



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:01 PM BST

PDB ID : 4V6Z  
EMDB ID: : EMD-2472  
Title : E. coli 70S-fMetVal-tRNAVal-tRNA<sup>f</sup>Met complex in classic pre-translocation state (pre1b)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 12.00 Å(reported)  
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

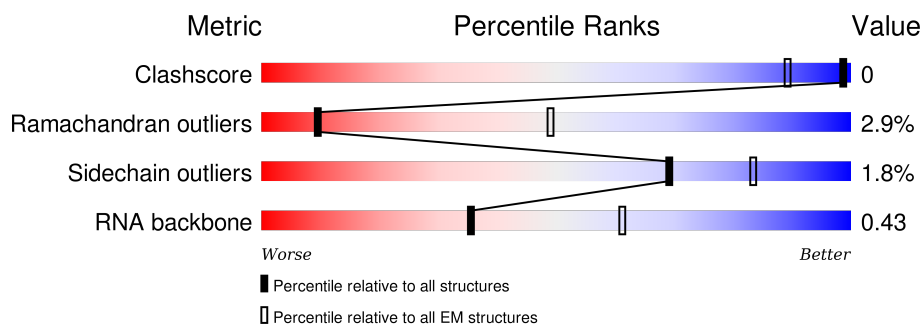
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.














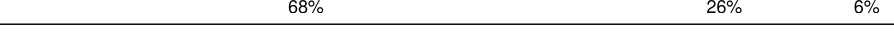

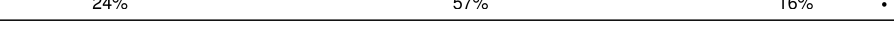

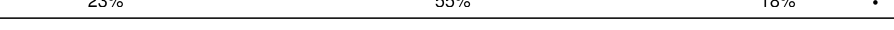



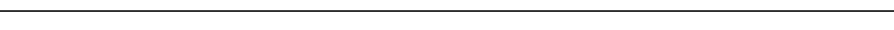

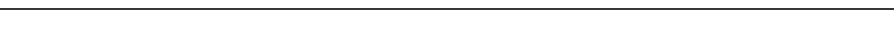
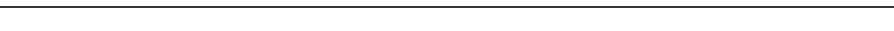


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AB	220	94% 6%
2	AC	208	89% 10%
3	AD	206	88% 11%
4	AE	152	89% 11% .
5	AF	101	87% 12% .
6	AG	152	93% 7%
7	AH	130	92% 7% .
8	AI	128	88% 11% .
























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Mol	Chain	Length	Quality of chain
9	AJ	100	 81% 16% .
10	AK	118	 90% 8% .
11	AL	124	 90% 10% .
12	AM	115	 84% 15% .
13	AN	101	 85% 14% .
14	AO	89	 87% 12% .
15	AP	81	 88% 12%
16	AQ	82	 91% 9%
17	AR	57	 88% 12%
18	AS	81	 91% 9%
19	AT	86	 86% 14%
20	AU	53	 68% 26% 6%
21	AA	1533	 13% 57% 25% 5%
22	A1	76	 24% 57% 16% .
23	A2	15	 33% 47% 20%
24	A3	77	 23% 55% 18% .
25	BC	273	 84% 14% .
26	BD	209	 88% 11% .
27	BE	201	 91% 9%
28	BF	179	 91% 8% .
29	BG	177	 89% 8% ..
30	BH	149	 94% 6%
31	BI	142	 93% 6% ..
32	BJ	142	 88% 12%
33	BK	123	 87% 11% ..

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

## 2 Entry composition

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
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

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
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

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
3	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	ACETYLATION	UNP P0A7W1
AE	159	NH2	-	AMIDATION	UNP P0A7W1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	ACETYLATION	UNP P02359
AG	152	NH2	-	AMIDATION	UNP P02359

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	ACETYLATION	UNP P0A7R5
AJ	103	NH2	-	AMIDATION	UNP P0A7R5

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	ACETYLATION	UNP P0AG63
AQ	83	NH2	-	AMIDATION	UNP P0AG63

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	ACETYLATION	UNP P0A7U3
AS	81	NH2	-	AMIDATION	UNP P0A7U3

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	ACETYLATION	UNP P68679
AU	54	NH2	-	AMIDATION	UNP P68679

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	ACETYLATION	UNP P0A7N9
B1	53	NH2	-	AMIDATION	UNP P0A7N9

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

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

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

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

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

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

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

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

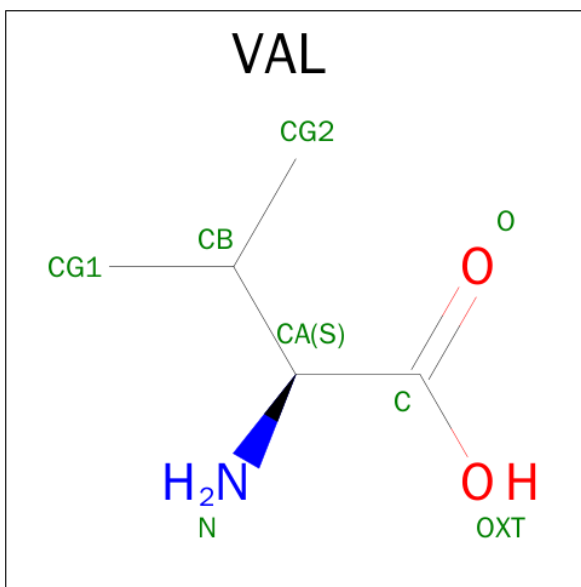
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

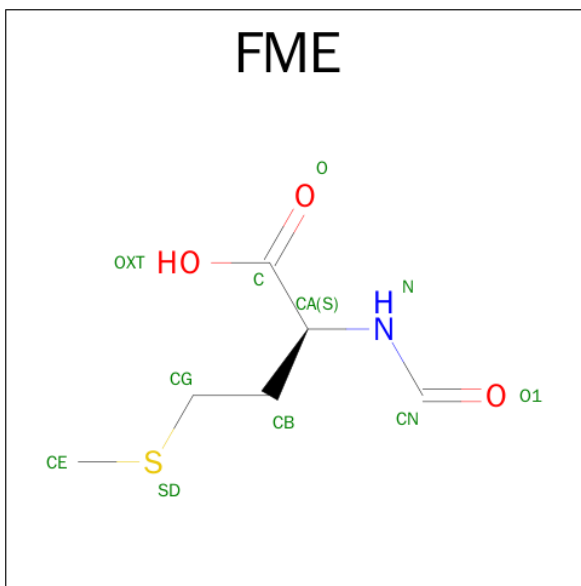
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



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

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).

