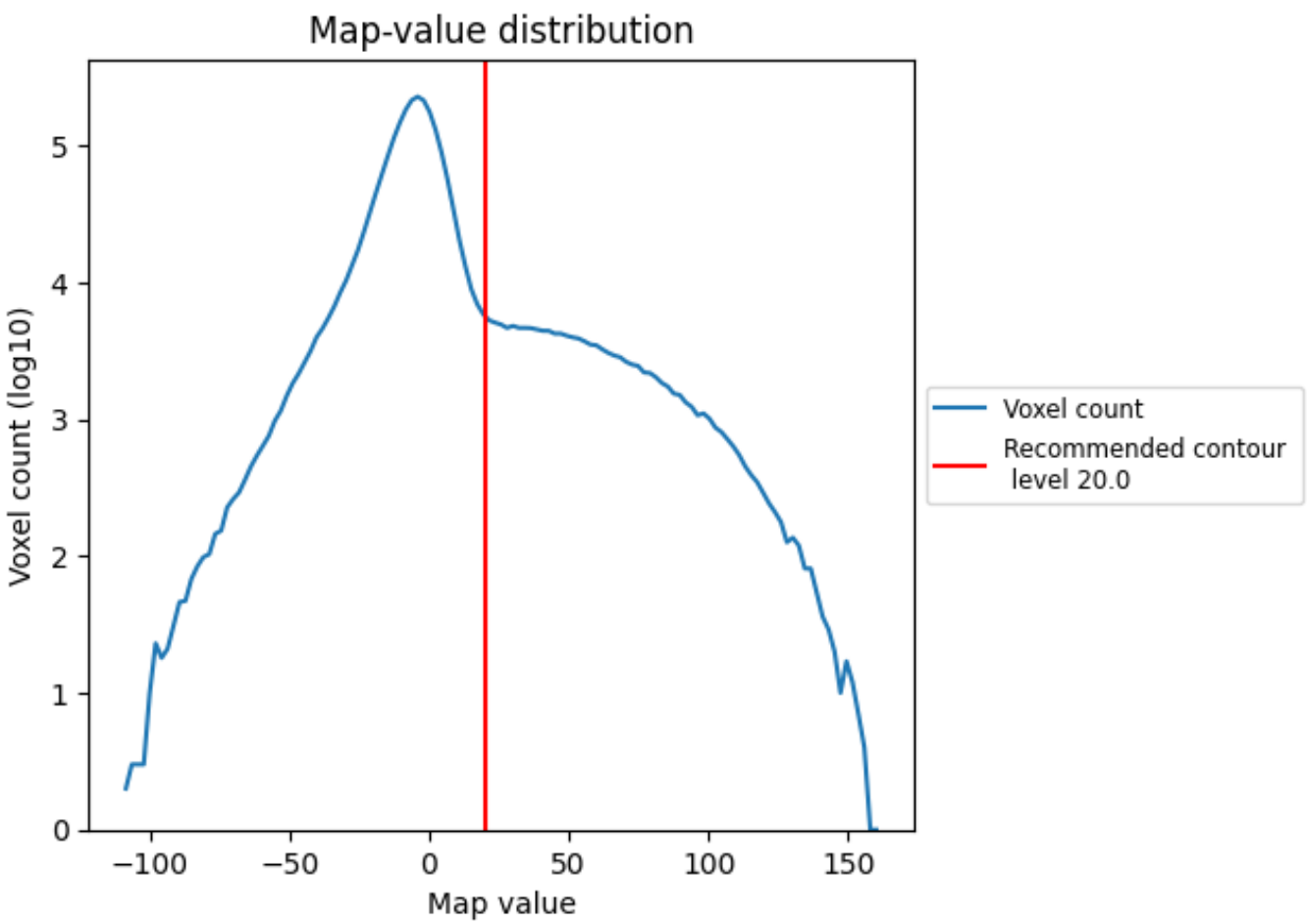
6.5 Mask visualisation (i)

