



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 11, 2019 – 08:46 AM EST

PDB ID : 4V6Y
EMDB ID: : EMD-1716
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in classic pre-translocation state (pre1a)
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/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

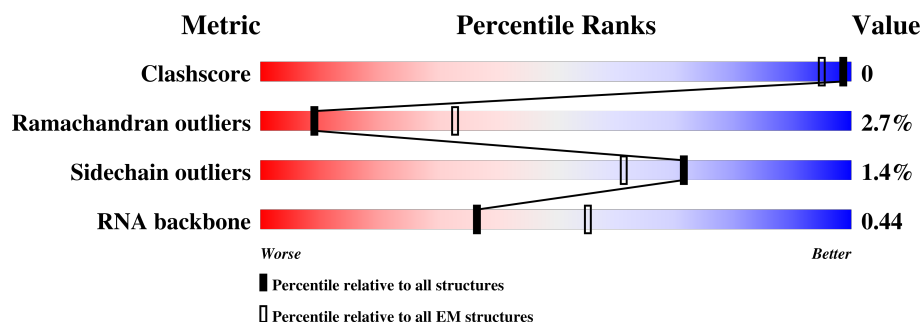
1 Overall quality at a glance

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.



















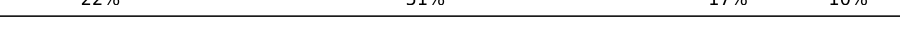





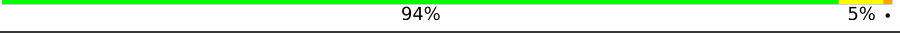
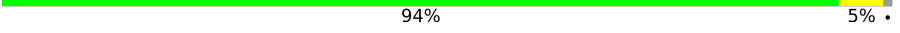

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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 ≥ 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	93% 7%
2	AC	208	92% 7%
3	AD	206	87% 12%
4	AE	152	89% 11% .
5	AF	101	87% 13%
6	AG	152	88% 13%
7	AH	130	91% 8% .
8	AI	128	81% 18% .











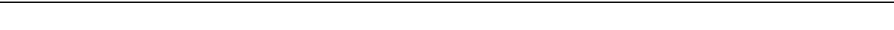

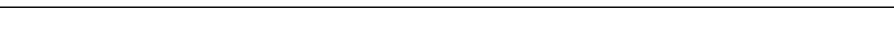
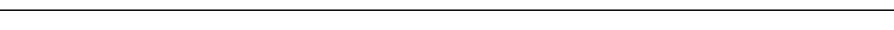
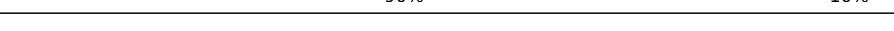








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Mol	Chain	Length	Quality of chain
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG	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	 85% 14% .
35	BM	136	 88% 12%
36	BN	121	 88% 12%
37	BO	117	 89% 10% .
38	BP	115	 83% 16% .
39	BQ	118	 84% 14% ..
40	BR	103	 89% 10% .
41	BS	110	 92% 8%
42	BT	94	 91% 7% .
43	BU	104	 90% 8% ..
44	BV	94	 95% 5%
45	BW	80	 88% 13%
46	BX	79	 84% 10% . .
47	BY	63	 90% 10%
48	BZ	59	 90% 7% ..
49	B0	57	 88% 11% .
50	B1	52	 88% 12%
51	B2	46	 76% 22% .
52	B3	65	 86% 12% .
53	B4	38	 89% 8% .
54	BA	2903	 16% 55% 24% .
55	BB	118	 15% 59% 19% 5% .
56	B5	234	 88% 6% . 5%

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 L35.

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 L36.

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 L2.

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 L3.

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 L4.

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 L5.

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 L6.

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 L9.

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 L11.

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 L13.

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 L14.

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 L15.

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 L16.

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 L17.

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 L18.

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 L19.

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 L20.

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 L21.

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 L22.

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 L23.

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 L24.

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 L25.

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 L27.

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 L28.

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 L29.

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 L30.

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 L32.

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 L33.

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 L34.

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		

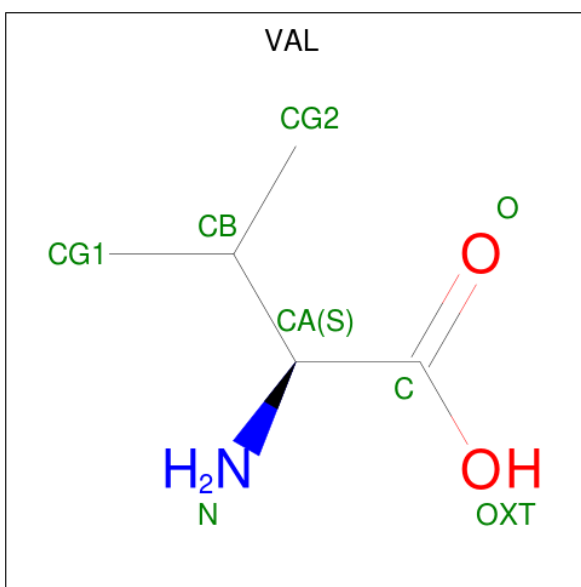
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

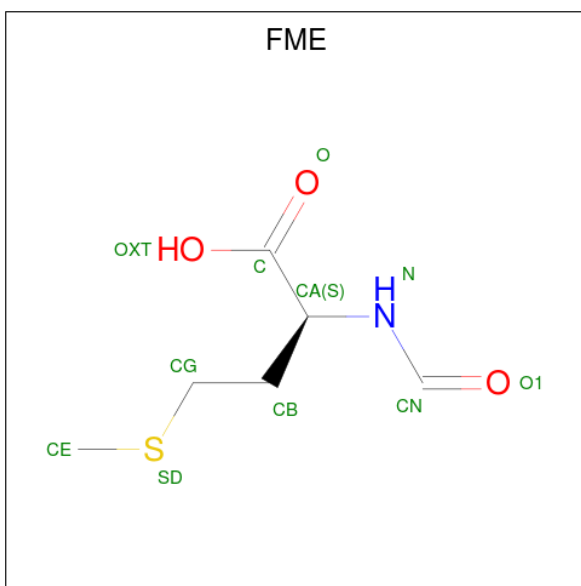
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



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: $\text{C}_6\text{H}_{11}\text{NO}_3\text{S}$).