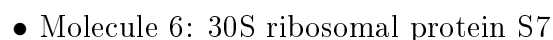
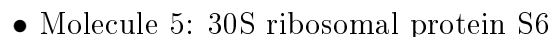
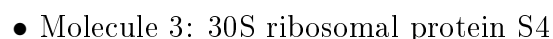
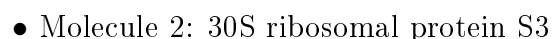


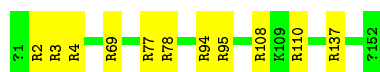
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	





- Molecule 1: 30S ribosomal protein S2





- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 7%



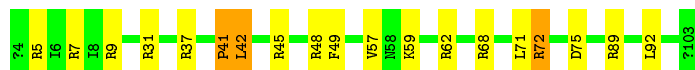
- Molecule 8: 30S ribosomal protein S9

Chain AI: 88% 11%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 81% 16%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 90% 8%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 90% 10%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 84% 15%

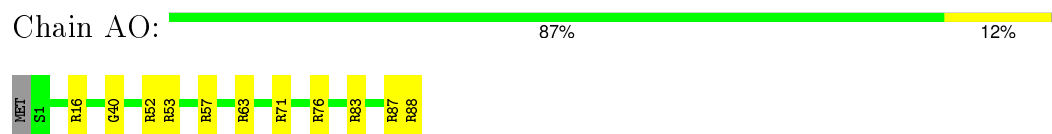


- Molecule 13: 30S ribosomal protein S14

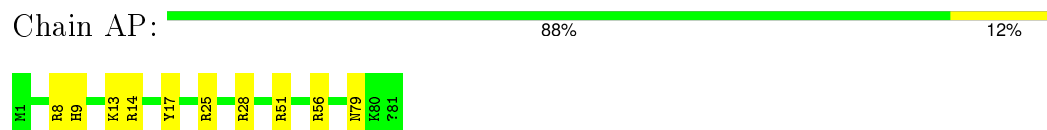
Chain AN: 85% 14%



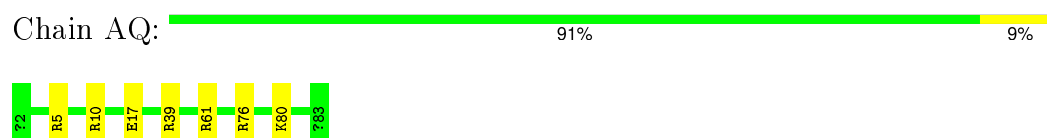
- Molecule 14: 30S ribosomal protein S15



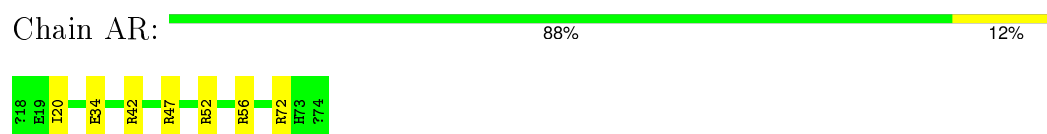
- Molecule 15: 30S ribosomal protein S16



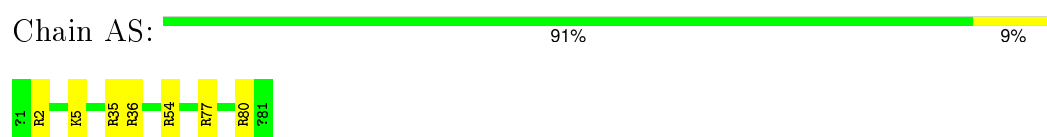
- Molecule 16: 30S ribosomal protein S17



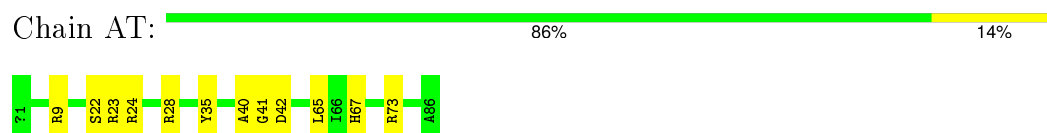
- Molecule 17: 30S ribosomal protein S18



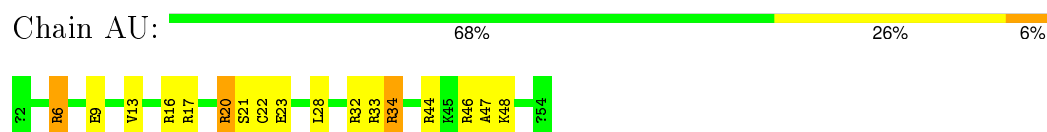
- Molecule 18: 30S ribosomal protein S19



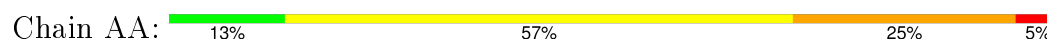
- Molecule 19: 30S ribosomal protein S20



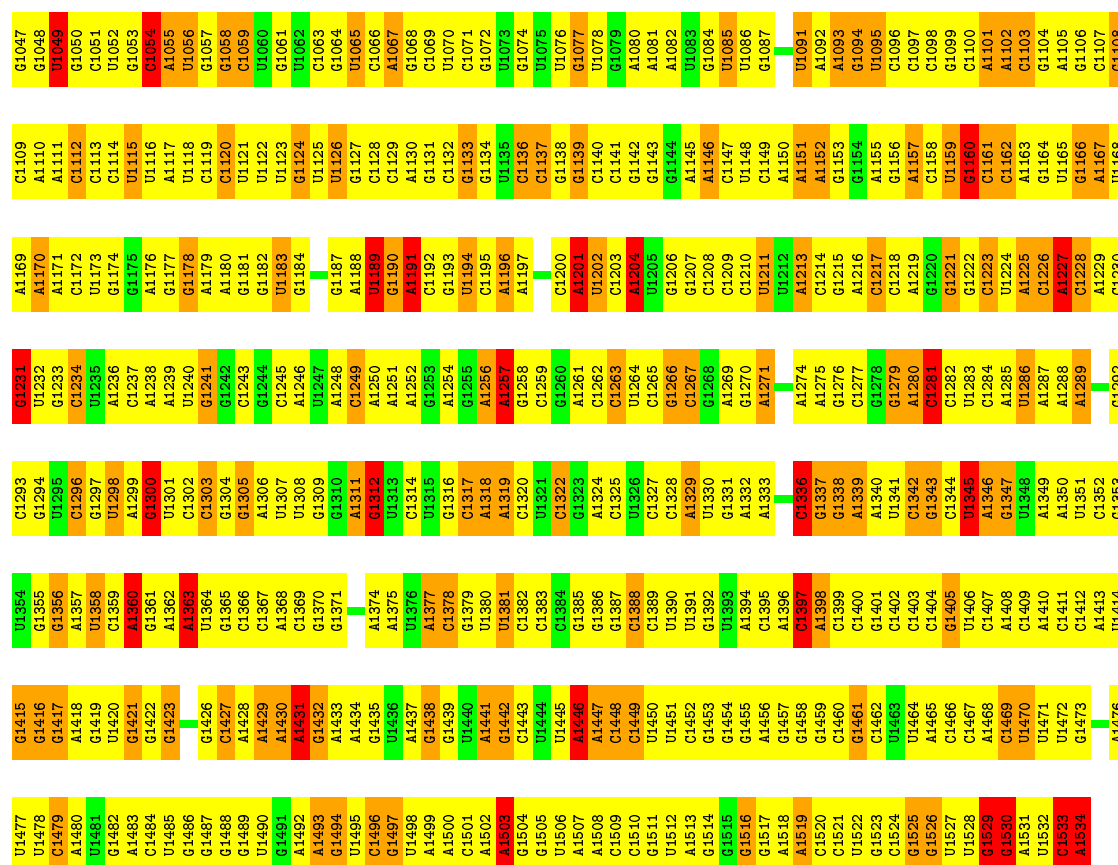
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA

