



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:51 pm GMT

PDB ID : 4V78
EMDB ID: : EMD-2475
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post3a)
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 : 20.00 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

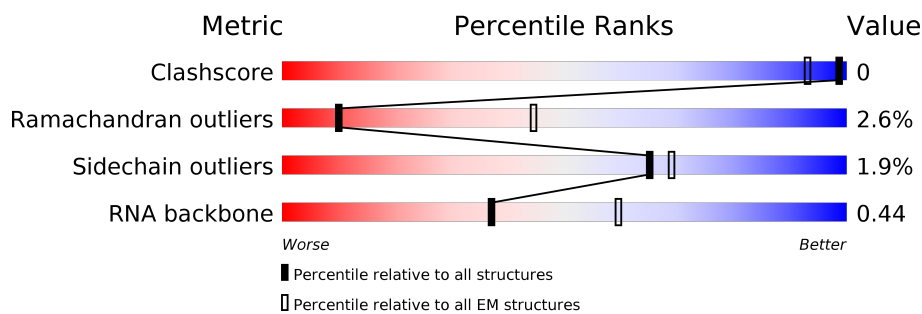
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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.

















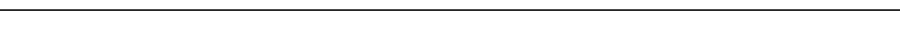

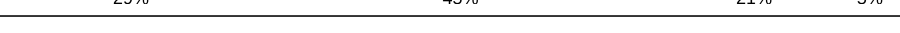


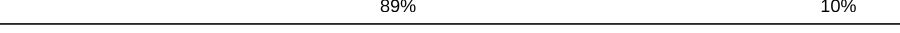


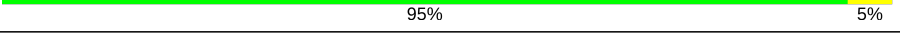
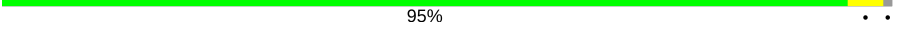

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	94% 5% .
2	AC	208	87% 13%
3	AD	206	86% 12% .
4	AE	152	94% 6%
5	AF	101	87% 13%
6	AG	152	88% 11% .
7	AH	130	92% 8% .
8	AI	128	84% 16%

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Mol	Chain	Length	Quality of chain
9	AJ	100	 86% 13% .
10	AK	118	 92% 7% .
11	AL	124	 85% 15% .
12	AM	115	 90% 10% .
13	AN	101	 87% 10% ..
14	AO	89	 88% 11% .
15	AP	81	 78% 22%
16	AQ	82	 90% 9% .
17	AR	57	 84% 16%
18	AS	81	 90% 9% .
19	AT	86	 86% 13% .
20	AU	53	 75% 25%
21	AA	1533	 24% 51% 21% .
22	A1	76	 28% 42% 30%
23	A2	15	 13% 47% 27% 13%
24	A3	77	 29% 45% 21% 5%
25	BC	273	 89% 9% .
26	BD	209	 90% 9%
27	BE	201	 89% 10%
28	BF	179	 89% 10% ..
29	BG	177	 89% 10% .
30	BH	149	 95% 5%
31	BI	142	 95% . .
32	BJ	142	 90% 10%
33	BK	123	 89% 11%

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Mol	Chain	Length	Quality of chain
34	BL	144	86% 13% ..
35	BM	136	90% 9% .
36	BN	121	88% 11% .
37	BO	117	87% 11% ..
38	BP	115	84% 15% .
39	BQ	118	85% 14% ..
40	BR	103	92% 8%
41	BS	110	92% 7% .
42	BT	94	91% 7% .
43	BU	104	88% 12% .
44	BV	94	95% 5%
45	BW	80	89% 10% .
46	BX	79	86% 11% .
47	BY	63	92% 8%
48	BZ	59	85% 12% ..
49	B0	57	77% 21% .
50	B1	52	87% 13%
51	B2	46	78% 22%
52	B3	65	85% 14% .
53	B4	38	87% 13%
54	BA	2903	22% 53% 21% .
55	BB	118	17% 61% 17% ..
56	B5	234	88% 7% 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 L2.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

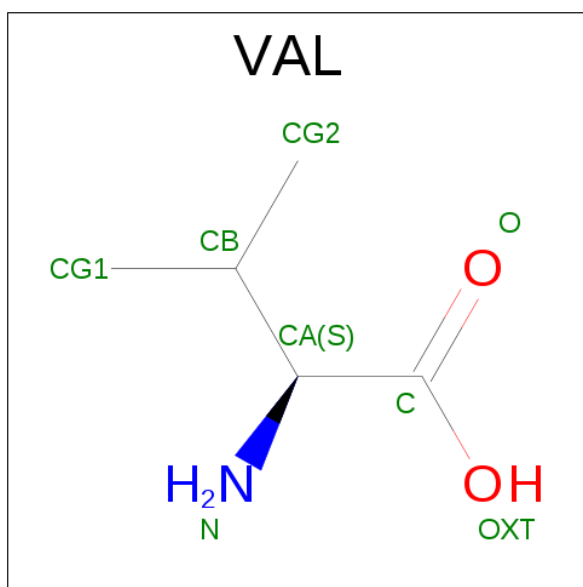
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

