



## wwPDB EM Validation Summary Report i

Nov 20, 2022 – 02:08 AM EST

PDB ID : 4V7A  
EMDB ID : EMD-1724  
Title : E. coli 70S-fMetVal-tRNAVal post-translocation complex (post4)  
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 : 9.00 Å(reported)  
Based on initial models : 2HGP, 3I1O, 2WRI, 2K4C

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

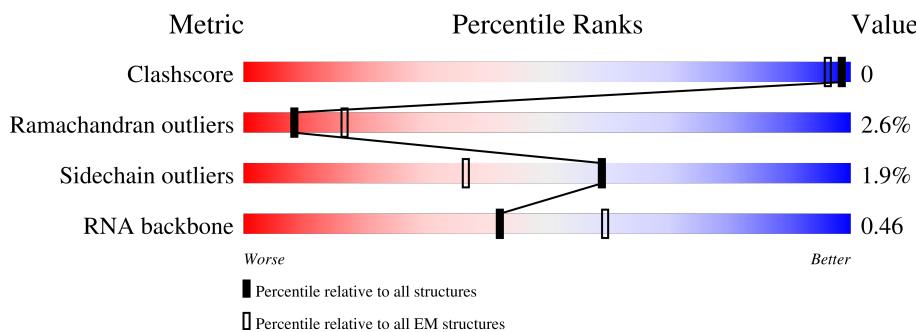
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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**

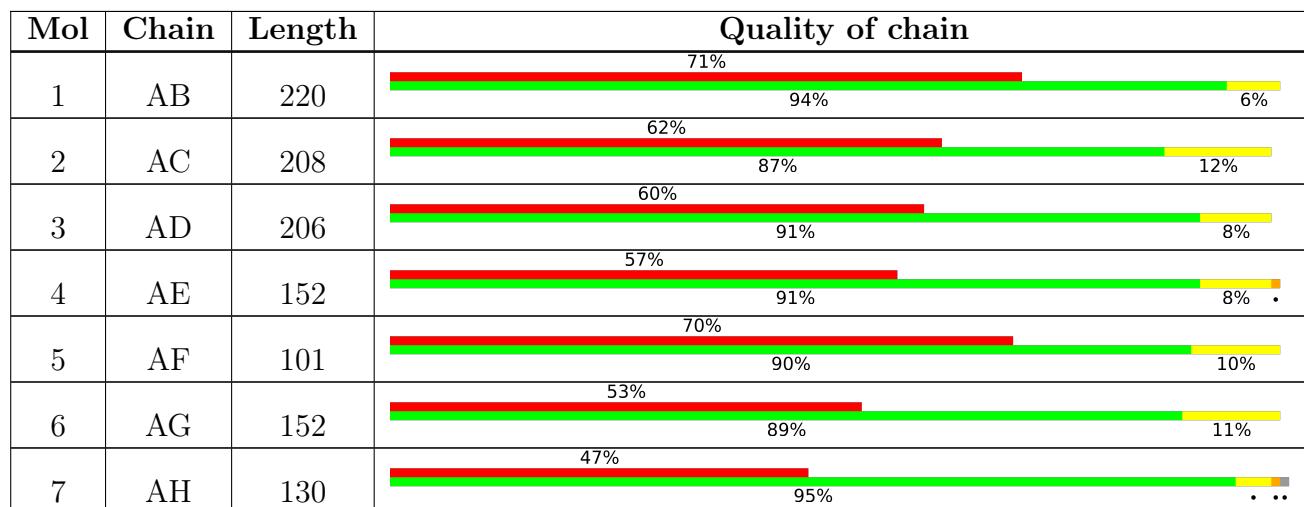
The reported resolution of this entry is 9.00 Å.

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.



Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain			
8	AI	128	41%	86%	14%	.
9	AJ	100	70%	86%	13%	.
10	AK	118	59%	92%	7%	.
11	AL	124	60%	83%	16%	.
12	AM	115	42%	87%	12%	.
13	AN	101	50%	86%	11%	..
14	AO	89	65%	84%	15%	.
15	AP	81	53%	91%	9%	.
16	AQ	82	60%	90%	9%	.
17	AR	57	44%	89%	7%	.
18	AS	81	56%	88%	11%	.
19	AT	86	63%	90%	10%	.
20	AU	53	72%	89%	9%	.
21	AA	1533	42%	55%	24%	.
22	A1	76	47%	70%	18%	.
23	A2	15	60%	40%	27%	.
24	BC	273	50%	88%	12%	.
25	BD	209	59%	89%	11%	.
26	BE	201	48%	91%	8%	.
27	BF	179	49%	84%	15%	..
28	BG	177	55%	90%	8%	..
29	BH	149	97%	94%	6%	.
30	BI	142	99%	96%	..	.
31	BJ	142	51%	91%	8%	.
32	BK	123	61%	85%	15%	.

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain				
33	BL	144	51%	83%	15%	..	
34	BM	136	55%	89%	10%	.	
35	BN	121	67%	83%	16%	.	
36	BO	117	39%	91%	9%	.	
37	BP	115	70%	90%	9%	..	
38	BQ	118	53%	87%	12%	.	
39	BR	103	68%	88%	12%		
40	BS	110	58%	89%	11%		
41	BT	94	67%	85%	15%		
42	BU	104	72%	90%	8%	..	
43	BV	94	51%	89%	11%		
44	BW	80	58%	79%	20%	.	
45	BX	79	61%	82%	13%	..	
46	BY	63	68%	90%	10%		
47	BZ	59	44%	86%	8%	..	
48	B0	57	60%	84%	14%	.	
49	B1	52	79%	87%	13%		
50	B2	46	61%	78%	22%		
51	B3	65	62%	85%	14%	.	
52	B4	38	55%	87%	11%	.	
53	BA	2903	50%	55%	25%	.	
54	BB	118	46%	53%	19%	5%	.
55	B5	234	21%	91%	6%	5%	

## 2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 146011 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AB	220	1708	1083	306	312	7	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	acetylation	UNP P0A7V0
AB	226	NH2	-	amidation	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AC	207	1625	1028	306	288	3	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	amidation	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AD	205	1643	1026	315	298	4	0	0

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	acetylation	UNP P0A7W1
AE	159	NH2	-	amidation	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AF	101	Total	C	N	O	S	
			818	515	149	148	6	

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			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
13	AN	100	Total	C	N	O	S	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AR	57	Total	C	N	O		0	1

There are 2 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P		0

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BC	272	Total	C	N	O	P	S	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BD	209	Total	C	N	O	S		0

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BE	201	Total	C	N	O	S		0

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BL	143	Total	C	N	O	S	0	0

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BN	121	Total	C	N	O	S	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 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BO	116	Total	C	N	O		0	0

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BP	114	Total	C	N	O	S	0	0

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BQ	117	Total	C	N	O		0	0

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BR	103	Total	C	N	O	S	0	0

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BS	110	Total	C	N	O	S	0	0

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BT	94	Total	C	N	O	S	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 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BU	103	Total	C	N	O		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 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BV	94	Total	C	N	O	S	0	0

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	80	Total	C	N	O	S	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 45 is a protein called 50S ribosomal protein L28.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

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

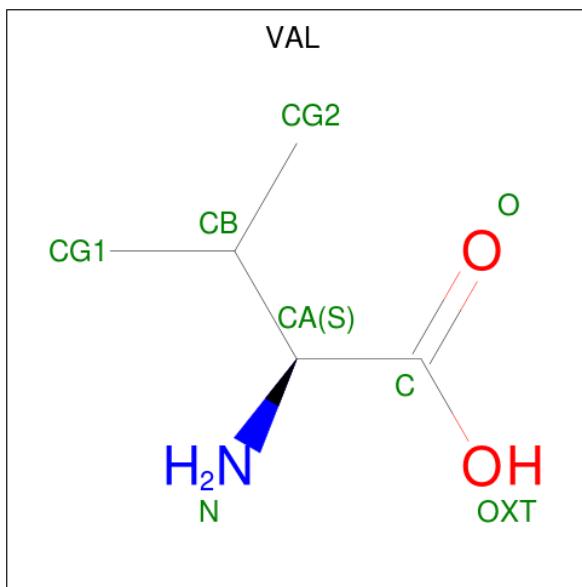
- Molecule 54 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 55 is a protein called 50S ribosomal protein L1.

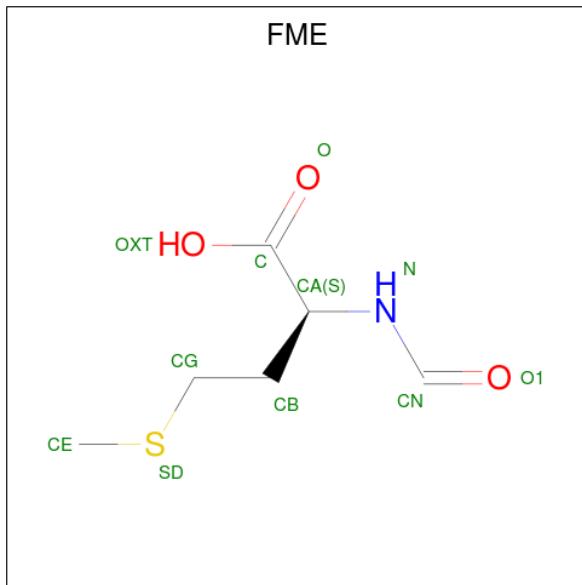
Mol	Chain	Residues	Atoms				AltConf	Trace
55	B5	223	Total	C	N	O	S	0
			1658	1038	302	312	6	0

- Molecule 56 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



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

- Molecule 57 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).

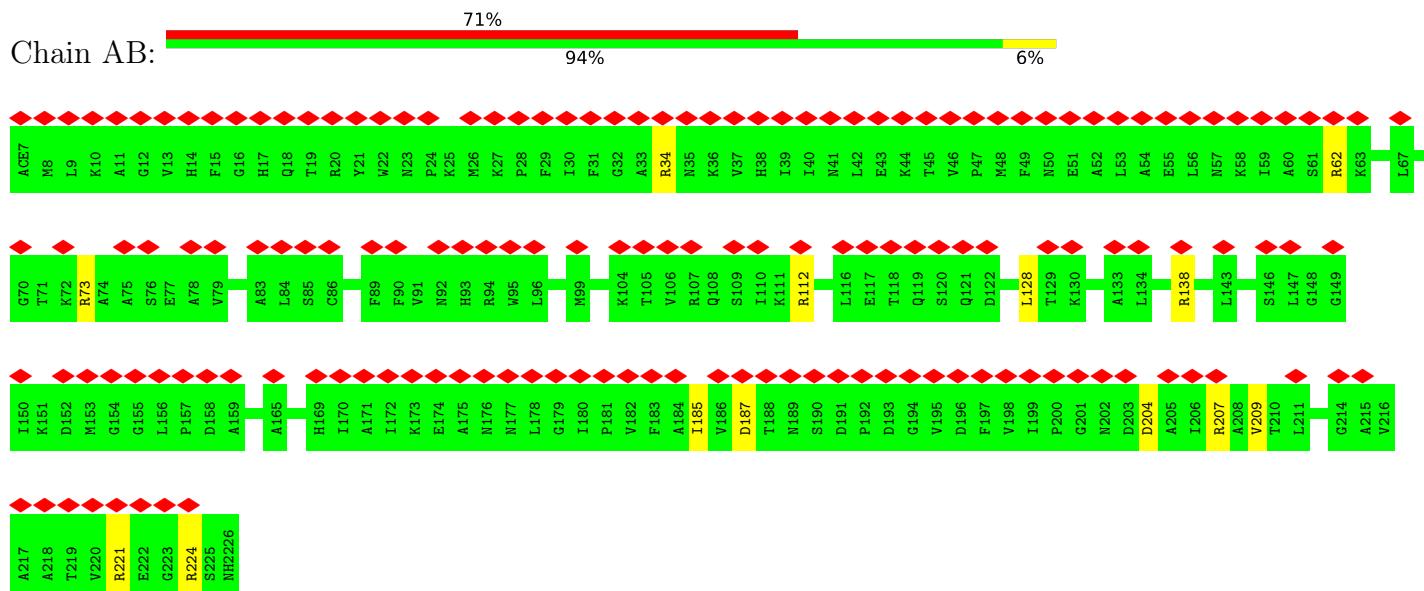


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	S
57	BA	1	10	6	1	2	1

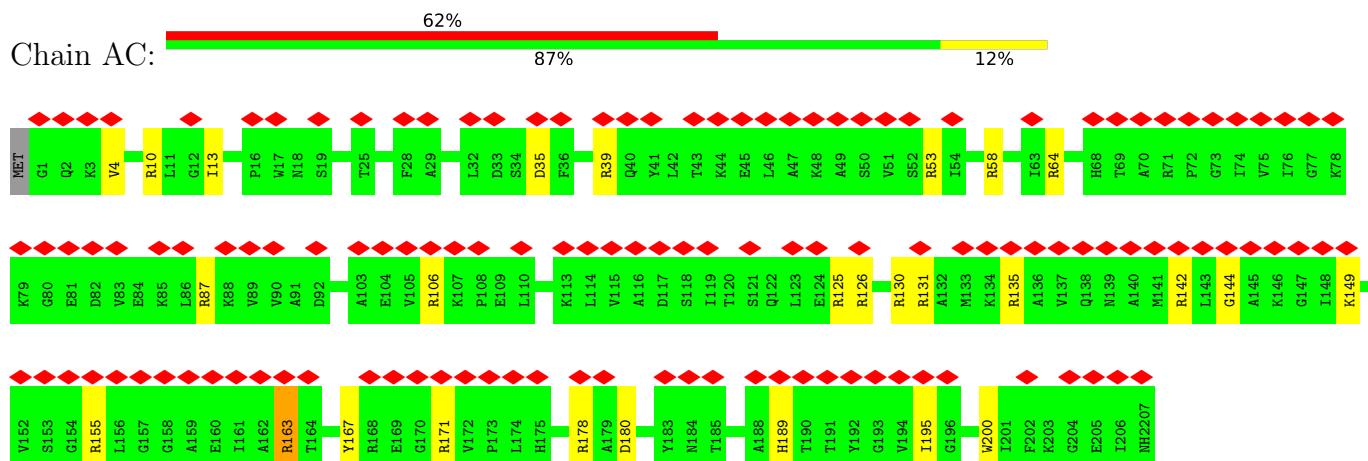
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

