



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:10 PM BST

PDB ID : 4V6Y
EMDB ID: : EMD-1716
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^fMet 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 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

A user guide is available at

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

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

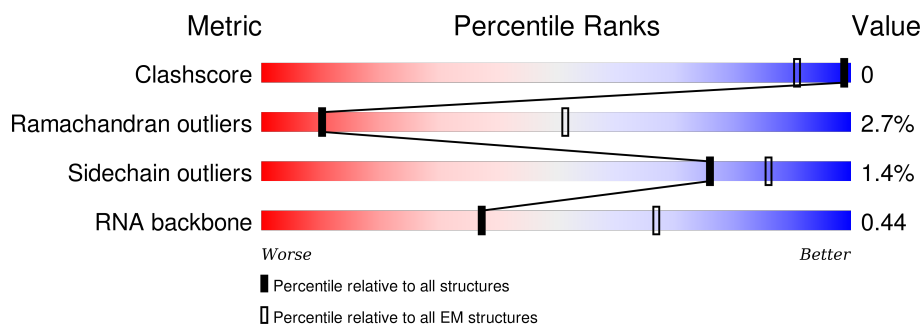
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 Å.

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











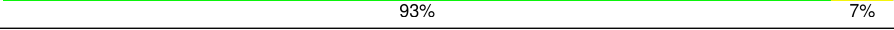


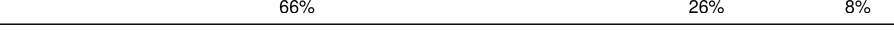

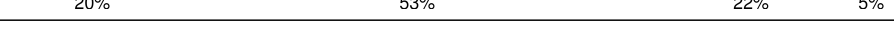

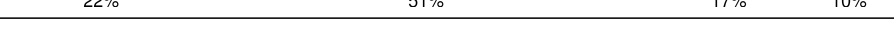



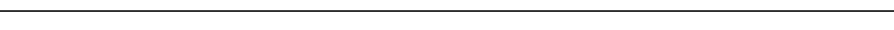

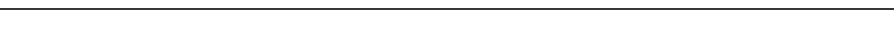
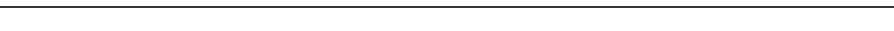


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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% .













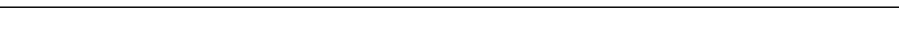



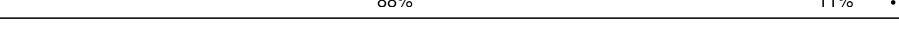






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Mol	Chain	Length	Quality of chain
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG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

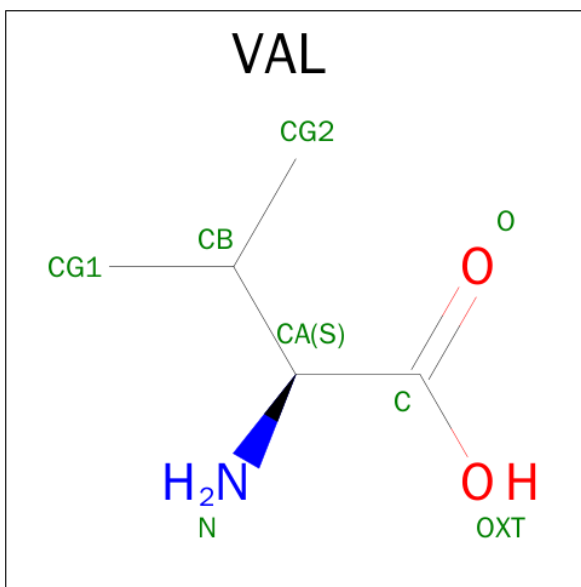
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

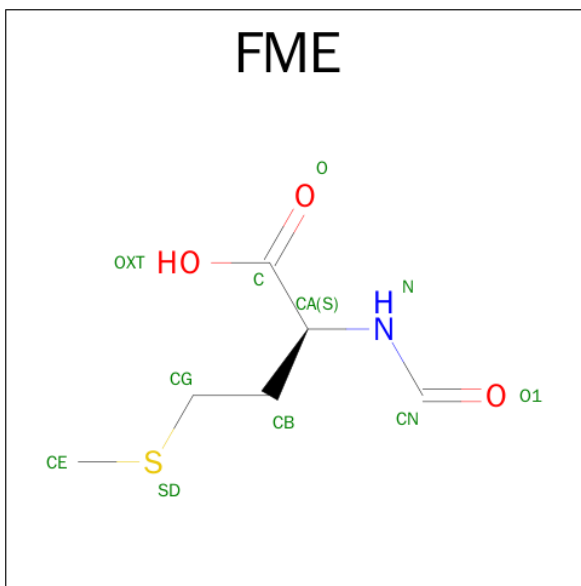
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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: $C_6H_{11}NO_3S$).

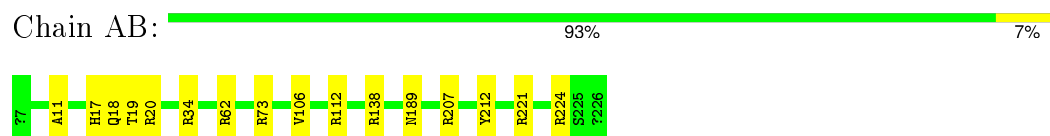


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

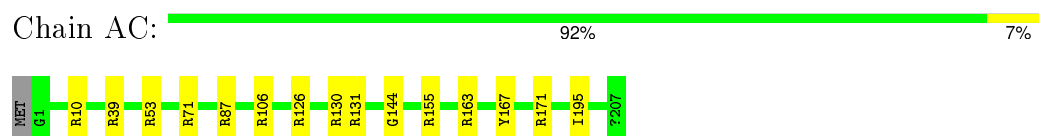
3 Residue-property plots [i](#)

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.