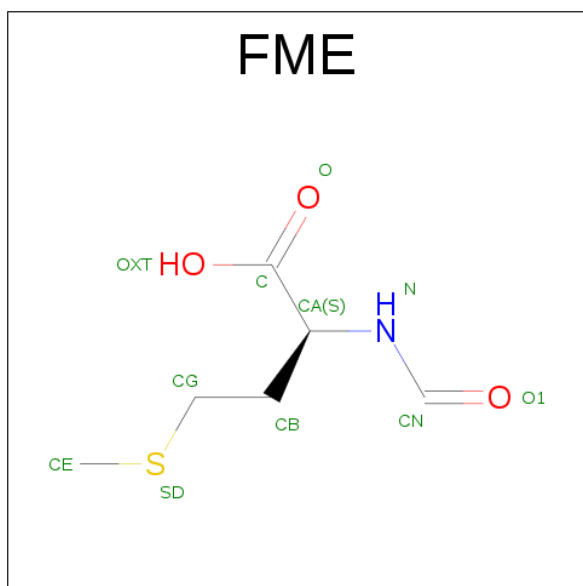
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: 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: $C_6H_{11}NO_3S$).

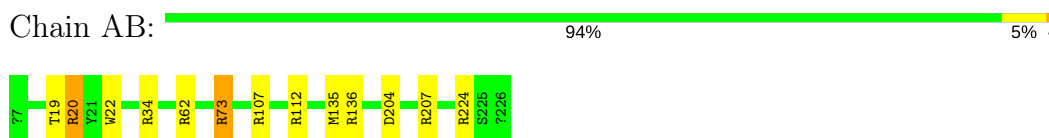


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

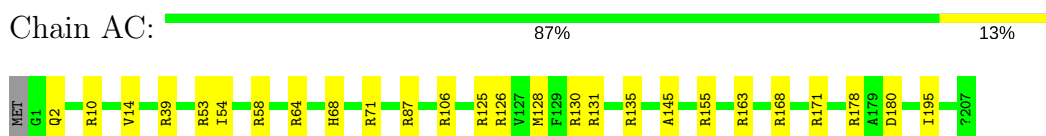
3 Residue-property plots

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.

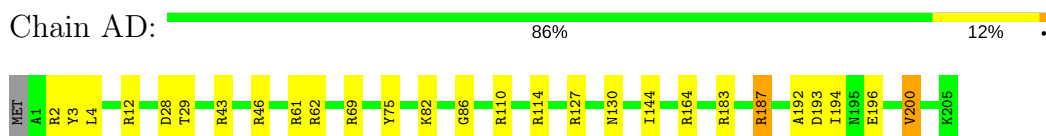
- Molecule 1: 30S ribosomal protein S2



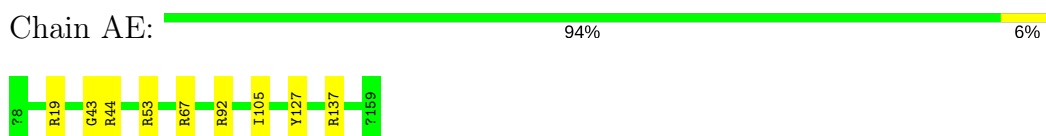
- Molecule 2: 30S ribosomal protein S3



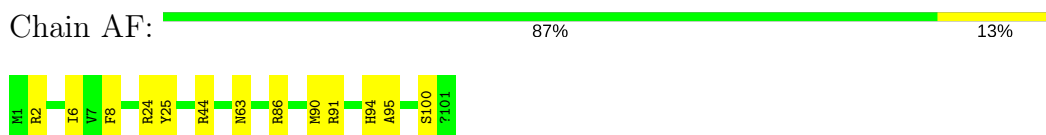
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7






- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI:  84% 16%



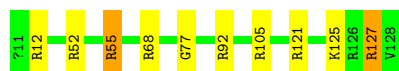
- Molecule 9: 30S ribosomal protein S10

Chain AJ: 86% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK:  92% 7% 1%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 85% 15%

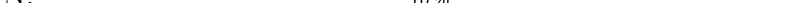


- Molecule 12: 30S ribosomal protein S13

Chain AM:  90% 10%



- Molecule 13: 30S ribosomal protein S14

Chain AN:  87% 10% ..