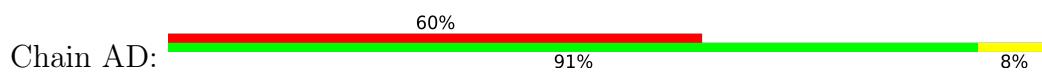
- Molecule 1: 30S ribosomal protein S2

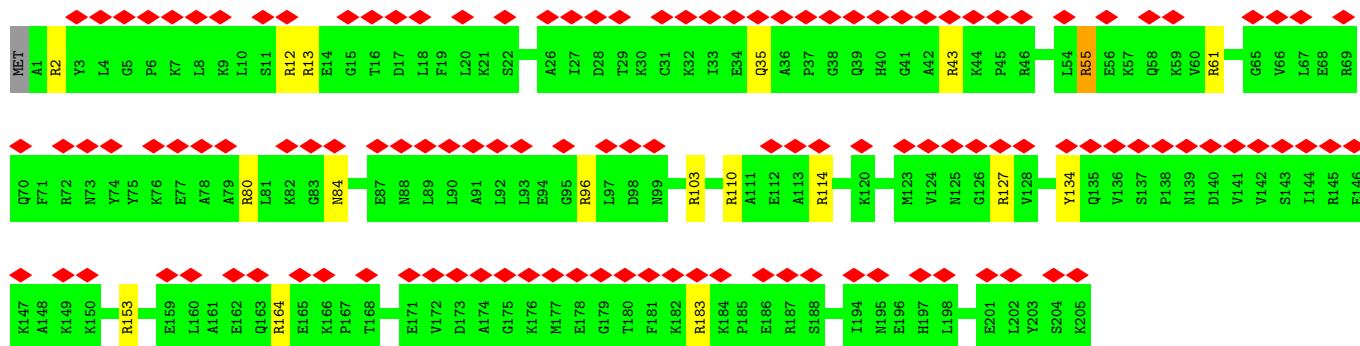


- Molecule 2: 30S ribosomal protein S3

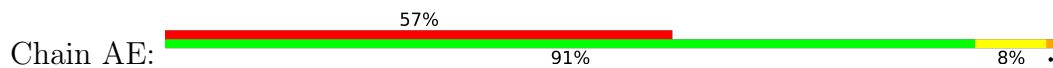


- Molecule 3: 30S ribosomal protein S4

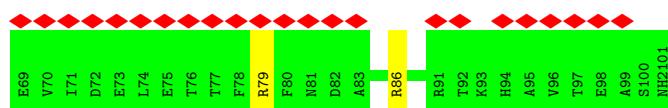
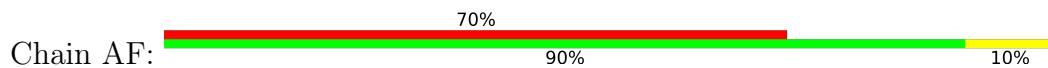




- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7



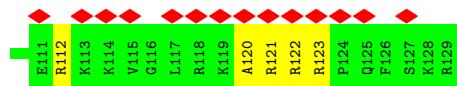
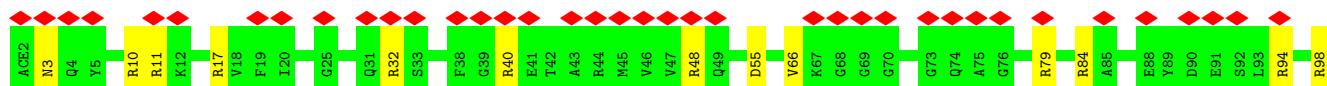
- Molecule 7: 30S ribosomal protein S8





- Molecule 8: 30S ribosomal protein S9

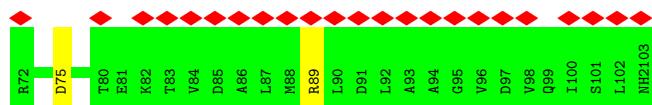
Chain AI:  41% 86%



- Molecule 9: 30S ribosomal protein S10

A horizontal bar chart titled "Chain AJ" showing the percentage distribution across four categories. The categories are represented by red bars of increasing length from left to right. The percentages are labeled above each bar: 70% (shortest bar), 86% (medium bar), 13% (longest bar), and 1% (barely visible bar). The bars are set against a white background with a light gray horizontal grid.

Category	Percentage
1	70%
2	86%
3	13%
4	1%



- Molecule 10: 30S ribosomal protein S11

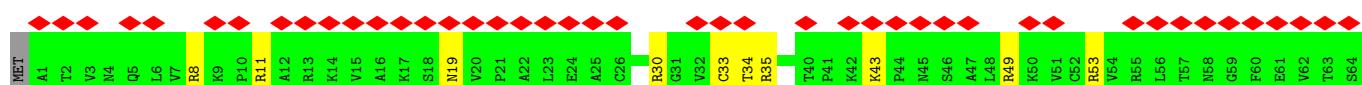
A horizontal bar chart illustrating the distribution of Chain AK across four categories. The categories are represented by colored bars: red, green, yellow, and orange. The percentages for each category are as follows:

Category	Percentage
Red	59%
Green	92%
Yellow	7%
Orange	•



- Molecule 11: 30S ribosomal protein S12

A horizontal bar chart illustrating the distribution of Chain AL across three categories. The categories are represented by colored bars: Red, Green, and Yellow. The Red bar accounts for 60% of the total, the Green bar for 83%, and the Yellow bar for 16%. The bars are positioned side-by-side, with the Green bar being the longest and the Yellow bar being the shortest.

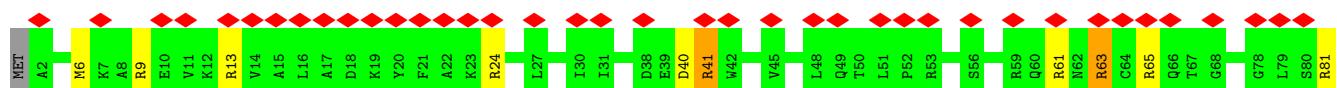
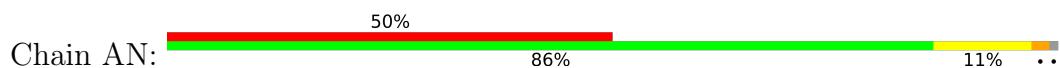




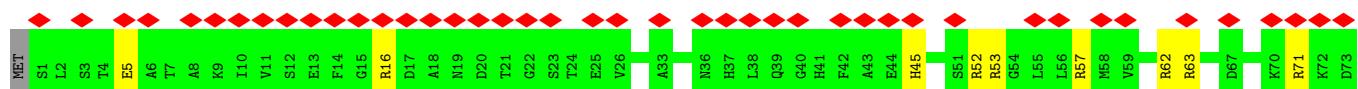
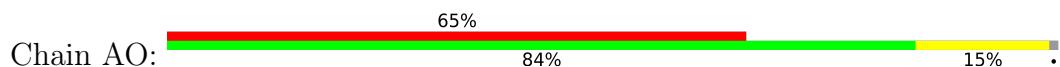
- Molecule 12: 30S ribosomal protein S13



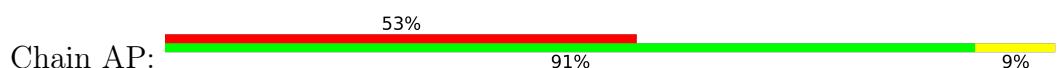
- Molecule 13: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S16

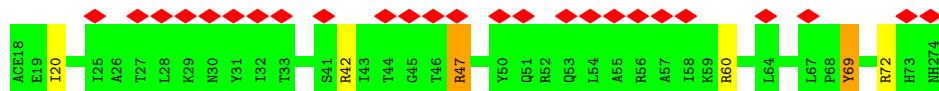
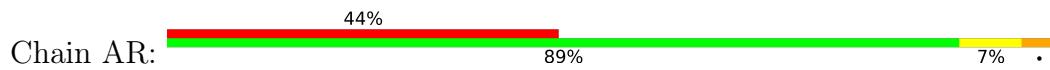


- Molecule 16: 30S ribosomal protein S17

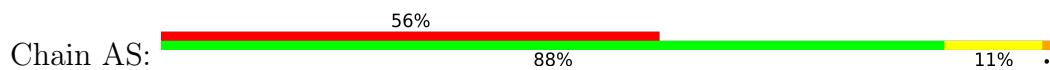




- Molecule 17: 30S ribosomal protein S18



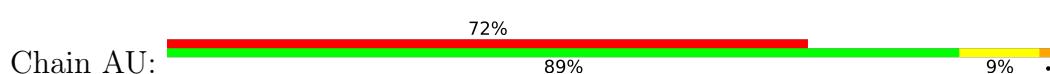
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20

