



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:55 PM BST

PDB ID : 4V77  
EMDB ID: : EMD-2474  
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post2b)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 17.00 Å(reported)  
Based on 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

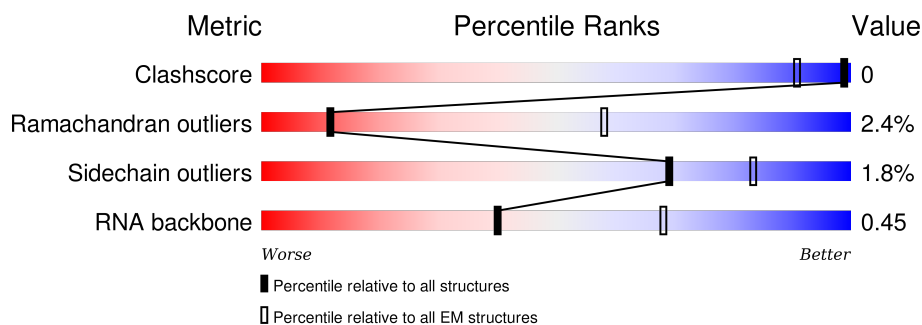
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 17.00 Å.

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













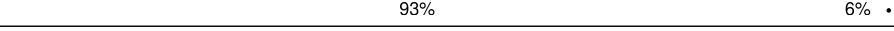
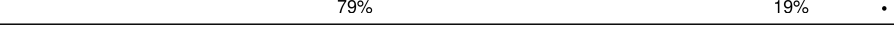
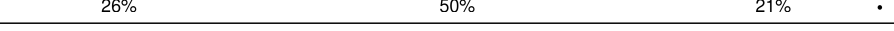
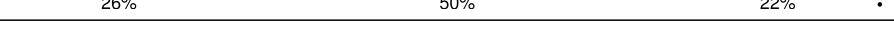





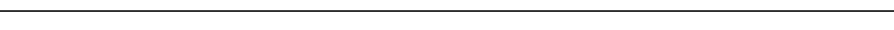

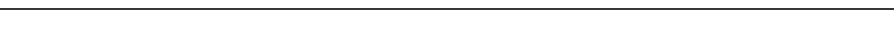
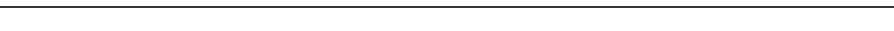


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	90% 9% .
3	AD	206	87% 12%
4	AE	152	91% 9%
5	AF	101	87% 13%
6	AG	152	88% 12% .
7	AH	130	92% 7% ..
8	AI	128	84% 16% .





















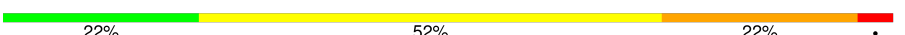
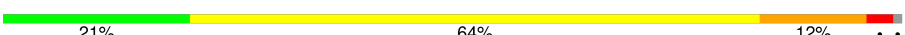

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Mol	Chain	Length	Quality of chain
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG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

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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\*P\*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		

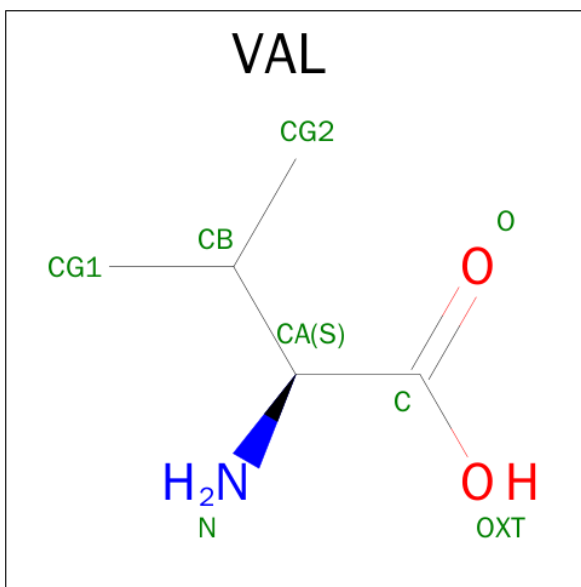
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

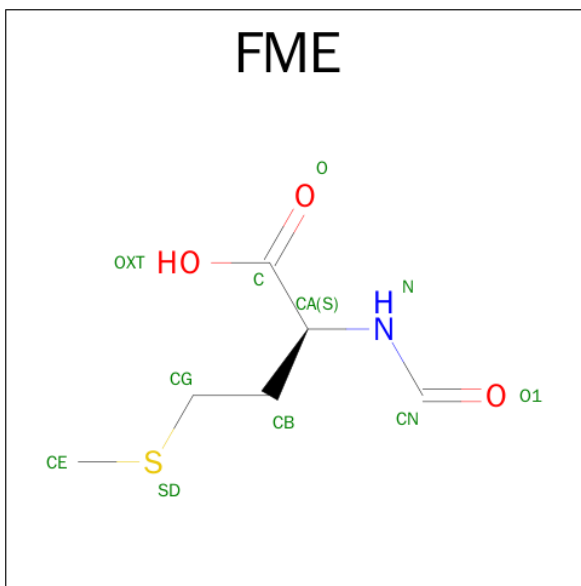
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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:  $C_6H_{11}NO_3S$ ).



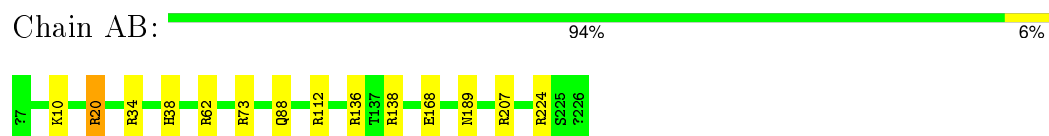
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



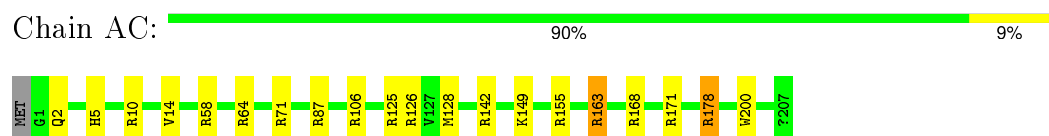
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

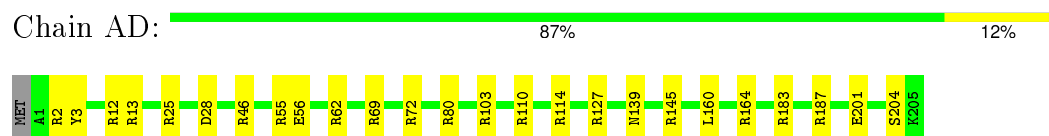
- Molecule 1: 30S ribosomal protein S2



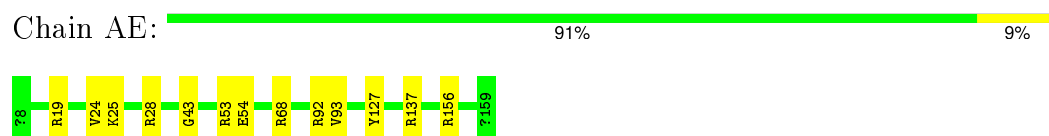
- Molecule 2: 30S ribosomal protein S3



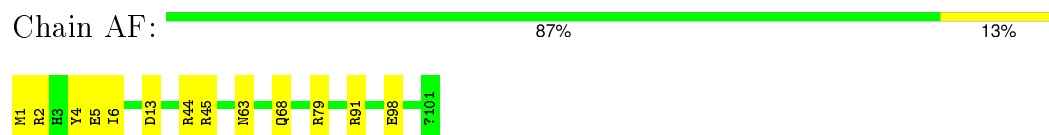
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 7% ..