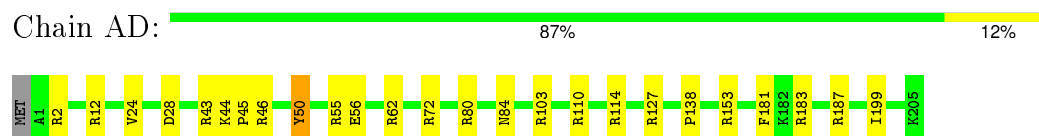
- Molecule 1: 30S ribosomal protein S2



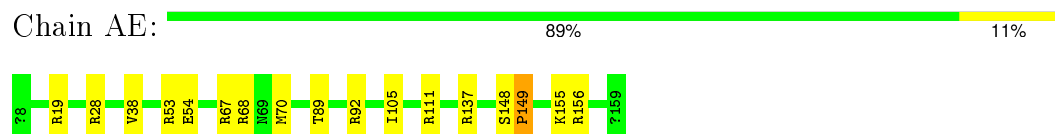
- Molecule 2: 30S ribosomal protein S3



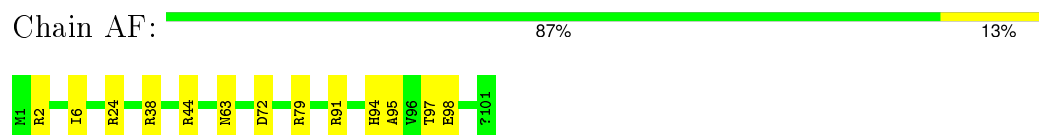
- Molecule 3: 30S ribosomal protein S4



- 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: 91% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 81% 18%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 84% 16%



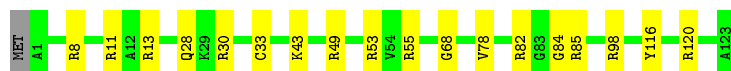
- Molecule 10: 30S ribosomal protein S11

Chain AK: 89% 11%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 85% 15%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%

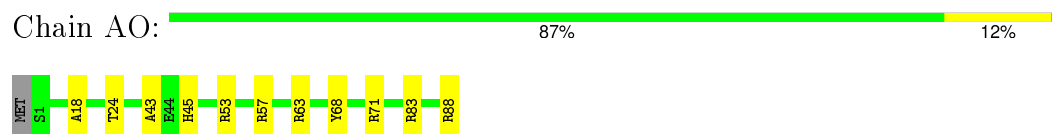


- Molecule 13: 30S ribosomal protein S14

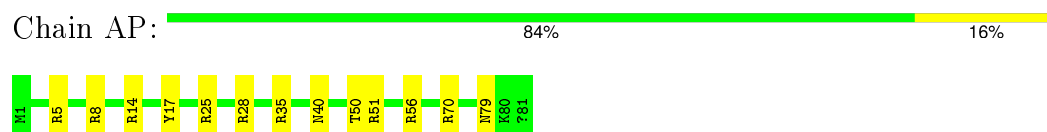
Chain AN: 86% 12%



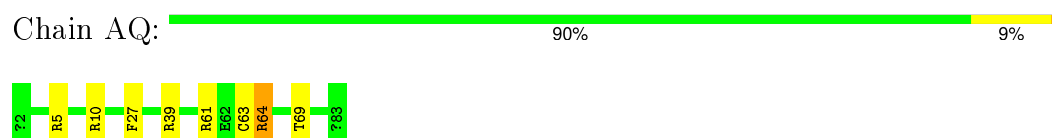
- Molecule 14: 30S ribosomal protein S15



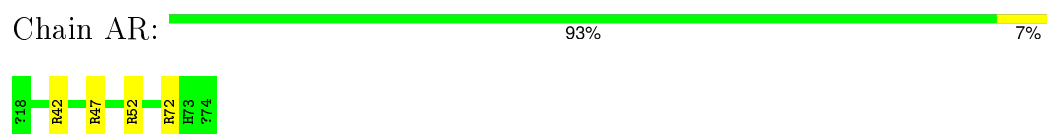
- Molecule 15: 30S ribosomal protein S16



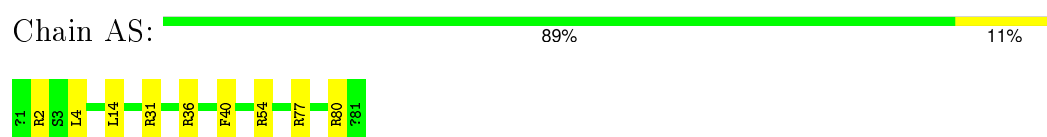
- Molecule 16: 30S ribosomal protein S17



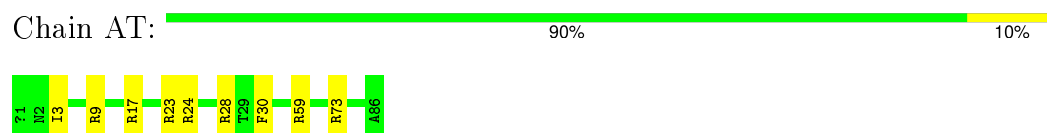
- Molecule 17: 30S ribosomal protein S18



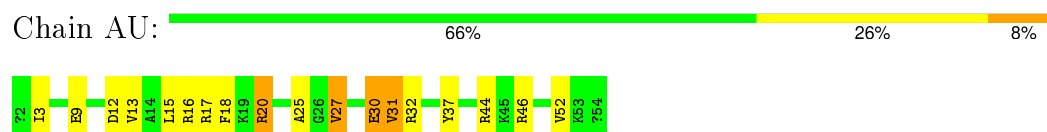
- Molecule 18: 30S ribosomal protein S19



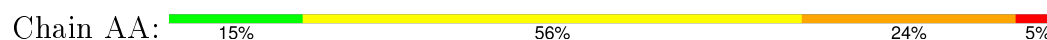
- Molecule 19: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S21