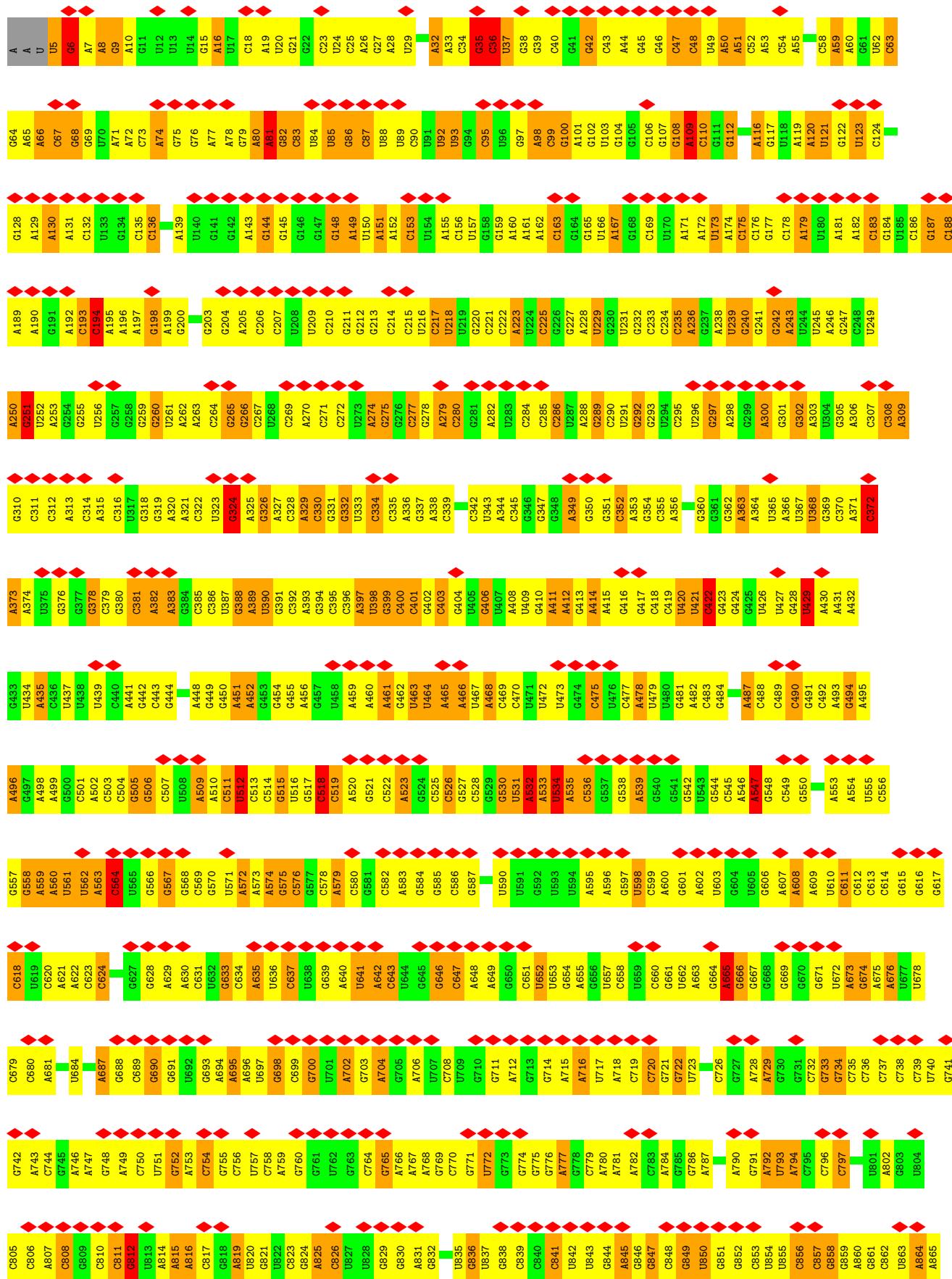


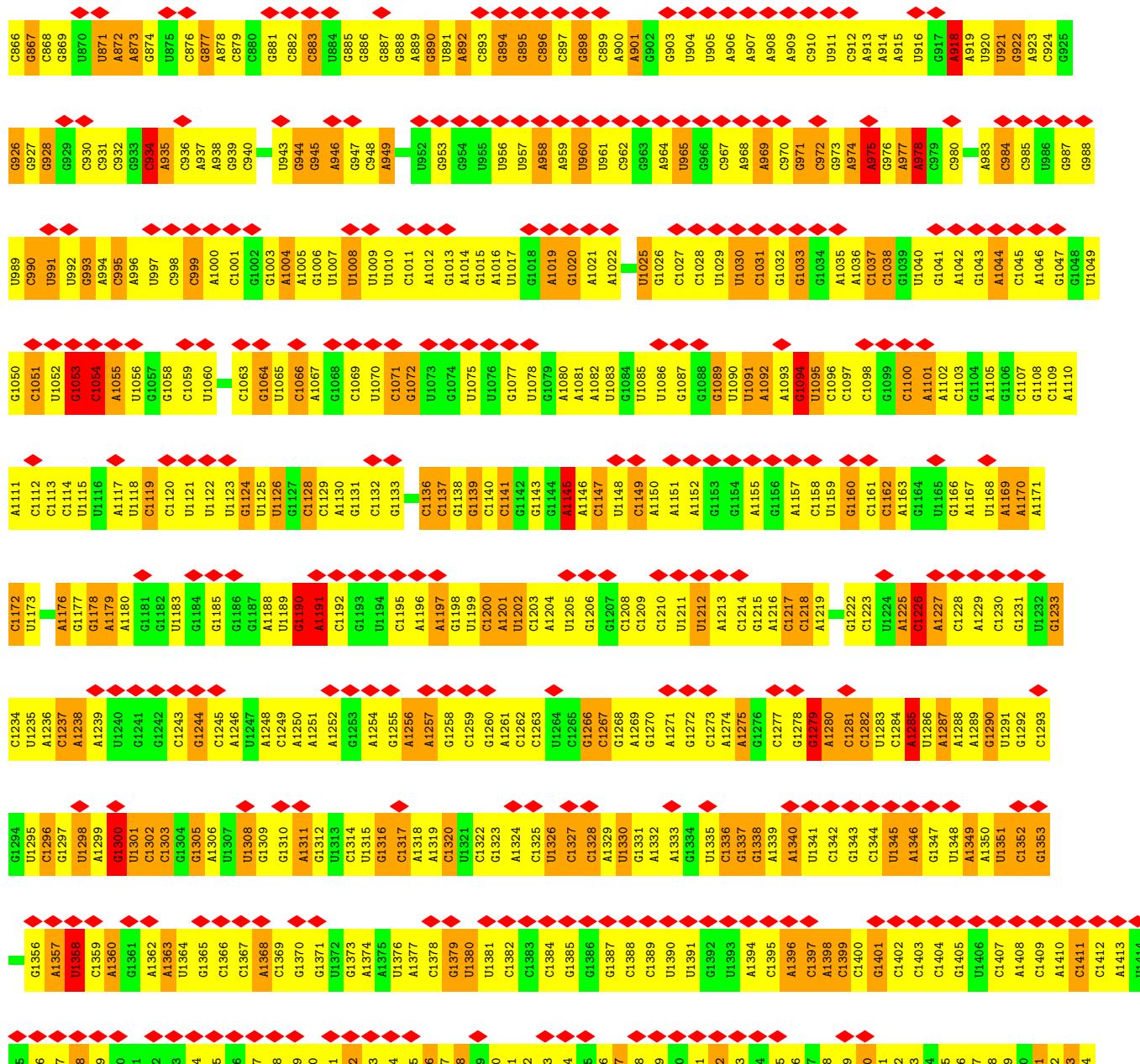
- Molecule 20: 30S ribosomal protein S21



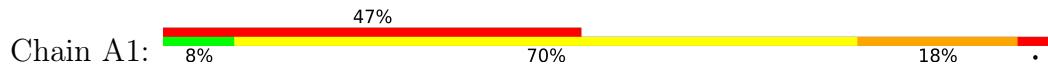
- Molecule 21: 16S ribosomal RNA







- Molecule 22: fMet-Val-tRNA-Val





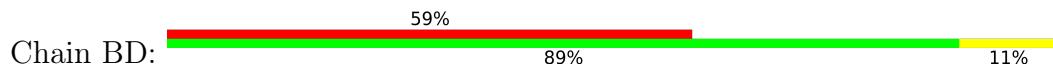
- Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

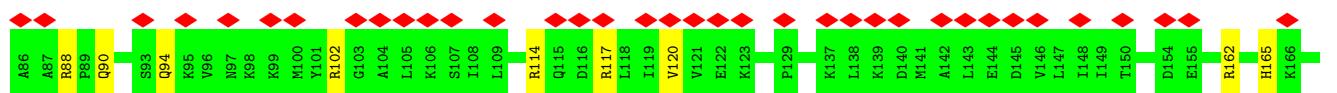


- Molecule 24: 50S ribosomal protein L2

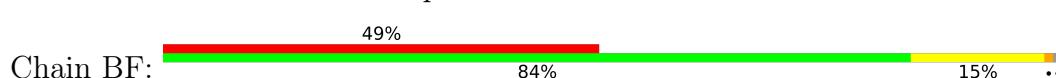


- Molecule 25: 50S ribosomal protein L3

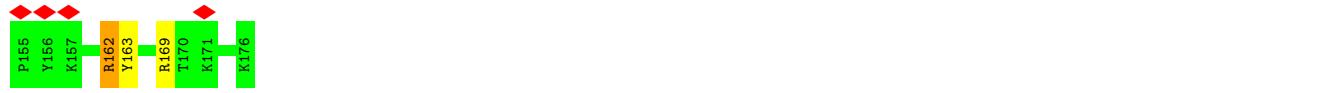
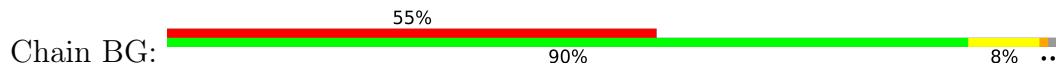




- Molecule 27: 50S ribosomal protein L5



- Molecule 28: 50S ribosomal protein L6



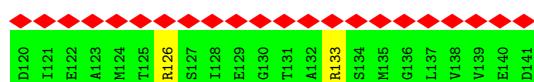
- Molecule 29: 50S ribosomal protein L9





- Molecule 30: 50S ribosomal protein L11

Chain BI:



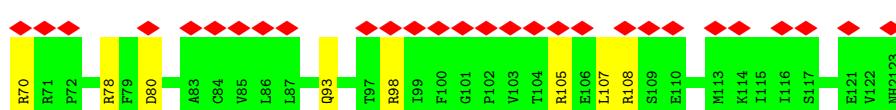
- Molecule 31: 50S ribosomal protein L13

Chain B.J.



- Molecule 32: 50S ribosomal protein L14

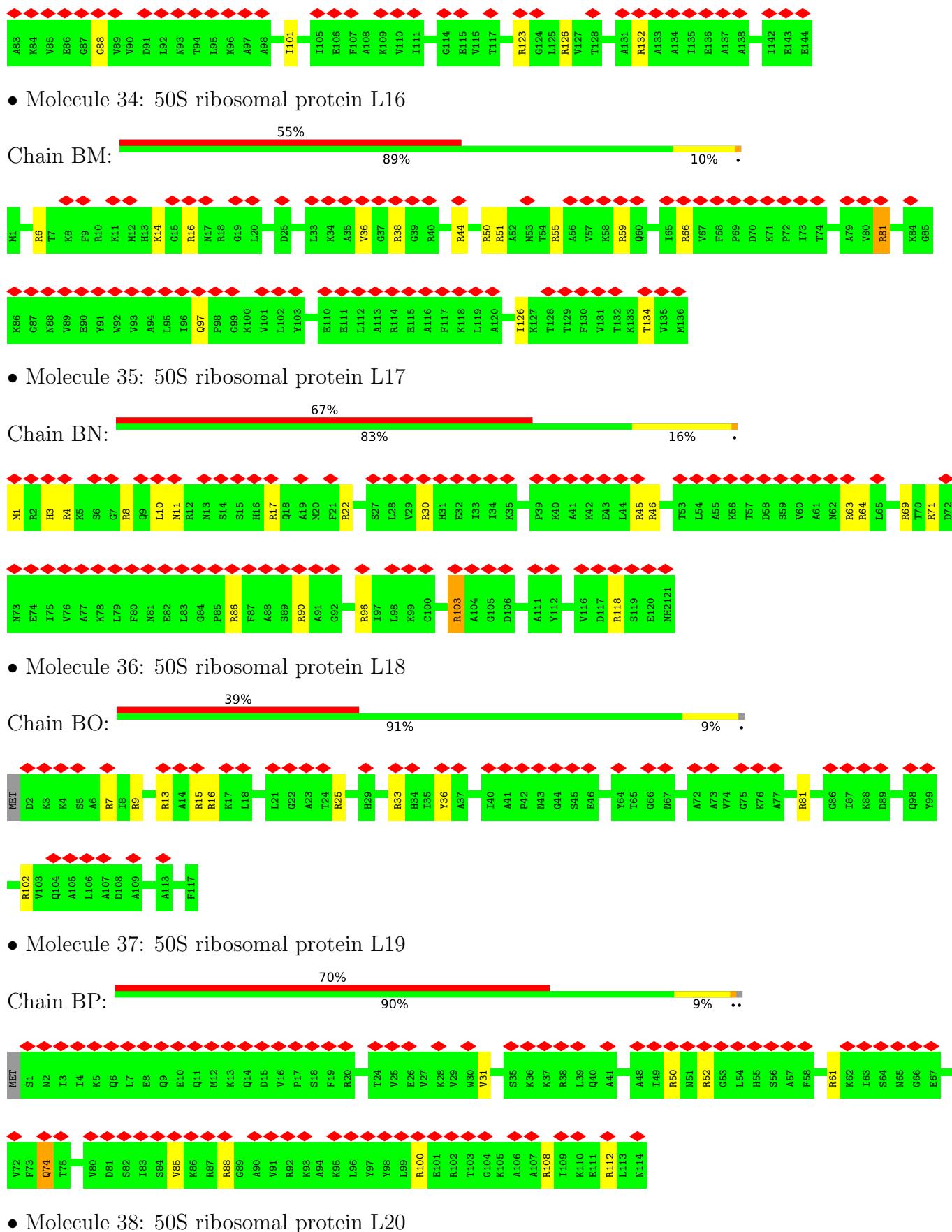
Chain BK

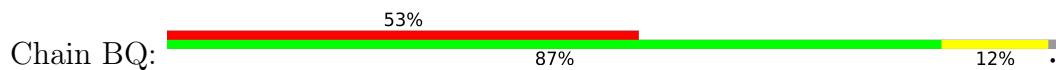


- Molecule 33: 50S ribosomal protein L15

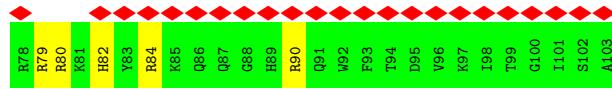
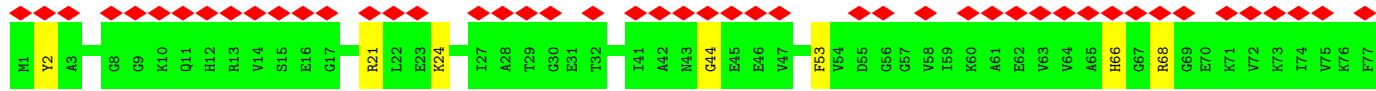
Chain BL



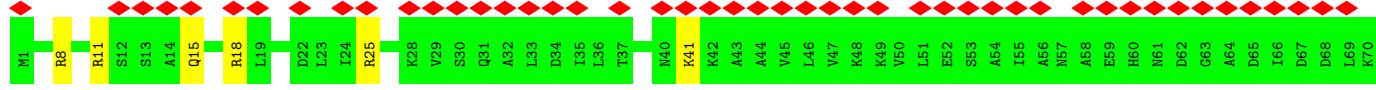




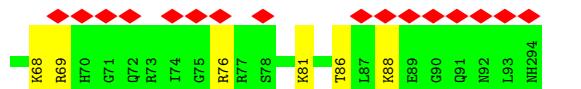
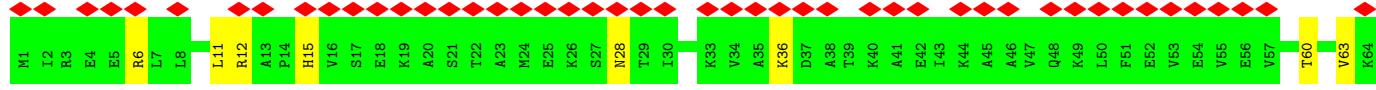
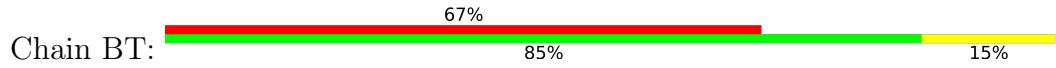
- Molecule 39: 50S ribosomal protein L21



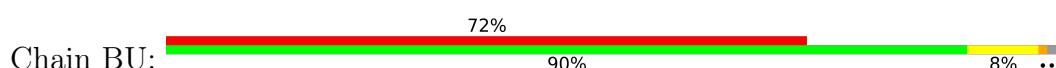
- Molecule 40: 50S ribosomal protein L22