- Molecule 8: 30S ribosomal protein S9

Chain AI: 84% 16% .



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 85% 15%



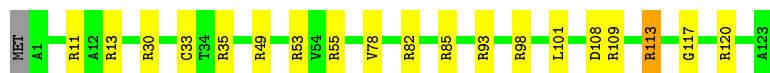
- Molecule 10: 30S ribosomal protein S11

Chain AK: 89% 8% ..



- Molecule 11: 30S ribosomal protein S12

Chain AL: 84% 15% ..



- Molecule 12: 30S ribosomal protein S13

Chain AM: 83% 15% ..

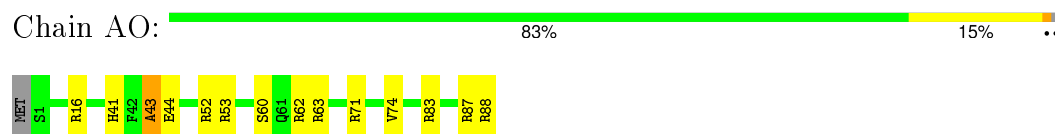


- Molecule 13: 30S ribosomal protein S14

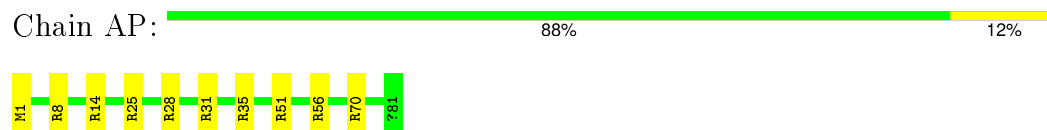
Chain AN: 85% 13% ..



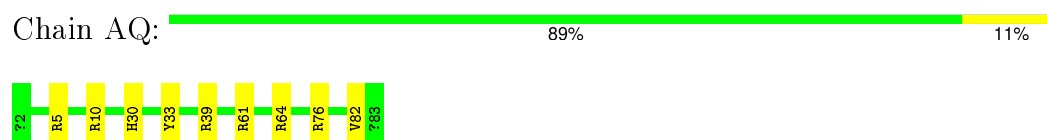
- Molecule 14: 30S ribosomal protein S15



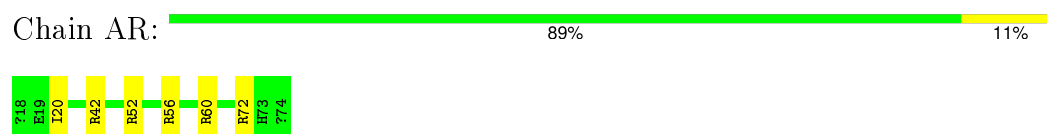
- Molecule 15: 30S ribosomal protein S16



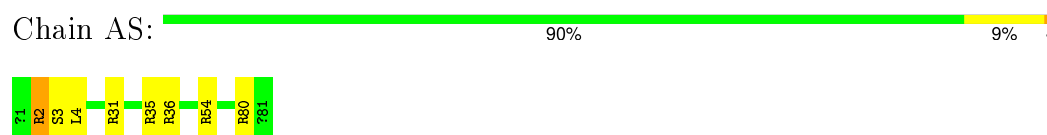
- Molecule 16: 30S ribosomal protein S17



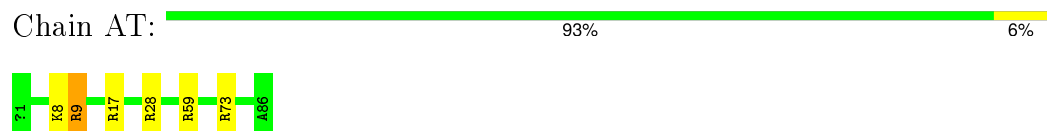
- Molecule 17: 30S ribosomal protein S18



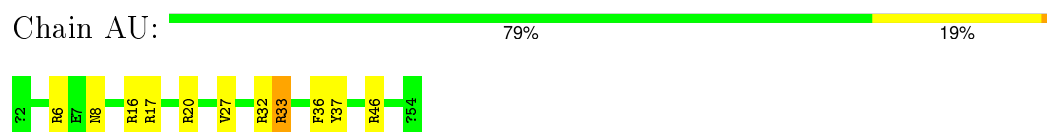
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



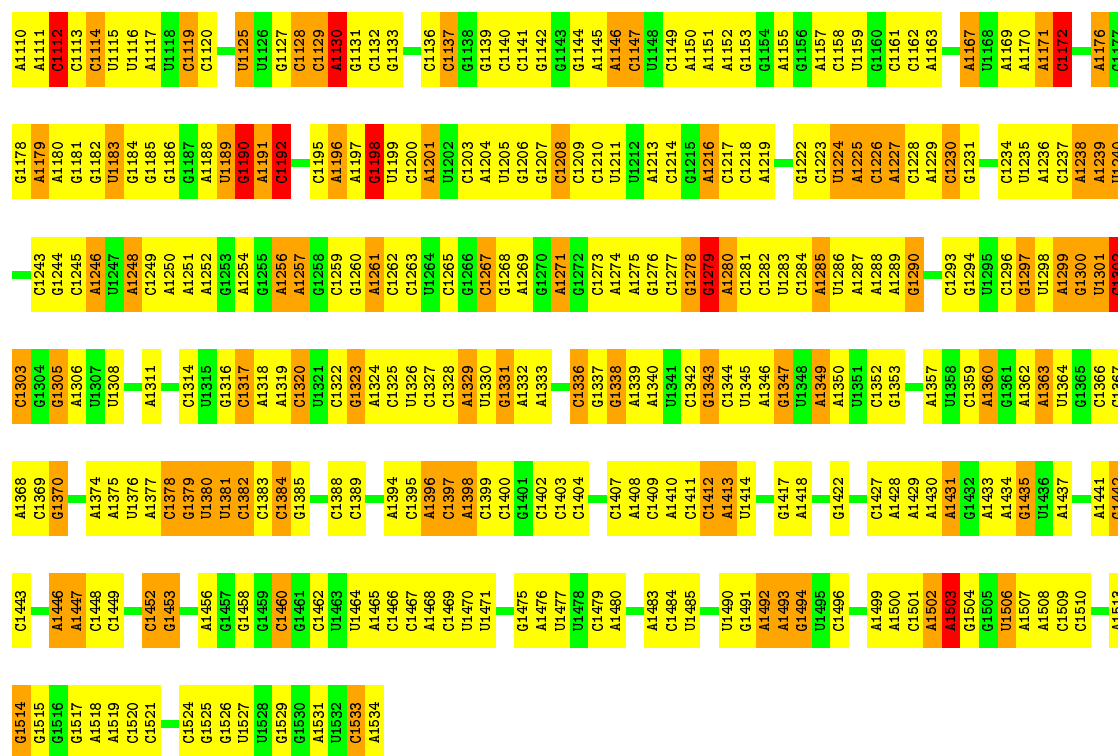
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA