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 the various outlier classes 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

Chain AB:  93% 7%



- Molecule 2: 30S ribosomal protein S3

Chain AC:  92% 7%



- Molecule 3: 30S ribosomal protein S4

Chain AD:  87% 12%



- Molecule 4: 30S ribosomal protein S5

Chain AE:  89% 11%




- Molecule 5: 30S ribosomal protein S6

Chain AF:  87% 13%



- Molecule 6: 30S ribosomal protein S7

Chain AG:  88% 13%



- Molecule 7: 30S ribosomal protein S8

Chain AH: 91% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 81% 18%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 84% 16%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 89% 11%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 85% 15%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%



- Molecule 13: 30S ribosomal protein S14

Chain AN: 86% 12%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  87% 12%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  84% 16%



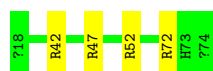
- Molecule 16: 30S ribosomal protein S17

Chain AQ:  90% 9%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  93% 7%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  89% 11%



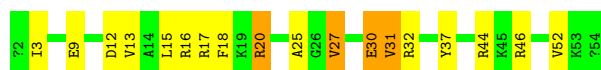
- Molecule 19: 30S ribosomal protein S20

Chain AT:  90% 10%




- Molecule 20: 30S ribosomal protein S21

Chain AU:  66% 26% 8%

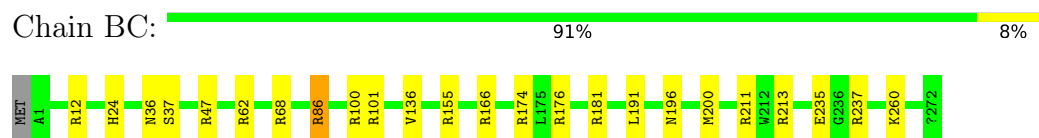


- Molecule 21: 16S ribosomal RNA

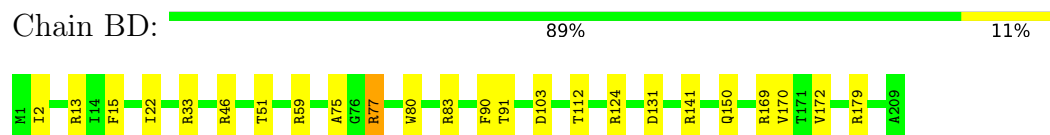
Chain AA:  15% 56% 24% 5%

A	C63	G126	G187	U249	C311	C372	A432	A493	C556	G616	C680	U740	A865	G926	U992
U	A64	G127	C188	A250	C312	A373	G433	C494	C557	G617	A681	G741	A802	G927	G993
U5	A65	A129	A189	G251	A313	A374	U434	C495	G558	C618	G682	G742	A803	G928	A994
G6	A66	A130	A190	U252	C314	U375	A435	A496	A559	U619	G683	A743	U804	G929	C995
A7	C67	A131	G191	C254	A315	G376	C436	C497	A560	G620	U684	G744	C805	C930	A996
A8	G68	A131	A192	G254	C316	G377	U437	A498	U561	A621	G685	G745	C806	C931	U997
G9	U70	C132	C193	G255	U317	G378	U438	A499	U562	A622	U686	A746	A807	G932	C998
A10	A71	C135	A195	U256	G319	G380	C440	C501	C564	G623	G687	A747	C808	G933	C999
G11	A72	C136	A196	G257	A320	C381	A441	A502	C565	G624	G688	A748	A809	G934	A1000
U12	C73	U137	A197	G260	A321	A382	G442	C503	G566	G625	G689	C750	C810	A935	C1001
U13	A74	G138	G198	U261	C322	A383	C443	C504	G567	G626	G690	U751	G812	G936	G1002
G15	G75	A139	A199	A262	U323	G384	G444	G505	G568	A629	U691	G752	U813	A937	G1003
A16	A77	G141	G200	A263	G324	C385	G445	C506	C569	G630	G693	A753	A814	G938	A1004
U17	A78	G142	G201	C264	G325	C386	G446	C507	G570	A631	U694	G754	A815	G939	G1005
C18	G79	C143	G202	G265	G326	U387	G447	U508	U571	U632	G695	G755	A816	C940	G1006
A19	A80	C143	G203	G266	A327	G388	A448	C508	A572	G633	A696	C756	C817	G941	C1011
U20	A81	G144	G204	C267	C328	A389	G449	A510	A573	C634	U697	U757	C818	U943	A1012
G21	G82	G145	A205	U268	C329	C390	A450	C511	A574	A635	G698	G758	A819	G944	G1013
G22	C83	G147	C206	C269	C330	C391	A451	U512	G575	U636	G699	A759	U820	A1014	A1014
C23	U84	C148	G207	A270	G331	C392	A452	C513	C576	C637	G700	G760	A815	A946	G1015
U24	U85	A149	U208	C271		A393	G453	C514	G577	U638	U701	G761	U822	G947	A1016
C25	G86	U150	U209	C272	C334	G384	G454	G515	C578	G639	A702	U762	C823	C948	U1017
A26	C87	U151	C210	U273	C335	C395	G455	U516	A579	A640	G703	G763	G824	A949	G1018
G27		A151	G211	A274	C336	C396	A456	U517	C580	U641	A704	G764	A825	G890	A1019
C90	C90	C153	G212	G275	A337	U398	U458	C518	G581	A642	G705	G765	C826	U891	G953
U91	U91	U154	G213	G276	A338	U398	A458	C519	C582	C643	A706	G766	U827	G954	A1021
			C214	C277	C339	C399	A459	A520	A583		U707	A767	U828	C893	A1022
		A155	C215	G278	U340	C400	A460	G521	G584	G646	G708	A768	G829	G894	U1023
G31	G34	C156	U216	A279	C341	C401	A461	C522	G585	C647	U709	G769	C830	G895	G1024
A32	C95	U157	C217	C280	C342	G402	G462	A523	C586	U648	G710	G770	A831	C896	A959
		G158	G220	G281	U343	C403	U463	C524	G587	A649	G711	G771	G832	G897	U960
U96	G97	C159	G221	A282	A344	G404	U464	C525	G588	C650	G712	G772	U833	G898	G1028
G34	A98	C160	C221	U283	C345	U405	A465	C526	U589	G651	G713	G773	G833	C899	U1029
C36	C99	A161	C222	C284	G346	G406	A466	G527	U590	U652	G714	G774	G838	A900	G963
U37	G100	A162	A223	C285	G347	U407	U467	C528	U591	U653	A715	G775	C839	A801	U1030
	A101	C163	G223	C286	G348	A408	A468	C529	G592	G654	A716	G776	C840	G902	G1031
G39	G102	G164	G226	U287	A349	U409	C469	C530	U593	A655	U717	G777	C841	G903	G1032
C40		G165	G227	A288	G350	G410	C470	U531	U594	G656	A718	G778	U842	U904	G1033
G41	G105	U166	U229	C289	G351	A411	U473	A532	A596	U657	C719	G779	U843	G905	A1035
C42	C42	C106	U229	G290	C352	A412	G474	A533	A597	C658	U720	A780	G844	A906	A1036
G43	G107	G168	G230	C291	A353	G413	C474	U534	G597	U659	G721	A781	A845	A907	C1037
	G108	C169	G231	G292	G354	A414	C475	A535	U598	C660	G722	A782	G846	C907	G1038
A44	A109	U170	G232	C293	C355	A415	U476	C536	C599		U723	G783	G847	A908	
G47	C110	C171	G233	U294	A356	G416	C477	C537	G600	A663	G724	A784	C848	G909	A1042
C48	G111	A172	C234	C295	G357	G417	A478	G538	G601	G664	G725	A785	C849	C910	G1043
U49	G112	U173	C235	U296	U358	C418	U479	A539	A602	A665	G726	G786	U850	C912	A1044
A50	G113	A174	A236	C297	G359	C419	U480	C540	U603	G666	G727	G787	U851	A913	C1045
A51	U114	C175	G237	A298	G360	U420	G481		G604		U728	U788	C852	A914	A1046
C52	G115	C176	A238	G299	G361	C421	C482	G544	U605	G669	A729	A789	C853	U916	G1047
A53	A116	G177	U239	A300	C362	U422	C483	C545	G606	G670	G730	U790	G854	C980	A1048
G54	G117	A179	G240		A363	G423	G484	A546	A607	G671	C731	A791	C855	U917	U1049
C55	U118	C178	G241		A364	G424	U485	A547	A608	U672	G732	A792	C856	A918	G1050
A56	A119	U180	G242	A303	U365	G425	U486	G548	A609	A673	G733	U793	G858	A919	C1051
U56	G120	U180	G242	U304	A366	G426	U487	G549	A610	G674	G734	A794	C859	A920	G983
G57	A121	A181	A243	G305	A367	U427	C488	G550	C611	A675	G735	A795	A860	U921	C984
C58	U121	C182	U244	A306	U367	U428	C489	G551	G612	A676	G736	C796	C861	G985	A1052
A59	G122	C183	G245	C307	U368	G428	C490	A553	C613	A677	G737	C797	C862	U989	G988
G60	U123	A184	A246	C308	G369	U429	C491	A554	C614	U678	G738	U798	U863	A922	A1053
C61	C124	U185	G247	A309	C370	A430	G491	A555	C615	U679	C739	C799	U864	C924	A1054
U62	U125	C186	C248	C310	A371	A431	C492	U556	C616	C680	C740		C865	C925	U1056