- Molecule 41: 50S ribosomal protein L23

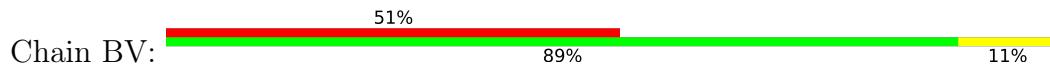


- Molecule 42: 50S ribosomal protein L24

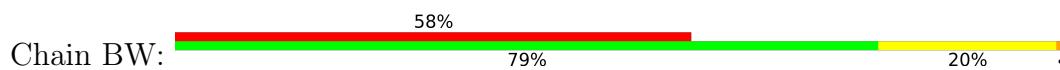




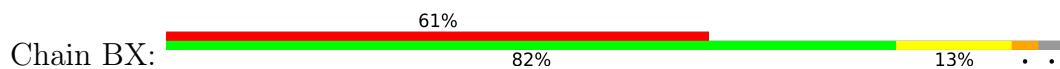
- Molecule 43: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L27



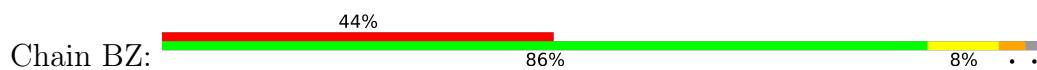
- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29

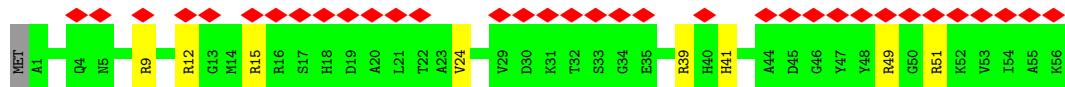
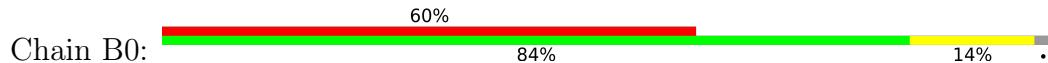


- Molecule 47: 50S ribosomal protein L30

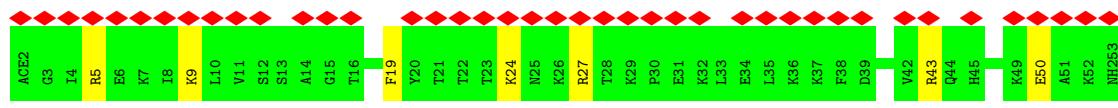
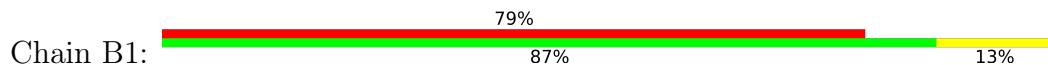




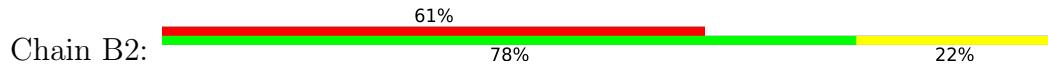
- Molecule 48: 50S ribosomal protein L32



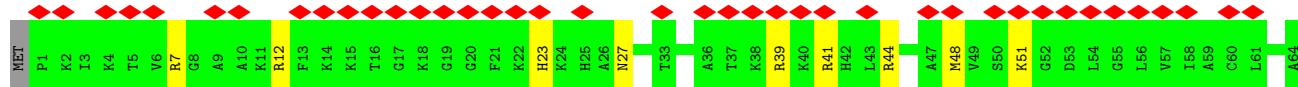
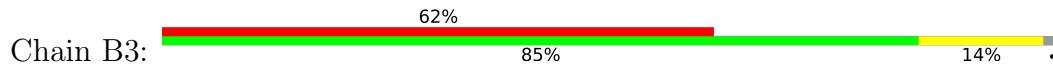
- Molecule 49: 50S ribosomal protein L33



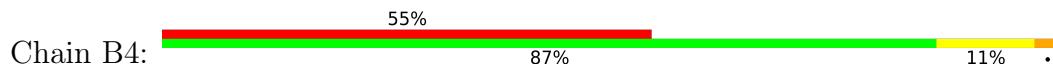
- Molecule 50: 50S ribosomal protein L34



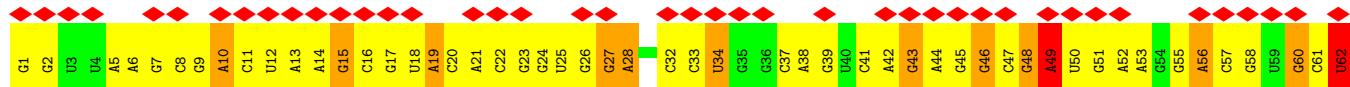
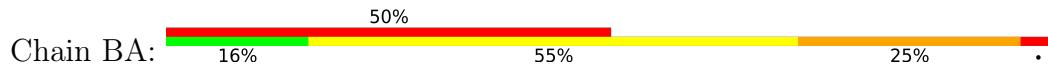
- Molecule 51: 50S ribosomal protein L35

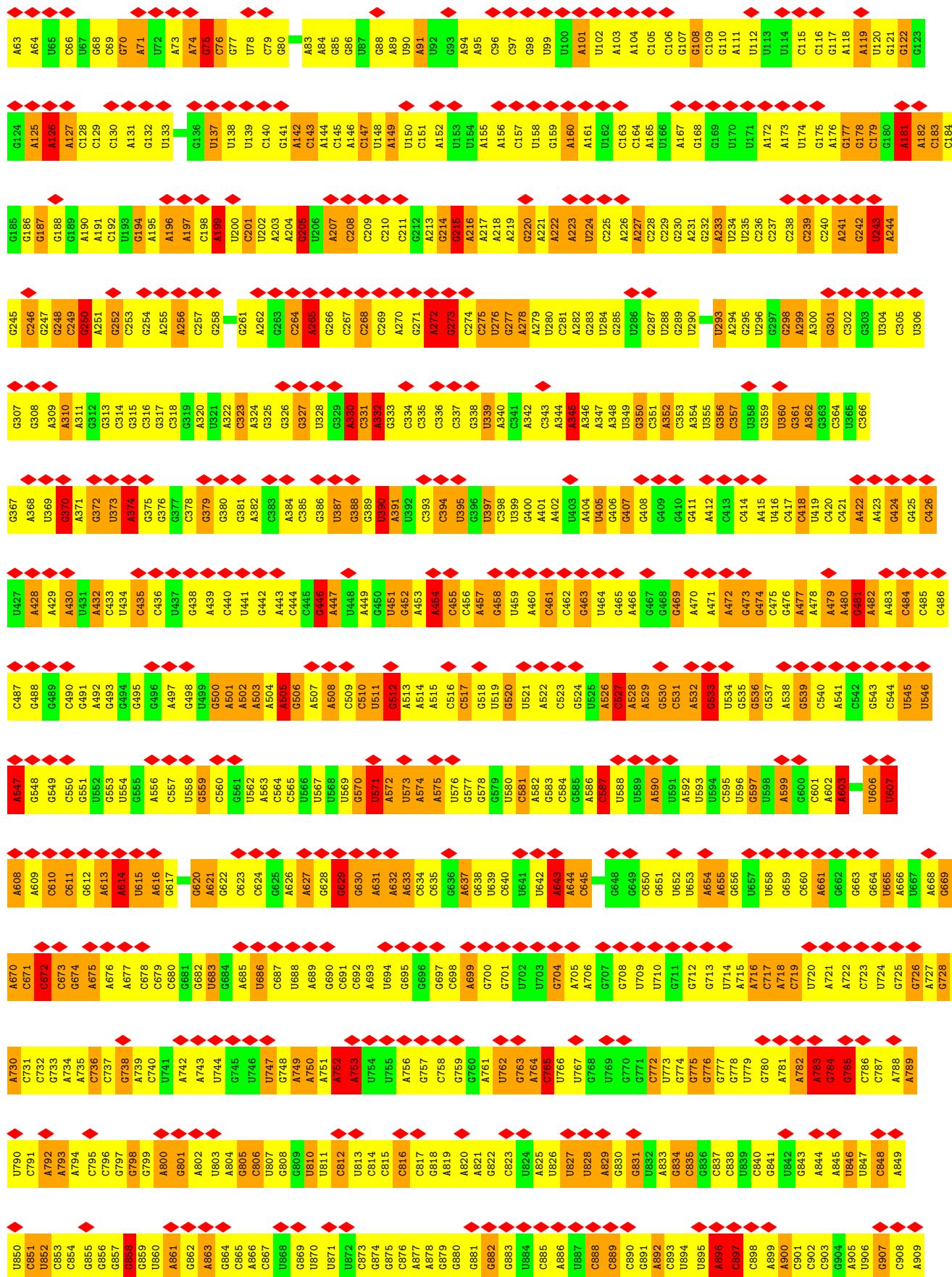


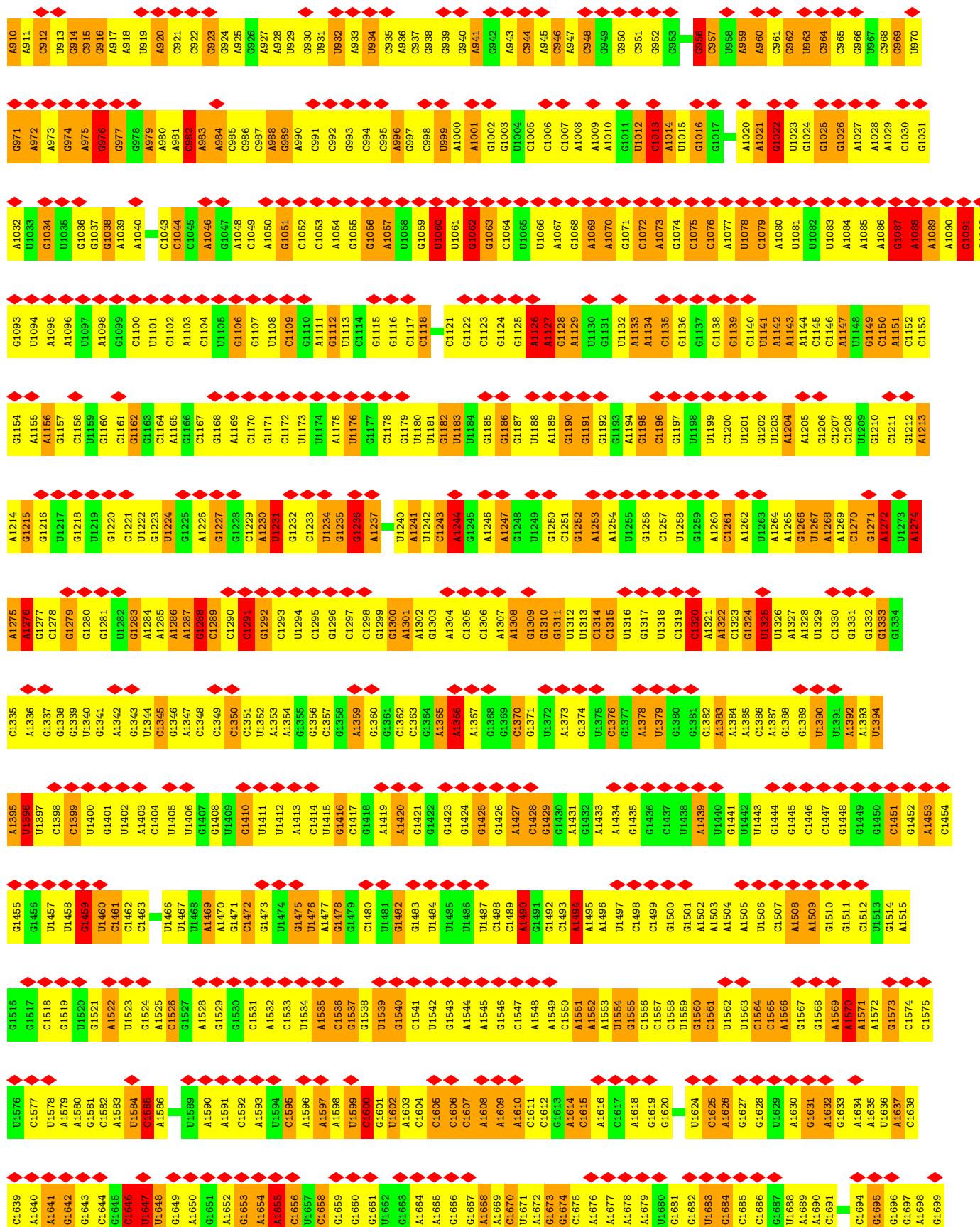
- Molecule 52: 50S ribosomal protein L36