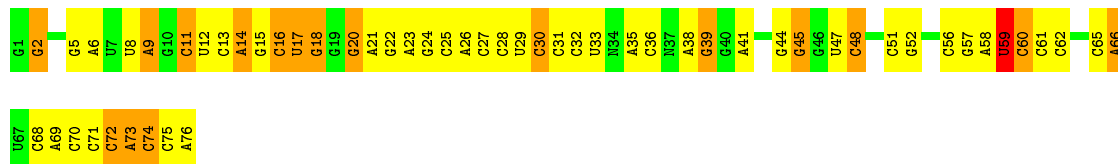


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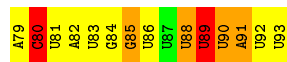
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 26% 50% 22%



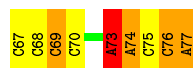
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

Chain A2: 7% 53% 27% 13%

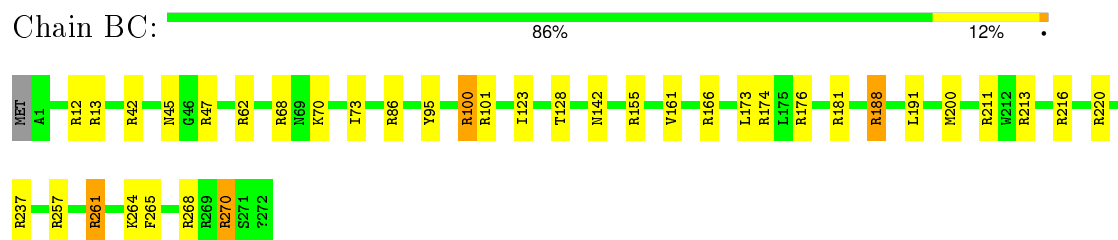


• Molecule 24: tRNA-fMet

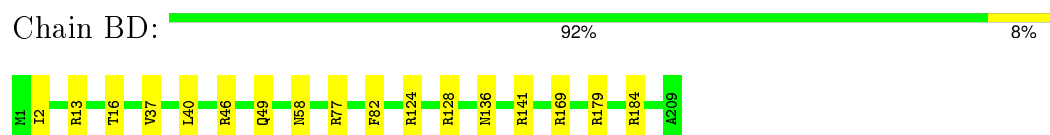
Chain A3: 29% 53% 16%



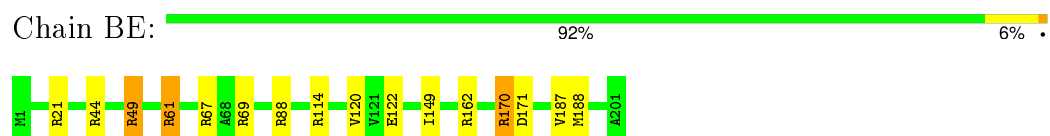
• Molecule 25: 50S ribosomal protein L2



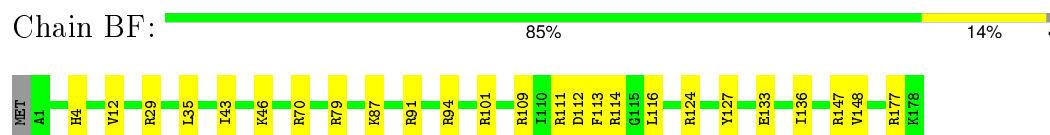
- Molecule 26: 50S ribosomal protein L3



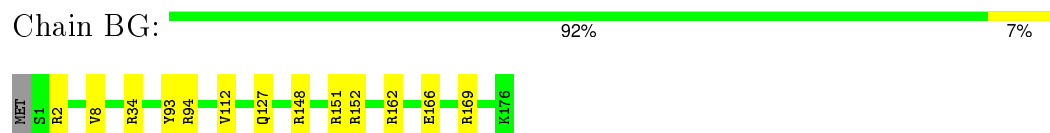
- Molecule 27: 50S ribosomal protein L4



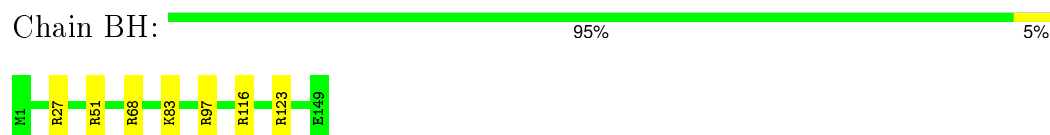
- Molecule 28: 50S ribosomal protein L5



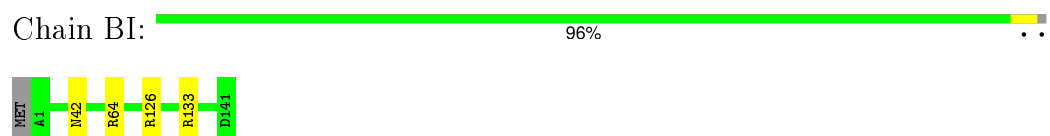
- Molecule 29: 50S ribosomal protein L6




- Molecule 30: 50S ribosomal protein L9

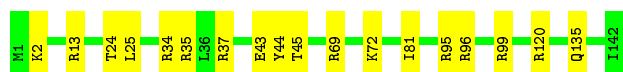


- Molecule 31: 50S ribosomal protein L11



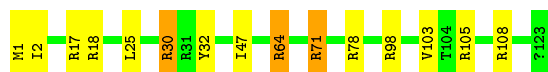
- Molecule 32: 50S ribosomal protein L13

Chain BJ:  87% 13%




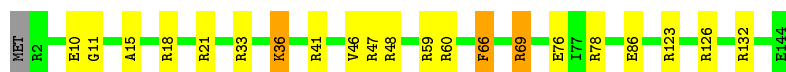
- Molecule 33: 50S ribosomal protein L14