- Molecule 14: 30S ribosomal protein S15

Chain AO:  88% 11%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  78% 22%




- Molecule 16: 30S ribosomal protein S17

Chain AQ:  90% 9%



- Molecule 17: 30S ribosomal protein S18

Chain AR:  84% 16%




- Molecule 18: 30S ribosomal protein S19

Chain AS:  90% 9%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  86% 13%



- Molecule 20: 30S ribosomal protein S21

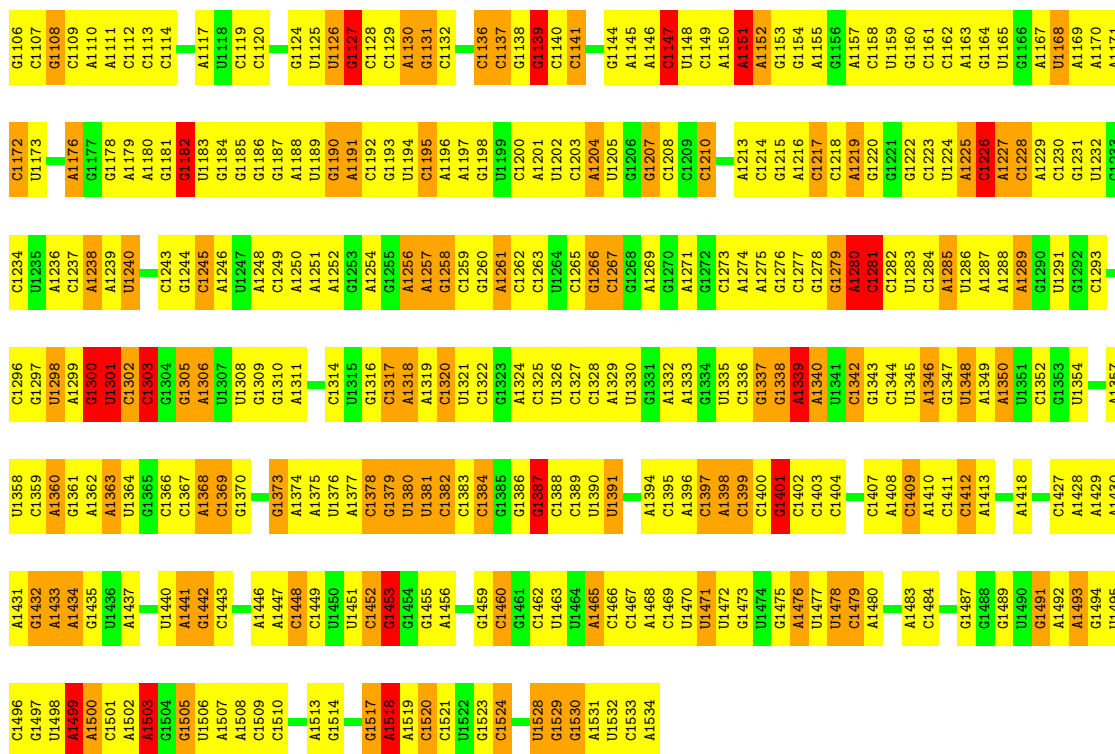
Chain AU:  75% 25%



- Molecule 21: 16S ribosomal RNA

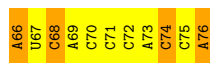
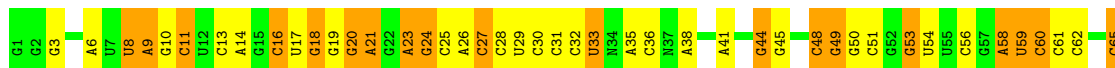
Chain AA:  24% 51% 21%