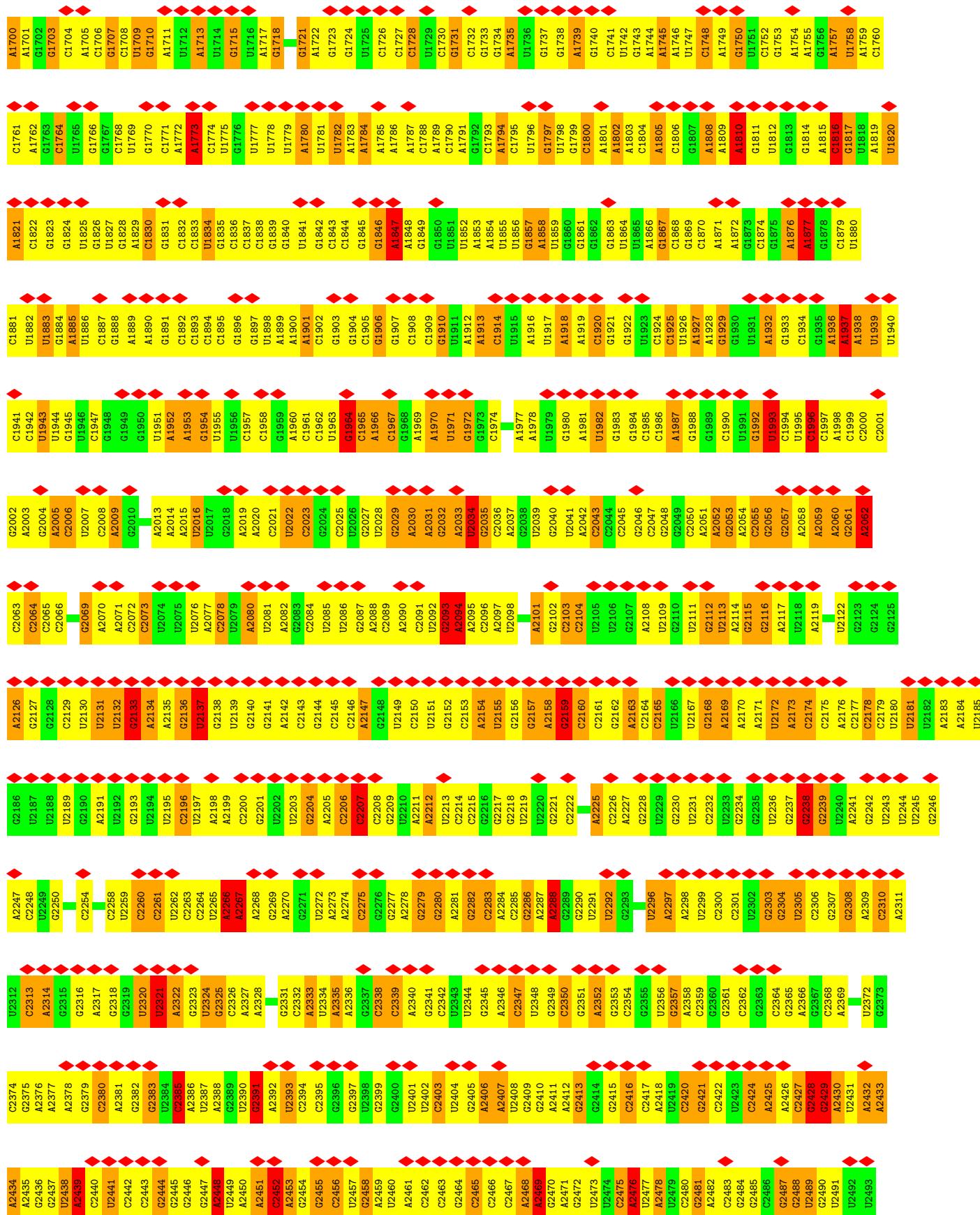


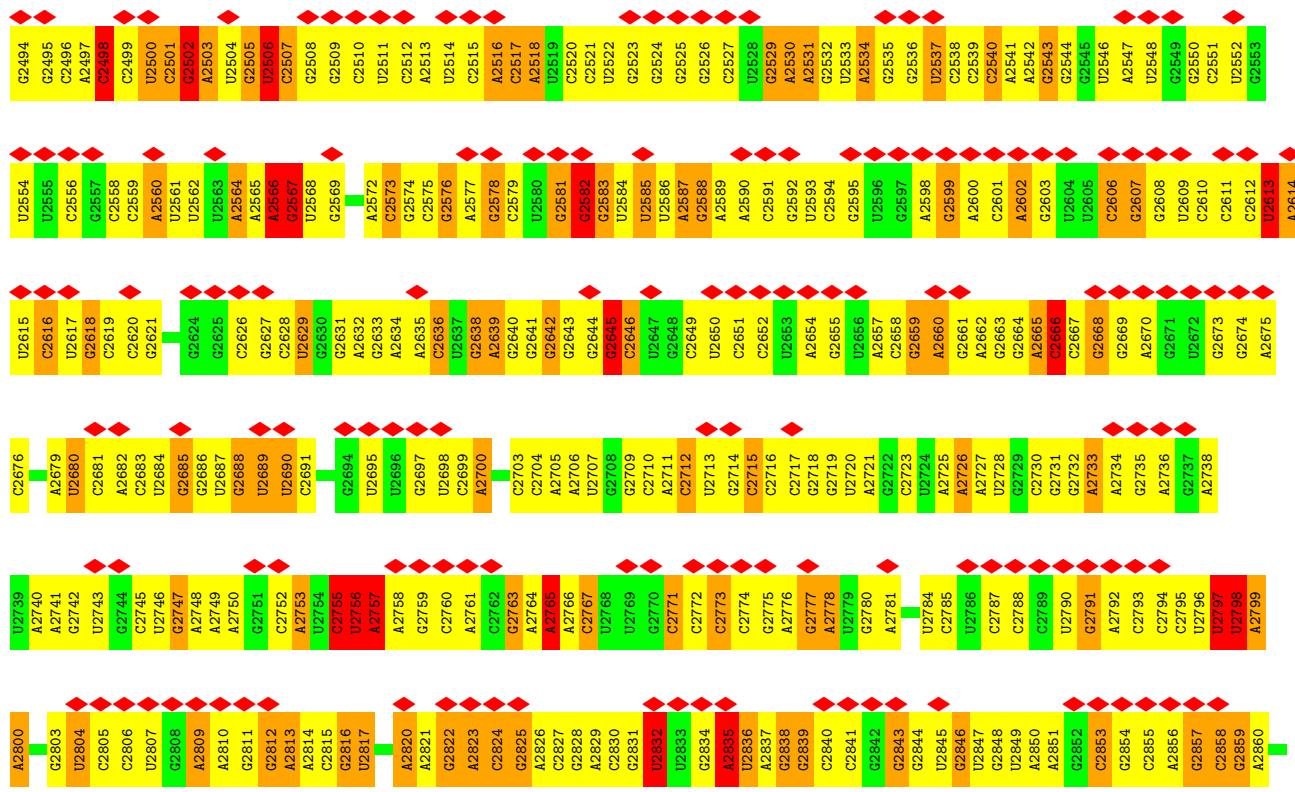
- Molecule 53: 23S ribosomal RNA







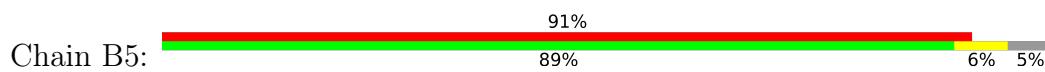




- Molecule 54: 5S ribosomal RNA



- Molecule 55: 50S ribosomal protein L1



K184	V124
L185	G125
K186	Q126
E187	L127
N188	G128
L189	Q129
E190	V130
A191	L131
L192	G132
L193	P133
V194	R134

K195	G135
L196	L136
K197	M137
K198	P138
A199	N139
K200	P140
P201	K141
	V142
A204	G143
K205	T144
G206	V145
	T146
V207	P147
Y208	N148
I209	
K210	V149
K211	A150
K212	E151
S213	A152
T214	V153
S215	K154
T216	M155
T217	A156
M218	K157
G219	A158
A220	G159
C221	Q160
V222	V161
A223	R162
V224	Y163
	R164
ASP	
GLN	N165
ALA	D166
GLY	
LEU	K167
SER	N168
ALA	G169
SER	
VAL	L170
ASN	L171
	H172
	T173
	T174
	L175
	G176
	K177
	H178
	D179
	F180
	D181
	A182
	D183

## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26429	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 ( $e^-/\text{\AA}^2$ )	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	223.953	Depositor
Minimum map value	-122.023	Depositor
Average map value	-0.756	Depositor
Map value standard deviation	22.478	Depositor
Recommended contour level	40.0	Depositor
Map size ( $\text{\AA}$ )	359.04, 359.04, 359.04	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.87, 1.87, 1.87	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: 7MG, FME, NH2, PSU, 5MU, ACE, 6MZ, CM0, 4SU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AB	0.69	0/1736	1.15	8/2340 (0.3%)
2	AC	0.77	0/1651	1.28	18/2225 (0.8%)
3	AD	0.80	0/1665	1.26	20/2227 (0.9%)
4	AE	0.72	0/1119	1.20	11/1506 (0.7%)
5	AF	0.76	0/835	1.23	7/1128 (0.6%)
6	AG	0.76	0/1188	1.28	12/1593 (0.8%)
7	AH	0.71	0/989	1.11	5/1326 (0.4%)
8	AI	0.83	0/1035	1.37	14/1377 (1.0%)
9	AJ	0.78	0/797	1.33	11/1079 (1.0%)
10	AK	0.76	0/894	1.26	9/1207 (0.7%)
11	AL	0.77	0/969	1.37	17/1300 (1.3%)
12	AM	0.79	0/884	1.35	11/1181 (0.9%)
13	AN	0.82	0/817	1.41	11/1088 (1.0%)
14	AO	0.72	0/722	1.29	13/964 (1.3%)
15	AP	0.84	0/648	1.28	7/870 (0.8%)
16	AQ	0.73	0/658	1.19	5/883 (0.6%)
17	AR	0.80	0/463	1.21	5/623 (0.8%)
18	AS	0.76	0/653	1.27	4/879 (0.5%)
19	AT	0.71	0/672	1.12	5/890 (0.6%)
20	AU	0.85	0/431	1.31	6/572 (1.0%)
21	AA	1.75	365/36759 (1.0%)	2.28	2447/57346 (4.3%)
22	A1	1.75	20/1668 (1.2%)	2.26	110/2595 (4.2%)
23	A2	1.66	1/343 (0.3%)	2.18	17/531 (3.2%)
24	BC	0.81	0/2121	1.35	26/2852 (0.9%)
25	BD	0.71	0/1586	1.18	9/2134 (0.4%)
26	BE	0.72	0/1571	1.19	11/2113 (0.5%)
27	BF	0.77	0/1444	1.26	16/1937 (0.8%)
28	BG	0.71	0/1343	1.18	10/1816 (0.6%)
29	BH	0.68	0/1122	1.16	7/1515 (0.5%)
30	BI	0.68	0/1046	1.07	5/1410 (0.4%)
31	BJ	0.75	0/1152	1.23	9/1551 (0.6%)
32	BK	0.76	0/947	1.23	10/1268 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	BL	0.79	0/1054	1.29	12/1403 (0.9%)
34	BM	0.80	0/1093	1.22	10/1460 (0.7%)
35	BN	0.83	0/973	1.44	18/1301 (1.4%)
36	BO	0.77	0/902	1.29	9/1209 (0.7%)
37	BP	0.78	0/929	1.25	9/1242 (0.7%)
38	BQ	0.81	0/960	1.36	14/1278 (1.1%)
39	BR	0.72	0/829	1.13	6/1107 (0.5%)
40	BS	0.70	0/864	1.28	10/1156 (0.9%)
41	BT	0.72	0/744	1.22	4/994 (0.4%)
42	BU	0.72	0/787	1.15	5/1051 (0.5%)
43	BV	0.74	0/766	1.27	8/1025 (0.8%)
44	BW	0.78	0/604	1.24	6/799 (0.8%)
45	BX	0.84	0/635	1.35	10/848 (1.2%)
46	BY	0.71	0/510	1.24	4/677 (0.6%)
47	BZ	0.73	0/453	1.31	6/605 (1.0%)
48	B0	0.80	0/450	1.26	8/599 (1.3%)
49	B1	0.73	0/417	1.14	3/556 (0.5%)
50	B2	0.89	0/380	1.58	10/498 (2.0%)
51	B3	0.79	0/513	1.23	6/676 (0.9%)
52	B4	0.80	0/303	1.35	6/397 (1.5%)
53	BA	1.77	819/69796 (1.2%)	2.30	4869/108888 (4.5%)
54	BB	1.74	17/2800 (0.6%)	2.24	176/4367 (4.0%)
55	B5	0.69	0/1673	1.11	8/2255 (0.4%)
All	All	1.54	1222/158363 (0.8%)	2.07	8093/236717 (3.4%)

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
18	AS	0	1
21	AA	0	328
22	A1	0	18
23	A2	0	2
53	BA	0	652
54	BB	0	27
All	All	0	1028

The worst 5 of 1222 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2078	C	C4-N4	-7.15	1.27	1.33
21	AA	1521	C	C4-N4	-7.01	1.27	1.33
53	BA	897	C	C4-N4	-6.68	1.27	1.33
21	AA	1214	C	C4-N4	-6.67	1.27	1.33
21	AA	637	C	C4-N4	-6.64	1.27	1.33

The worst 5 of 8093 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BA	323	C	O4'-C1'-N1	14.98	120.18	108.20
53	BA	1932	A	N1-C6-N6	-13.12	110.73	118.60
53	BA	800	A	N1-C6-N6	-12.78	110.93	118.60
21	AA	1502	A	N1-C6-N6	-12.44	111.14	118.60
53	BA	219	A	N1-C6-N6	-12.42	111.15	118.60

There are no chirality outliers.