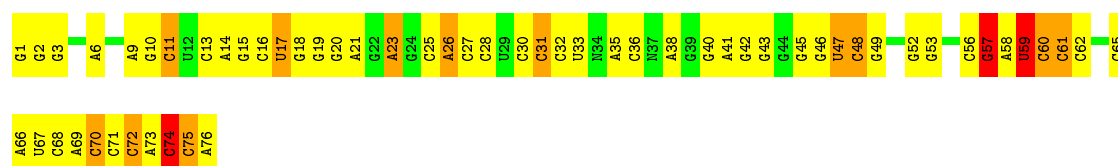




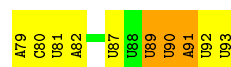
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 24% 57% 16%



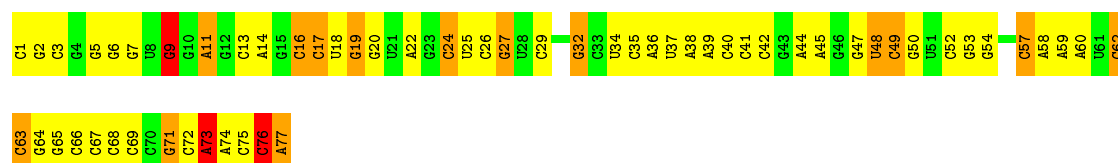
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

Chain A2: 33% 47% 20%

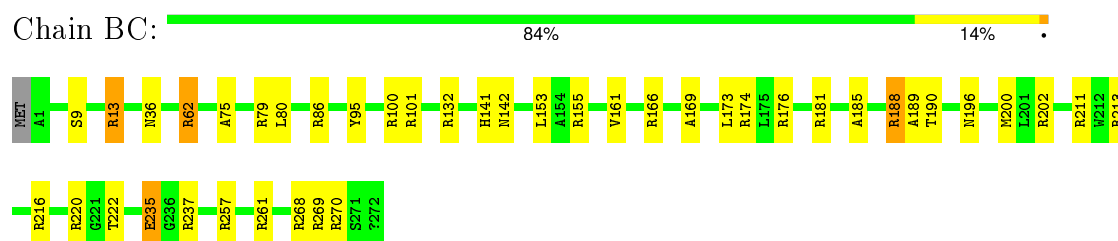


• Molecule 24: tRNA-fMet

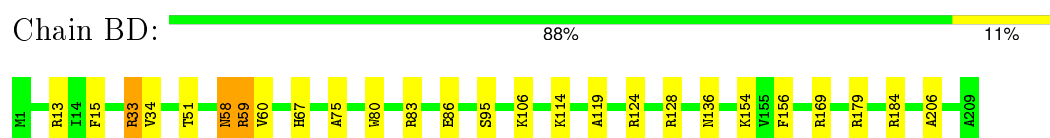
Chain A3: 23% 55% 18%



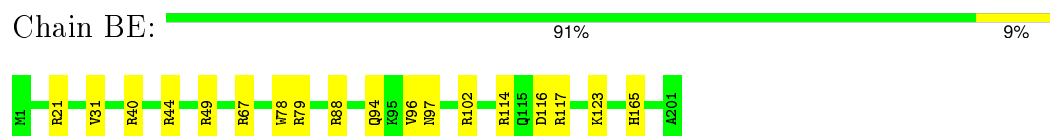
- Molecule 25: 50S ribosomal protein L2



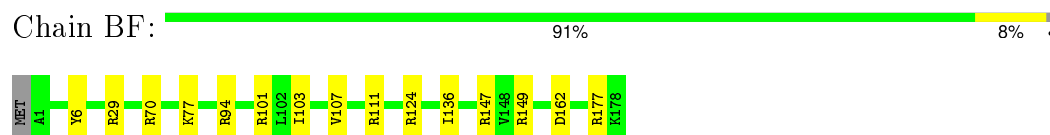
- Molecule 26: 50S ribosomal protein L3



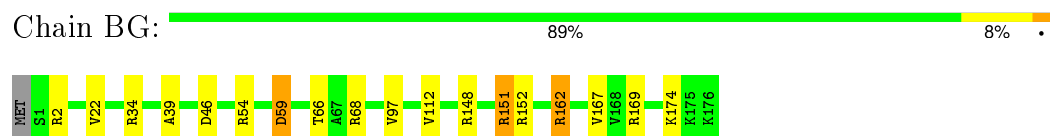
- Molecule 27: 50S ribosomal protein L4



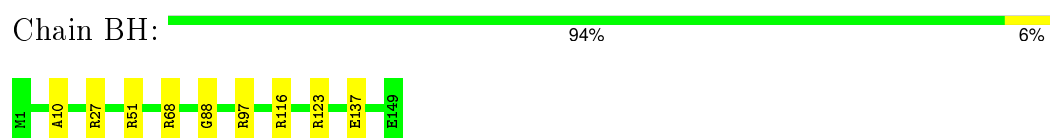
- Molecule 28: 50S ribosomal protein L5



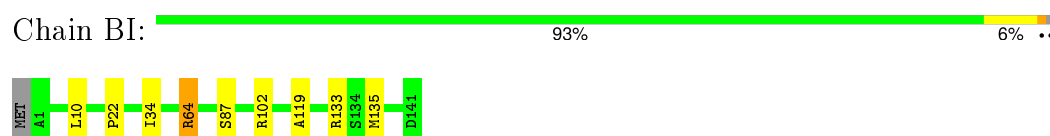
- Molecule 29: 50S ribosomal protein L6



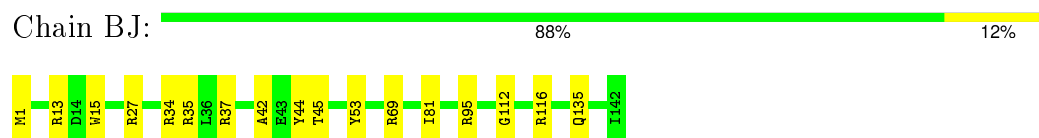
- Molecule 30: 50S ribosomal protein L9



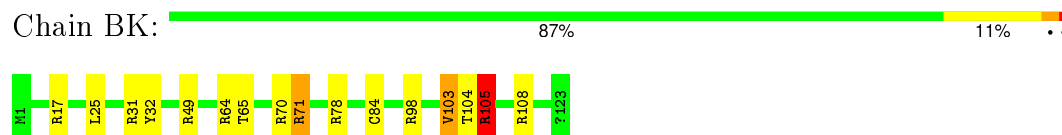
- Molecule 31: 50S ribosomal protein L11