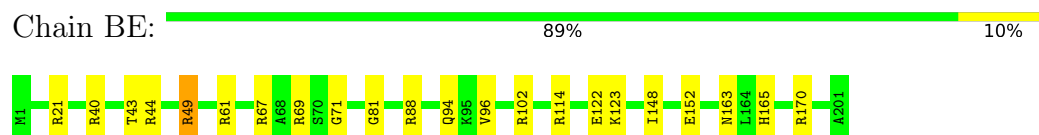
- Molecule 25: 50S ribosomal protein L35



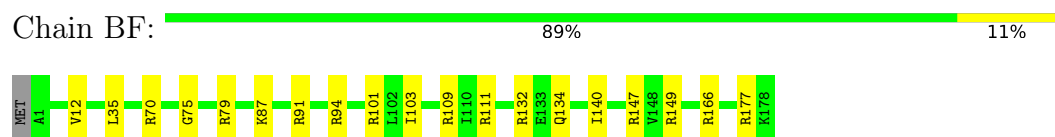
- Molecule 26: 50S ribosomal protein L36



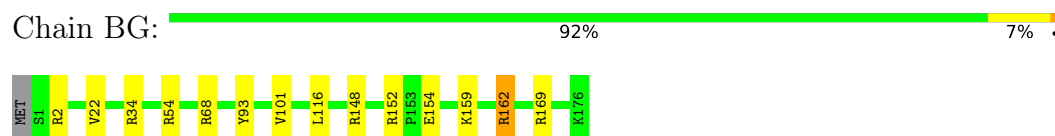
- Molecule 27: 50S ribosomal protein L2



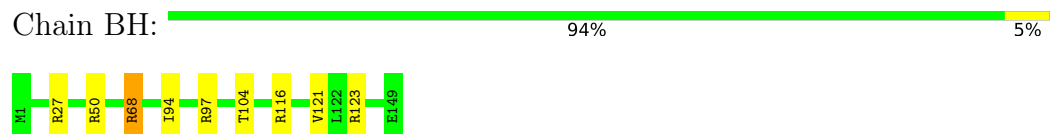
- Molecule 28: 50S ribosomal protein L3



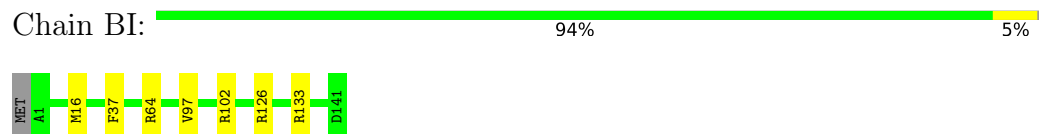
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9

Chain BJ:  91% 8%




- Molecule 33: 50S ribosomal protein L11

Chain BK:  90% 10%



- Molecule 34: 50S ribosomal protein L13

Chain BL:  85% 14%




- Molecule 35: 50S ribosomal protein L14

Chain BM:  88% 12%



- Molecule 36: 50S ribosomal protein L15

Chain BN:  88% 12%




- Molecule 37: 50S ribosomal protein L16

Chain BO:  89% 10%




- Molecule 38: 50S ribosomal protein L17

Chain BP:  83% 16%



- Molecule 39: 50S ribosomal protein L18

Chain BQ:  84% 14%



- Molecule 40: 50S ribosomal protein L19

Chain BR: 89% 10% .



- Molecule 41: 50S ribosomal protein L20

Chain BS: 92% 8%



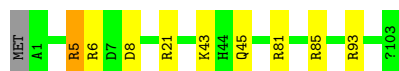
- Molecule 42: 50S ribosomal protein L21

Chain BT: 91% 7% .



- Molecule 43: 50S ribosomal protein L22

Chain BU: 90% 8% ..



- Molecule 44: 50S ribosomal protein L23

Chain BV: 95% 5%



- Molecule 45: 50S ribosomal protein L24

Chain BW: 88% 13%

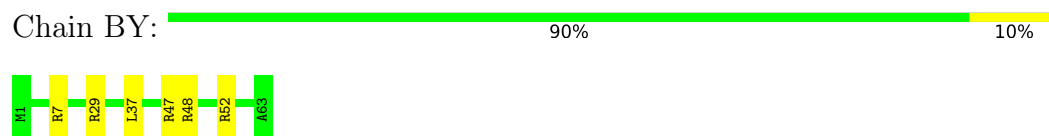


- Molecule 46: 50S ribosomal protein L25

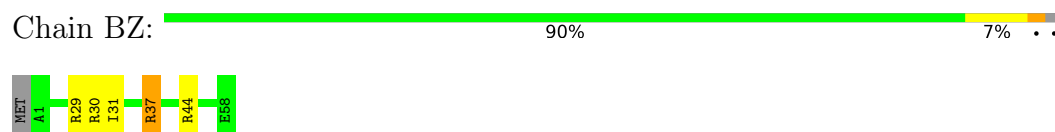
Chain BX: 84% 10% . .