5 of 1028 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	21	G	Sidechain
21	AA	35	G	Sidechain
21	AA	36	C	Sidechain
21	AA	6	G	Sidechain
18	AS	74	ALA	Peptide

## 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	1	0
2	AC	1625	0	1699	2	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	1	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16108	7	0
22	A1	1627	0	808	0	0
23	A2	309	0	158	0	0
24	BC	2083	0	2157	0	0
25	BD	1565	0	1616	0	0
26	BE	1552	0	1619	0	0
27	BF	1420	0	1460	1	0
28	BG	1323	0	1374	0	0
29	BH	1111	0	1148	0	0
30	BI	1032	0	1088	0	0
31	BJ	1129	0	1162	1	0
32	BK	939	0	1012	1	0
33	BL	1045	0	1117	2	0
34	BM	1074	0	1157	1	0
35	BN	961	0	1000	0	0
36	BO	892	0	923	0	0
37	BP	917	0	965	0	0
38	BQ	947	0	1022	0	0
39	BR	816	0	839	1	0
40	BS	857	0	922	0	0
41	BT	739	0	807	0	0
42	BU	780	0	834	0	0
43	BV	753	0	780	0	0
44	BW	599	0	614	0	0
45	BX	625	0	655	0	0
46	BY	509	0	543	0	0
47	BZ	449	0	491	1	0
48	B0	444	0	461	0	0
49	B1	413	0	444	1	0
50	B2	377	0	418	0	0
51	B3	504	0	574	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B4	302	0	343	0	0
53	BA	62317	0	30428	10	0
54	BB	2504	0	1247	0	0
55	B5	1658	0	1751	0	0
56	A1	7	0	8	0	0
57	BA	10	0	10	1	0
All	All	146011	0	97443	27	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 27 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)
53:BA:2644:G:H2'	53:BA:2645:G:C8	2.46	0.51
53:BA:1287:A:H2'	53:BA:1288:G:C2	2.47	0.50
49:B1:9:LYS:HE3	49:B1:19:PHE:CD2	2.49	0.48
21:AA:292:G:C5	21:AA:293:G:H1'	2.48	0.47
33:BL:54:GLN:HE21	53:BA:2428:G:N2	2.11	0.47

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%)	193 (88%)	24 (11%)	1 (0%)	29 69
2	AC	205/208 (99%)	186 (91%)	11 (5%)	8 (4%)	3 23
3	AD	203/206 (98%)	192 (95%)	9 (4%)	2 (1%)	15 55
4	AE	150/152 (99%)	141 (94%)	5 (3%)	4 (3%)	5 31
5	AF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15 55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	AG	150/152 (99%)	138 (92%)	8 (5%)	4 (3%)	5 31
7	AH	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19 60
8	AI	126/128 (98%)	115 (91%)	9 (7%)	2 (2%)	9 44
9	AJ	98/100 (98%)	87 (89%)	8 (8%)	3 (3%)	4 27
10	AK	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	9 42
11	AL	121/124 (98%)	111 (92%)	6 (5%)	4 (3%)	4 26
12	AM	112/115 (97%)	94 (84%)	15 (13%)	3 (3%)	5 31
13	AN	98/101 (97%)	89 (91%)	7 (7%)	2 (2%)	7 38
14	AO	86/89 (97%)	78 (91%)	8 (9%)	0	100 100
15	AP	79/81 (98%)	73 (92%)	6 (8%)	0	100 100
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	12 48
17	AR	55/57 (96%)	51 (93%)	2 (4%)	2 (4%)	3 25
18	AS	79/81 (98%)	73 (92%)	3 (4%)	3 (4%)	3 24
19	AT	84/86 (98%)	74 (88%)	7 (8%)	3 (4%)	3 25
20	AU	51/53 (96%)	47 (92%)	4 (8%)	0	100 100
24	BC	270/273 (99%)	245 (91%)	17 (6%)	8 (3%)	4 28
25	BD	207/209 (99%)	174 (84%)	21 (10%)	12 (6%)	1 18
26	BE	199/201 (99%)	182 (92%)	13 (6%)	4 (2%)	7 38
27	BF	176/179 (98%)	143 (81%)	26 (15%)	7 (4%)	3 23
28	BG	174/177 (98%)	152 (87%)	18 (10%)	4 (2%)	6 34
29	BH	147/149 (99%)	131 (89%)	15 (10%)	1 (1%)	22 63
30	BI	139/142 (98%)	128 (92%)	11 (8%)	0	100 100
31	BJ	140/142 (99%)	129 (92%)	6 (4%)	5 (4%)	3 25
32	BK	121/123 (98%)	105 (87%)	11 (9%)	5 (4%)	3 23
33	BL	141/144 (98%)	117 (83%)	14 (10%)	10 (7%)	1 14
34	BM	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	10 46
35	BN	119/121 (98%)	103 (87%)	13 (11%)	3 (2%)	5 32
36	BO	114/117 (97%)	108 (95%)	6 (5%)	0	100 100
37	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	5 31
38	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9 42
39	BR	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	7 38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	BS	108/110 (98%)	97 (90%)	10 (9%)	1 (1%)	17 57
41	BT	92/94 (98%)	73 (79%)	11 (12%)	8 (9%)	1 11
42	BU	101/104 (97%)	86 (85%)	10 (10%)	5 (5%)	2 20
43	BV	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	6 35
44	BW	78/80 (98%)	62 (80%)	8 (10%)	8 (10%)	0 8
45	BX	75/79 (95%)	64 (85%)	8 (11%)	3 (4%)	3 23
46	BY	61/63 (97%)	55 (90%)	4 (7%)	2 (3%)	4 26
47	BZ	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	8 40
48	B0	54/57 (95%)	50 (93%)	3 (6%)	1 (2%)	8 38
49	B1	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	7 38
50	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6 34
51	B3	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
52	B4	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2 19
55	B5	221/234 (94%)	211 (96%)	8 (4%)	2 (1%)	17 57
All	All	5876/6008 (98%)	5278 (90%)	447 (8%)	151 (3%)	8 31

5 of 151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	105	ILE
24	BC	206	LYS
25	BD	9	VAL
25	BD	150	GLN
25	BD	188	LEU

### 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%)	169 (99%)	1 (1%)	86 92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	85 (98%)	2 (2%)	50	70
6	AG	123/123 (100%)	122 (99%)	1 (1%)	81	89
7	AH	104/105 (99%)	103 (99%)	1 (1%)	76	86
8	AI	105/105 (100%)	102 (97%)	3 (3%)	42	64
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	50	70
10	AK	90/90 (100%)	88 (98%)	2 (2%)	52	71
11	AL	103/104 (99%)	101 (98%)	2 (2%)	57	75
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	80 (96%)	3 (4%)	35	59
14	AO	76/77 (99%)	74 (97%)	2 (3%)	46	66
15	AP	65/65 (100%)	64 (98%)	1 (2%)	65	80
16	AQ	74/74 (100%)	73 (99%)	1 (1%)	67	80
17	AR	48/48 (100%)	47 (98%)	1 (2%)	53	72
18	AS	70/70 (100%)	67 (96%)	3 (4%)	29	53
19	AT	65/65 (100%)	64 (98%)	1 (2%)	65	80
20	AU	44/44 (100%)	43 (98%)	1 (2%)	50	70
24	BC	216/217 (100%)	214 (99%)	2 (1%)	78	87
25	BD	164/164 (100%)	162 (99%)	2 (1%)	71	83
26	BE	165/165 (100%)	161 (98%)	4 (2%)	49	69
27	BF	149/150 (99%)	144 (97%)	5 (3%)	37	60
28	BG	137/138 (99%)	134 (98%)	3 (2%)	52	71
29	BH	114/114 (100%)	113 (99%)	1 (1%)	78	87
30	BI	109/110 (99%)	108 (99%)	1 (1%)	78	87
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	78	87
32	BK	103/103 (100%)	98 (95%)	5 (5%)	25	50
33	BL	102/103 (99%)	100 (98%)	2 (2%)	55	74
34	BM	109/109 (100%)	106 (97%)	3 (3%)	43	65
35	BN	100/100 (100%)	98 (98%)	2 (2%)	55	74
36	BO	86/87 (99%)	85 (99%)	1 (1%)	71	83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BP	99/100 (99%)	98 (99%)	1 (1%)	76	86
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	82 (98%)	2 (2%)	49	69
40	BS	93/93 (100%)	91 (98%)	2 (2%)	52	71
41	BT	80/80 (100%)	78 (98%)	2 (2%)	47	68
42	BU	83/84 (99%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	76 (97%)	2 (3%)	46	66
44	BW	59/59 (100%)	55 (93%)	4 (7%)	16	41
45	BX	67/68 (98%)	65 (97%)	2 (3%)	41	63
46	BY	55/55 (100%)	55 (100%)	0	100	100
47	BZ	48/49 (98%)	45 (94%)	3 (6%)	18	43
48	B0	47/48 (98%)	46 (98%)	1 (2%)	53	72
49	B1	45/45 (100%)	44 (98%)	1 (2%)	52	71
50	B2	38/38 (100%)	37 (97%)	1 (3%)	46	66
51	B3	51/52 (98%)	48 (94%)	3 (6%)	19	45
52	B4	34/34 (100%)	34 (100%)	0	100	100
55	B5	173/181 (96%)	167 (96%)	6 (4%)	36	59
All	All	4842/4870 (99%)	4748 (98%)	94 (2%)	59	75

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	BL	39	LYS
43	BV	12	GLN
34	BM	97	GLN
39	BR	2	TYR
44	BW	39	GLN

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

Mol	Chain	Res	Type
52	B4	37	GLN

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	195 (12%)	46 (3%)
22	A1	73/76 (96%)	7 (9%)	2 (2%)
23	A2	14/15 (93%)	4 (28%)	2 (14%)
53	BA	2902/2903 (99%)	455 (15%)	123 (4%)
54	BB	116/118 (98%)	19 (16%)	2 (1%)
All	All	4635/4645 (99%)	680 (14%)	175 (3%)

5 of 680 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	8	A
21	AA	9	G
21	AA	16	A
21	AA	32	A

5 of 175 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	BA	1266	G
53	BA	2062	A
53	BA	1289	C
53	BA	1625	C
53	BA	2288	A

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

6 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	7MG	A1	46	22	22,26,27	5.57	1 (4%)	29,39,42	1.41	1 (3%)
22	5MU	A1	54	22	19,22,23	0.77	0	28,32,35	1.41	3 (10%)
22	CM0	A1	34	23,22	22,26,27	1.30	2 (9%)	28,37,40	1.10	1 (3%)
22	6MZ	A1	37	22	18,25,26	1.10	1 (5%)	16,36,39	1.30	2 (12%)

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	0.85	0	22,30,33	1.02	1 (4%)
22	4SU	A1	7	22	18,21,22	1.44	1 (5%)	26,30,33	0.87	1 (3%)

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	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
22	CM0	A1	34	23,22	-	3/12/30/31	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
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-25.87	1.31	1.46
22	A1	7	4SU	C5-C4	-5.02	1.36	1.42
22	A1	34	CM0	O5-C5	-4.69	1.25	1.36
22	A1	37	6MZ	C8-N7	-2.50	1.30	1.34
22	A1	34	CM0	O8-C8	-2.04	1.23	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	N9-C8-N7	5.65	111.47	103.38
22	A1	54	5MU	C5M-C5-C6	-3.75	117.84	122.85
22	A1	37	6MZ	C9-N6-C6	3.12	125.56	122.87
22	A1	54	5MU	C6-C5-C4	3.02	120.55	118.03
22	A1	37	6MZ	C2-N1-C6	2.90	119.08	116.59

There are no chirality outliers.

All (4) 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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	A1	55	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	C6-C5-O5-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	FME	BA	3001	56	8,9,10	0.59	0	7,9,11	1.39	1 (14%)
56	VAL	A1	101	57,22	4,6,7	0.49	0	6,7,9	1.45	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
57	FME	BA	3001	56	-	2/7/9/11	-
56	VAL	A1	101	57,22	-	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(°)	Ideal(°)
56	A1	101	VAL	O-C-CA	-3.52	115.55	124.78
57	BA	3001	FME	C-CA-N	2.50	114.25	109.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	3001	FME	1	0

## 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.

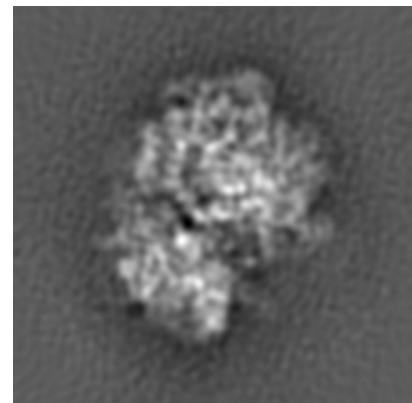
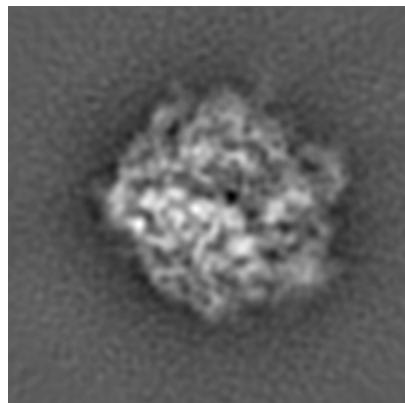
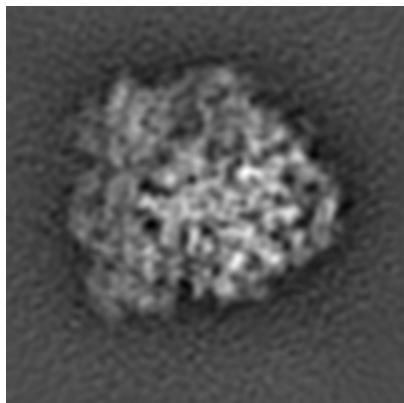
## 6 Map visualisation i

This section contains visualisations of the EMDB entry EMD-1724. 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