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

7 Map analysis (i)

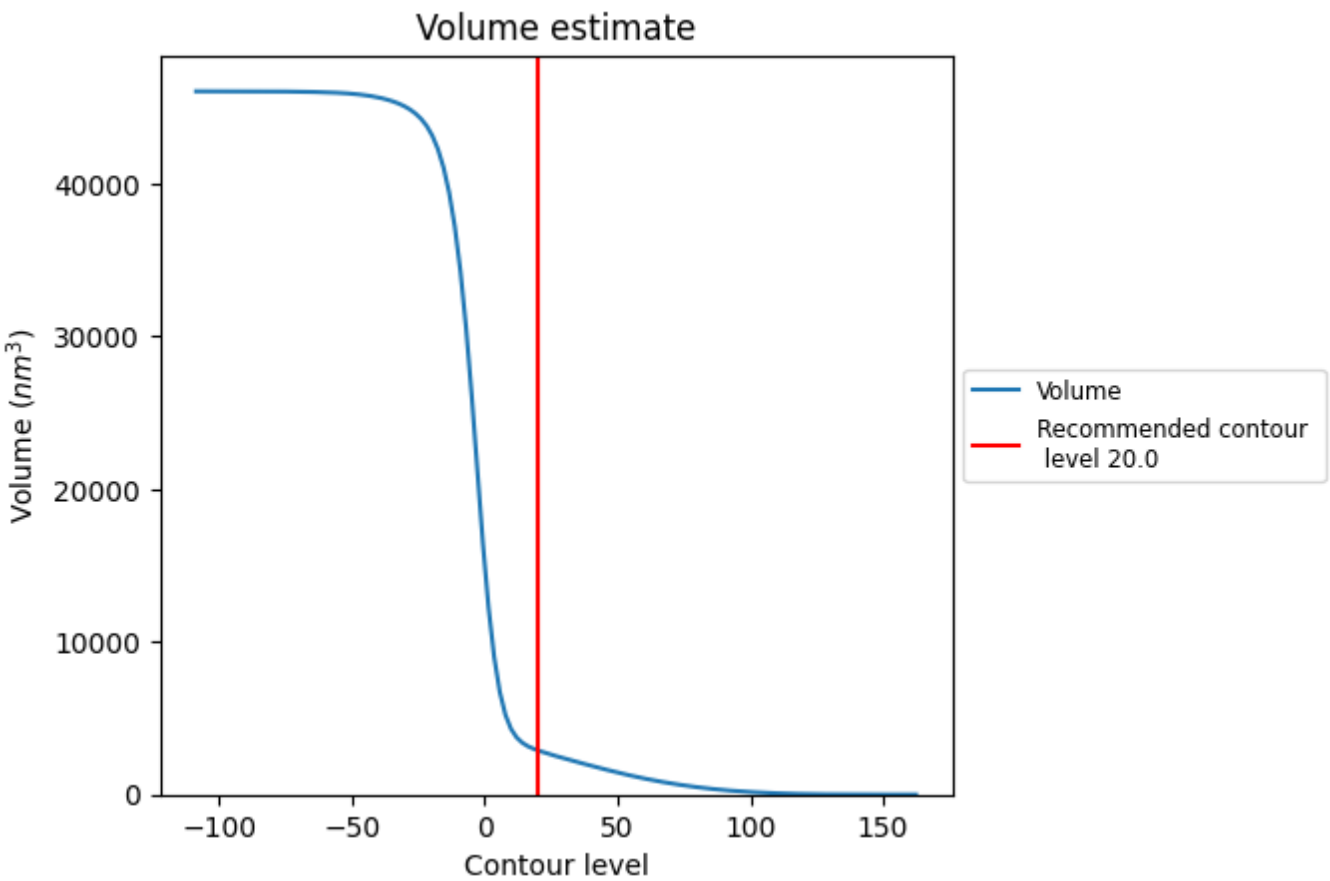
This section contains the results of statistical analysis of the map.