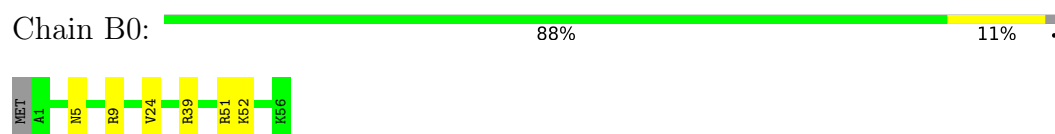
- Molecule 47: 50S ribosomal protein L27



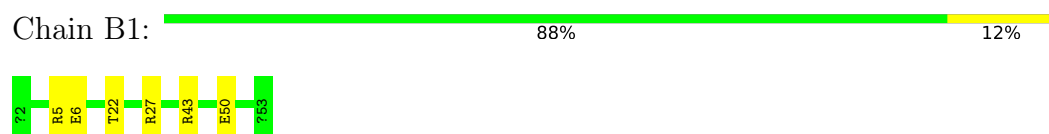
- Molecule 48: 50S ribosomal protein L28



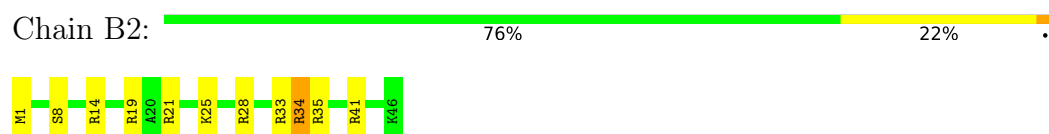
- Molecule 49: 50S ribosomal protein L29



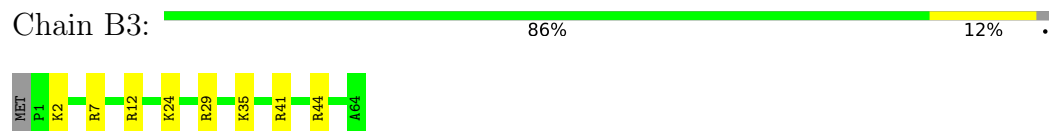
- Molecule 50: 50S ribosomal protein L30



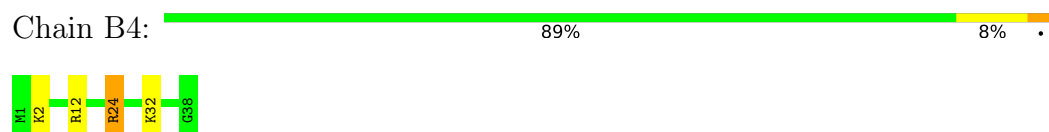
- Molecule 51: 50S ribosomal protein L32



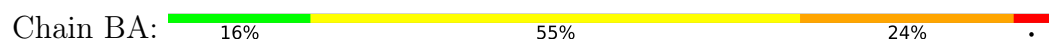
- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

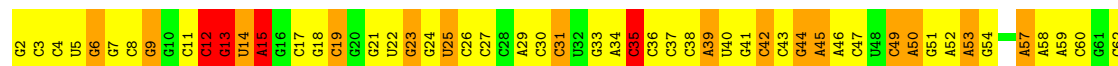


- Molecule 54: 23S ribosomal RNA



A1001	G938	G874	G809	U744	C680	G820	U558	G496	C436	G372	G312	G248	G188	A125	A63	G1
C1005	G939	G875	U810	G745	G681	A621	G559	A497	U437	U373	G313	C249	G189	A126	A64	G2
C1006	G940	A876	U811	U746	G684	G823	G560	G498	A438	A374	G314	G250	G190	A127	U66	U4
C1007	A941	A877	C812	U747	G684	G823	G561	G499	A439	A374	G315	A251	A191	C128	G66	U3
A1008	G942	A878	U813	G748	G685	C824	U562	A501	U440	G377	G316	G252	C192	C129	U67	A5
A1009	G943	A879	C814	A749	U686	G825	A563	A502	U441	G378	G317	G253	U193	C130	G68	A6
A1010	G944	G880	C815	A750	C687	G826	C564	A503	A442	G379	G318	G254	G194	A131	G69	G7
A1011	A945	A751	C816	A752	U686	A827	C565	A504	A443	G381	G319	A255	A195	G134	G70	C8
G1011	C946	A752	G817	A753	A689	G828	U566	A505	C444	G382	A320	A256	A196	A10	A71	C9
U1012	A947	U753	G818	U754	G690	G829	U567	A506	C445	A383	A321	C257	A197	U72	U72	A10
C1013	C948	A754	A819	U755	C691	G830	U568	G506	C446	A384	A322	G257	C198	G136	A73	C11
A1014	G949	U756	A820	U756	C692	A831	U569	A507	C447	A385	C323	A262	A199	G137	A74	U12
U1015	G950	A756	A821	U756	A693	A832	G570	A508	U448	G386	A324	G263	G200	C140	G75	A13
G1016	C951	G757	G822	G757	U694	A833	U571	C509	A449	U387	G325	A264	C201	G141	G77	A14
	G952		G695		G695	C834	A572	C510	A450	G388	G326	A265	U202	G142	G78	G15
						C835	U573		U451	G389	G327	A266	A203	A143	G79	G16
U1019						A836	A574	A513	A452	U390	U328	C268	G205	C144	U82	U18
A1020	G956	G760	A825	A761	A699	A837	A575	A514	A453	A391	G329	C269	G206	C145	A83	A19
A1021	C957	U762	U826	A761	G700	G838	U576	A515	A454	U392	A330	A270	A207	C146	A21	C20
G1022	U958	U762	U827	U762	G701	U839	G577	C516	C455	C393	C331	A271	C208	C147	A84	G21
U1023	U885	G763	U828	G763	G702	U840	G578	G517	C456	C394	A332	G272	C209	A148	G85	G22
G1024	A896	A764	A829	A764	U703	U841	G579	U518	A457	U395	G333	A273	C210	A149	G86	G23
G1025	C897	G765	G830	G765	G704	U842	U580	U519	C458	U396	G334	G274	C211	U150	U87	G24
U1026	C898		G831		G704	U843	U581	G520	A459	U397	G335	C275	G212	C151	G88	
A1027	C899		A832		A705	A643	C581	U521	U460	C398	C336	C276	A213	A152	A89	
A1028	A900	G770	A833	G770	A706	A644	A582	G522	C461	U399	C337	U276	G214	U153	U90	G27
A1029	C901	C772	G834	C772	G707	C845	G583	A523	C462	G400	G338	G277	G215	U154	A91	A28