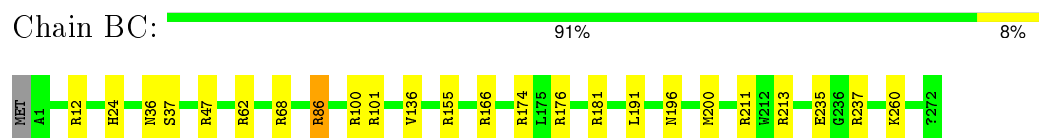
- Molecule 21: 16S ribosomal RNA



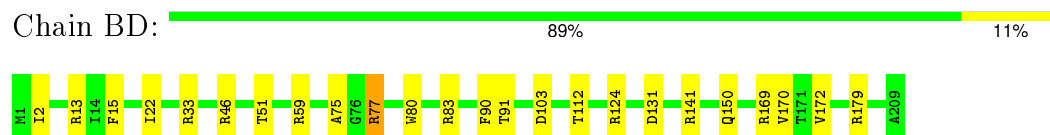




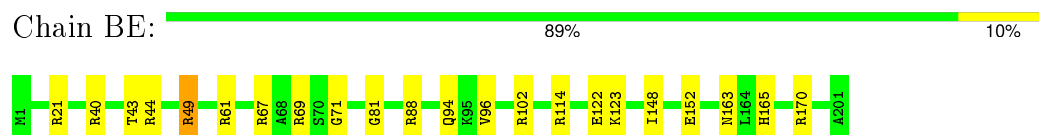

- Molecule 25: 50S ribosomal protein L35



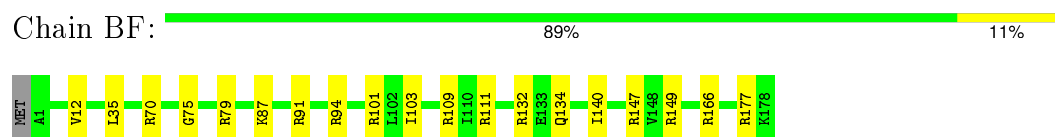
- Molecule 26: 50S ribosomal protein L36



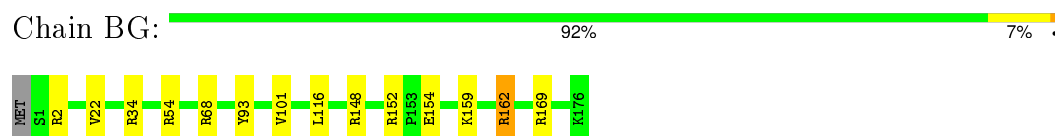
- Molecule 27: 50S ribosomal protein L2



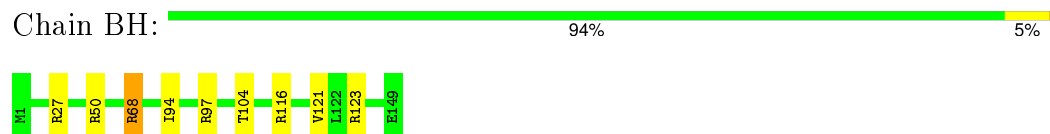
- Molecule 28: 50S ribosomal protein L3



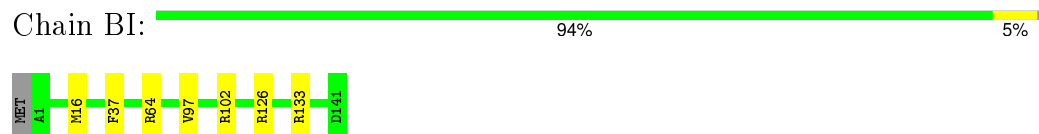
- Molecule 29: 50S ribosomal protein L4



- 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%



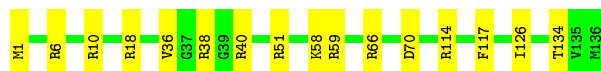
- Molecule 34: 50S ribosomal protein L13

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%



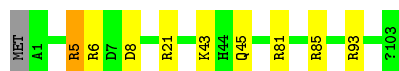
- Molecule 42: 50S ribosomal protein L21

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%

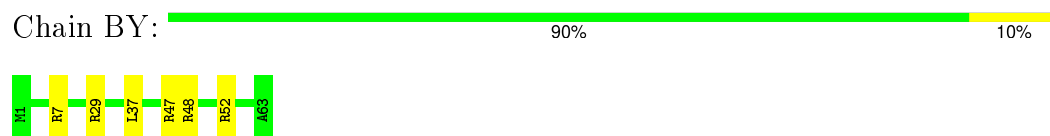


- Molecule 46: 50S ribosomal protein L25

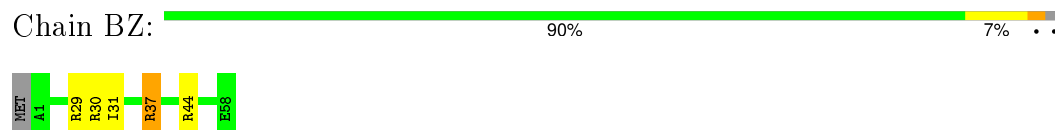
Chain BX: 84% 10% . .



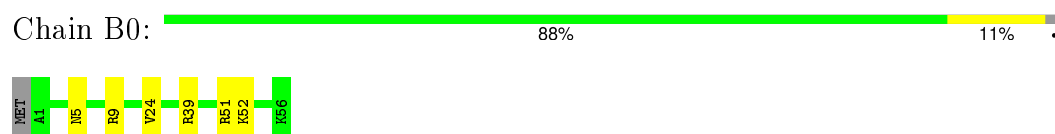
- Molecule 47: 50S ribosomal protein L27



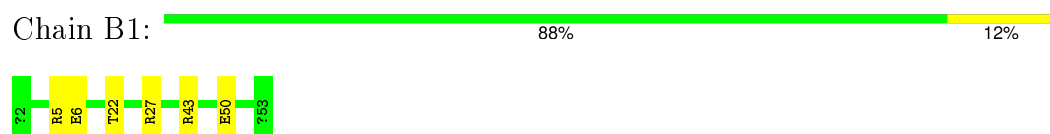
- Molecule 48: 50S ribosomal protein L28