G1039	A975	C910	G846	A777	G711	A642	G577	C514	A451	U390	U323		A196	C132	G64	A
U1040	G976	U911	G847	G778	A712	G643	C578	G515	A452	G391	G324		A197	C135	A65	A
G1041	A977	C912	G848	C779	G713	G646	C580	U516	G455	C392	A325		G198		A66	U
A1042	A978	A913	G849	A780	G714	G647	C581	C519	A456	A393	G326		G199	C136	C67	U
G1043	C979	A914	U850	A781	A715	G648	C582	C519		G395	A327		G200	U137	G68	G6
A1044	C980	A915	C851	A782	A716	A648	C583	C520	A459	C396	C328		G201	G138	G69	A7
G1045	G981		G852	C783	U717	A649	A583	A520	A460	A397	A329		G202	A139	U70	A8
G1046	U982	A918	C853	A784	C718	G650	G584	G521	A461	U398	C330		A205	U140	A71	G9
A1047	A983	A919		G785	A719	C651	G585	C522	A462	U399			C206	G141	A72	A10
G1048	C984	U920	C856	C786	C720	G652	C586	A523	A463	G399	C334		C207	G142	G73	G11
U1049	C985	U921	C857	A787	G721	A655	G587	G524	U463	C400	C334		U208	A143	A74	G12
G1050		G922	G858		G722	G656	G588	C525	U464	C401	C335		U209	G144		U13
C1051	A923	A923	G859	A790	U723	U657	G589	C526	A465	G402	A336		C210		A77	U14
U1052	C924	C924	A860	G791	G724	C658	U590	G527	A466	C403	G337		G211	G148	A78	G15
G1053	G925	G925	C861	A792	G725	U659	U591	C528	U467	G404	A338		G212	A149	G79	G16
C1054	G926	U921	C862	U793	C726	C660		G529	A468	U405	C339		G213	U150	A80	U17
A1055	U992	G927	G863	C794	G727	G661	A595	U530	C469	G406	U340		C214	A151	A81	C18
U1056	G933	G928	U864	C795	A728	U662	A596	G531	C470	U407	C341		C215	A152	G82	A19
G1057	A994	G929	A865	C796	A729	A663	G597	A532	U471	U408	C342		U216	G153	G83	U20
C1058	C995	C930	C866	C797	G730	G664	U598	A533	U472	U409	U343		C217	U154	U84	G21
G1059	A996	C931	C867		G731	A665	C599	A534	U473	G410	A344		C221	A155	U85	G22
U1060	U997	C932	C868	G800	G732	G666	A600	A535	C474	A411	C345		C222	U156	U86	C23
G1061	C998	G933	C869	U801	G733	G667	G601	C536	C475	A412	G346		C223	U157	C87	U24
U1062	A999	C934	U870	A802	G734	G668	A602	G537	U476	G413	G347		A223	G158		C25
C1063	C1000	A935	U871		G735	G669	G603	G538	C477	A414	G348		G224	G159	G90	A26
G1064	C1001	C936	A872		C736	G670	U603	A539	A478	A415	A349		C225	A160	U91	C27
U1065		A937	A873	C806	C737		A607	G542	U479	G416	G350		G226	A161	U92	A28
C1066	A1004	A938	G874	A807	G738	A673	A608	U543		G417	G351		G227	U162	U93	U29
A1067	G1006	G939	U875	C808	G739	G674	A609	U544	A482	C418	C352		A228	C163	G94	C36
G1068	G1005	C940	C876	G809	U740	A675	U610	G544	C483	C419	C353		U229	C95	G95	G31
C1069	U1007	G941	G877	C810	G741	A676	C611	C545	C484	U420	G354		G230	U166	U96	A32
U1070	U1008	G942	A878	C811	G742	U677	C612	A546	U485	U421	C355		G231	A167	G97	A33
C1071	U1009		C879	G812	G743	U678	C613	A547	U486	C422	A356		G232	G168	A98	C34
G1072	U1010	G945	C880	U813	C744	C679	G614	G548	A487	G423	G357		C233	U170	G99	C35
U1078	C1011	A946	G881	A814	G745	C680	G615	C549	C488	G424	U358		C234	G100	G100	C36
G1079	A1012	G950	C882	A815	A746	A681	G616		C489	U425	G359		G235	A171	A101	U37
A1080	U1013	C948	C883	A816	A747		G617	A553	C490	G426	G362		A236	A172	G102	G38
A1081	A1014	A949	U884	C817	G748	A887	C618	A554	C491	U427	A363		G237	U173		G39
U1082	G1015	U951	G885	G818	A749	G688	U619	U555	C492	G428	A364		A238	A174	C106	C40
U1083	U1016	G951	C886	A819	C750	C889	C620	C556	A493	U429	U365		G239	C175	G107	G41
G1084		G954		U820	U751		A621	G557	C494	A430	A366		U239	G176	G108	C42
U1085	A1019		A889	G821	G752	U692	A622	G558	A495	A431	U367		G240	C177	A109	C43
	G1020	A958	G890	U822	A753	G693	C623	A559	A496	A432	U368		G242	C178	G110	A44
A1092	A1021	A959	A892	G823	C754	A694	C624	A560	G497	G433	G369		U244	A179	G111	
G1093	A1022	U960	C893	G824	C756	A695	U625	U561	A498	U434	C370		U245	U180	G112	
C1094	U1023	U961		A825	G757	A696	G626	U562	A499	A435	A371		A246	A181		C47
U1095	U1025	C962	C896	C826	C758	U697	G627	A563	G500	C436	C372		U247	A182	G115	C48
C1096	G1026	G963	C897	U827	A759	G698	G628	C564	C501	U437	A373		G248	C183	G116	U49
C1097	C1027	A964	C898	U828	G760	C699	A629	U565	A502	U438	A374		C249	G184	A51	A50
U1098	U1028	U965	C899	G829	G761	G700	A630	G566	C503	U439	C379		U250	U185	C52	
G1099	U1029	G966	A900	A831	C764	A702	C631	G567	C504	C440	C379		A251	C186	A119	A53
C1100	U1030	C967	A901		G765	G703	G633	G568	G505	A441	G380		G252	G187	U121	C54
A1101	G1032	A969	G903	C840	A766	A704	C634	C570	C507	C443	C381		A253	C188		A55
C1102		C970		C841	A767	G705	A635	U571	U508	G444	A383		G254	G189	C124	
G1103	A1035	G971	A906	U842	G768	U707	G637	U572	A509	G445	G384		G255	A190	U125	C58
U1105	A1036	C972	A907	U843	C770	U708		A573	C510	A448	C385		U256	G191	G128	A60
	C1038	A974	A908	G844	C776	U709	A640	G574	C511	G449	C386		G257	A192	U129	A61
			A909	A845		G710		G575	C512	A450	C396		G258	C193	A130	U62
								C576	C513	G450	A389		G259	A195	A131	C63



• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 28% 42% 30%



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

Chain A2: 13% 47% 27% 13%



• Molecule 24: tRNA-fMet

Chain A3: 29% 45% 21% 5%



• Molecule 25: 50S ribosomal protein L2

Chain BC: 89% 9%



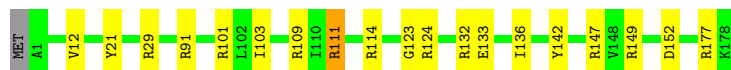
- Molecule 26: 50S ribosomal protein L3



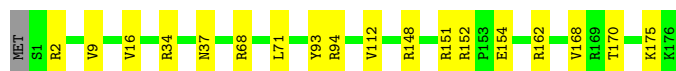
- Molecule 27: 50S ribosomal protein L4



- Molecule 28: 50S ribosomal protein L5



- Molecule 29: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L9



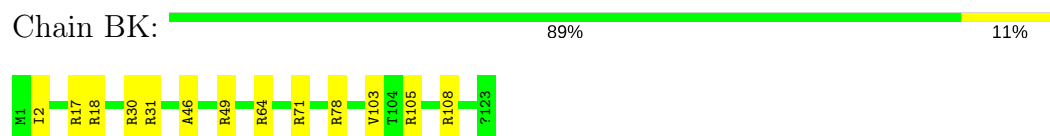
- Molecule 31: 50S ribosomal protein L11



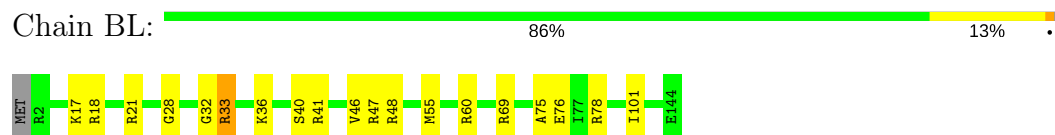
- Molecule 32: 50S ribosomal protein L13



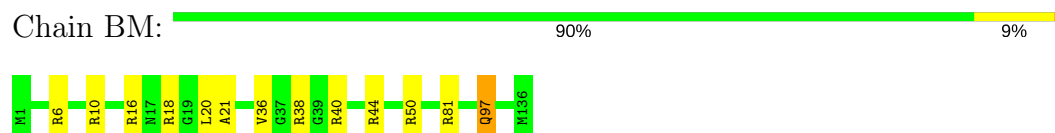
- Molecule 33: 50S ribosomal protein L14



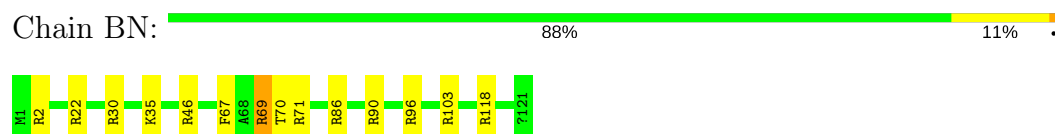
- Molecule 34: 50S ribosomal protein L15



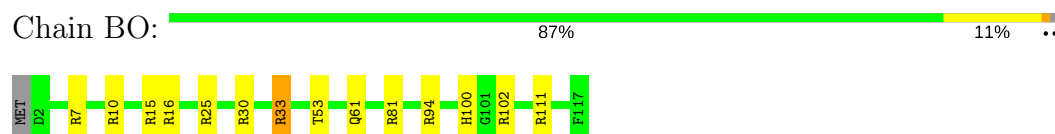
- Molecule 35: 50S ribosomal protein L16



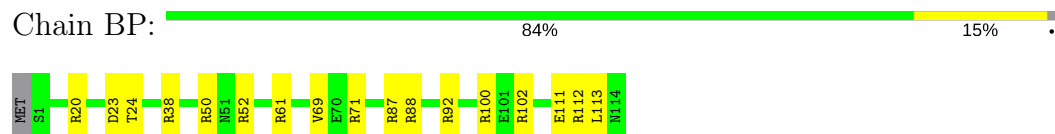
- Molecule 36: 50S ribosomal protein L17



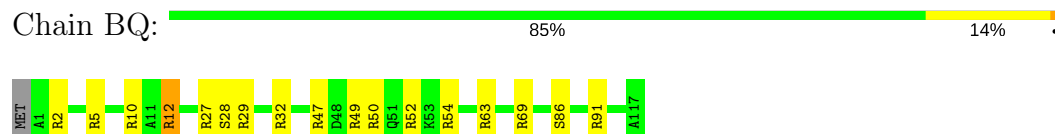
- Molecule 37: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L20



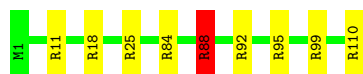
- Molecule 40: 50S ribosomal protein L21

Chain BR:  92% 8%



- Molecule 41: 50S ribosomal protein L22

Chain BS:  92% 7%




- Molecule 42: 50S ribosomal protein L23

Chain BT:  91% 7%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  88% 12%



- Molecule 44: 50S ribosomal protein L25

Chain BV:  95% 5%



- Molecule 45: 50S ribosomal protein L27

Chain BW:  89% 10%



- Molecule 46: 50S ribosomal protein L28

Chain BX:  86% 11%



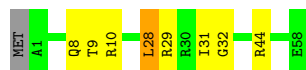
- Molecule 47: 50S ribosomal protein L29

Chain BY:  92% 8%



- Molecule 48: 50S ribosomal protein L30

Chain BZ: 85% 12% . .



- Molecule 49: 50S ribosomal protein L32

Chain B0: 77% 21% .