G1030	C902	U773	C835	U773	U710	U646	C584	G524	C463	A401	U339	A278	G216	U155	A92	C31
U1031	G903	G774		G774	U710	G647	G585	G530	A469	G402	A340	A279	A216	A156	U92	
A1032	G904	G775	C838	G775	G711	G648	A586	A532	U470	A410	A346	A280	A222	A161	G97	
U1033	A905	G776	U839	G776	G712	U649	C587	U526	U465	A403	A341	G281	A217	A157	G93	C32
G1034		G777	C840	G777	G712	C850	U588	A527	A466	A404	A342	C282	A218	C157	A94	C33
U1035					A715	G851	U589	A528	C467	U405	A343	A283	A219	U158	A95	U34
A972	A973				A716	U852	A590	A529	C468	G406	A344	G284	G220	G159	G96	
A973	A974	G780	A844	G780	C717	U853	U591	G530	A470	G410	A345	U284	A221	A160	C97	G35
A974	A975	A781	A845	A781	C717	A854	A592	A531	U471	A411	A347	U285	A222	A161	G98	G36
A1040	G976	A782	U846	A782	C719	A855	U593	A532	A471	A412	A348	U286	A223	U162	U99	A38
G1041	G977	G783	C848	G783	U720	G856	U594	G533	A472	C413	U349	G287	U224	C163	U100	G39
G1042	G978	G785	A849	G785	A721	U857	C595		G473	C414	G350		G225	C164	U101	U40
C1043	A979	C786	U850	C786	A722	U858	U596	G536	C474	C415	G351	U290	A226	A165	U102	C41
A980	A980	C787	C851	C787	C723	G859	G597	G537	C475	A415	A352	G291	A227	U166	A103	A42
A981	C981	A788		A788	U724	C660	U598	A538	C476	A416	A353	U292	C228	U167	A104	A43
C982	A982	A789	C854	A789	G725	A661	A599	G539	A477	C417	C353	U293	C229	G168	C105	A44
A1046	A983	U790	G855	U790	G726	G662	G600	C540	A478	C418	A354	A294	G230	G169	C106	A44
G1047	A984	C791	C856	C791	A727	G663	C601	A541	A479	U419	U355	G295	A231	U170	G107	G46
A1048	A984	U792	G857	U792	G726	G664	A602	C542	A480	C420	G356	U296	G232	U171	G108	C47
C1049	C985	A792		A792	G726	U665	A603	G543	C481	C421	C357	G297	A233	A172	C109	C48
A1050	C986	A793	G858	A793	G729	U666	G604	C544	A482	A422	U358	G298	U234	A173	G110	A49
G1051	C987	A794	C859	A794	A730	A666	G605	U545	A483	G423	G359	A299	U235	U174	A11	G50
C1052	A988	C795	U860	C795	C731	U667	G606	U546	C484	A424	U360	A300	G236	G175	U51	U51
C1053	G989	G796	A861	G796	C732	A668	U606	A547	C485	G425	G361	G301	C237	A176	A52	
A1054	A990	G797	C862	G797	G733	G669	U607	A547	C486	C426	A362	C302	C238	G177	A53	
G1055	C991	A928	A863	A928	A734	A870	A608	G548	C487	U427	G363	G303	C239	G178	A54	
U1056	C992	U929	G864	C992	C671	C871	A609	G549	C488	A428	C364	G304	C240	C179	G55	
G993	A993	G801	C865	A993	C672	C872	C610	C550	U489	A429	C365	U304	A241	G180	A56	
U1058	C994	A802	A866	A802	C737	C873	C611	G551	C489	A430	C366	U306	G242	A181	C57	
G1059	C995	U803	C867	U803	G738	G874	G612	U552	C490	U431	C367	G307	U243	A182	G58	
U1060	A996	A804	U868	A804	G739	A875	A613	G553	C491	U432	A368	G308	A244	C183	U59	
	C997	G805	G869	G805	C740	A876	A614	U554	A492	A432	A369	G309	A245	C184	G60	
C1064	C998	C806	U870	C806	U741	A877	U615	G555	C493	C433	U369	A309	G246	G185	C61	
U1065	U999	U807	A742	U807	A742	C878	A616	A556	C494	U434	G370	A310	C246	G185	G123	
U1066	A1000	G808	A743	G808	A743	C879		C557	C495	C435	A371	A311	G247		U62	