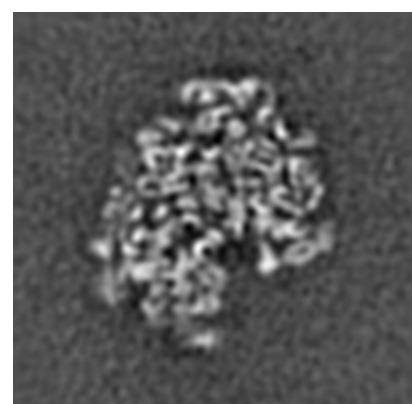
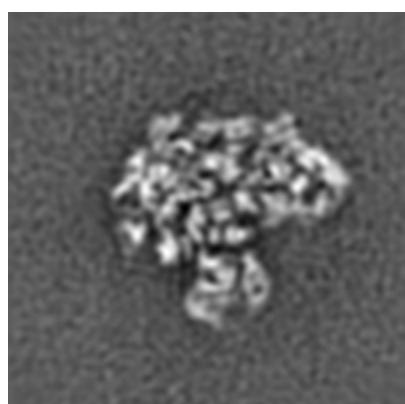
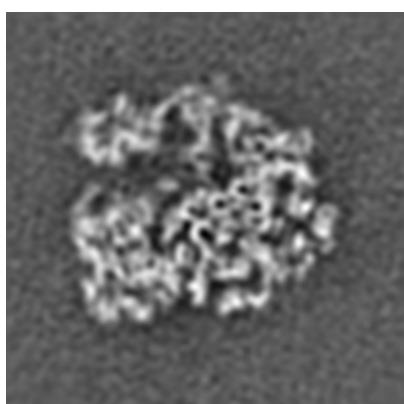
#### 6.1.1 Primary map



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

### 6.2 Central slices i

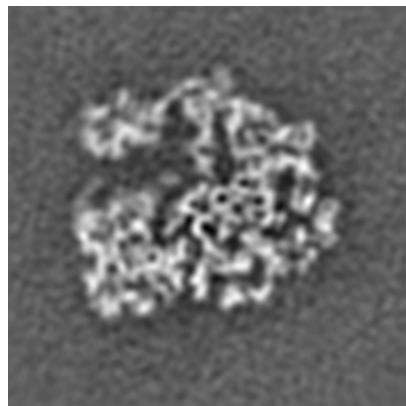
#### 6.2.1 Primary map



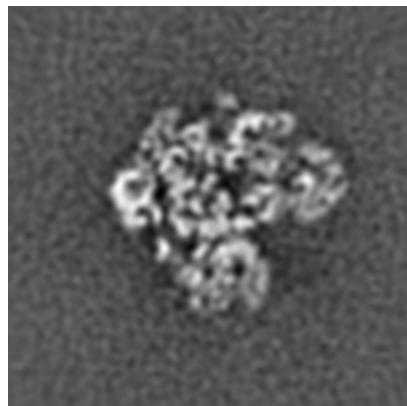
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices [\(i\)](#)

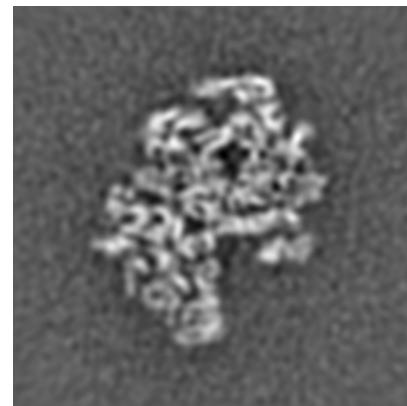
#### 6.3.1 Primary map



X Index: 97



Y Index: 92

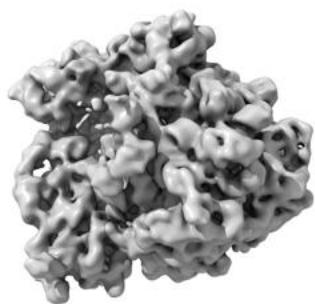


Z Index: 91

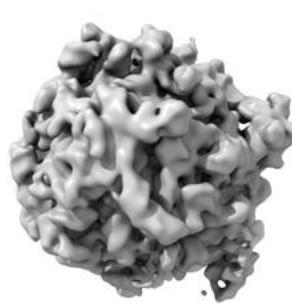
The images above show the largest variance slices of the map in three orthogonal directions.

### 6.4 Orthogonal surface views [\(i\)](#)

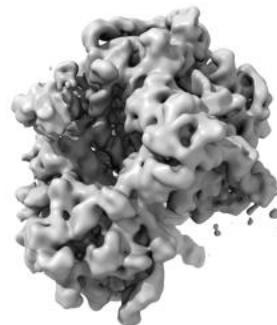
#### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 40.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

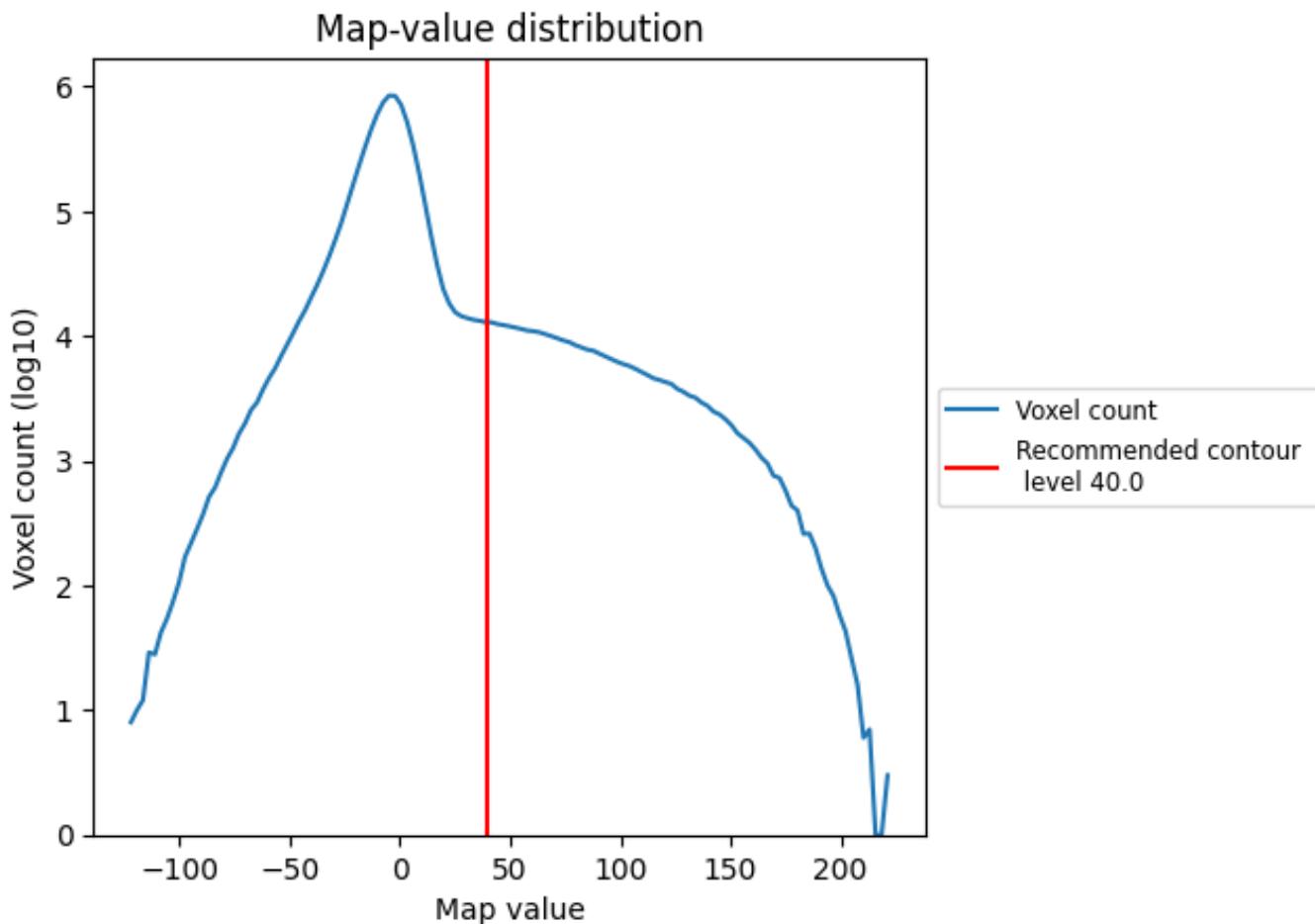
## 6.5 Mask visualisation

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

## 7 Map analysis (i)

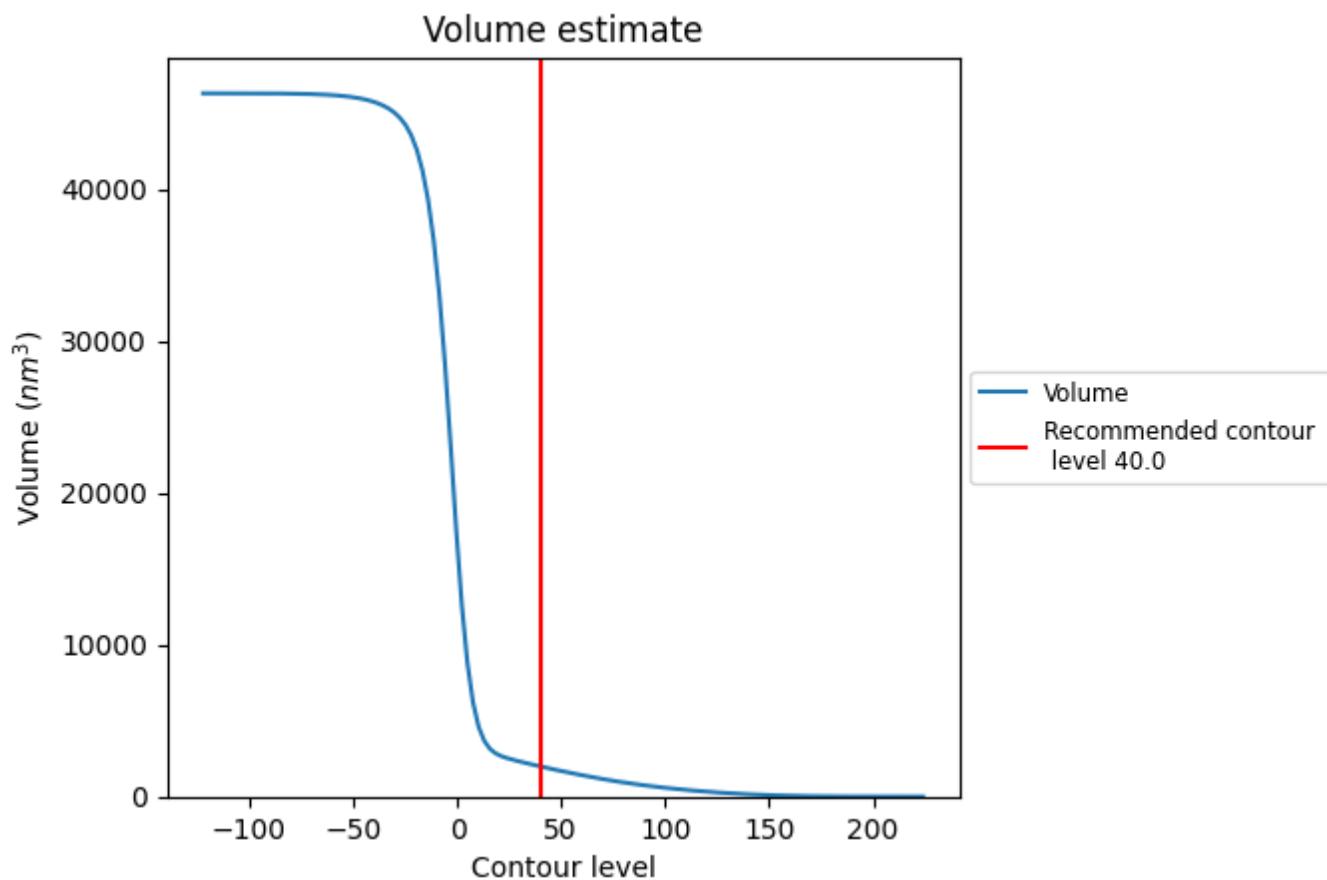
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution (i)