- Molecule 50: 50S ribosomal protein L33

Chain B1: 87% 13%



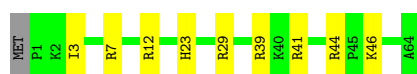
- Molecule 51: 50S ribosomal protein L34

Chain B2: 78% 22%



- Molecule 52: 50S ribosomal protein L35

Chain B3: 85% 14% .



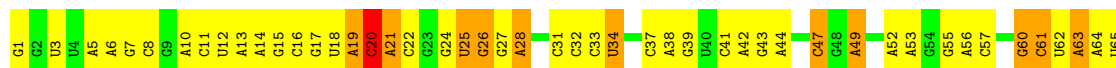
- Molecule 53: 50S ribosomal protein L36

Chain B4: 87% 13%



- Molecule 54: 23S ribosomal RNA

Chain BA: 22% 53% 21% .

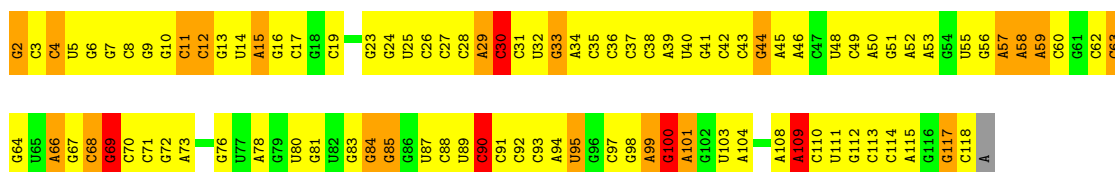





A2095	G2035	G1972	C1909	G1845	A1784	G1723	G1661	C1595	A1469	A1403	G1339	A1274	U1209	C1146
C2096	C2036	G1973	C1912	G1846	A1785	G1726	G1662	A1596	A1470	C1404	U1340	A1275	G1210	A1147
A2097	A2037	G1974	A1912	A1847	A1786	C1727	G1663	A1597	G1471		A1341	A1276	G1211	U1148
U2098	G2038	G1975	A1913	A1848	A1787	C1728	A1664	A1598	C1472	U1409	A1342	A1277	G1212	G1149
U2099	U2039	G1976	G1914	G1849	C1788	C1729	A1665	G1600	G1473	U1410	G1343	C1278	A1213	C1150
G2100	G2040	A1977	U1915	G1850	A1789	U1729		U1599	U1474	U1411	U1344	G1279	A1214	A1151
A2101	U2041	A1978	A1916	U1851	C1790	C1730		G1601	G1475	U1412	G1345		G1215	C1152
G2102	A2042	U1979	U1917	U1852	A1791	G1731	A1668	U1602	U1476	A1413	G1346	A1284		C1153
G2103	C2043	G1980	A1918	A1853	G1792	C1732	A1669	G1540	A1477	A1414	A1347	A1285	G1218	G1154
C2104	C2044	A1981	A1919	A1854	C1793	G1733	C1670	U1542	G1478	U1415	A1348	A1286	U1219	A1155
	C2045	U1982	G1920		A1794	G1734	U1671	C1605	G1479	G1416	A1349	A1287	U1220	A1156
G2046	G2046	G1983	G1924	A1857	C1795	A1735	A1672	A1544	A1480	C1417	C1350	G1288	C1221	G1157
C2047	A1858	U1984	U1916	G1858	U1796	U1736	G1673	C1607	U1481	G1418	C1351	G1289	U1222	C1158
G2048	U1859	G1797	C1925	U1859	G1797	G1737	G1674	A1608	G1482	A1419	U1352	C1290		U1159
G2049	U1926	U1798	C1926	G1860	U1798	G1738	C1675	A1609		A1420	A1353	C1291	G1226	G1160
C2050	A1927	G1799	U1927	G1861	U1799	A1739	A1676	A1610	U1485	A1421	A1354	G1292	G1227	C1161
A2051	A1928	A1800	A1928	G1862	A1800	G1740	A1677	A1549		G1422	G1355	C1293	G1228	G1162
A2052	G1929	A1801	G1930	U1864	A1801	C1741	A1678	C1550	C1488	G1423	G1356	U1294	C1229	G1163
G2063	U1930	A1802	U1930	A1865	A1802	U1742	A1679	A1551	C1489	G1424	C1357	A1230	A1230	C1164
A2054	A1866	A1803	U1931	A1867	A1803	G1743	U1680	A1552	A1490	G1425	G1358	G1296	U1231	A1165
C2065	G1867	C1804	A1932	G1867	C1804	A1744	U1681	A1553	G1491	G1426	C1359		U1232	G1166
G2056	C1868	A1805	G1933	C1868	A1805	A1745	G1682	U1554	G1492	C1427	C1362	G1298	U1233	C1167
G2057	G1869	C1806	C1934	G1869	C1806	A1746	U1683	G1555	C1493	C1428	G1363	G1299	U1234	G1168
A2058	C1870	G1807	G1935	C1870	G1807	U1747	U1684	C1556	A1494		G1364	G1300	G1235	A1169
A2059	A1871	A1808	A1936	A1871	A1808	C1748	C1685	C1557	A1495	A1431	G1365	A1301	G1236	G1170
	A1872	A1809	A1937	A1872	A1809	A1749	C1686	C1558	A1496	G1432	A1366	A1302	A1237	G1171
A2060	G1873	A1810	A1938	C1873	A1810	G1750	G1687	C1559	U1497	A1433	A1367	G1303		G1172
G2061	C1874	G1811	U1939	U1880	G1811	U1751	U1688	G1560	A1504	A1434	A1367	A1304	U1240	U1173