C1996	G1935	C1874	G1811	C1686	C1625	U1563	A1503	U1440	C1376	U1316	G1256	G1193	A1129	A1067
G1997	A1936	G1875	U1812	C1686	A1626	C1564	A1504	G1441	G1377	G1317	C1257	A1194	U1130	G1068
A1998	A1937	A1876	G1813	A1689	G1627	C1565	A1505	U1442	U1378	U1318	U1258	G1195	G1131	A1069
C1999	A1938	A1877	G1814	A1690	G1628	A1566	A1506	U1443	U1379	C1319	G1259	C1196	U1132	A1070
C2001	U1939	C1878	A1815	C1691	U1629	G1567	C1507	G1444	G1390	G1320	C1260	A1133	A1133	G1071
G2002	U1940	C1879	A1816	U1692	A1630	G1568	A1508	G1445	G1381	A1321	C1261	U1198	A1134	C1072
A2003	C1941	U1880	G1817	C1697	G1631	A1569	A1509	C1446	G1382	A1322	A1262	U1199	C1135	A1073
G2004	C1942	C1881	U1818	C1697	A1632	A1570	G1510	C1447	A1383	C1323	U1263	C1200	C1140	C1076
A2005	U1943	A1819	U1819	A1698	G1633	A1571	G1511	G1448	A1384	G1324	A1264	U1201	U1141	U1077
C2006	U1944	A1882	A1820	G1699	A1634	A1572	C1512	G1449	A1385	U1325	A1265	G1202	U1142	U1078
U2007	G1945	C1883	G1821	A1700	A1635	G1573	G1513	G1450	C1386	U1326	C1266	U1203	A1143	C1079
C2008	U1946	A1885	C1822	A1701	U1636	C1574	G1514	G1451	A1387	A1327	U1267	A1204	A1144	A1080
A2009	C1947	U1886	G1823	G1702	A1637	C1575	A1515	G1452	G1388	A1328	A1268	A1205	C1145	U1081
G2010	C1947	C1887	C1823	G1703	C1638	U1576	G1516	A1453	G1389	U1329	A1269	G1206	C1146	U1082
U2011	G1950	G1888	G1826	C1764	A1639	C1577	G1517	C1454	U1390	C1330	C1270	C1207	A1147	U1083
U2012	U1951	A1889	U1827	A1705	A1640	U1578	C1518	G1455	U1391	G1331	G1271	C1208	C1147	A1084
G2013	A1952	C1890	G1828	C1706	A1641	A1579	G1519	G1456	A1392	U1332	A1272	U1209	U1148	A1085
A2014	G1953	G1891	A1829	G1707	G1642	A1580	U1520	U1457	A1393	G1333	U1273	G1210	G1149	A1086
U2015	U1954	C1892	C1830	C1708	G1643	G1581	G1521	U1458	U1394	G1334	A1274	C1211	C1150	A1087
U2016	U1955	C1893	G1831	U1709	C1644	C1582	A1522	G1459	A1395	C1335	A1275	G1212	A1151	A1088
U2017	U1956	C1894	G1832	G1710	G1645	A1583	G1523	U1460	U1396	A1336	A1276	C1152	C1152	G1089
G2018	C1957	A1895	C1833	A1711	C1646	U1584	G1524	C1461	U1397	G1337	G1277	A1214	C1153	A1090
A2019	U1958	G1896	U1834	U1712	A1647	C1585	A1525	C1462	C1398	G1338	C1278	G1215	G1154	A1091
U2020	G1959	A1773	G1835	A1713	U1648	A1586	C1526	G1463	C1399	G1339	C1279	G1216	A1155	G1091
A2021	A1960	U1898	C1836	U1714	G1649	G1587	G1527	G1464	U1400	U1340	G1280	U1217	A1156	C1092
C2021	C1961	A1899	C1837	G1715	A1650	G1588	A1528	G1465	G1401	G1341	G1281	G1218	G1157	G1093
U2022	U1962	A1900	G1840	U1716	G1651	U1589	G1529	U1466	U1402	A1342	U1282	U1219	C1158	U1094
C2023	C1963	U1889	U1841	A1717	A1652	A1590	C1530	U1467	A1403	G1343	G1283	G1220	A1159	U1101
G2024	G1964	A1902	G1842	G1718	G1653	A1591	C1531	U1468	U1404	U1344	C1284	C1221	G1160	A1096
C2025	C1965	G1903	C1843	G1719	C1654	C1592	A1532	A1469	U1405	C1345	A1285	U1222	C1161	U1097
U2026	A1966	G1904	C1843	U1720	A1655	A1593	C1533	A1470	U1406	G1346	U1286	G1223	G1163	A1098
G2027	C1967	C1905	C1844	G1721	C1656	U1594	U1534	G1471	G1407	A1347	A1287	U1224	G1163	G1099
C2029	U1968	G1906	A1847	A1722	U1657	C1595	A1535	G1472	G1408	G1346	G1288	G1225	C1164	C1100
A2030	A1969	U1907	A1848	G1723	C1658	A1596	C1536	U1473	U1409	C1349	G1289	A1226	A1165	U1101
C2031	C1970	A1784	C1849	G1724	G1661	A1597	G1537	U1474	A1413	C1350	C1290	G1227	G1166	C1102
G2032	U1971	A1786	G1850	U1725	G1662	A1598	C1538	G1475	U1419	C1351	G1228	C1229	C1167	A1103
A2033	G1972	A1787	G1851	G1726	U1662	U1599	U1539	U1476	C1414	U1352	G1292	G1229	G1168	C1104
U2034	G1973	C1788	U1851	C1727	G1663	C1600	G1540	A1477	U1415	A1353	C1293	A1230	A1169	U1105
G2035	C1974	U1812	U1852	C1728	A1664	G1601	C1541	C1477	U1416	A1354	U1294	C1233	C1170	C1108
C2036	G1975	A1853	A1853	U1729	A1665	U1602	U1542	U1487	C1417	G1355	C1295	G1171	G1172	C1109
A2037	U1976	A1854	C1854	G1730	G1666	A1603	G1543	U1481	G1418	G1356	G1296	G1236	U1173	G1110
G2038	C1977	U1855	U1855	G1731	A1667	C1604	A1544	G1482	A1419	C1357	C1297	A1237	U1174	A1111
U2039	A1978	U1856	G1857	C1732	A1668	C1605	A1545	C1485	A1420	G1358	G1298	G1238	A1175	G1112
C2042	U1979	U1917	C1857	G1733	A1669	C1606	G1546	U1486	G1421	A1359	G1299	G1238	U1176	U1113
G2043	A1980	C1918	A1858	G1734	C1670	C1607	C1547	U1486	G1422	G1360	G1300	C1233	U1177	C1114
C2044	A1981	U1919	U1859	A1735	A1671	A1608	A1548	U1487	A1301	G1361	A1301	A1241	G1177	G1115
G2045	U1982	C1920	G1860	U1736	U1672	A1609	A1549	C1488	A1302	C1362	A1302	U1242	C1178	G1116
U2046	G1983	G1921	G1861	G1737	G1673	A1610	C1550	C1489	A1427	C1363	G1303	G1179	G1179	C1117
C2047	G1984	G1799	G1862	G1738	G1674	C1611	A1551	A1490	C1428	G1364	A1304	A1244	U1180	C1118
G2048	C1985	C1800	G1863	A1739	C1675	C1612	A1552	G1491	G1429	A1365	C1305	G1245	U1181	U1119
U2049	U1986	A1801	U1864	G1740	A1676	G1613	A1553	G1492	G1430	A1366	C1306	A1246	U1182	G1120
C2050	A1987	U1926	U1865	C1741	A1677	A1614	C1493	C1493	A1431	A1367	A1307	A1247	U1183	C1121
G2051	G1988	A1803	A1866	U1742	A1678	C1615	G1555	A1494	A1432	G1368	G1308	G1248	G1186	G1122
A2052	C1989	C1804	G1867	G1743	A1679	A1616	C1556	A1495	A1433	G1369	A1309	U1249	G1187	C1123
U2053	G1990	A1805	C1868	A1745	U1680	C1617	C1557	A1496	A1434	C1370	G1310	G1250	G1187	G1124
G2054	U1991	C1806	G1869	A1746	G1681	A1618	U1497	U1497	G1435	G1371	G1311	G1251	U1188	G1125
A2055	G1992	G1807	C1870	A1746	G1682	G1619	C1559	C1498	G1436	U1372	U1312	G1252	A1189	G1126
C2056	U1993	A1808	A1871	U1747	U1683	G1620	G1560	C1499	C1437	A1373	U1313	A1253	G1190	A1127
G2057	C1994	C1748	A1872	C1748	G1684	C1561	U1561	C1499	U1438	G1374	U1314	U1254	G1191	G1128
	U1995	C1934	G1873	A1749	C1685	U1624	U1562	A1502	A1439	U1375	C1315	G1192	G1192	