Chain BK:  88% 10%



- Molecule 34: 50S ribosomal protein L15

Chain BL:  85% 13%



- Molecule 35: 50S ribosomal protein L16

Chain BM:  85% 15%



- Molecule 36: 50S ribosomal protein L17

Chain BN:  88% 12%




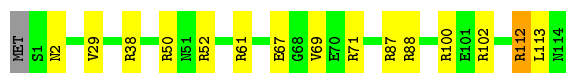
- Molecule 37: 50S ribosomal protein L18

Chain BO:  87% 11%




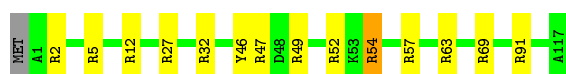
- Molecule 38: 50S ribosomal protein L19

Chain BP:  86% 12%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  87% 11%



- Molecule 40: 50S ribosomal protein L21

Chain BR: 91% 9%



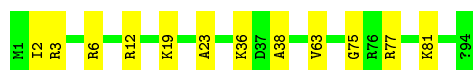
- Molecule 41: 50S ribosomal protein L22

Chain BS: 92% 8%



- Molecule 42: 50S ribosomal protein L23

Chain BT: 87% 13%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 87% 12% ..



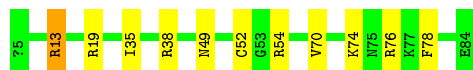
- Molecule 44: 50S ribosomal protein L25

Chain BV: 91% 9%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 86% 13% .



- Molecule 46: 50S ribosomal protein L28

Chain BX: 86% 10% ..





- Molecule 47: 50S ribosomal protein L29

Chain BY:  92% 8%




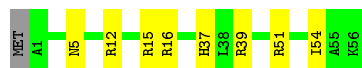
- Molecule 48: 50S ribosomal protein L30