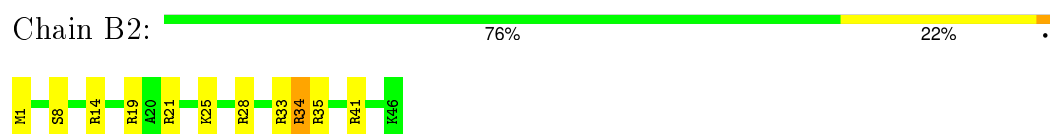
- Molecule 49: 50S ribosomal protein L29



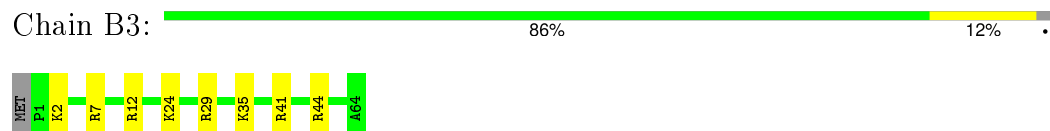
- Molecule 50: 50S ribosomal protein L30



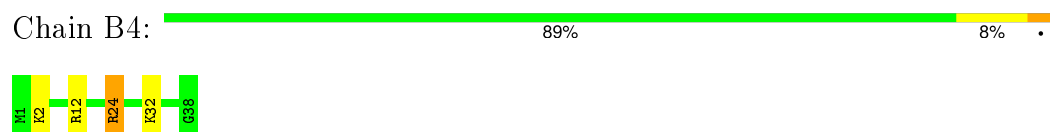
- Molecule 51: 50S ribosomal protein L32



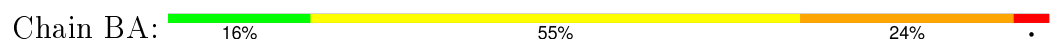
- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