● Molecule 56: 50S ribosomal protein L1

Chain B5: 88% 6% • 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14235	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor

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	1.11	13/2340 (0.6%)
10	AK	0.80	0/894	1.27	12/1207 (1.0%)
11	AL	0.80	0/969	1.25	13/1300 (1.0%)
12	AM	0.82	0/884	1.29	13/1181 (1.1%)
13	AN	0.82	0/817	1.25	9/1088 (0.8%)
14	AO	0.77	0/722	1.18	6/964 (0.6%)
15	AP	0.82	0/648	1.42	14/870 (1.6%)
16	AQ	0.71	0/658	1.18	8/883 (0.9%)
17	AR	0.77	0/463	1.19	5/623 (0.8%)
18	AS	0.80	0/653	1.23	7/879 (0.8%)
19	AT	0.75	0/672	1.18	7/890 (0.8%)
2	AC	0.76	0/1651	1.17	14/2225 (0.6%)
20	AU	0.87	0/431	1.59	8/572 (1.4%)
21	AA	1.88	441/36759 (1.2%)	2.29	2411/57346 (4.2%)
22	A1	1.89	18/1668 (1.1%)	2.23	102/2595 (3.9%)
23	A2	1.67	1/343 (0.3%)	2.18	19/531 (3.6%)
24	A3	1.93	26/1722 (1.5%)	2.27	102/2685 (3.8%)
25	BC	0.79	0/2121	1.28	19/2852 (0.7%)
26	BD	0.72	0/1586	1.23	12/2134 (0.6%)
27	BE	0.71	0/1571	1.17	11/2113 (0.5%)
28	BF	0.77	0/1444	1.18	13/1937 (0.7%)
29	BG	0.72	0/1343	1.16	7/1816 (0.4%)
3	AD	0.76	0/1665	1.23	21/2227 (0.9%)
30	BH	0.67	0/1122	1.14	6/1515 (0.4%)
31	BI	0.69	0/1046	1.11	7/1410 (0.5%)
32	BJ	0.74	0/1152	1.23	9/1551 (0.6%)
33	BK	0.76	0/947	1.23	11/1268 (0.9%)
34	BL	0.76	0/1054	1.28	14/1403 (1.0%)
35	BM	0.79	0/1093	1.27	11/1460 (0.8%)
36	BN	0.80	0/973	1.26	12/1301 (0.9%)
37	BO	0.80	0/902	1.28	10/1209 (0.8%)
38	BP	0.77	0/929	1.26	9/1242 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.80	0/960	1.37	17/1278 (1.3%)
4	AE	0.70	0/1119	1.12	11/1506 (0.7%)
40	BR	0.73	0/829	1.22	9/1107 (0.8%)
41	BS	0.71	0/864	1.18	7/1156 (0.6%)
42	BT	0.73	0/744	1.19	5/994 (0.5%)
43	BU	0.70	0/787	1.17	6/1051 (0.6%)
44	BV	0.72	0/766	1.12	5/1025 (0.5%)
45	BW	0.73	0/604	1.25	4/799 (0.5%)
46	BX	0.82	0/635	1.47	14/848 (1.7%)
47	BY	0.70	0/510	1.22	5/677 (0.7%)
48	BZ	0.73	0/453	1.27	4/605 (0.7%)
49	B0	0.78	0/450	1.25	4/599 (0.7%)
5	AF	0.79	0/835	1.15	7/1128 (0.6%)
50	B1	0.75	0/417	1.10	3/556 (0.5%)
51	B2	0.91	0/380	1.45	8/498 (1.6%)
52	B3	0.73	0/513	1.24	6/676 (0.9%)
53	B4	0.72	0/303	1.25	3/397 (0.8%)
54	BA	1.74	667/69796 (1.0%)	2.28	4747/108888 (4.4%)
55	BB	1.83	58/2800 (2.1%)	2.30	198/4367 (4.5%)
56	B5	0.68	0/1673	1.14	10/2255 (0.4%)
6	AG	0.77	0/1188	1.24	16/1593 (1.0%)
7	AH	0.74	0/989	1.11	7/1326 (0.5%)
8	AI	0.85	0/1035	1.33	20/1377 (1.5%)
9	AJ	0.78	0/797	1.39	16/1079 (1.5%)
All	All	1.56	1211/160085 (0.8%)	2.06	8067/239402 (3.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	AN	0	1
14	AO	0	1
21	AA	0	342
22	A1	0	13
23	A2	0	5
24	A3	0	19
3	AD	0	1
4	AE	0	1
46	BX	0	1
54	BA	0	646

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	23
56	B5	0	1
All	All	0	1054

The worst 5 of 1211 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2048	G	C2-N2	-6.80	1.27	1.34
24	A3	75	C	N3-C4	-6.76	1.29	1.33
21	AA	1063	C	C4-N4	-6.70	1.27	1.33
23	A2	80	C	C4-N4	-6.68	1.27	1.33
55	BB	113	C	C4-N4	-6.68	1.27	1.33

The worst 5 of 8067 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	34	A	N1-C6-N6	-13.76	110.34	118.60
54	BA	323	C	O4'-C1'-N1	13.51	119.01	108.20
54	BA	547	A	O4'-C1'-N9	12.98	118.58	108.20
54	BA	1943	U	O4'-C1'-N1	12.88	118.50	108.20
54	BA	1340	U	O4'-C1'-N1	12.80	118.44	108.20

There are no chirality outliers.

5 of 1054 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	5	U	Sidechain
3	AD	44	LYS	Peptide
4	AE	148	SER	Peptide
13	AN	69	ARG	Sidechain
14	AO	68	TYR	Sidechain

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	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	1	0
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	1	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	1	0
21	AA	32828	0	16011	4	0
22	A1	1627	0	802	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	811	2	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	1	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	2	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	1	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	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	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	1	0
52	B3	504	0	574	3	0
53	B4	302	0	343	0	0
54	BA	62317	0	30495	12	0
55	BB	2504	0	1187	0	0
56	B5	1658	0	1751	1	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	98156	28	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 28 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BL:64:PHE:CE2	52:B3:24:LYS:HE2	2.40	0.56
20:AU:30:GLU:H	20:AU:31:VAL:HG22	1.72	0.54
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.30	0.49
56:B5:19:LYS:HE3	56:B5:21:TYR:CE2	2.46	0.49
52:B3:2:LYS:HE3	54:BA:242:G:C8	2.51	0.45

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	199 (91%)	17 (8%)	2 (1%)	19	61
2	AC	205/208 (99%)	187 (91%)	15 (7%)	3 (2%)	11	51
3	AD	203/206 (98%)	184 (91%)	14 (7%)	5 (2%)	6	39
4	AE	150/152 (99%)	132 (88%)	14 (9%)	4 (3%)	5	38
5	AF	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	5	35
6	AG	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	8	45
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	6	40
8	AI	126/128 (98%)	113 (90%)	7 (6%)	6 (5%)	2	26
9	AJ	98/100 (98%)	90 (92%)	4 (4%)	4 (4%)	3	29
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	19	61
11	AL	121/124 (98%)	108 (89%)	7 (6%)	6 (5%)	2	26
12	AM	112/115 (97%)	100 (89%)	9 (8%)	3 (3%)	5	38
13	AN	98/101 (97%)	83 (85%)	12 (12%)	3 (3%)	4	35
14	AO	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	7	41
15	AP	79/81 (98%)	67 (85%)	8 (10%)	4 (5%)	2	25
16	AQ	80/82 (98%)	75 (94%)	3 (4%)	2 (2%)	6	39
17	AR	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
18	AS	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	13	54
19	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	14	56
20	AU	51/53 (96%)	32 (63%)	9 (18%)	10 (20%)	0	2
25	BC	270/273 (99%)	246 (91%)	18 (7%)	6 (2%)	7	42
26	BD	207/209 (99%)	177 (86%)	19 (9%)	11 (5%)	2	25
27	BE	199/201 (99%)	179 (90%)	11 (6%)	9 (4%)	3	28
28	BF	176/179 (98%)	150 (85%)	20 (11%)	6 (3%)	4	33
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	10	49
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	12	52
31	BI	139/142 (98%)	130 (94%)	7 (5%)	2 (1%)	12	52
32	BJ	140/142 (99%)	122 (87%)	15 (11%)	3 (2%)	8	43
33	BK	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
34	BL	141/144 (98%)	127 (90%)	10 (7%)	4 (3%)	5	37
35	BM	134/136 (98%)	118 (88%)	11 (8%)	5 (4%)	4	31
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	10	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	19	61
38	BP	112/115 (97%)	94 (84%)	11 (10%)	7 (6%)	1	21
39	BQ	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	6	38
40	BR	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	8	45
41	BS	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	19	61
42	BT	92/94 (98%)	71 (77%)	17 (18%)	4 (4%)	3	28
43	BU	101/104 (97%)	88 (87%)	10 (10%)	3 (3%)	5	35
44	BV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
45	BW	78/80 (98%)	60 (77%)	15 (19%)	3 (4%)	3	30
46	BX	75/79 (95%)	64 (85%)	9 (12%)	2 (3%)	5	38
47	BY	61/63 (97%)	53 (87%)	7 (12%)	1 (2%)	11	50
48	BZ	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	9	47
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2	24
50	B1	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3	29
51	B2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	B3	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	11	50
53	B4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2	24
56	B5	221/234 (94%)	207 (94%)	12 (5%)	2 (1%)	19	61
All	All	5876/6008 (98%)	5263 (90%)	456 (8%)	157 (3%)	9	38