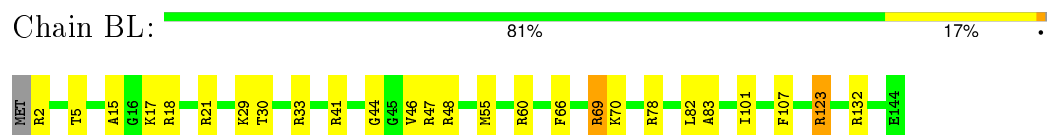
- Molecule 32: 50S ribosomal protein L13



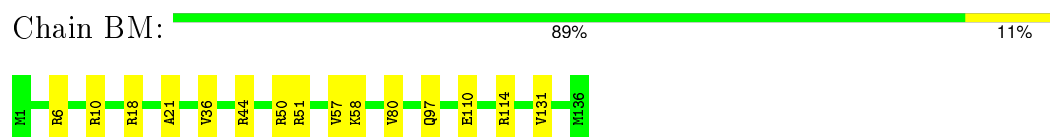
- Molecule 33: 50S ribosomal protein L14



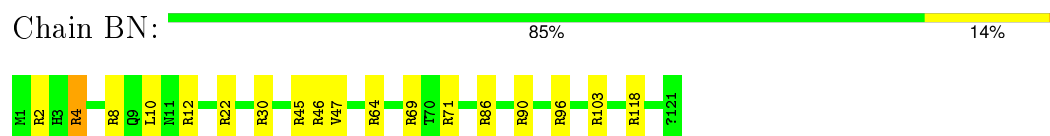
- Molecule 34: 50S ribosomal protein L15



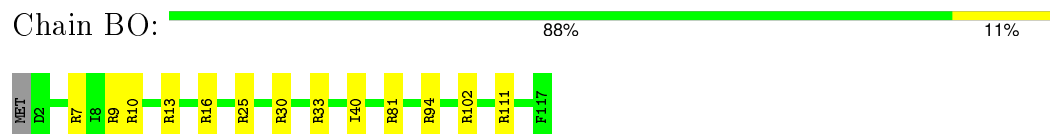
- Molecule 35: 50S ribosomal protein L16



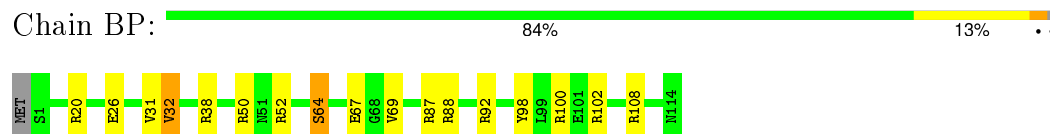
- Molecule 36: 50S ribosomal protein L17




- Molecule 37: 50S ribosomal protein L18

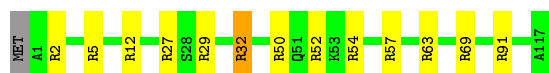


- Molecule 38: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  88% 10% ..




- Molecule 40: 50S ribosomal protein L21

Chain BR:  89% 11%



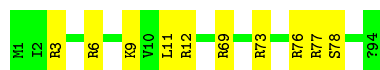
- Molecule 41: 50S ribosomal protein L22

Chain BS:  90% 10%



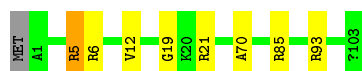
- Molecule 42: 50S ribosomal protein L23

Chain BT:  89% 11%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  91% 7% ..




- Molecule 44: 50S ribosomal protein L25

Chain BV:  93% 7%




- Molecule 45: 50S ribosomal protein L27

Chain BW:  84% 13% .



- Molecule 46: 50S ribosomal protein L28

Chain BX:  84% 13% . .





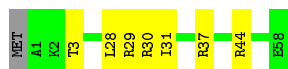
- Molecule 47: 50S ribosomal protein L29

Chain BY: 92% 8%



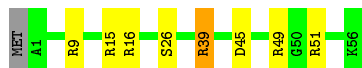
- Molecule 48: 50S ribosomal protein L30

Chain BZ: 86% 12%



- Molecule 49: 50S ribosomal protein L32

Chain B0: 84% 12%



- Molecule 50: 50S ribosomal protein L33

Chain B1: 83% 17%



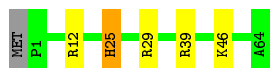
- Molecule 51: 50S ribosomal protein L34