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.

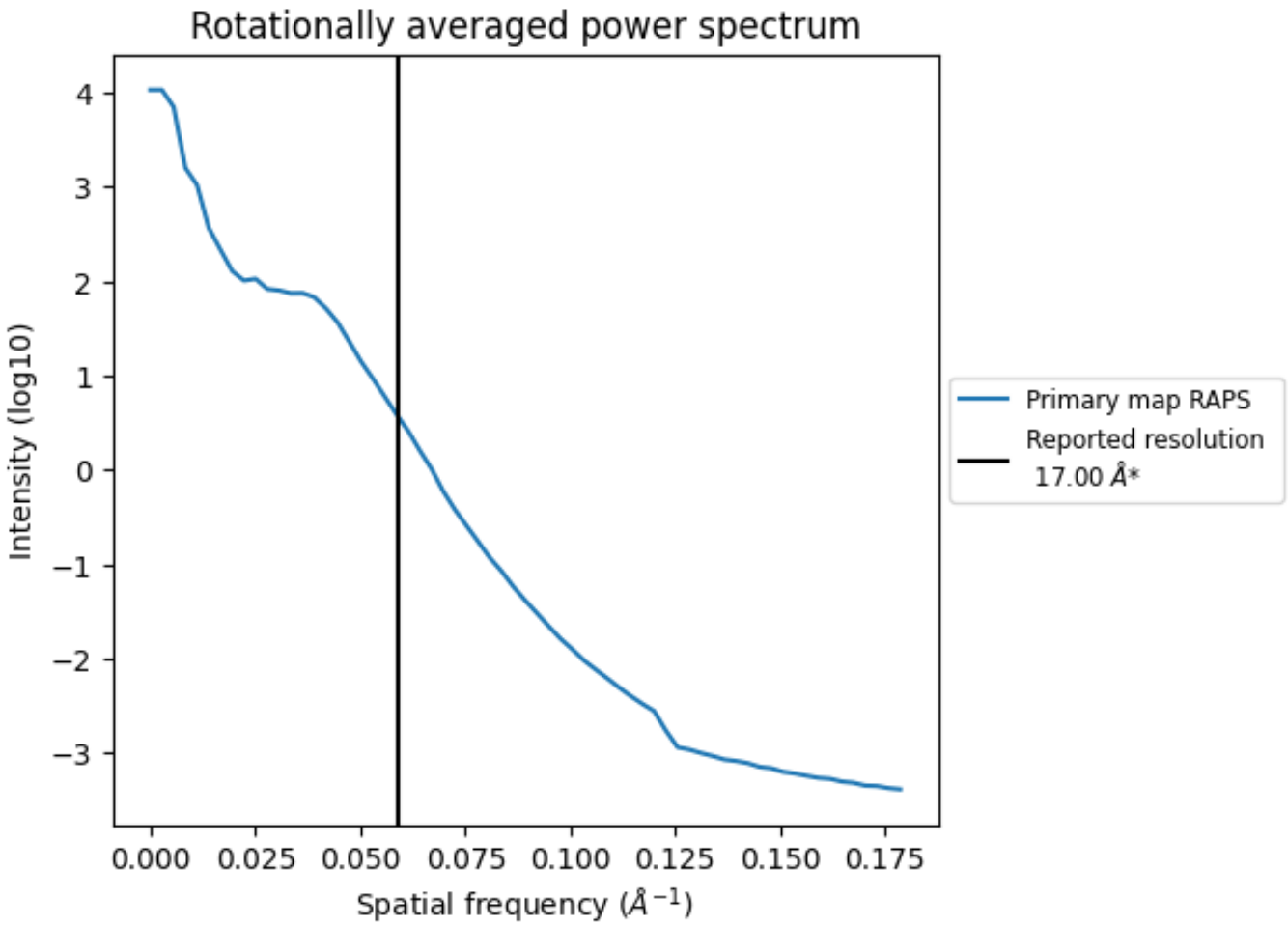
7.2 Volume estimate (i)