Chain BZ:  86% 12%



- Molecule 49: 50S ribosomal protein L32

Chain B0:  84% 14%




- Molecule 50: 50S ribosomal protein L33

Chain B1:  92% 8%




- Molecule 51: 50S ribosomal protein L34

Chain B2:  74% 26%



- Molecule 52: 50S ribosomal protein L35

Chain B3:  86% 12%



- Molecule 53: 50S ribosomal protein L36

Chain B4:  92% 8%

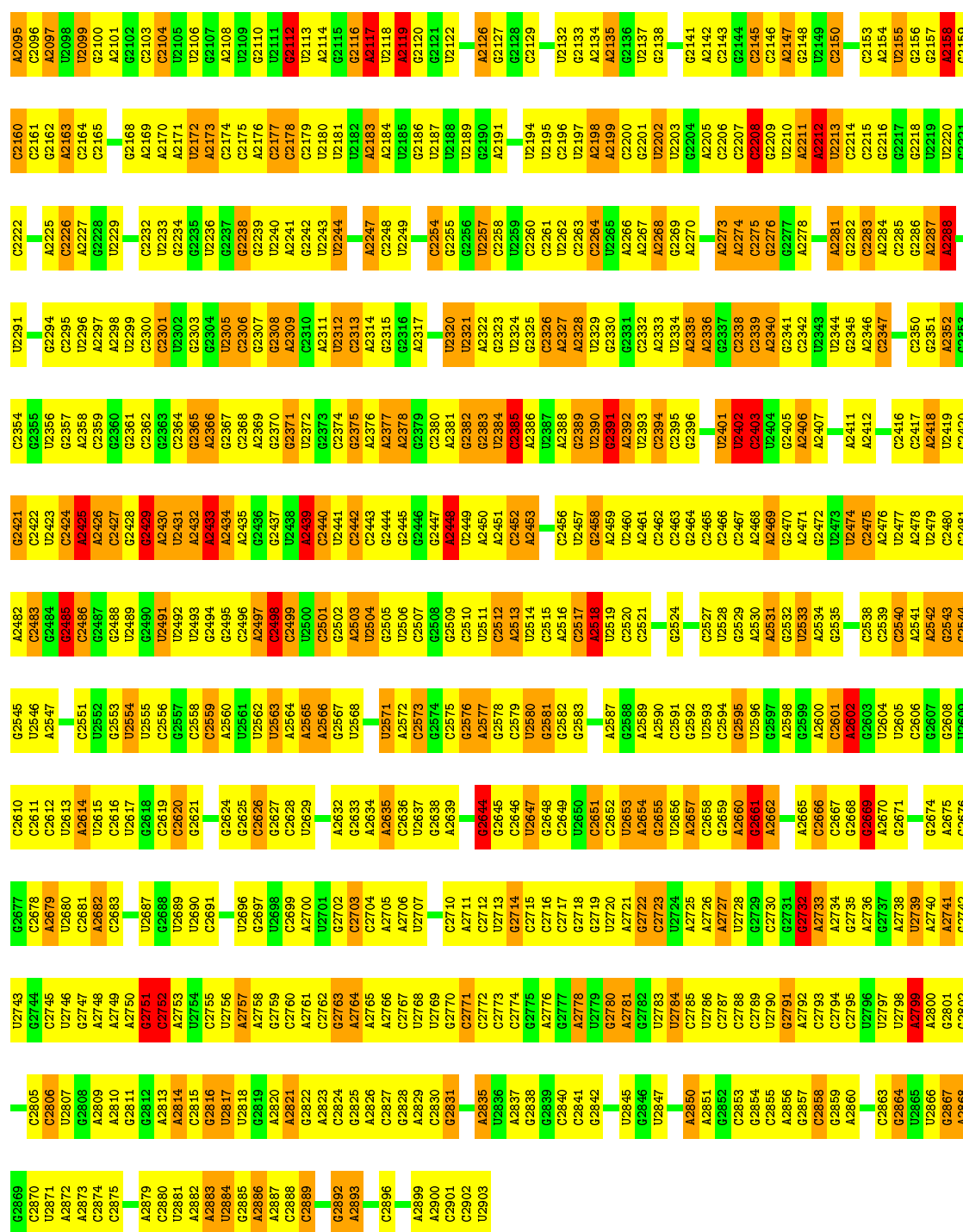


- Molecule 54: 23S ribosomal RNA

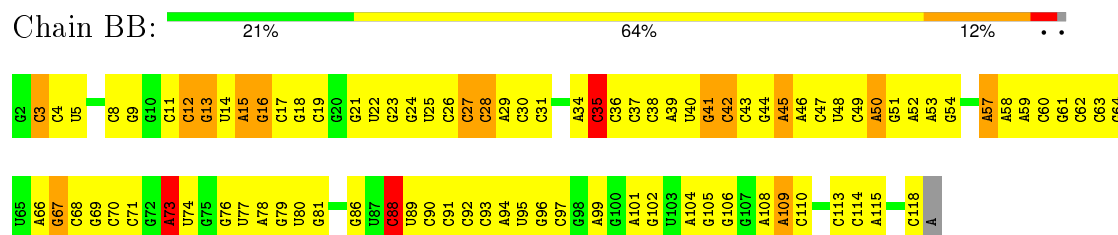
Chain BA:  22% 52% 22%

G1024	C957	A896	G831	G768	G704	A643	C581	A515	U451	U387	G254	A195	A127	A63	G1
G1025	U958	C997	U832	G768	A705	A644	A582	C516	G452	G388	A255	A196	C128	A64	U4
G1026	A959	C998	A833	C772	A706	U646	G583	C517	A453	U390	A256	A197	C129	U65	A5
A1027	A960	A989	G834	U773		U647	C584		A454	G389	C257	A198	C130	C66	A6
A1028	C961	A900	C835	G774	U709	G647	G585	G520	C455	A391	A262	A199	A131	U67	G7
A1029	G962	C901	G836	G775	U710		A586	U521	C456	U392	G263	U200	G132	G68	C8
C1030	U963	C902	G837	G776			C587	A522	A457	C393	G264	U202	U133	C69	G9
C1031	C964	G903	C838	G777	U714	C850	U588	C523	G458	C394	G265	C201	G134	G70	
A1032	C965	A905	U839	G778	A715	G851	U589		U459	U395	A266	U202		A71	A10
U1033			C840	U779	A716	U653	A590	A526	A460	G396	C267	A204	U138	U72	C11
G1034			G841	U780	C717	A654	U591	C527	C461	U397	C268	A205	U139	A73	U12
U1035			U842	A781	C718	A655	A592	A528	C462	C398	C269	G206	C140	A74	A13
			G843	A782	C719	G856	U593	A529	G463	U399	A270	A207	G141	G75	A14
A1039	G971	A909	A844	A783	U720	U657	U594	G530	U464	G400	C271	A208	A142	C76	G15
A1040	A972	A912	A845	G784	A721	U658	C595	C531	G465	A401	G272	C209	C143	G77	C16
G1041	A973	C912	U846	G785	A722	U659	U596	A532	A466	A402	G273	C210	A144	U78	G17
G1042	G974	U913	U847	C786	C723	C660	G597	G533	C467	U403	G274	C211	C145	U79	U18
C1043	A975	G914	C848	C787	U724	A661	U598	U534		A404	C275	G212	A146	A19	A19
			A849	A788	G725	G662	A599	G535	A470	U405	C276	A213	C147	C20	C20
			U850	A789	G726	G663	G600	G536	A471		U276	A213	U148	A21	A21
			C851	U790	A727	G664	C601	G537	A472	G408	G277	G214	U149	C22	C22
			U852	A791	G728	U665	A602	A538	G473		A278	G215	U150	G85	G23
			C853	A792	G729	A666	A603	G539	G474	G411	A279	A216	U151	U87	G24
			C854	A793	A730	U667		C540	C475	A412	U280	A217	A152	U25	U25
			G855	A794	C731	A668	U606	A541	G476	C413	C281	A218		G26	G26
			G856	C795	C732	G669	U607	C542	A477	C414	A282	A219		G27	G27
			G857	G796	G733	A670	A608	G543	A478	A415	G283	G220	U155	A91	A28
			C858		A734	C671	A609	U545	A479	U416	U284	A221	C157	U92	U29
			G859		A735	C672	C610	U546	A480	C417	G285	A222	U158	G93	G30
			U860	G799	G736	C673	C611	U547	A481	C418	U286	A223	G159	A94	C31
			A861	A800	C737	G674	G612	A547	A482	U419	G287	U224	A160	A95	C32
			G862	A802	G738	A675	A613	G548	A483	C420	U288	C225	A161	C96	C33
			C863	U803	A739	A676	A614	G549	C484	C421	G289	A226	U162	C97	
			C864	A804	C740	A677	U615	G550	C485	A422	U290	A227	U163	G98	
			C865	G805	U741	C678	A616	G551	C486	A423	G291	C228	C164	U99	
			A866	C806	A742	C679	G617		C487		A294	C229	A165	C97	C37
			C867	A743	A743	C680		U554	G488	G426		G230	U166	A100	A38
				U744	U744	G681	G620	G555	G489	U427	A294	A231	A167	A101	G39
			U870	G809	G745	U682	A621	A556	C490	A428	A299	G232	G168	U102	U40
			U871	U810	U746	G683	G622	C557	G491	A429	A300	A233	G169	A103	C41
			C872	U811	U747	U684	C623	U558	A492	A430	C301	U234	U170	A104	A42
			C873	U812	G748	A685	C624	G559	G493	U431	C302	U235	U171	C105	G43
				U813	A749	U686	G625	G560		A432	G303	C236	A172	C106	A44
				C815	A750	C687	A626		A497	C433	U304	C237	A173	G107	G45
			A877	C816	A751	U688	A627	A563		U434	C305	C238	U174	C109	G46
			A878	C817	A752	A689	G628	C564	G500	C435	U306	C239	G175	G110	C47
			G879	C818	A753	G690	G629	C565		C436	U307	C240	A176	G111	A49
				G818		C691	A630	U566	A502	U437	G308	A241	G177	A112	U50
			U884	A819	G756	C692	A631	U567	A503	G438	A309	G242	G178	U113	G51
			C885	A820	G757	A693	A632	U568	A504	A439	U310	G243	C179	U114	A52
				A821	C758	U694	A633	U569	A505	C440	A311	A244	G180	C115	A53
			U887	G759	G759	G695	C634	G370		A443	G312	G245	A181	C116	G54
			C888	G760	G760	U696	C635	U571	A507	A444	G313	G246	A182	G117	G55
			C889	A761	G761	G697	C636	U572	A508	C445	C314	G247	C183	A118	A56
			C890	U824	U762	A698	A637	U573	C509	G446	G315	G248	C184	A119	C57
			C891	A825	G763	A699	G638	A574	C510	G447	C316	G249		U120	G58
			G891	U826	G763	G700	U639	A575	U511	A447	G317	G250	G189	G121	U59
			U827	U827	A764	G701	C640	A576	U512	U448	G318	A251	A190	G60	
			U828	U765	C766	U702	U641	A577	A513	U449	C319	G252	A191	C61	C61
			A829	U766	U766	U702	U641	G578	A514	G450	G320	G253	C192	A126	U62
			G830	U767		U703	U642								