Chain B2: 74% 26%



- Molecule 52: 50S ribosomal protein L35

Chain B3: 91% 6%

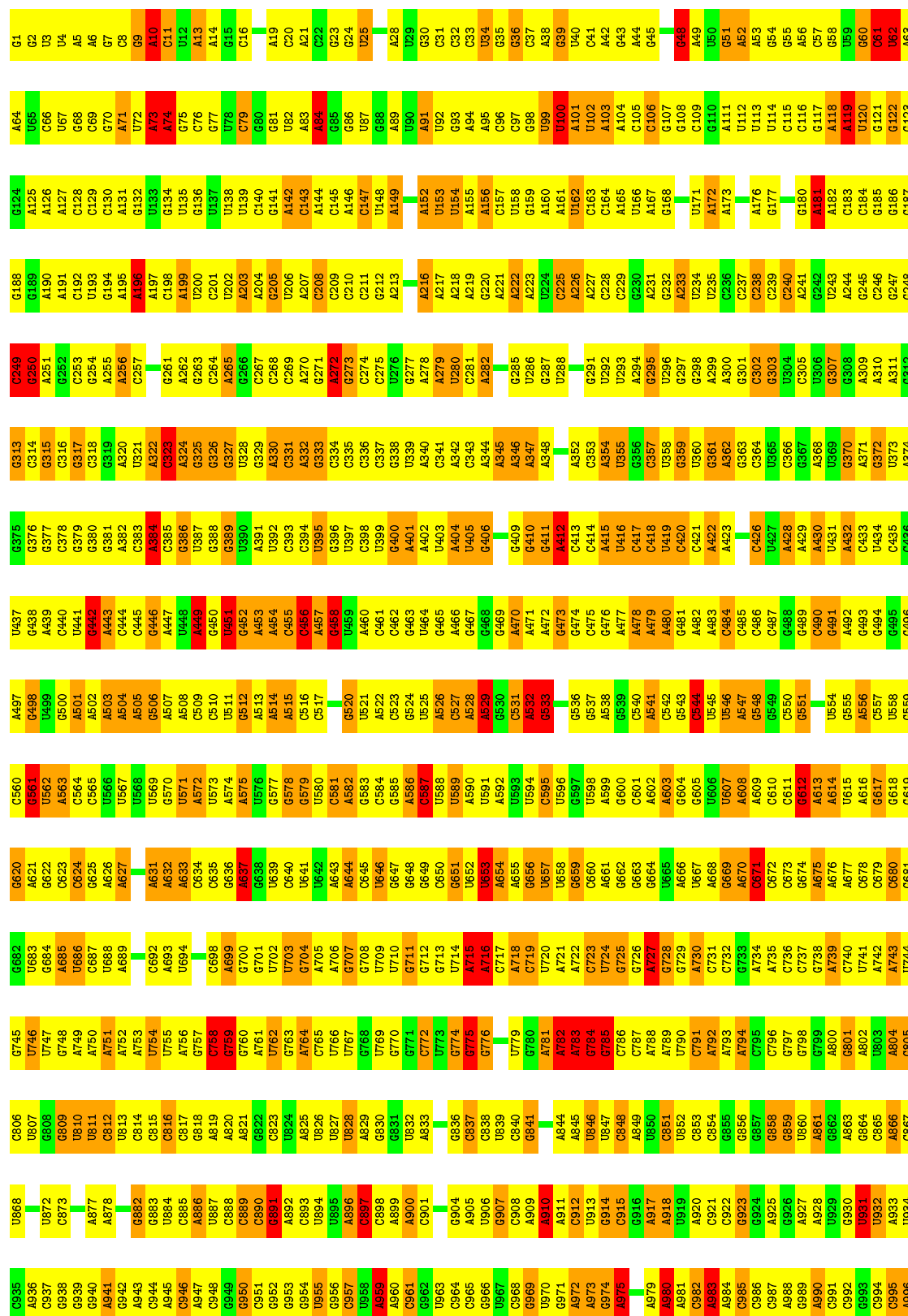



- Molecule 53: 50S ribosomal protein L36

Chain B4: 87% 13%



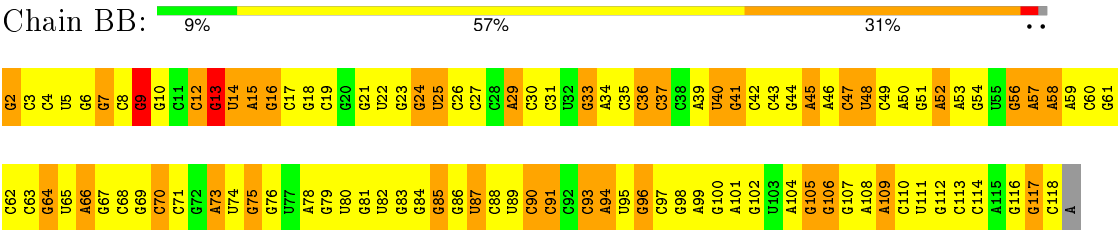
## ● Molecule 54: 23S ribosomal RNA

Chain BA: 