The volume at the recommended contour level is 2895 nm^3; this corresponds to an approximate mass of 2615 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}

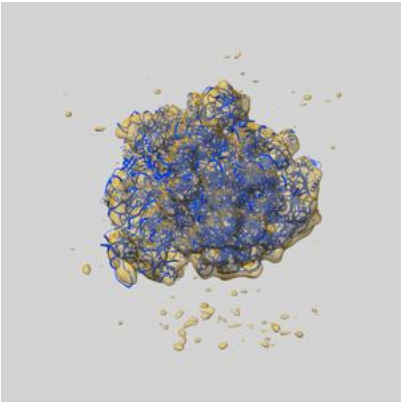
8 Fourier-Shell correlation (i)

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

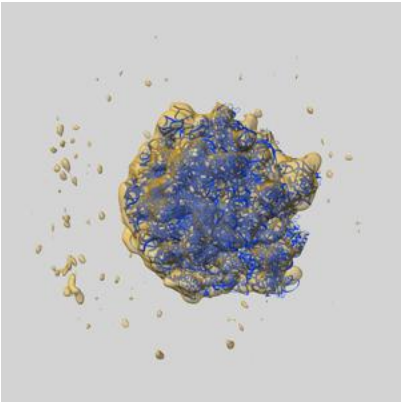
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1720 and PDB model 4V74. Per-residue inclusion information can be found in section 3 on page 17.

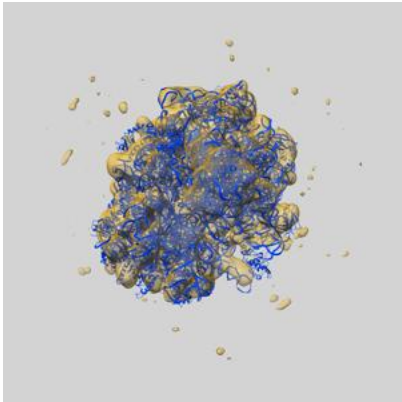
9.1 Map-model overlay (i)