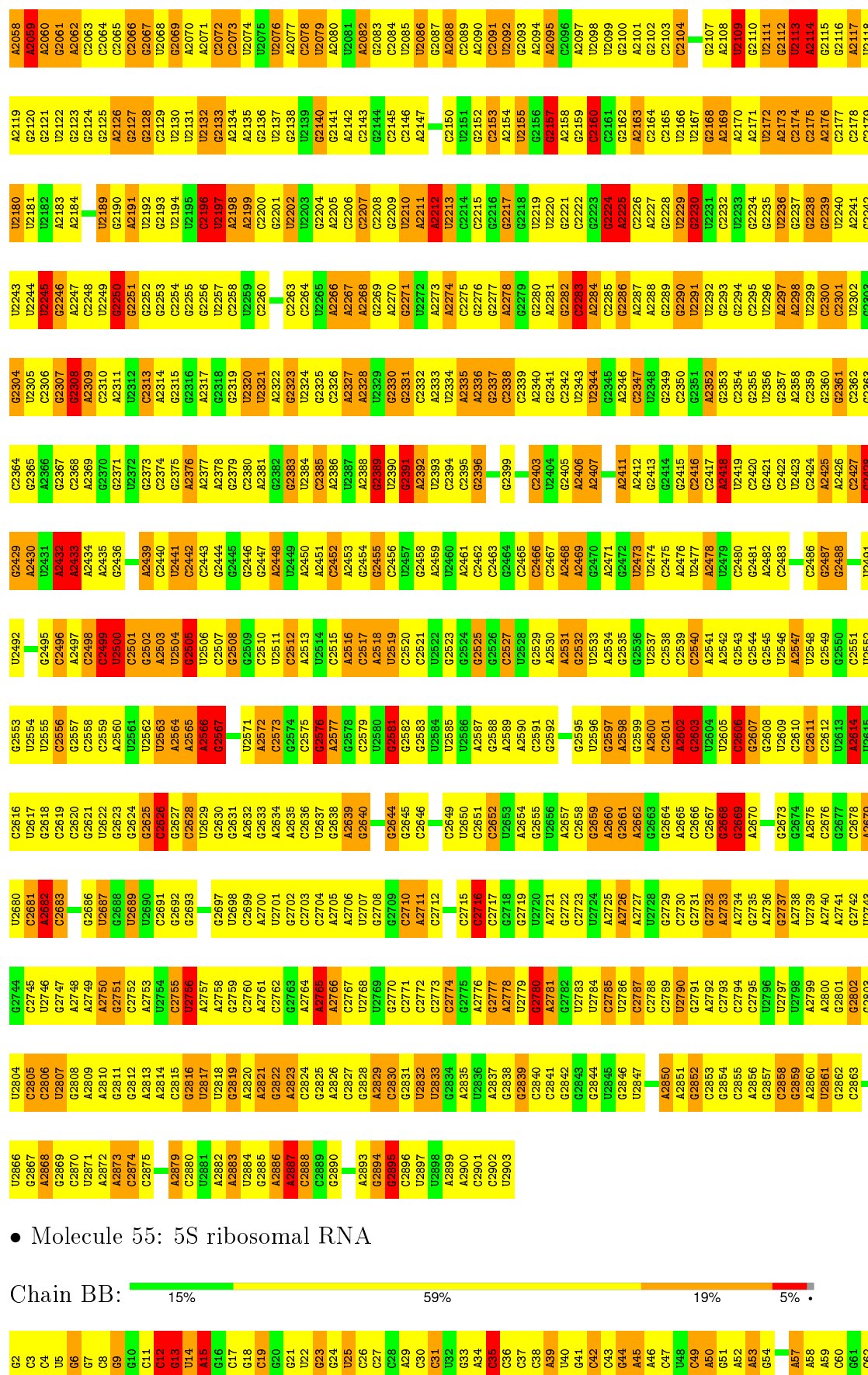


- Molecule 54: 23S ribosomal RNA



A1001	G938	G809	U744	C680	G620	U558	G496	C436	G372	G312	G248	G188	A125	A63	G1
C1005	G939	U810	G745	G681	A621	G559	A497	U437	U373	G313	C249	G189	A126	A64	G2
C1006	G940	U811	U746	G684	G622	C560	G498	G438	A374	G314	C250	A190	A127	U66	U3
C1007	G941	C812	U747	G684	G623	G561	U499	A439		C315	A251	A191	U128	C66	U4
A1008	G942	U813	G748	G685	C824	U562	G500	U440	G377	G316	G252	C192	C129	U67	A5
A1009	G943	C814	A749	U686	G625	A563	A501	U441	G378	G317	C253	U193	C130	G68	A6
A1010	G944	C815	A750	C687	A626	C564	A502	U442		C318	G254	G194	A131	C69	G7
A1011	G945	C816	A751	U688	A627	C565	A503	U443	G381	G319	A255	A195		G70	C8
U1012	G946	C817	A752	G689	G628	U566	A504	U444	A382	A320	A256	A196	G134	A71	G9
C1013	G947	U818	A753	G690	G629	U567	A505	U445	A383	U321	C257	A197	U135	U72	A10
G948	A947	A819	U754	C691	G630	U568	G506	U446	A384	U322		C198	G136	A73	C11
G949	A948	A820	U755	C692	A631	U569	A507	U447	C385	C323		A199		A74	U12
A1014	G949	A821	A756	A693	A632	G570	A508	U448	G386	A324		U200		G75	U13
U1015	G950	G822	G757	U694	A633	U571	C509	U449	U387	G325		C201	C140	C76	A14
G1016	G951	G823	G758	G695	C634	A572	C510	U450	G388	G326		U202	G142	G77	C16
	G952	C824		G695	C635	U573		U451	G389	G327		A203	A143	G78	C17
U1019		U823	G759		C636	A574		U452	U390	U328		C204	U139	C79	G18
A1020	G956	U824	G760	C698	A637	A575	A513	A453	A391	G329		G205	A144	U82	A19
A1021	C957	A825	A761	A699	G638	U576	A514	A454	U392	A330		U206	C145	A83	C20
G1022	U958	U826	U762	G700	U639	G577	A515	C455	C393	C331		A207	C146	A84	A21
U1023	U959	U827	G763	G701	U640	G578	C516	C456	C394	A332		C208	C147	G85	G22
A1024	A960	U828	A764	U702	U641	U579	G518	A457	U395	G333		C209	U148	G86	G23
G1025	C961	C830	C765	G703	U642	U580	U519	A458	G396	C334		C210	A149	U87	C24
		G831		G704	U643	C581	G520	U459	U397	G335		C211	U150	G88	
A1027	C964	U832	G770	A705	A643	C582	U521	U460	C398	C356		G212	C151	G89	
A1028	C965	A833	G771	A706	A644	A582	A522	C461	U399	C337		A213	A152	A89	
A1029	C966	C834	C772	G707	C645	G583	A523	C462	G400	G338		G214	U153	U90	G27
	C967	C835	U773		U646	C584	G524	C463	A401	U339		G215	U154	U91	A28
G1030	C968	U836	G774	U710	G647	U585	G525	C464	A402	A340		A216	U155	U92	C31
A1032	G969	G837	G775	G711	G648	A586	U526	U464	A403	A341		A217	A156	G93	G32
U1033	G970	C838	G776	G712	G649	C587	A527	C465	U404	A342		A218	C157	G94	C33
G1034	G971	C839	G777	G713	C650	U588	C528	C466	U405	C343		A219	U158	U95	U34
U1035	A972	C840			G651	U589	A529	C467	G406	A344		G220	G159	C96	G35
				A715	U652	A590	U530	C468		A345		A221	A160	G97	G36
A1039	A973	A844	G780	C717	U653	U591	G531	C469	G410	A346		A222	A161	C98	C37
A1040	G974	A845	A781	C718	A654	A592	A532	C470	G411	A347		A223	U162	U99	A38
A1041	A975	U846	A782	A719	A655	U593	A533	C471	G412	A348		A224	C163	U100	G39
G1042	G976	U847	A783	U720	G656	U594		C472	C413	U349		C225	C164	A101	U40
	G977	A848	G784	U721	U657	C595		C473	C414	G350		A226	A165	U102	C41
G1043	G978	A849	G785	A722	U658	U596		C474	C415	C351		A227	U166	A103	A42
A1045	A979	U850	C786	C723	G659	G597		C475	A416	A352		C228	U167	A104	G43
C1046	C981	C854	C787	U724	C660	U598	A538	C476	C417	A353		C229	G168	C105	A44
A1048	A981	U855	A788	G725	A661	A599	G539	C477	C418	A354		G230	G169	C106	G45
G1047	C982	C856	A789	G726	A662	G600	C540	C478	U419	U355		A231	U170	G107	G46
A1049	A983	U857	U790	G727	G663	C601	C541	C479	C420	G356		G232	U171	G108	C47
	C984	C858	G791	U728	U664	A602	C542	C480	C421	C357		A233	A172	C109	G48
C1049	C985	A863	A792	G729	U665	A603	G543	C481	A422	U358		U235	A173	G110	A49
A1050	C986	G860	A793	C730	A666	G604	C544	C482	G423	G359		C236	U174	A111	G51
G1051	C987	U861	C794	A731	U667	G605	U545	A483	A424	U360		A300	G175	A52	A53
C1052	A988	C862	C795	G732	U668	U606	U546	C484	G425	U361		G301	A176	A54	
A1054	C989	U863	G796	C733	G669	U607	A547	C485	G426	G361		C302	G177	U114	
G1055	A990	A864	G797	G734	A670	A608	G548	C486	C427	A362		C238	G178	C115	A55
	C991	C865		A735	C671	A609	G549	C487	U428	G363		C239	G179	C116	G54
U1056	G992	U866	A800	C736	C672	C610	C550	C488	A429	C364		C240	C179	G117	G55
	C993	C867	G801	C737	C673	C611	G551	C489	A430	U365		A241	G180	A118	A56
A1058	G994	U867	A802	G738	C674	C612	U552	C490	U431	C366		G242	A181	A119	C57
C1059	C995	C868	C803	G739	A675	G613	G553	C491	A432	G367		U243	A182	U120	G58
U1060	A996	U868	A804	A739	G676	A614	U554	C492	A433	A368		A244	C183	G121	U59
	C997	C869	G805	C740	A677	A615	U555	A493	A434	U369		G245	C184	G122	G60
C1064	U998	U870	C806	U741	A678	U616	G556	C494	U435	G370		C246	G185	G123	C61
U1065	A1000	C873	G808	A743	C679	A617	C557	C495	C435	A371		G247		G124	U62