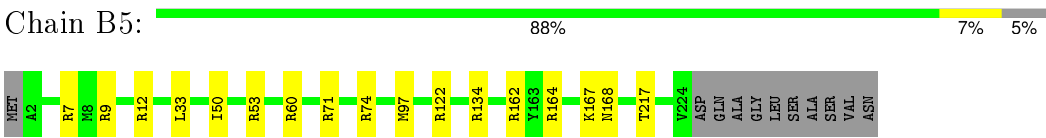
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C2036	C1974	U1911	U1781	G1650	U1589	U1460	U1589	G1334	U1274	G1211	G1150	A1090
A2037	G1975	G1912	U1782	G1651	A1590	C1461	U1397	G1335	A1275	G1212	A1151	G1091
G2038	U1976	C1913	A1783	G1652	A1591	C1462	C1398	G1336	A1276	A1213	C1152	C1092
U2039	A1977	G1914	A1784	G1653	A1592	C1463	C1399	G1337	A1277	A1214	C1153	G1093
G2040	A1978	C1915	A1785	G1654	A1593	G1464	U1400	G1338	G1278	G1215	G1154	U1094
U2041	A1979	U1916	A1786	A1655	U1594		G1401	G1339	G1279	G1216	A1155	A1095
A2042	U1980	U1917	A1787	C1656	A1595		U1402	U1340	G1280	U1217	A1156	A1096
C2043	A1981	A1913	C1788	A1657	C1536	A1470	A1403	G1341	G1281	G1218	G1157	U1097
C2044	U1982	A1914	A1789	C1658	A1596	G1471	A1404	G1342	U1282	U1219	C1158	A1098
C2045		G1920	A1790		A1597	C1472	U1405	G1343	G1283	G1220	U1159	G1099
G2046	C1985	G1921	A1791	U1662	U1598		U1406	U1344	A1284	C1221	G1160	G1100
C2047	C1986		G1792	G1663	C1600	G1475	G1407	C1345	A1285	U1222	C1161	U1101
	A1987	C1924	C1793	A1664	G1601	U1476	G1408	G1346	A1286	G1223	G1162	C1102
C2050		C1925	U1794	A1665	U1602	U1477	U1409	A1347	A1287		G1163	A1103
A2051	U1990	U1926	C1795		A1603	G1478		C1348	G1288		C1164	C1104
A2052	G1992	A1928	U1796	A1668	C1604	G1479	A1413	C1349	C1289		A1165	U1105
G2053	G1993	G1929	G1797	A1669	C1605		C1414	C1350	C1290	G1228	G1166	G1106
A2054	C1994	G1930	A1798	A1670	C1606		U1415	C1351	G1291	A1230	C1167	G1107
G2055	U1995	U1931	G1799	A1671	C1547		G1416	C1352	G1292	U1231	G1168	U1108
G2056	U1996	G1932	A1800	G1672	A1608		C1417	A1353	C1293	G1232	A1169	C1109
G2057	C1997	A1933	A1801	G1673	A1548		G1418	A1354	U1294	C1233	C1170	G1110
A2058	A1998	G1934	A1739	G1674	A1610		A1419	G1355	G1295	U1234	G1171	A1111
C2059	C1999	C1935	A1802	G1675	A1551		A1420	G1356	G1296	G1235	G1172	G1112
A2060	C2000	U1936	C1804	A1676	C1612		G1428	C1357	C1297	G1236	U1173	U1113
G2061	C2001	A1937	A1805	A1677	G1613		G1429	G1358	C1298	A1237	U1174	C1114
C2062	G2002	U1943	G1743	A1678	U1554		G1430	A1359	G1299	G1238	A1175	G1115
G2063	G2003	U1944	A1744	C1685	G1615		A1431	A1360	G1300	U1239	G1176	G1116
C2064	A2003	G1945	A1745	C1686	C1556		G1432	A1367	G1239	U1240	G1177	C1117
G2065	G2004	U1946	G1751	G1687	G1622		A1433	G1368	A1307	A1246	U1184	C1123
C2066	C2005	C1947	C1752	G1687	U1563		A1434	G1369	A1308	A1247	G1185	G1124
G2067	C2006	U1942	G1753	U1688	C1564		A1502	C1370	G1309	G1248	G1186	G1125
U2068	U2007	G1943	A1754	A1689	C1565		A1503	G1371			G1187	A1126
G2069	C2008	U1944	A1755	A1690	A1566		A1504	U1372	G1310	C1251	U1188	A1127
A2070	A2009	G1945	G1750	C1685	G1567		A1505	A1373	U1312	G1252	A1189	G1128
G2071	G2010	U1946	U1751	C1686	U1568		U1506	G1374	U1313	A1253	G1190	A1129
C2072	U2011	C1947	C1752	G1687	A1569		A1507	U1375	G1314	G1254	G1191	U1130
C2073	G2012	U1951	G1753	U1688	C1570		A1508	C1376	C1315	U1255	G1192	G1131
U2074	A2013	A1952	A1754	A1689	A1571		A1509	G1377	U1316	G1256	G1193	U1132
U2075	A2014	G1953	A1755	A1690	A1572		U1441	U1378	C1257	C1257	A1194	A1133
A2076	A2015	C1954	G1756	C1691	G1573		U1442	U1379	U1318	U1258	G1195	A1134
G2077	U2016	U1955	A1757	U1692	A1574		G1443	G1380	C1319	G1259	C1196	C1135
C2078	U2017	G1956	U1758	U1693	C1575		G1444	G1381	G1320	A1260	G1197	G1136
U2079	G2018	U1956	A1759	C1694	U1576		G1445	G1382	A1321	C1261	U1198	G1137
A2080	A2019	C1957	C1760	G1695	C1577		U1446	A1383	A1322	A1262	U1199	G1138
U2081	A2020	U1958	C1761		U1578		U1447	A1384	C1323	U1263	C1200	G1139
A2082	C2021	G1959	A1762	G1699	G1579		U1448	A1385	G1324	A1264	U1201	C1140
G2083	C2022	A1960	G1763	A1700	A1580		G1451	C1386	U1325	A1265	G1202	U1141
C2084	C2023	C1961	C1764	A1701	G1581		G1452	A1387	G1326	G1266	U1203	A1142
U2085	G2024	U1962	U1765		A1641		G1453	G1388	A1327	U1267	A1204	A1143
G2086	C2025	U1963	C1768	G1702	A1637		C1454		A1328	A1268	A1205	A1144
G2087	U2026	G1964		G1703	C1638		G1455		U1329	A1269	G1206	C1145
A2088	G2027	U1965	A1772	A1704	A1579		G1456		U1330	C1270	C1146	C1146
C2089	U2028	A1966	A1773	G1706	A1640		G1457					
A2090	G2029	C1967	C1774				G1458					
C2091	A2030	G1968	U1775	G1708	A1583		C1459					
U2092	A2031	A1969	G1776	G1709	U1584		G1460					
G2093	C2032	U1970	U1777	G1710	A1585		G1461					
A2094	A2033	U1971	U1778	A1711	A1586		U1457					