X



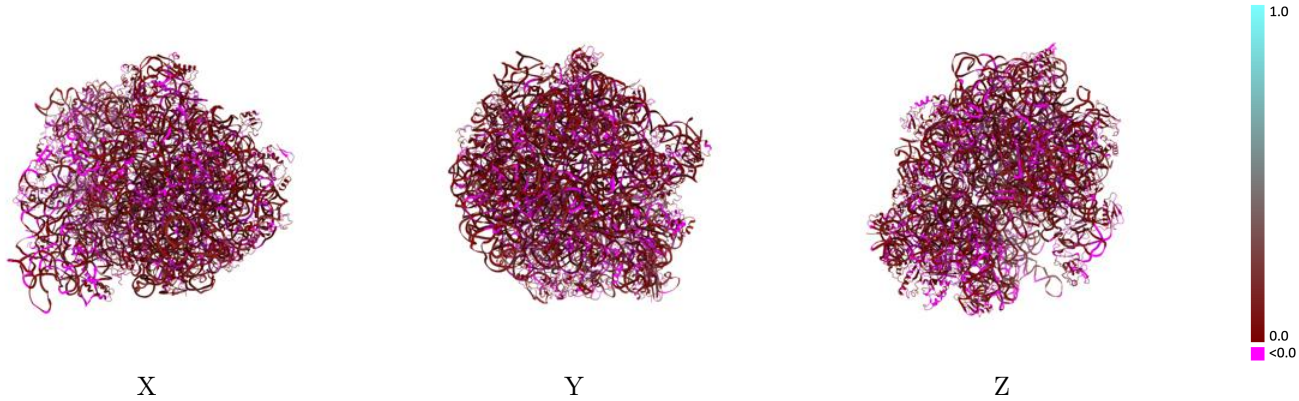
Y



Z

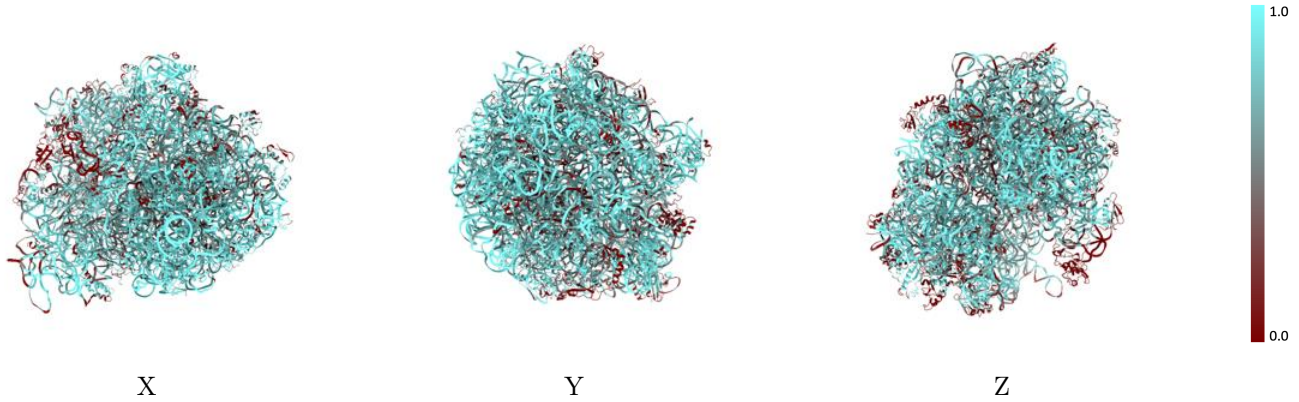
The images above show the 3D surface view of the map at the recommended contour level 20.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