C1996	G1995	C1874	G1811	G1750	C1686	C1625	U1563	A1503	U1440	C1376	U1316	G1256	G1193	A1129	A1067
A1996	A1936	C1875	U1812	U1751	C1687	A1626	C1564	A1504	G1441	G1377	G1317	C1257	A1194	U1130	G1068
A1998	A1937	A1876	G1813	C1752	G1627	G1627	C1565	A1505	U1442	A1378	U1318	A1258	A1195	G1131	A1069
A1999	A1938	A1877	G1814	G1753	A1628	A1628	A1566	A1506	U1443	U1379	C1319	G1259	C1196	U1132	A1070
C2001	U1940	C1878	A1815	A1764	G1629	U1629	G1567	C1507	G1444	G1390	G1320	A1260	A1197	A1133	G1071
C2002	G1941	U1880	C1816	A1755	U1692	A1630	G1568	A1508	G1445	G1381	A1321	C1261	U1198	A1134	C1072
A2003	C1942	C1881	G1817	G1756	C1691	G1631	A1569	A1509	C1446	G1382	A1322	A1262	U1199	C1135	A1073
C2004	U1943	A1819	U1818	U1757	G1697	A1632	A1570	G1510	C1447	A1383	C1323	U1263	C1200	C1140	C1076
C2005	U1944	A1820	A1819	U1758	A1698	G1633	A1571	G1511	G1448	A1384	G1324	A1264	U1201	U1141	U1077
C2006	G1945	A1821	G1820	A1759	A1699	A1634	A1572	C1512	G1449	A1385	U1325	A1265	U1202	U1142	U1078
U2007	U1946	C1822	A1821	C1760	G1700	A1635	G1573	C1513	G1450	C1386	U1326	G1266	U1203	U1143	C1079
C2008	U1947	A1762	G1823	C1761	A1701	U1636	C1574	G1514	G1451	A1387	A1327	A1267	A1204	A1143	A1080
A2009	C1947	A1763	G1823	A1762	G1702	A1637	C1575	A1515	G1452	G1388	A1328	A1268	A1205	A1144	U1081
C2010	G1950	C1887	C1826	G1763	G1703	C1638	U1576	G1516	A1453	G1389	U1329	A1269	G1206	C1145	U1082
U2011	U1951	A1888	U1827	C1764	C1704	C1639	C1577	G1517	C1454	U1391	G1330	C1270	U1207	C1146	U1083
C2012	A1952	A1889	A1827	U1765	A1705	A1640	U1578	C1518	G1455	U1390	G1331	G1271	C1208	A1147	U1084
A2013	A1953	A1890	G1828	G1766	C1706	A1641	A1579	G1519	G1456	A1392	G1332	A1272	U1148	U1148	A1085
A2014	G1954	A1829	A1830	G1767	G1707	G1642	A1580	A1526	U1457	A1393	G1333	U1273	G1210	G1149	A1090
A2015	U1955	C1893	G1831	C1768	C1708	G1643	G1581	G1521	U1458	U1394	G1334	A1274	C1211	C1150	A1086
U2016	U1956	C1894	G1832	U1769	U1709	C1644	C1582	A1522	G1459	A1395	C1335	A1275	G1212	A1151	G1087
U2017	C1957	A1895	A1833	G1770	G1710	G1645	A1583	G1523	U1460	U1396	C1336	A1276	G1213	C1152	A1088
C2018	C1958	G1834	U1834	C1771	A1711	C1646	U1584	G1524	C1461	U1397	G1337	G1277	A1214	C1153	A1089
A2019	G1959	A1772	U1835	A1772	U1712	C1647	C1585	A1525	G1462	C1398	G1338	C1278	G1215	G1154	A1090
A2020	A1960	C1773	G1836	A1773	A1713	G1648	A1586	A1526	G1463	C1399	G1339	C1279	G1216	A1155	G1091
C2021	C1961	C1774	C1836	C1774	U1714	A1649	G1587	G1527	G1464	U1400	U1340	G1280	U1217	A1156	C1092
U2022	U1962	A1899	C1837	U1775	G1715	A1650	G1588	A1528	G1465	G1401	G1341	G1281	G1218	G1157	G1093
C2023	C1963	A1900	G1840	U1776	U1716	G1651	U1589	G1529	U1466	U1402	A1342	U1282	U1219	C1158	U1094
G2024	G1964	C1902	U1841	U1779	A1717	A1652	A1590	G1530	U1467	A1403	G1343	G1283	G1220	U1159	A1095
C2025	C1965	A1903	G1842	A1780	G1718	G1653	A1591	C1531	U1468	C1404	U1344	A1284	C1221	A1165	A1096
A2026	A1966	G1904	C1843	G1781	U1720	A1654	C1592	A1532	A1469	U1405	C1345	A1285	U1222	C1161	U1097
C1967	C1967	U1905	C1844	U1782	U1721	C1656	A1593	C1533	A1470	U1406	G1346	A1286	G1223	G1162	A1098
G2029	U1968	G1906	U1851	U1783	G1722	C1657	U1594	U1534	G1471	A1407	A1347	A1287	U1224	G1163	G1099
A2030	A1969	A1907	A1852	A1783	G1723	C1658	C1595	A1535	G1472	G1408	G1348	G1288	G1225	C1164	C1100
A2031	C1970	C1908	A1853	A1784	G1724	A1660	A1596	G1536	U1473	U1409	C1349	G1289	A1226	A1165	U1101
G2032	U1971	A1786	G1849	A1785	U1725	A1661	A1597	G1537	U1474	A1413	C1350	C1290	G1227	G1166	C1102
A2033	G1972	A1787	G1850	A1787	C1726	U1662	A1598	G1538	G1475	C1414	C1351	G1291	G1228	C1167	A1103
U2034	G1973	C1788	U1851	U1788	C1727	G1663	U1599	U1539	U1476	U1415	U1352	G1292	C1229	G1168	C1104
G2035	C1974	A1789	A1852	A1789	C1728	A1664	C1600	G1540	A1477	U1416	A1353	C1293	A1230	A1169	U1105
C2036	G1975	C1790	U1853	C1790	U1729	A1665	G1601	C1541	C1480	G1416	A1354	U1294	C1233	C1170	U1108
A2037	U1976	A1791	A1854	G1730	C1730	G1666	A1602	G1542	U1481	C1417	G1355	G1295	G1236	C1172	C1109
G2038	A1977	G1922	U1855	G1731	A1731	G1667	C1604	A1544	G1482	A1419	C1357	G1297	A1237	U1174	G1110
U2039	A1978	C1793	U1856	G1732	A1732	A1668	C1605	A1545	G1486	G1421	G1358	C1298	A1238	A1175	A1111
C2042	U1979	A1794	G1857	U1917	G1733	A1669	C1606	G1546	U1486	G1422	G1360	G1299	G1238	U1176	G1112
C2043	A1980	C1795	A1858	C1794	G1734	C1670	C1607	C1547	U1487	G1423	G1361	G1300	A1241	U1177	U1113
C2044	A1981	A1796	U1859	A1735	A1671	A1671	A1608	A1548	U1488	G1426	C1362	A1301	U1242	C1178	C1114
C2045	U1982	C1920	G1860	U1736	A1672	A1672	A1609	A1549	C1489	A1427	C1363	A1302	U1243	G1179	G1115
G2046	G1983	G1921	G1861	G1737	G1673	G1674	A1610	C1550	A1490	C1428	G1364	A1304	C1243	G1179	G1116
C2047	G1984	G1799	G1862	G1738	A1738	C1675	C1612	A1551	G1491	G1429	A1365	C1305	G1245	U1180	C1117
C2048	C1985	C1800	G1863	A1739	A1739	C1675	A1562	A1562	U1486	G1430	A1366	C1306	G1246	U1181	C1118
G2049	U1986	A1801	U1864	G1740	G1740	A1676	G1613	A1563	G1492	A1431	A1367	A1307	A1247	G1182	U1119
C2050	A1987	U1926	U1865	C1741	C1741	A1677	A1614	U1554	C1493	A1431	G1367	A1307	A1247	U1183	G1120
A2051	G1988	A1803	A1866	U1742	U1742	A1678	C1615	G1555	A1494	G1432	G1368	A1308	G1248	G1186	C1121
C2052	U1989	C1804	G1867	G1743	G1743	A1679	A1616	G1556	A1495	A1433	G1369	G1309	U1249	G1187	C1122
G2053	C1990	A1806	C1868	A1744	A1744	A1680	C1617	C1557	A1496	A1496	C1370	G1310	G1250	G1187	C1123
A2054	U1991	G1930	G1869	A1745	A1745	G1681	A1613	C1568	U1497	G1435	G1371	G1311	G1251	U1188	G1124
G1992	G1992	C1807	C1870	A1746	A1746	G1682	G1619	U1559	C1498	G1436	U1372	U1312	G1252	A1189	G1125
C2055	U1993	A1808	A1871	U1747	U1747	U1683	G1620	G1560	C1499	C1437	A1373	U1313	A1253	G1190	A1126
G2056	C1994	A1872	A1872	C1748	C1748	G1684	G1620	C1561	U1438	U1438	G1374	U1314	A1254	G1191	A1127
G2057	U1995	C1934	G1873	A1810	A1749	C1685	U1624	U1562	A1502	A1439	U1375	C1315	U1255	G1192	G1128