# 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	0.72	0/1736	1.05	12/2340 (0.5%)
10	AK	0.74	0/894	1.20	12/1207 (1.0%)
11	AL	0.76	0/969	1.32	18/1300 (1.4%)
12	AM	0.76	0/884	1.23	16/1181 (1.4%)
13	AN	0.79	0/817	1.32	12/1088 (1.1%)
14	AO	0.73	0/722	1.12	9/964 (0.9%)
15	AP	0.76	0/648	1.22	9/870 (1.0%)
16	AQ	0.71	0/658	1.14	6/883 (0.7%)
17	AR	0.81	0/463	1.28	6/623 (1.0%)
18	AS	0.78	0/653	1.29	8/879 (0.9%)
19	AT	0.71	0/672	1.08	6/890 (0.7%)
2	AC	0.72	0/1651	1.12	14/2225 (0.6%)
20	AU	0.83	0/431	1.48	10/572 (1.7%)
21	AA	1.52	2/36759 (0.0%)	2.21	1934/57346 (3.4%)
22	A1	1.53	0/1668	2.22	92/2595 (3.5%)
23	A2	1.51	0/343	2.43	24/531 (4.5%)
24	A3	1.53	0/1722	2.18	82/2685 (3.1%)
25	BC	0.75	0/2121	1.27	26/2852 (0.9%)
26	BD	0.68	0/1586	1.11	8/2134 (0.4%)
27	BE	0.68	0/1571	1.12	9/2113 (0.4%)
28	BF	0.76	0/1444	1.21	13/1937 (0.7%)
29	BG	0.69	0/1343	1.13	10/1816 (0.6%)
3	AD	0.77	0/1665	1.23	21/2227 (0.9%)
30	BH	0.67	0/1122	1.08	6/1515 (0.4%)
31	BI	0.66	0/1046	1.02	3/1410 (0.2%)
32	BJ	0.72	0/1152	1.19	11/1551 (0.7%)
33	BK	0.73	0/947	1.28	10/1268 (0.8%)
34	BL	0.74	0/1054	1.32	14/1403 (1.0%)
35	BM	0.75	0/1093	1.22	14/1460 (1.0%)
36	BN	0.77	0/973	1.31	14/1301 (1.1%)
37	BO	0.75	0/902	1.25	11/1209 (0.9%)
38	BP	0.73	0/929	1.20	10/1242 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.79	0/960	1.30	14/1278 (1.1%)
4	AE	0.70	0/1119	1.09	9/1506 (0.6%)
40	BR	0.72	0/829	1.19	7/1107 (0.6%)
41	BS	0.65	0/864	1.13	7/1156 (0.6%)
42	BT	0.68	0/744	1.21	5/994 (0.5%)
43	BU	0.70	0/787	1.14	6/1051 (0.6%)
44	BV	0.72	0/766	1.18	6/1025 (0.6%)
45	BW	0.75	0/604	1.27	5/799 (0.6%)
46	BX	0.76	0/635	1.32	10/848 (1.2%)
47	BY	0.67	0/510	1.24	6/677 (0.9%)
48	BZ	0.68	0/453	1.21	4/605 (0.7%)
49	B0	0.72	0/450	1.18	5/599 (0.8%)
5	AF	0.74	0/835	1.09	5/1128 (0.4%)
50	B1	0.72	0/417	1.04	2/556 (0.4%)
51	B2	0.80	0/380	1.47	10/498 (2.0%)
52	B3	0.71	0/513	1.20	5/676 (0.7%)
53	B4	0.70	0/303	1.17	2/397 (0.5%)
54	BA	1.40	0/69796	2.22	4069/108888 (3.7%)
55	BB	1.40	0/2800	2.18	144/4367 (3.3%)
56	B5	0.66	0/1673	1.12	11/2255 (0.5%)
6	AG	0.75	0/1188	1.21	17/1593 (1.1%)
7	AH	0.70	0/989	1.10	9/1326 (0.7%)
8	AI	0.81	0/1035	1.28	20/1377 (1.5%)
9	AJ	0.72	0/797	1.21	14/1079 (1.3%)
All	All	1.28	2/160085 (0.0%)	2.00	6842/239402 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	1
10	AK	0	1
14	AO	0	1
2	AC	0	1
21	AA	0	350
22	A1	0	16
23	A2	0	5
24	A3	0	17
26	BD	0	1
27	BE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	BO	0	1
5	AF	0	1
54	BA	0	705
55	BB	0	21
All	All	0	1122

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1382	C	C4-N4	-5.09	1.29	1.33
21	AA	476	U	C5'-C4'	5.08	1.57	1.51

The worst 5 of 6842 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1932	A	N1-C6-N6	-13.19	110.69	118.60
54	BA	371	A	N1-C6-N6	-12.55	111.07	118.60
21	AA	1239	A	N1-C6-N6	-12.45	111.13	118.60
54	BA	2432	A	N1-C6-N6	-12.35	111.19	118.60
54	BA	1635	A	N1-C6-N6	-12.24	111.26	118.60

There are no chirality outliers.

5 of 1122 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	20	ARG	Sidechain
2	AC	178	ARG	Sidechain
5	AF	4	TYR	Sidechain
10	AK	121	ARG	Peptide
14	AO	43	ALA	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AC	1625	0	1699	1	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	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	16520	1	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	2	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	1	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	1	0
43	BU	780	0	834	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	1	0
53	B4	302	0	343	0	0
54	BA	62317	0	31345	4	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99663	14	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 14 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BA:889:C:H1'	54:BA:890:C:C6	2.44	0.52
42:BT:19:LYS:HA	42:BT:23:ALA:HB3	1.92	0.52
21:AA:577:G:H1'	21:AA:816:A:C4	2.49	0.47
2:AC:149:LYS:HE3	2:AC:200:TRP:CZ3	2.50	0.46
54:BA:680:C:H2'	54:BA:681:G:C8	2.52	0.44