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	149	PRO
6	AG	11	ILE
6	AG	56	SER
8	AI	110	VAL
9	AJ	57	VAL

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%)	63	83
2	AC	170/171 (99%)	170 (100%)	0	100	100
3	AD	172/173 (99%)	169 (98%)	3 (2%)	63	83
4	AE	113/113 (100%)	111 (98%)	2 (2%)	62	82
5	AF	87/87 (100%)	85 (98%)	2 (2%)	53	76
6	AG	123/123 (100%)	121 (98%)	2 (2%)	65	84
7	AH	104/105 (99%)	104 (100%)	0	100	100
8	AI	105/105 (100%)	102 (97%)	3 (3%)	45	70
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	89 (99%)	1 (1%)	76	88
11	AL	103/104 (99%)	102 (99%)	1 (1%)	78	89
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	82 (99%)	1 (1%)	74	87
14	AO	76/77 (99%)	74 (97%)	2 (3%)	49	73
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	73 (99%)	1 (1%)	69	85
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	69 (99%)	1 (1%)	69	85
19	AT	65/65 (100%)	64 (98%)	1 (2%)	67	85
20	AU	44/44 (100%)	41 (93%)	3 (7%)	17	48
25	BC	216/217 (100%)	213 (99%)	3 (1%)	69	85
26	BD	164/164 (100%)	160 (98%)	4 (2%)	52	75
27	BE	165/165 (100%)	162 (98%)	3 (2%)	62	82
28	BF	149/150 (99%)	147 (99%)	2 (1%)	71	86
29	BG	137/138 (99%)	134 (98%)	3 (2%)	55	77
30	BH	114/114 (100%)	112 (98%)	2 (2%)	62	82
31	BI	109/110 (99%)	108 (99%)	1 (1%)	81	90
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	81	90
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	58	79
35	BM	109/109 (100%)	107 (98%)	2 (2%)	62	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	78	89
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	58	79
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	76	88
40	BR	84/84 (100%)	82 (98%)	2 (2%)	52	75
41	BS	93/93 (100%)	92 (99%)	1 (1%)	76	88
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	82 (99%)	1 (1%)	74	87
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	57 (97%)	2 (3%)	40	66
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%)	47 (98%)	1 (2%)	56	78
49	B0	47/48 (98%)	47 (100%)	0	100	100
50	B1	45/45 (100%)	44 (98%)	1 (2%)	55	77
51	B2	38/38 (100%)	35 (92%)	3 (8%)	13	43
52	B3	51/52 (98%)	51 (100%)	0	100	100
53	B4	34/34 (100%)	33 (97%)	1 (3%)	45	70
56	B5	173/181 (96%)	170 (98%)	3 (2%)	63	83
All	All	4842/4870 (99%)	4774 (99%)	68 (1%)	71	85

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	BD	91	THR
29	BG	34	ARG
51	B2	25	LYS
26	BD	103	ASP
27	BE	152	GLU

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

Mol	Chain	Res	Type
29	BG	110	HIS

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Mol	Chain	Res	Type
46	BX	31	ASN
44	BV	88	HIS
10	AK	100	ASN
45	BW	56	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	264 (17%)	77 (5%)
22	A1	74/76 (97%)	14 (18%)	6 (8%)
23	A2	14/15 (93%)	5 (35%)	2 (14%)
24	A3	76/77 (98%)	14 (18%)	7 (9%)
54	BA	2902/2903 (99%)	451 (15%)	146 (5%)
55	BB	116/118 (98%)	12 (10%)	3 (2%)
All	All	4711/4722 (99%)	760 (16%)	241 (5%)

5 of 760 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U

5 of 241 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	330	A
54	BA	1069	A
54	BA	2565	A
54	BA	372	G
54	BA	532	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	2.35	3 (20%)	15,37,40	3.63	4 (26%)
22	6MZ	A1	37	22	17,25,26	1.10	1 (5%)	15,36,39	1.61	2 (13%)
22	7MG	A1	46	22	20,26,27	1.76	3 (15%)	24,39,42	1.54	2 (8%)
22	5MU	A1	54	22	13,22,23	1.33	2 (15%)	14,32,35	3.30	1 (7%)
22	PSU	A1	55	22	16,21,22	1.34	2 (12%)	20,30,33	4.75	5 (25%)
22	4SU	A1	7	22	13,21,22	1.23	1 (7%)	14,30,33	2.69	2 (14%)
24	H2U	A3	21	24	17,21,22	1.53	3 (17%)	20,30,33	1.15	2 (10%)
24	OMC	A3	33	24	15,22,23	1.38	2 (13%)	20,31,34	1.10	1 (5%)
24	5MU	A3	55	24	13,22,23	1.36	3 (23%)	14,32,35	3.45	1 (7%)
24	PSU	A3	56	24	16,21,22	1.39	3 (18%)	20,30,33	4.64	7 (35%)
24	4SU	A3	8	24	13,21,22	1.29	1 (7%)	14,30,33	2.97	3 (21%)

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	-	2/6/30/31	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	7MG	A1	46	22	-	1/7/37/38	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	-	3/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/3/25/26	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	34	CM0	O5-C5	-7.22	1.23	1.37
22	A1	46	7MG	C8-N9	-5.55	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C2-N3	-3.65	1.31	1.38
22	A1	34	CM0	O5'-C5'	-3.50	1.39	1.44
24	A3	21	H2U	C4-N3	-3.37	1.32	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	55	PSU	N1-C2-N3	-14.43	116.96	128.43
24	A3	56	PSU	N1-C2-N3	-13.12	118.00	128.43
24	A3	55	5MU	C4-N3-C2	12.38	125.60	115.14
22	A1	54	5MU	C4-N3-C2	11.89	125.18	115.14
22	A1	55	PSU	C4-N3-C2	11.80	125.11	115.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	34	CM0	C4-C5-O5-C7
22	A1	34	CM0	C6-C5-O5-C7
24	A3	56	PSU	O4'-C1'-C5-C6
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	C2'-C1'-C5-C6

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
58	FME	BA	3001	57	9,9,10	0.85	1 (11%)	6,9,11	1.22	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	FME	BA	3001	57	-	0/6/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3001	FME	CA-C	2.14	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	O-C-CA	-2.58	119.20	125.11

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.