• Molecule 55: 5S ribosomal RNA

Chain BB: 15% 59% 19% 5%





- 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, Not provided	Depositor
Number of images	14235	Depositor
Resolution determination method	FSC at 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	161000	Depositor
Image detector	4k CCD camera (TVIPS)	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
54:BA:780:G:C6	54:BA:782:A:C2	3.05	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%)	21	67
2	AC	205/208 (99%)	187 (91%)	15 (7%)	3 (2%)	13	57
3	AD	203/206 (98%)	184 (91%)	14 (7%)	5 (2%)	7	46
4	AE	150/152 (99%)	132 (88%)	14 (9%)	4 (3%)	6	45
5	AF	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	5	42
6	AG	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	9	51
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	7	47
8	AI	126/128 (98%)	113 (90%)	7 (6%)	6 (5%)	3	32
9	AJ	98/100 (98%)	90 (92%)	4 (4%)	4 (4%)	3	35
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	21	67
11	AL	121/124 (98%)	108 (89%)	7 (6%)	6 (5%)	3	31
12	AM	112/115 (97%)	100 (89%)	9 (8%)	3 (3%)	6	45
13	AN	98/101 (97%)	83 (85%)	12 (12%)	3 (3%)	5	42
14	AO	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	8	48
15	AP	79/81 (98%)	67 (85%)	8 (10%)	4 (5%)	2	30
16	AQ	80/82 (98%)	75 (94%)	3 (4%)	2 (2%)	7	46
17	AR	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
18	AS	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	15	60
19	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	16	61
20	AU	51/53 (96%)	32 (63%)	9 (18%)	10 (20%)	0	3
25	BC	270/273 (99%)	246 (91%)	18 (7%)	6 (2%)	8	49
26	BD	207/209 (99%)	177 (86%)	19 (9%)	11 (5%)	2	29
27	BE	199/201 (99%)	179 (90%)	11 (6%)	9 (4%)	3	33
28	BF	176/179 (98%)	150 (85%)	20 (11%)	6 (3%)	5	40
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	11	55
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	14	58
31	BI	139/142 (98%)	130 (94%)	7 (5%)	2 (1%)	14	58
32	BJ	140/142 (99%)	122 (87%)	15 (11%)	3 (2%)	9	50
33	BK	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
34	BL	141/144 (98%)	127 (90%)	10 (7%)	4 (3%)	6	44
35	BM	134/136 (98%)	118 (88%)	11 (8%)	5 (4%)	4	38
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	11	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	21	67
38	BP	112/115 (97%)	94 (84%)	11 (10%)	7 (6%)	2	25
39	BQ	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	7	45
40	BR	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	9	51
41	BS	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	21	67
42	BT	92/94 (98%)	71 (77%)	17 (18%)	4 (4%)	3	34
43	BU	101/104 (97%)	88 (87%)	10 (10%)	3 (3%)	5	42
44	BV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
45	BW	78/80 (98%)	60 (77%)	15 (19%)	3 (4%)	4	37
46	BX	75/79 (95%)	64 (85%)	9 (12%)	2 (3%)	6	45
47	BY	61/63 (97%)	53 (87%)	7 (12%)	1 (2%)	12	56
48	BZ	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	11	53
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2	28
50	B1	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	4	35
51	B2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	B3	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	12	56
53	B4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2	28
56	B5	221/234 (94%)	207 (94%)	12 (5%)	2 (1%)	21	67
All	All	5876/6008 (98%)	5263 (90%)	456 (8%)	157 (3%)	10	45