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%)	202 (93%)	16 (7%)	0	100	100
2	AC	205/208 (99%)	190 (93%)	13 (6%)	2 (1%)	19	65
3	AD	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	19	65
4	AE	150/152 (99%)	135 (90%)	10 (7%)	5 (3%)	5	40
5	AF	99/101 (98%)	87 (88%)	8 (8%)	4 (4%)	4	35
6	AG	150/152 (99%)	134 (89%)	14 (9%)	2 (1%)	15	60
7	AH	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AI	126/128 (98%)	119 (94%)	4 (3%)	3 (2%)	7	47
9	AJ	98/100 (98%)	93 (95%)	3 (3%)	2 (2%)	9	51
10	AK	116/118 (98%)	105 (90%)	8 (7%)	3 (3%)	7	45
11	AL	121/124 (98%)	106 (88%)	10 (8%)	5 (4%)	3	35
12	AM	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	4	38
13	AN	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	9	51
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	4	39
15	AP	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
16	AQ	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	7	46
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	11	53
18	AS	79/81 (98%)	69 (87%)	10 (13%)	0	100	100
19	AT	84/86 (98%)	72 (86%)	10 (12%)	2 (2%)	7	47
20	AU	51/53 (96%)	36 (71%)	11 (22%)	4 (8%)	1	20
25	BC	270/273 (99%)	244 (90%)	22 (8%)	4 (2%)	13	57
26	BD	207/209 (99%)	182 (88%)	19 (9%)	6 (3%)	6	43
27	BE	199/201 (99%)	185 (93%)	7 (4%)	7 (4%)	4	39
28	BF	176/179 (98%)	149 (85%)	16 (9%)	11 (6%)	2	25
29	BG	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	17	63
30	BH	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	26	71
31	BI	139/142 (98%)	125 (90%)	14 (10%)	0	100	100
32	BJ	140/142 (99%)	125 (89%)	10 (7%)	5 (4%)	4	38
33	BK	121/123 (98%)	106 (88%)	9 (7%)	6 (5%)	3	31
34	BL	141/144 (98%)	118 (84%)	15 (11%)	8 (6%)	2	28
35	BM	134/136 (98%)	128 (96%)	2 (2%)	4 (3%)	5	42
36	BN	119/121 (98%)	105 (88%)	13 (11%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	21	67
38	BP	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	4	38
39	BQ	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
40	BR	101/103 (98%)	88 (87%)	11 (11%)	2 (2%)	9	51
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	10	52
42	BT	92/94 (98%)	75 (82%)	13 (14%)	4 (4%)	3	34
43	BU	101/104 (97%)	85 (84%)	9 (9%)	7 (7%)	1	23
44	BV	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	17	63
45	BW	78/80 (98%)	60 (77%)	13 (17%)	5 (6%)	2	25
46	BX	75/79 (95%)	67 (89%)	7 (9%)	1 (1%)	15	60
47	BY	61/63 (97%)	53 (87%)	8 (13%)	0	100	100
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	29
49	B0	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	10	52
50	B1	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	4	35
51	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	3	33
52	B3	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	12	56
53	B4	36/38 (95%)	28 (78%)	7 (19%)	1 (3%)	6	44
56	B5	221/234 (94%)	205 (93%)	13 (6%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5257 (90%)	478 (8%)	141 (2%)	12	47

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	AG	5	VAL
11	AL	108	ASP
19	AT	9	ARG
26	BD	2	ILE
27	BE	69	ARG

### 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%)	176 (98%)	4 (2%)	60	83
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%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	84 (97%)	3 (3%)	44	75
6	AG	123/123 (100%)	120 (98%)	3 (2%)	57	82
7	AH	104/105 (99%)	101 (97%)	3 (3%)	50	78
8	AI	105/105 (100%)	103 (98%)	2 (2%)	65	86
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	86 (96%)	4 (4%)	35	69
11	AL	103/104 (99%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	68 (97%)	2 (3%)	50	78
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	207 (96%)	9 (4%)	36	70
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%)	147 (99%)	2 (1%)	76	89
29	BG	137/138 (99%)	135 (98%)	2 (2%)	72	88
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	84	93
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	54	80
33	BK	103/103 (100%)	100 (97%)	3 (3%)	50	78
34	BL	102/103 (99%)	99 (97%)	3 (3%)	50	78
35	BM	109/109 (100%)	107 (98%)	2 (2%)	66	87

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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%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	60	83
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	93 (100%)	0	100	100
42	BT	80/80 (100%)	78 (98%)	2 (2%)	55	81
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
45	BW	59/59 (100%)	57 (97%)	2 (3%)	44	75
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%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68	87
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	69	87

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

Mol	Chain	Res	Type
25	BC	173	LEU
27	BE	171	ASP
45	BW	49	ASN
25	BC	188	ARG
26	BD	16	THR

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

Mol	Chain	Res	Type
13	AN	62	ASN

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Mol	Chain	Res	Type
26	BD	134	HIS
34	BL	99	ASN
38	BP	55	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	240 (15%)	90 (5%)
22	A1	73/76 (96%)	9 (12%)	2 (2%)
23	A2	14/15 (93%)	7 (50%)	2 (14%)
24	A3	76/77 (98%)	9 (11%)	5 (6%)
54	BA	2902/2903 (99%)	458 (15%)	137 (4%)
55	BB	116/118 (98%)	12 (10%)	3 (2%)
All	All	4711/4722 (99%)	735 (15%)	239 (5%)

5 of 735 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	32	A
21	AA	39	G

5 of 239 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	322	A
54	BA	931	U
54	BA	2439	A
54	BA	428	A
54	BA	670	A

## 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	1.94	3 (20%)	18,37,40	3.08	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.85	0	15,36,39	1.58	1 (6%)
22	7MG	A1	46	22	20,26,27	2.21	3 (15%)	23,39,42	2.17	2 (8%)
22	5MU	A1	54	22	13,22,23	1.26	2 (15%)	16,32,35	4.43	2 (12%)
22	PSU	A1	55	22	15,21,22	1.07	1 (6%)	16,30,33	3.31	4 (25%)
22	4SU	A1	7	22	12,21,22	0.95	0	15,30,33	2.18	2 (13%)
24	H2U	A3	21	24	17,21,22	1.39	2 (11%)	23,30,33	1.46	4 (17%)
24	OMC	A3	33	24	15,22,23	1.09	0	20,31,34	0.89	0
24	5MU	A3	55	24	13,22,23	1.06	1 (7%)	16,32,35	4.69	2 (12%)
24	PSU	A3	56	24	15,21,22	1.15	1 (6%)	16,30,33	3.50	5 (31%)
24	4SU	A3	8	24	12,21,22	1.16	1 (8%)	15,30,33	2.23	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 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.24	1.33	1.45
22	A1	34	CM0	O5-C5	-5.97	1.25	1.37
24	A3	21	H2U	C4-N3	-3.70	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C2-N3	-3.18	1.32	1.38
22	A1	46	7MG	C8-N7	-2.72	1.31	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	55	5MU	C5-C4-N3	-12.71	114.68	125.35
22	A1	54	5MU	C5-C4-N3	-12.19	115.12	125.35
24	A3	8	4SU	C5-C4-N3	-7.82	115.27	123.56
22	A1	7	4SU	C5-C4-N3	-7.55	115.56	123.56
22	A1	46	7MG	C5-C6-N1	-6.68	113.44	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	0.55	0	5,7,9	1.37	2 (40%)
58	FME	BA	3001	57	8,9,10	0.78	0	5,9,11	1.33	1 (20%)

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	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	O-C-CA	-2.79	118.07	125.69
57	A1	101	VAL	O-C-CA	-2.17	119.76	125.69
57	A1	101	VAL	C-CA-N	2.05	114.48	109.95

There are no chirality outliers.

There are no torsion outliers.

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.