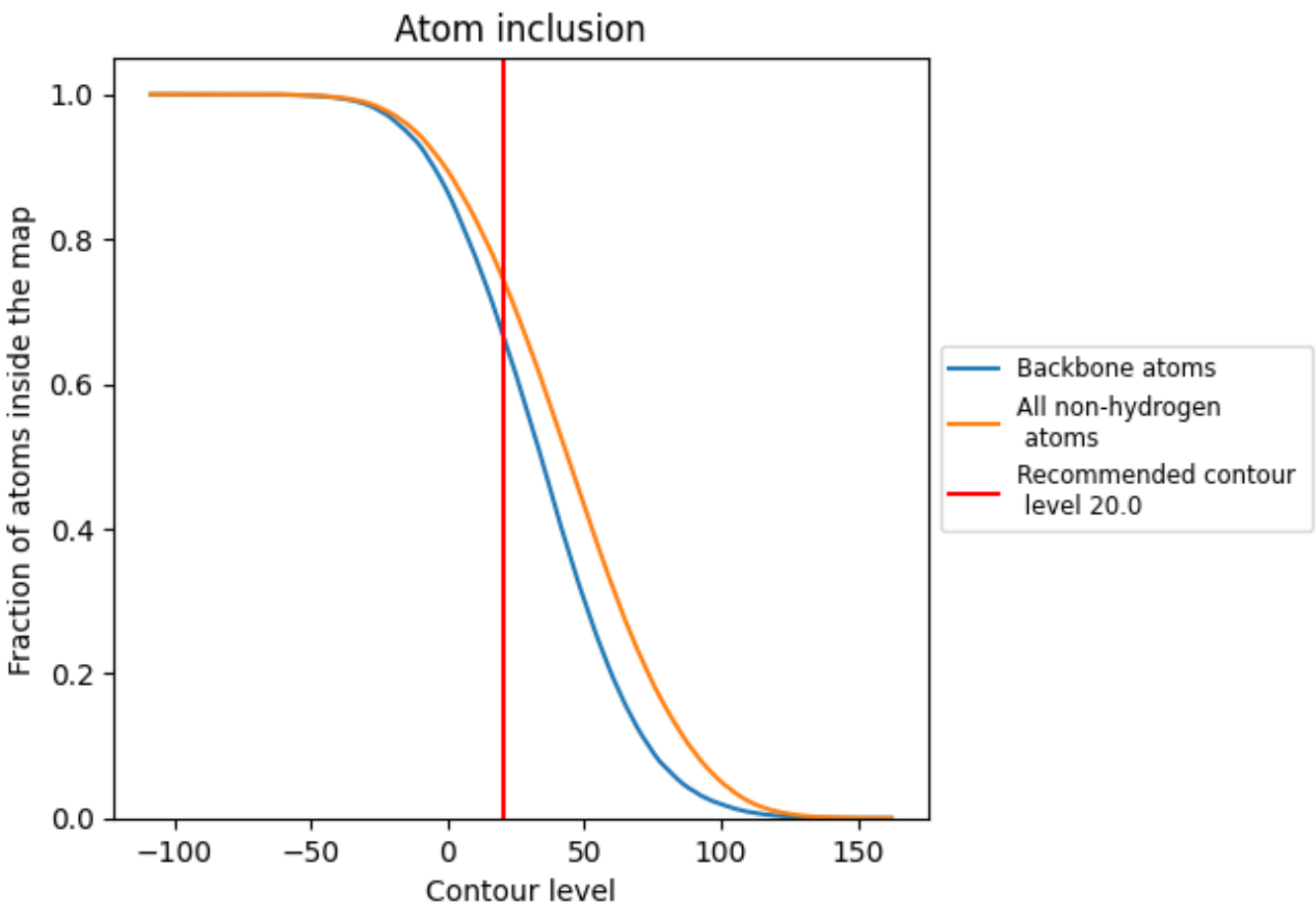
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (20.0).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 75% 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 (20.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7471	0.0520
A1	0.6958	0.0570
A2	0.7735	0.0820
A3	0.7095	0.0620
AA	0.8142	0.0590
AB	0.5495	0.0480
AC	0.4725	0.0200
AD	0.5572	0.0210
AE	0.5534	0.0290
AF	0.8130	0.0430
AG	0.7018	0.0390
AH	0.6573	0.0280
AI	0.6239	0.0300
AJ	0.7696	0.0250
AK	0.7088	0.0460
AL	0.6167	0.0240
AM	0.6734	0.0350
AN	0.5581	0.0250
AO	0.9087	0.0320
AP	0.5251	-0.0030
AQ	0.6472	0.0240
AR	0.6606	0.0150
AS	0.7276	0.0360
AT	0.7132	-0.0010
AU	0.5550	0.0350
B0	0.6822	0.0130
B1	0.7005	0.0550
B2	0.4676	0.0060
B3	0.4521	-0.0330
B4	0.6473	0.0220
B5	0.5695	0.0360
BA	0.8149	0.0680
BB	0.8850	0.0740
BC	0.4536	-0.0050
BD	0.6378	0.0320

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Chain	Atom inclusion	Q-score
BE	0.6184	0.0150
BF	0.7332	0.0500
BG	0.5775	0.0360
BH	0.1414	0.0060
BI	0.0000	-0.0000
BJ	0.6791	0.0210
BK	0.5449	0.0280
BL	0.6457	0.0230
BM	0.5873	0.0190
BN	0.8299	0.0250
BO	0.8389	0.0260
BP	0.5484	0.0270
BQ	0.5738	-0.0130
BR	0.7064	0.0470
BS	0.6316	0.0290
BT	0.7109	0.0300
BU	0.6641	0.0110
BV	0.6707	0.0320
BW	0.5344	-0.0070
BX	0.6339	0.0030
BY	0.5252	0.0260
BZ	0.6384	0.0530