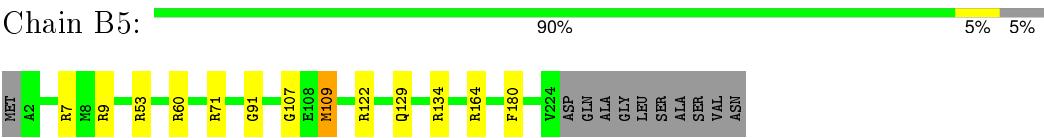
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A1919	A1858	A1794	A1735	G1673	A1610	C1550	A1490	G1429	G1369	G1309	G1248	U1188	G1124	G1063	C998
C1920	U1859	C1795	U1736	G1674	C1611	A1551	G1491	A1430	C1370	G1310	G1250	G1190	G1125	G1064	U999
U1923	G1861	G1797	U1737	G1675	C1612	A1552	C1492	A1431	G1371	G1311	G1251	G1191	A1126	U1065	A1000
G1924	G1862	G1798	G1738	A1677	A1614	U1554	C1493	A1432	U1372	U1312	G1252	G1192	G1127	U1066	A1001
C1925	G1863	G1799	A1739	A1678	C1615	G1555	A1495	A1434	A1373	U1313	G1253	G1193	G1128	A1067	G1002
U1926	U1864	C1800	G1740	A1679	A1616	C1556	A1496	A1435	G1374	C1314	A1254	G1194	U1130	G1068	
A1927	U1865	A1801	C1741	U1680	C1617	C1557	U1497	G1436	U1375	C1315	A1255	G1195	U1131	A1069	C1005
A1928	A1866	A1802	U1742	G1681	A1618	C1558	C1498	A1437	G1377	G1317	G1256	C1196	U1132	G1071	C1006
G1929	G1867	G1803	G1743	G1682	G1619	U1559	C1499	A1438	A1378	U1318	G1257	C1197	A1133	C1072	C1007
G1930	C1868	C1804	A1744	U1683	G1620	G1560	G1500	A1439	G1379	G1319	U1258	U1198	A1134	A1073	A1008
U1931	G1869	A1805	A1745	U1684	U1621	C1561	G1501	U1440	G1380	C1320	G1259	U1199	G1135	A1074	A1009
A1932	C1870	C1806	A1746	C1685	U1622	U1562	A1502	G1441	G1381	A1321	A1260	C1200		C1075	A1010
G1933	A1871	G1807	U1747	C1686	U1624	U1563	A1503	U1442	G1382	A1322	G1261	U1201	G1138	G1076	G1011
C1934	A1872	A1808	C1748	G1687	C1625	C1564	A1504	U1443	A1383	A1323	A1262	G1202	G1139	A1077	U1012
G1935	C1873	A1809	A1749	U1688	A1626	C1565	A1505	G1444	G1384	G1324	U1263	U1203	C1140	U1078	C1013
A1936	G1874	A1810	G1750	A1689	G1627	A1566	U1506	G1445	A1385	U1325	A1264	A1204	U1141	C1079	A1014
A1937	G1875		U1751	A1690	G1628	G1567	C1507	G1446	C1386	U1326	A1265	A1205	A1143	A1080	A1020
A1938	A1876	G1813	C1752	C1691	U1629	U1568	A1508	C1447	A1387	A1327	G1266	G1206	A1144	U1081	A1021
U1939	A1877	G1814	G1753	U1692	A1630	G1569	A1509	G1448	G1388	A1328	U1267	C1207	A1145	U1082	G1022
U1940	G1878	A1815	A1754	U1693	G1631	U1570	G1510	G1449	G1389	U1329	A1268	C1208	C1146	U1083	U1023
C1941	C1879	A1816	A1755	C1694	A1632	A1571	G1511	G1450	U1390	G1330	A1269	U1209	C1145	A1084	G1024
C1942	U1880	G1817	G1756	G1695	G1633	A1572	C1512	G1451	U1391	G1331	G1270	G1210	A1147	A1085	G1025
U1943	C1881	U1818	A1757	G1696	A1634	G1573	U1513	G1452	A1392	G1332	G1271	G1211	U1148	A1086	G1026
U1944	U1882	A1819	U1758	G1697	A1635	C1574	G1514	A1453	A1393	G1333	A1272	G1212	G1149	G1087	A1027
G1945	U1883	U1820	A1759	U1698	U1636	C1575	G1515	C1454	U1394	G1334	U1273	A1213	C1150	A1088	A1028
U1946	G1884	A1821	C1760	G1699	A1637	U1576	G1516	G1455	A1395	A1335	A1274	A1214	A1151	A1089	A1029
C1947	G1885	C1822	C1761	U1700	C1638	C1577	G1517	G1456	U1396	A1336	A1275	G1215	C1152	A1090	C1030
G1948	U1886	G1823	A1762	A1701	G1639	U1578	C1518	U1457	U1397	G1337	A1276	G1216	C1153	G1091	G1031
G1949	A1887	G1824	G1763	G1702	A1640	A1579	G1519	U1458	C1398	G1338	G1277	U1217	G1154	A1092	A1032
G1950	G1888	U1825	C1764	G1703	A1641	A1580	U1520	G1459	C1399	G1339	C1278	G1218	A1155	G1093	U1033
U1951	U1889	G1826	U1765	C1704	G1642	G1581	G1521	U1460	U1400	U1340		U1219	A1156	U1094	G1034
A1952	G1890	U1827	G1766	A1705	G1643	C1582	A1522	C1461	G1401	G1341	G1281	G1220	G1157	A1095	U1035
A1953	G1891	G1828	C1767	C1706	C1644	U1583	U1523	A1462	U1402	A1342	U1282	C1221	C1158	A1096	G1036
G1954	C1892	A1829	C1768	G1707	G1645	U1584	G1524	C1463	A1403	G1343	G1283	U1222	U1159	U1097	G1037
U1955	C1893	C1830	U1769	C1708	C1646	C1585	A1525	G1464	C1404	U1344	A1284	G1223	G1160	A1098	G1038
U1956	C1894	U1831	G1770	U1709	U1647	A1586	C1526	G1465	U1405	C1345	A1285	U1224	C1161	G1099	A1039
C1957	G1895	G1832	C1771	G1710	U1648	G1587	G1527	U1466	U1406	G1346	A1286	G1225		C1100	A1040
G1958	G1896	C1833	A1772	A1711	G1649	G1588	A1528	U1467	G1407	A1347	A1287	A1226	C1164	G1041	G1047
G1959		U1834	A1773	U1712	A1650	U1589	G1529	U1468	G1408	C1348	G1288	G1227	A1165	G1042	G1042
A1960	A1899	G1835	C1774	A1713	G1651	A1590	C1530	U1469	U1409	C1349	G1289	G1228	G1166	A1103	C1043
A1901	A1900	A1836	U1775	U1714	A1652	A1591	C1531	A1470	U1408	C1350	G1290	C1229	G1167	C1044	G1044
G1962	C1902	G1837	G1776	G1715	G1653	C1592	A1532	G1471	U1411	C1351	G1291	A1230	G1168	U1105	G1045
U1963	G1903	C1838	U1777	U1716	A1654	A1593	C1533	C1472	U1412	U1352	G1292	U1231	A1169	A1046	A1046
G1964	G1964		U1778	U1717	A1655	U1594	U1534	G1475	A1413	A1353	C1293	G1232	C1170	G1047	
A1965	G1904	C1843	U1779	G1718	C1656	C1595	A1535	U1476	C1414	A1354	U1294	C1233	G1171	A1048	A1048
A1966	G1905	U1844	A1780	G1719	U1657	A1596	C1536	A1477	U1415	G1355	C1295	U1234	C1172	C1049	C1049
G1967	G1906	G1845	U1781	U1720	C1658	A1597	G1537	G1478	G1416	G1356	G1296	G1235	U1173	A1050	A1050
G1968	G1907	G1846	U1782	G1721		A1598	G1538	G1479	C1417	C1357	G1297	G1236	U1174	G1051	G1051
A1969	C1908	A1847	A1783	A1722	U1662	U1599	U1539	G1479	G1418	G1358	C1298	A1237	A1175	C1052	C1052
A1970	G1909	G1848	G1723	G1723	G1663	C1600	G1540	A1480	A1419	A1359	G1299	G1238	U1176	C1053	C1053
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G1972	U1911	G1849	U1785	U1725	A1665	U1602	U1542	G1482	G1421	G1361	A1301	U1240	G1178	G1055	G1055
G1973	G1912	A1850	A1787	G1726	G1666	G1603	G1543	G1483	G1422	C1362	A1302	A1241	G1179	G1056	G1056
C1974	A1913	U1851	C1788	C1727	G1667	C1604	A1544	U1484	G1423	C1363	G1303	U1242	U1180	C1117	A1057
G1975	C1914	U1852	A1789	C1728	A1668	C1605	A1545	U1485	G1424	G1364	A1304	C1243	U1181	U1119	U1058
U1976	U1915	A1853	C1790	C1729	A1669	C1606	G1546	U1486	G1425	A1365	C1305	A1244		G1120	G1059
A1977	A1916	U1854	A1791	U1730	C1670	C1607	C1547	U1487	G1426	A1366	C1306	G1245		C1121	U1060
A1978	U1917		G1792	G1731	U1671	A1608	A1548	C1488	A1427	A1367	A1307	A1246	G1186	G1122	U1061

G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903
G2834	A2835	A2836	A2837	G2838	G2839	G2840	G2841	G2842	G2843
G2774	G2775	G2776	G2777	A2778	A2779	G2780	A2781	G2782	G2783
G2714	G2715	G2716	G2717	G2718	G2719	G2720	A2721	G2722	G2723
C2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661
G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601
G2538	G2539	A2540	A2541	G2542	G2543	G2544	G2545	G2546	G2547
G2529	A2530	A2531	A2532	A2533	A2534	A2535	G2536	G2537	G2538
C2467	A2468	A2469	G2470	A2471	G2472	G2473	G2474	G2475	G2476
A2407	G2408	G2409	G2410	A2411	A2412	G2413	G2414	G2415	G2416
A2346	C2347	G2348	G2349	G2350	G2351	A2352	G2353	G2354	G2355
C2285	G2286	A2287	A2288	G2289	G2290	G2291	G2292	G2293	G2294
A2225	C2226	A2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234
A2163	C2164	G2165	U2166	G2167	G2168	A2169	A2170	G2171	A2172
U2099	G2100	A2101	G2102	C2103	C2104		G2107	A2108	U2109
U2039	G2040	A2041	A2042	C2043	C2044	C2045	G2046	G2047	G2048
U1979	G1980	A1981	U1982	G1983	G1984	C1985	C1986	C1987	G1988