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%)	68	87
2	AC	170/171 (99%)	170 (100%)	0	100	100
3	AD	172/173 (99%)	169 (98%)	3 (2%)	68	87
4	AE	113/113 (100%)	111 (98%)	2 (2%)	66	87
5	AF	87/87 (100%)	85 (98%)	2 (2%)	58	83
6	AG	123/123 (100%)	121 (98%)	2 (2%)	70	88
7	AH	104/105 (99%)	104 (100%)	0	100	100
8	AI	105/105 (100%)	102 (97%)	3 (3%)	50	78
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	89 (99%)	1 (1%)	80	91
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%)	82 (99%)	1 (1%)	78	90
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	73 (99%)	1 (1%)	74	89
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	69 (99%)	1 (1%)	74	89
19	AT	65/65 (100%)	64 (98%)	1 (2%)	72	88
20	AU	44/44 (100%)	41 (93%)	3 (7%)	20	57
25	BC	216/217 (100%)	213 (99%)	3 (1%)	74	89
26	BD	164/164 (100%)	160 (98%)	4 (2%)	57	82
27	BE	165/165 (100%)	162 (98%)	3 (2%)	66	87
28	BF	149/150 (99%)	147 (99%)	2 (1%)	76	89
29	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
30	BH	114/114 (100%)	112 (98%)	2 (2%)	66	87
31	BI	109/110 (99%)	108 (99%)	1 (1%)	84	93
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	84	93
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	63	85
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%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	82 (98%)	2 (2%)	57	82
41	BS	93/93 (100%)	92 (99%)	1 (1%)	80	91
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	82 (99%)	1 (1%)	78	90
44	BV	78/78 (100%)	78 (100%)	0	100	100
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%)	47 (98%)	1 (2%)	61	84
49	B0	47/48 (98%)	47 (100%)	0	100	100
50	B1	45/45 (100%)	44 (98%)	1 (2%)	60	83
51	B2	38/38 (100%)	35 (92%)	3 (8%)	15	51
52	B3	51/52 (98%)	51 (100%)	0	100	100
53	B4	34/34 (100%)	33 (97%)	1 (3%)	50	78
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68	87
All	All	4842/4870 (99%)	4774 (99%)	68 (1%)	76	89

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	2.11	2 (13%)	18,37,40	3.11	4 (22%)
22	6MZ	A1	37	22	17,25,26	1.11	2 (11%)	15,36,39	1.32	1 (6%)
22	7MG	A1	46	22	20,26,27	2.32	3 (15%)	23,39,42	2.16	2 (8%)
22	5MU	A1	54	22	13,22,23	1.14	1 (7%)	16,32,35	4.32	2 (12%)
22	PSU	A1	55	22	15,21,22	1.30	3 (20%)	16,30,33	3.26	3 (18%)
22	4SU	A1	7	22	12,21,22	1.06	1 (8%)	15,30,33	2.10	1 (6%)
24	H2U	A3	21	24	17,21,22	1.43	3 (17%)	23,30,33	1.17	2 (8%)
24	OMC	A3	33	24	15,22,23	1.14	1 (6%)	20,31,34	0.77	0
24	5MU	A3	55	24	13,22,23	1.16	2 (15%)	16,32,35	4.51	3 (18%)
24	PSU	A3	56	24	15,21,22	1.24	1 (6%)	16,30,33	3.36	4 (25%)
24	4SU	A3	8	24	12,21,22	1.19	1 (8%)	15,30,33	2.24	2 (13%)

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 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.92	1.32	1.45
22	A1	34	CM0	O5-C5	-7.10	1.23	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C2-N3	-3.54	1.31	1.38
24	A3	21	H2U	C4-N3	-3.36	1.32	1.37
24	A3	56	PSU	O4'-C1'	-3.02	1.39	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	55	5MU	C5-C4-N3	-12.36	114.97	125.35
22	A1	54	5MU	C5-C4-N3	-11.87	115.39	125.35
24	A3	8	4SU	C5-C4-N3	-7.87	115.21	123.56
22	A1	7	4SU	C5-C4-N3	-7.27	115.85	123.56
22	A1	46	7MG	C5-C6-N1	-7.03	112.93	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	0.73	0	5,7,9	1.51	1 (20%)
58	FME	BA	3001	57	8,9,10	0.47	0	5,9,11	1.21	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
57	A1	101	VAL	O-C-CA	-2.84	117.93	125.69
58	BA	3001	FME	O-C-CA	-2.38	119.20	125.69

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.