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

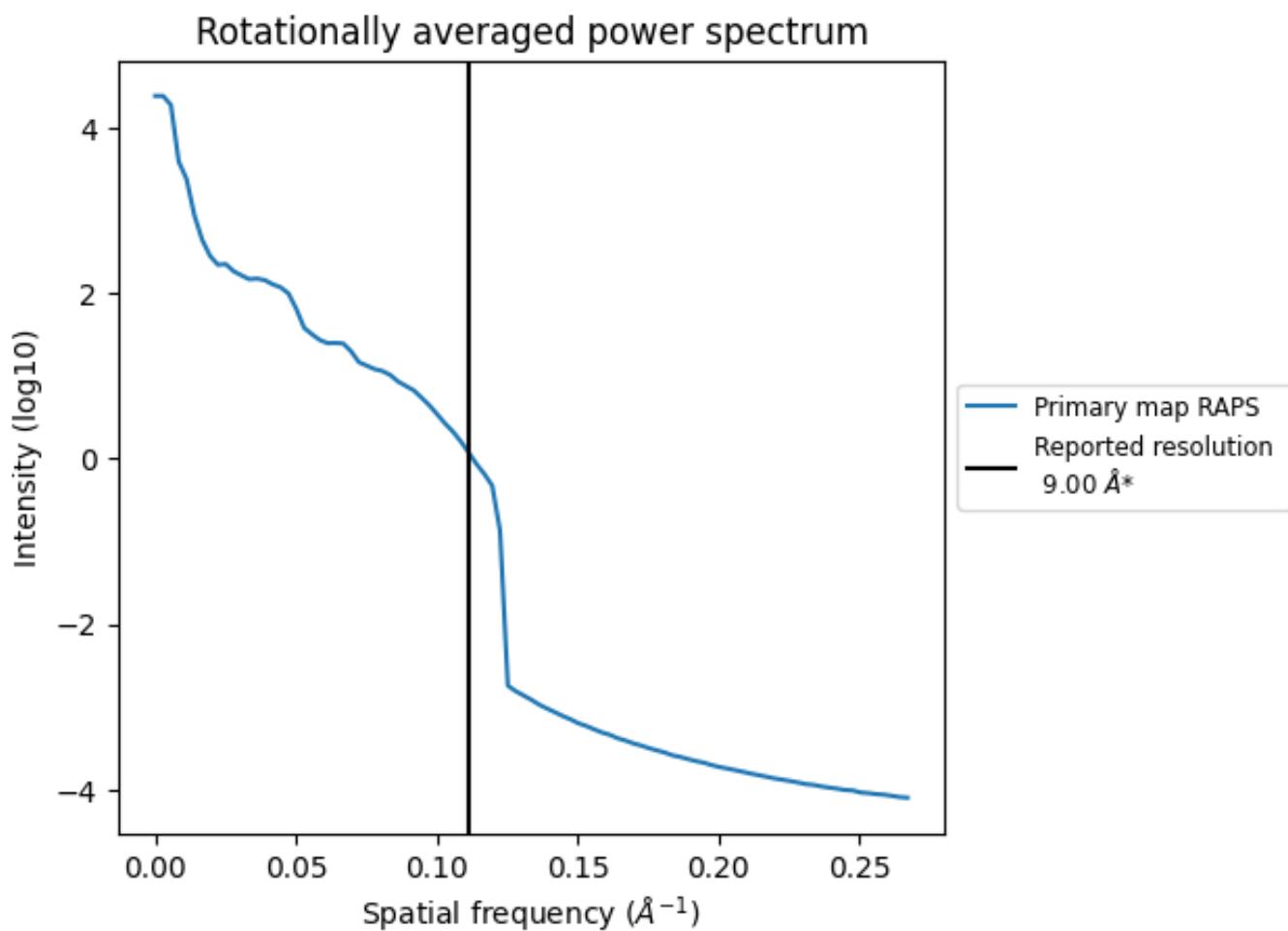
## 7.2 Volume estimate (i)



The volume at the recommended contour level is  $1986 \text{ nm}^3$ ; this corresponds to an approximate mass of 1794 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  $0.111 \text{ \AA}^{-1}$

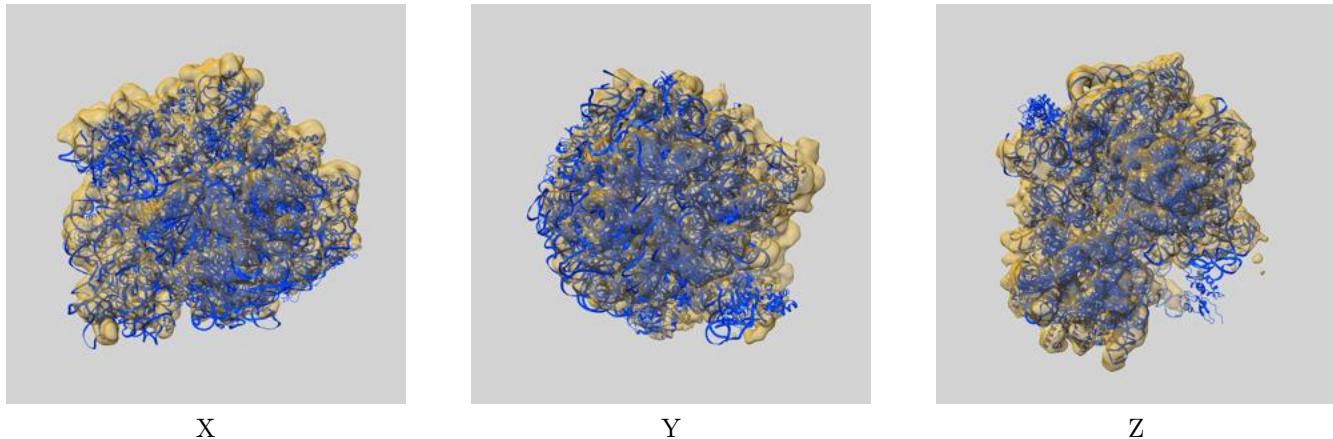
## 8 Fourier-Shell correlation

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

## 9 Map-model fit (i)

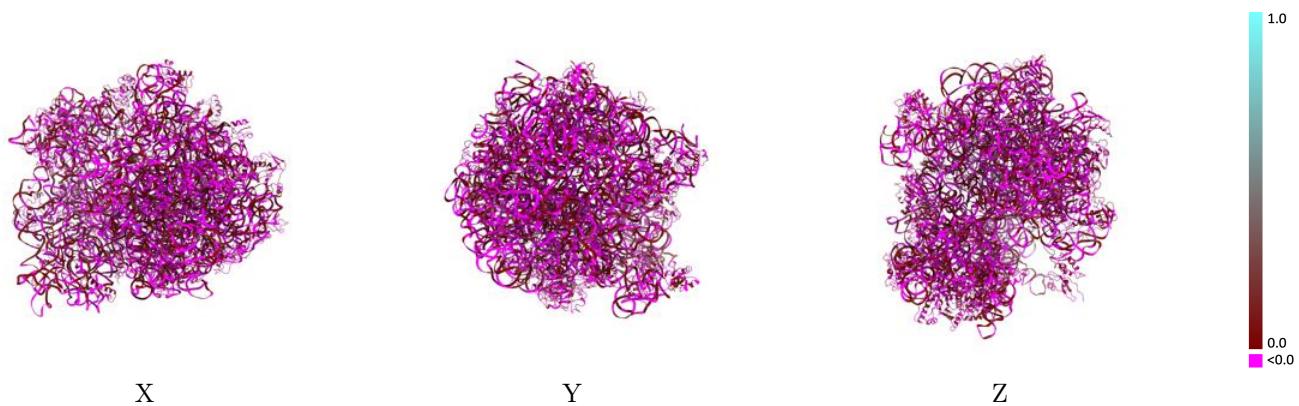
This section contains information regarding the fit between EMDB map EMD-1724 and PDB model 4V7A. Per-residue inclusion information can be found in section 3 on page 17.

### 9.1 Map-model overlay (i)



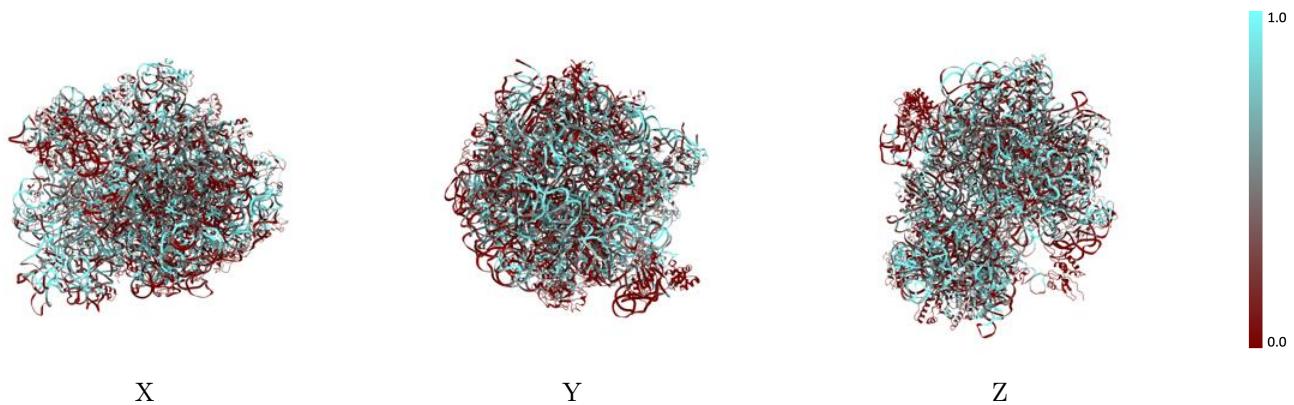
The images above show the 3D surface view of the map at the recommended contour level 40.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



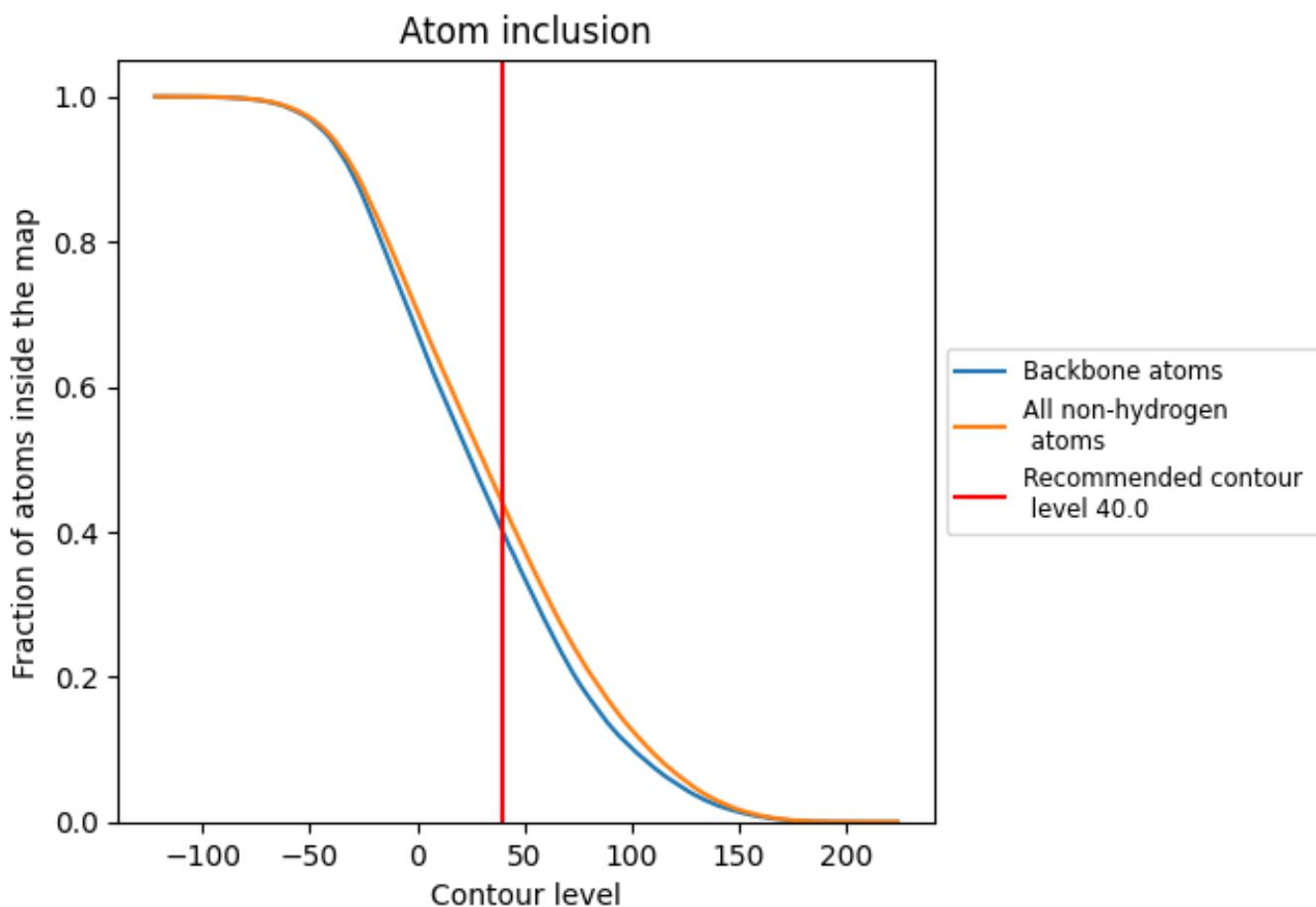
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (40.0).

## 9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 40% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (40.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4381	-0.0050
A1	0.4504	0.0020
A2	0.3236	-0.0520
AA	0.5085	-0.0040
AB	0.2664	-0.0000
AC	0.3559	-0.0030
AD	0.3421	-0.0160
AE	0.4300	0.0150
AF	0.2811	-0.0160
AG	0.4368	0.0260
AH	0.4792	-0.0000
AI	0.5392	0.0110
AJ	0.3010	0.0130
AK	0.3965	-0.0220
AL	0.3898	-0.0020
AM	0.5243	0.0280
AN	0.4625	0.0020
AO	0.3174	-0.0060
AP	0.4344	0.0060
AQ	0.3622	-0.0190
AR	0.4875	0.0390
AS	0.4375	0.0020
AT	0.3696	-0.0400
AU	0.2518	-0.0130
B0	0.3808	0.0110
B1	0.2005	-0.0140
B2	0.3634	-0.0360
B3	0.3401	-0.0240
B4	0.4418	-0.0230
B5	0.0337	0.0060
BA	0.4545	-0.0070
BB	0.4772	-0.0150
BC	0.4546	0.0110
BD	0.3836	-0.0090
BE	0.4579	-0.0020



*Continued on next page...*

Continued from previous page...

Chain	Atom inclusion	Q-score
BF	0.4678	0.0020
BG	0.4025	0.0180
BH	0.0283	-0.0480
BI	0.0000	0.0060
BJ	0.4182	0.0070
BK	0.3753	-0.0060
BL	0.4409	-0.0070
BM	0.4376	-0.0040
BN	0.3218	-0.0170
BO	0.5423	-0.0110
BP	0.2455	-0.0350
BQ	0.4449	0.0000
BR	0.3087	-0.0060
BS	0.3840	0.0010
BT	0.3375	-0.0040
BU	0.2708	-0.0030
BV	0.4634	-0.0050
BW	0.3918	-0.0280
BX	0.3577	-0.0250
BY	0.2455	-0.0170
BZ	0.4783	0.0010