● Molecule 55: 5S ribosomal RNA



● Molecule 56: 50S ribosomal protein L1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, FME, ACE, H2U, CM0, 6MZ, NH2, 4SU, 7MG, PSU

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  >2	RMSZ	# Z  >2
1	AB	0.76	0/1736	1.10	10/2340 (0.4%)
10	AK	0.85	0/894	1.20	10/1207 (0.8%)
11	AL	0.85	0/969	1.25	13/1300 (1.0%)
12	AM	0.84	0/884	1.30	14/1181 (1.2%)
13	AN	0.88	1/817 (0.1%)	1.43	16/1088 (1.5%)
14	AO	0.86	0/722	1.26	12/964 (1.2%)
15	AP	0.88	0/648	1.25	6/870 (0.7%)
16	AQ	0.78	0/658	1.13	5/883 (0.6%)
17	AR	0.85	0/463	1.25	8/623 (1.3%)
18	AS	0.84	0/653	1.26	8/879 (0.9%)
19	AT	0.79	0/672	1.24	8/890 (0.9%)
2	AC	0.81	0/1651	1.19	17/2225 (0.8%)
20	AU	0.96	0/431	1.57	12/572 (2.1%)
21	AA	2.03	752/36759 (2.0%)	2.33	2571/57346 (4.5%)
22	A1	2.04	28/1668 (1.7%)	2.30	106/2595 (4.1%)
23	A2	1.81	3/343 (0.9%)	2.39	25/531 (4.7%)
24	A3	2.06	38/1722 (2.2%)	2.29	111/2685 (4.1%)
25	BC	0.85	0/2121	1.31	31/2852 (1.1%)
26	BD	0.77	0/1586	1.22	10/2134 (0.5%)
27	BE	0.75	0/1571	1.20	13/2113 (0.6%)
28	BF	0.79	0/1444	1.21	11/1937 (0.6%)
29	BG	0.76	0/1343	1.18	10/1816 (0.6%)
3	AD	0.83	0/1665	1.27	20/2227 (0.9%)
30	BH	0.72	0/1122	1.10	7/1515 (0.5%)
31	BI	0.71	0/1046	1.07	3/1410 (0.2%)
32	BJ	0.77	0/1152	1.24	12/1551 (0.8%)
33	BK	0.79	0/947	1.30	11/1268 (0.9%)
34	BL	0.82	0/1054	1.36	14/1403 (1.0%)
35	BM	0.84	0/1093	1.24	9/1460 (0.6%)
36	BN	0.89	0/973	1.43	19/1301 (1.5%)
37	BO	0.85	0/902	1.32	11/1209 (0.9%)
38	BP	0.85	0/929	1.42	13/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.86	0/960	1.33	14/1278 (1.1%)
4	AE	0.79	0/1119	1.16	9/1506 (0.6%)
40	BR	0.79	0/829	1.18	6/1107 (0.5%)
41	BS	0.76	0/864	1.20	8/1156 (0.7%)
42	BT	0.77	0/744	1.27	8/994 (0.8%)
43	BU	0.78	0/787	1.20	5/1051 (0.5%)
44	BV	0.75	0/766	1.17	6/1025 (0.6%)
45	BW	0.84	0/604	1.29	5/799 (0.6%)
46	BX	0.87	0/635	1.39	11/848 (1.3%)
47	BY	0.77	0/510	1.26	4/677 (0.6%)
48	BZ	0.84	0/453	1.29	5/605 (0.8%)
49	B0	0.85	0/450	1.33	7/599 (1.2%)
5	AF	0.79	0/835	1.15	7/1128 (0.6%)
50	B1	0.77	0/417	1.21	4/556 (0.7%)
51	B2	0.98	0/380	1.49	10/498 (2.0%)
52	B3	0.76	0/513	1.16	4/676 (0.6%)
53	B4	0.86	0/303	1.39	5/397 (1.3%)
54	BA	1.91	1309/69796 (1.9%)	2.32	5106/108888 (4.7%)
55	BB	2.03	85/2800 (3.0%)	2.33	222/4367 (5.1%)
56	B5	0.71	0/1673	1.10	10/2255 (0.4%)
6	AG	0.81	0/1188	1.19	11/1593 (0.7%)
7	AH	0.80	0/989	1.09	8/1326 (0.6%)
8	AI	0.88	0/1035	1.34	14/1377 (1.0%)
9	AJ	0.81	0/797	1.22	11/1079 (1.0%)
All	All	1.71	2216/160085 (1.4%)	2.09	8646/239402 (3.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AK	0	1
2	AC	0	2
21	AA	0	365
22	A1	0	10
23	A2	0	1
24	A3	0	14
25	BC	0	2
33	BK	0	1
34	BL	0	1
54	BA	0	666

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	30
8	AI	0	1
All	All	0	1094

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

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

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

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

There are no chirality outliers.

5 of 1094 planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	2	0
20	AU	429	0	453	0	0
21	AA	32828	0	15886	9	0
22	A1	1627	0	798	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	801	1	0
25	BC	2083	0	2157	2	0
26	BD	1565	0	1616	3	0
27	BE	1552	0	1619	1	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	2	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	1	0
51	B2	377	0	418	1	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	30186	21	0
55	BB	2504	0	1181	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	97702	45	0

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

The worst 5 of 45 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AT:40:ALA:HB1	19:AT:41:GLY:HA2	1.81	0.62
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
26:BD:154:LYS:HE3	26:BD:156:PHE:CE1	2.46	0.51
54:BA:931:U:C5	54:BA:1167:C:H1'	2.46	0.50
21:AA:5:U:H4'	21:AA:6:G:C6	2.46	0.50

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	195 (89%)	22 (10%)	1 (0%)	34	77
2	AC	205/208 (99%)	191 (93%)	12 (6%)	2 (1%)	19	65
3	AD	203/206 (98%)	185 (91%)	15 (7%)	3 (2%)	13	57
4	AE	150/152 (99%)	134 (89%)	9 (6%)	7 (5%)	3	32
5	AF	99/101 (98%)	86 (87%)	6 (6%)	7 (7%)	1	22
6	AG	150/152 (99%)	143 (95%)	7 (5%)	0	100	100
7	AH	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
8	AI	126/128 (98%)	110 (87%)	12 (10%)	4 (3%)	5	41
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	30
10	AK	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	21	67
11	AL	121/124 (98%)	111 (92%)	10 (8%)	0	100	100
12	AM	112/115 (97%)	98 (88%)	12 (11%)	2 (2%)	11	53
13	AN	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	19	65
14	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	16	61
15	AP	79/81 (98%)	68 (86%)	7 (9%)	4 (5%)	2	30
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	7	46
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	11	53
18	AS	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
19	AT	84/86 (98%)	74 (88%)	8 (10%)	2 (2%)	7	47
20	AU	51/53 (96%)	27 (53%)	14 (28%)	10 (20%)	0	3
25	BC	270/273 (99%)	238 (88%)	21 (8%)	11 (4%)	3	35
26	BD	207/209 (99%)	178 (86%)	18 (9%)	11 (5%)	2	29
27	BE	199/201 (99%)	177 (89%)	17 (8%)	5 (2%)	7	46
28	BF	176/179 (98%)	151 (86%)	21 (12%)	4 (2%)	8	48
29	BG	174/177 (98%)	152 (87%)	13 (8%)	9 (5%)	2	30
30	BH	147/149 (99%)	132 (90%)	13 (9%)	2 (1%)	14	58
31	BI	139/142 (98%)	125 (90%)	10 (7%)	4 (3%)	6	43
32	BJ	140/142 (99%)	125 (89%)	8 (6%)	7 (5%)	3	31
33	BK	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	7	46
34	BL	141/144 (98%)	117 (83%)	12 (8%)	12 (8%)	1	18
35	BM	134/136 (98%)	117 (87%)	12 (9%)	5 (4%)	4	38
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	11	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
38	BP	112/115 (97%)	91 (81%)	15 (13%)	6 (5%)	2	29
39	BQ	115/118 (98%)	100 (87%)	15 (13%)	0	100	100
40	BR	101/103 (98%)	94 (93%)	3 (3%)	4 (4%)	4	35
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	10	52
42	BT	92/94 (98%)	78 (85%)	11 (12%)	3 (3%)	5	40
43	BU	101/104 (97%)	85 (84%)	12 (12%)	4 (4%)	4	35
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	65 (83%)	6 (8%)	7 (9%)	1	17
46	BX	75/79 (95%)	70 (93%)	3 (4%)	2 (3%)	6	45
47	BY	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	12	56
48	BZ	56/59 (95%)	50 (89%)	4 (7%)	2 (4%)	4	38
49	B0	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	10	52
50	B1	50/52 (96%)	43 (86%)	3 (6%)	4 (8%)	1	19
51	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
52	B3	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	5	41
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5249 (89%)	458 (8%)	169 (3%)	9	43

5 of 169 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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%)	68	87
2	AC	170/171 (99%)	167 (98%)	3 (2%)	66	87
3	AD	172/173 (99%)	168 (98%)	4 (2%)	58	83
4	AE	113/113 (100%)	110 (97%)	3 (3%)	52	79
5	AF	87/87 (100%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	123 (100%)	0	100	100
7	AH	104/105 (99%)	102 (98%)	2 (2%)	65	86
8	AI	105/105 (100%)	105 (100%)	0	100	100
9	AJ	86/86 (100%)	82 (95%)	4 (5%)	32	68
10	AK	90/90 (100%)	88 (98%)	2 (2%)	60	83
11	AL	103/104 (99%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	88 (97%)	3 (3%)	45	76
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	62 (95%)	3 (5%)	33	68
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	51	78
26	BD	164/164 (100%)	161 (98%)	3 (2%)	66	87
27	BE	165/165 (100%)	163 (99%)	2 (1%)	78	90
28	BF	149/150 (99%)	148 (99%)	1 (1%)	88	94
29	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
30	BH	114/114 (100%)	113 (99%)	1 (1%)	84	93
31	BI	109/110 (99%)	106 (97%)	3 (3%)	51	78
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	99 (96%)	4 (4%)	39	72
34	BL	102/103 (99%)	101 (99%)	1 (1%)	82	92
35	BM	109/109 (100%)	106 (97%)	3 (3%)	51	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	82	92
37	BO	86/87 (99%)	85 (99%)	1 (1%)	78	90
38	BP	99/100 (99%)	95 (96%)	4 (4%)	38	71
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	90 (97%)	3 (3%)	46	76
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	83 (100%)	0	100	100
44	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
45	BW	59/59 (100%)	55 (93%)	4 (7%)	20	57
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	45 (96%)	2 (4%)	35	70
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	33 (97%)	1 (3%)	50	78
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68	87
All	All	4842/4870 (99%)	4756 (98%)	86 (2%)	69	87

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

Mol	Chain	Res	Type
26	BD	33	ARG
31	BI	22	PRO
49	B0	45	ASP
26	BD	124	ARG
28	BF	162	ASP

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

Mol	Chain	Res	Type
18	AS	51	HIS

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Mol	Chain	Res	Type
32	BJ	77	HIS
18	AS	56	HIS
13	AN	62	ASN
26	BD	134	HIS

### 5.3.3 RNA ⓘ

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

5 of 747 RNA backbone outliers are listed below:

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

5 of 220 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	384	A
54	BA	764	A
54	BA	2529	G
54	BA	405	U
54	BA	548	G

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	CM0	A1	34	22,23	15,26,27	2.11	4 (26%)	18,37,40	3.24	4 (22%)
22	6MZ	A1	37	22	17,25,26	0.87	0	15,36,39	1.30	1 (6%)
22	7MG	A1	46	22	20,26,27	2.23	3 (15%)	23,39,42	2.22	2 (8%)
22	5MU	A1	54	22	13,22,23	0.98	1 (7%)	16,32,35	4.08	2 (12%)
22	PSU	A1	55	22	15,21,22	1.28	2 (13%)	16,30,33	3.45	5 (31%)
22	4SU	A1	7	22	12,21,22	1.12	1 (8%)	15,30,33	2.33	3 (20%)
24	H2U	A3	21	24	17,21,22	1.41	2 (11%)	23,30,33	1.25	4 (17%)
24	OMC	A3	33	24	15,22,23	1.22	1 (6%)	20,31,34	0.83	0
24	5MU	A3	55	24	13,22,23	1.30	2 (15%)	16,32,35	4.22	3 (18%)
24	PSU	A3	56	24	15,21,22	1.20	2 (13%)	16,30,33	3.41	5 (31%)
24	4SU	A3	8	24	12,21,22	1.45	3 (25%)	15,30,33	2.14	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	22,23	-	0/6/30/31	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/3/25/26	0/2/2/2
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/3/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/5/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/3/25/26	0/2/2/2
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/3/25/26	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.43	1.33	1.45
22	A1	34	CM0	O5-C5	-6.31	1.24	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C2-N3	-3.44	1.31	1.38
24	A3	21	H2U	C4-N3	-3.28	1.32	1.37
22	A1	46	7MG	C8-N7	-2.87	1.30	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-11.73	115.51	125.35
24	A3	55	5MU	C5-C4-N3	-11.46	115.73	125.35
24	A3	8	4SU	C5-C4-N3	-7.56	115.55	123.56
22	A1	7	4SU	C5-C4-N3	-7.52	115.58	123.56
22	A1	46	7MG	C5-C6-N1	-6.87	113.16	123.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	5,6,7	0.62	0	5,7,9	1.66	2 (40%)
58	FME	BA	3001	57	8,9,10	0.81	0	5,9,11	1.21	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	-	0/4/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-2.85	117.91	125.69
57	A1	101	VAL	C-CA-N	2.37	115.19	109.95

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.