A2062	A1875	A1812	U1940	C1880	A1812	C1752	A1689	C1561	U1506	G1435	C1368	C1305	A1241	U1174
C2063	G1876	G1813	C1941	A1876	G1813	C1753	A1690	U1562	G1507	G1436	G1369	C1306	U1242	A1175
C2064	A1877	A1814	C1942	A1877	A1814	A1754	C1691	U1563	A1508	G1437	C1370	A1307	G1243	U1176
C2065	G1878	A1815	U1943	C1878	A1815	A1755	U1692	C1564	A1502	U1438	G1371	A1308		G1177
G2066	C1879	C1816	U1944	U1880	C1816	G1756	U1693	C1565	U1503	U1439	U1372		G1244	C1178
C2067	A1880	A1817	G1945	C1880	A1817	A1757	C1694	A1566	A1504		A1373		G1245	C1179
U2068	C1881	U1818	U1946	C1881	U1818	U1758	G1695	G1567	U1505	U1442	C1376	U1312	A1247	U1180
A2135	C1882	A1819	U1947	C1882	A1819	A1759	G1696	A1568	U1506	U1443	G1377	U1313	A1248	U1181
G2136	G1883	U1820	C1948	G1883	U1820	C1760	G1697	A1569	C1507	G1444	G1378	C1314	U1249	G1182
A2071	G1884	A1821	G1949	A1885	A1821	C1761	A1698	A1570	A1508	G1445	C1379	C1315	G1250	U1183
C2072	A1886	C1822	G1950	A1886	C1822	G1762	G1699	A1571	A1509	C1446	U1379		C1251	U1184
U2139	C1887	G1823	U1951	C1887	G1823	A1763	U1700	A1572	G1510	G1447	G1380		G1252	G1185
G2140	G1888	G1824	A1952	G1888	G1824	C1764	A1701	G1573	G1511	G1448		C1319	A1253	G1186
G2141	A1889	U1825	A1953	A1889	U1825	U1765		C1574	G1512		G1381	A1320	A1254	U1187
A2142	A1890	G1826	G1954	A1890	G1826	G1766	A1705	U1575	G1513	G1451	A1383	A1321		U1188
C2143	G1891	U1827	U1955	G1891	U1827	G1767	C1706	U1576	G1514	G1452	A1384	A1322	G1257	A1189
C2144	C1892	G1828	U1956	C1892	G1828	C1768	G1707	C1577	A1515	A1453	A1385	C1323	U1258	G1190
C2145	A1893	A1829	C1957	A1893	A1829	U1769	G1708	U1578	G1516	C1454	C1386	G1324	G1259	G1191
C2146	C1894	C1830	C1958	C1894	C1830	G1770	C1708	A1579	G1517	G1455	C1387	G1325	A1260	G1192
A2147	C1895	G1831	G1959	C1895	G1831	C1771	U1709	C1646	C1518	G1456	U1326	U1326	C1261	G1193
U2149	A1960	C1832	A1960	C1896	C1832	A1772	G1710	U1647		U1457	A1327	A1262	A1194	A1194
C2150	C1961	C1833	C1961	U1898	C1833	A1773	A1711	C1582	U1458	U1458	A1328		U1263	G1195
U2151	C1962		C1962	A1899		C1774	U1712	C1583	A1522	G1459	U1329		A1264	C1196
U2085	U1963	C1836	U1963	A1900	C1836	U1775	A1713	A1584	U1523	G1460	U1330	A1265		G1197
U2086	A1901	C1837	A1901	C1897	C1837	U1776	U1714	G1651	G1524	A1461	G1331	A1266	C1200	U1201
G2087	C1902	C1838	C1902	G1903	C1838	U1777	G1715	A1586	A1525	C1462	G1332	U1267	G1266	
A2088	G1903	G1839	G1903	G1904	G1839	U1778	U1716	G1653	G1527	C1463	G1333	A1268	G1267	
G2089	C1967	U1840	C1967	G1904	U1840	U1779	A1717	A1590	A1528	G1463	G1334	A1269	A1269	A1204
A2090	G1968	C1905	G1968	C1905	U1841	A1780	A1720	A1591	G1529	G1465	C1335		C1270	A1205
C2091	A1969	G1906	G1969	A1969	G1842	U1781	G1721	C1592	G1530	U1466	A1336		G1271	G1206
U2092	A1970	C1843	A1970	G1907	C1843	U1782	A1722	A1593	G1531	U1467	G1337		A1272	C1207
G2093	A2031	U2032	A2031	C1908	C1844	A1783		U1594	A1532	U1468	U1402		U1273	C1208



Chain BB:  17% 61% 17% 5%



- Molecule 56: 50S ribosomal protein L1

Chain B5:

88%

7%

5%



4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	AB	0.67	0/1736	1.06	12/2340 (0.5%)
10	AK	0.73	0/894	1.10	8/1207 (0.7%)
11	AL	0.73	0/969	1.29	17/1300 (1.3%)
12	AM	0.72	0/884	1.36	14/1181 (1.2%)
13	AN	0.75	0/817	1.18	10/1088 (0.9%)
14	AO	0.70	0/722	1.18	7/964 (0.7%)
15	AP	0.74	0/648	1.27	11/870 (1.3%)
16	AQ	0.66	0/658	1.17	7/883 (0.8%)
17	AR	0.76	0/463	1.17	6/623 (1.0%)
18	AS	0.72	0/653	1.19	7/879 (0.8%)
19	AT	0.67	0/672	1.13	6/890 (0.7%)
2	AC	0.70	0/1651	1.18	18/2225 (0.8%)
20	AU	0.83	0/431	1.48	7/572 (1.2%)
21	AA	1.61	27/36759 (0.1%)	2.23	2065/57346 (3.6%)
22	A1	1.63	0/1668	2.16	80/2595 (3.1%)
23	A2	1.49	0/343	2.31	18/531 (3.4%)
24	A3	1.64	0/1722	2.26	102/2685 (3.8%)
25	BC	0.73	0/2121	1.28	21/2852 (0.7%)
26	BD	0.65	0/1586	1.19	14/2134 (0.7%)
27	BE	0.66	0/1571	1.22	14/2113 (0.7%)
28	BF	0.72	0/1444	1.18	12/1937 (0.6%)
29	BG	0.65	0/1343	1.14	9/1816 (0.5%)
3	AD	0.74	0/1665	1.20	17/2227 (0.8%)
30	BH	0.62	0/1122	1.08	5/1515 (0.3%)
31	BI	0.63	0/1046	1.03	4/1410 (0.3%)
32	BJ	0.71	0/1152	1.22	10/1551 (0.6%)
33	BK	0.70	0/947	1.23	10/1268 (0.8%)
34	BL	0.72	0/1054	1.29	10/1403 (0.7%)
35	BM	0.71	0/1093	1.19	9/1460 (0.6%)
36	BN	0.75	0/973	1.34	12/1301 (0.9%)
37	BO	0.71	0/902	1.27	13/1209 (1.1%)
38	BP	0.70	0/929	1.22	11/1242 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.76	0/960	1.30	16/1278 (1.3%)
4	AE	0.66	0/1119	1.03	7/1506 (0.5%)
40	BR	0.68	0/829	1.18	8/1107 (0.7%)
41	BS	0.63	0/864	1.22	10/1156 (0.9%)
42	BT	0.62	0/744	1.19	7/994 (0.7%)
43	BU	0.65	0/787	1.21	6/1051 (0.6%)
44	BV	0.66	0/766	1.06	4/1025 (0.4%)
45	BW	0.71	0/604	1.26	7/799 (0.9%)
46	BX	0.72	0/635	1.28	7/848 (0.8%)
47	BY	0.65	0/510	1.24	5/677 (0.7%)
48	BZ	0.67	0/453	1.23	5/605 (0.8%)
49	B0	0.72	0/450	1.30	7/599 (1.2%)
5	AF	0.71	0/835	1.12	7/1128 (0.6%)
50	B1	0.68	0/417	1.10	2/556 (0.4%)
51	B2	0.79	0/380	1.49	9/498 (1.8%)
52	B3	0.70	0/513	1.23	6/676 (0.9%)
53	B4	0.69	0/303	1.35	5/397 (1.3%)
54	BA	1.48	61/69796 (0.1%)	2.23	4183/108888 (3.8%)
55	BB	1.48	1/2800 (0.0%)	2.19	150/4367 (3.4%)
56	B5	0.62	0/1673	1.09	11/2255 (0.5%)
6	AG	0.72	0/1188	1.27	17/1593 (1.1%)
7	AH	0.69	0/989	1.07	8/1326 (0.6%)
8	AI	0.77	0/1035	1.21	13/1377 (0.9%)
9	AJ	0.71	0/797	1.16	9/1079 (0.8%)
All	All	1.34	89/160085 (0.1%)	2.01	7075/239402 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AK	0	1
21	AA	0	374
22	A1	0	20
23	A2	0	5
24	A3	0	13
25	BC	0	1
26	BD	0	1
3	AD	0	1
31	BI	0	1
35	BM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	BN	0	1
54	BA	0	623
55	BB	0	30
All	All	0	1072

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2507	C	C4-N4	-5.63	1.28	1.33
21	AA	742	G	C2-N2	-5.58	1.28	1.34
21	AA	756	C	C4-N4	-5.57	1.28	1.33
54	BA	2164	C	C4-N4	-5.44	1.29	1.33
21	AA	984	C	C4-N4	-5.43	1.29	1.33

The worst 5 of 7075 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1617	C	N3-C2-O2	-16.02	110.69	121.90
54	BA	640	C	N3-C2-O2	-15.80	110.84	121.90
24	A3	73	A	N1-C6-N6	-13.57	110.46	118.60
54	BA	1847	A	N1-C6-N6	-13.18	110.69	118.60
54	BA	323	C	O4'-C1'-N1	12.86	118.49	108.20

There are no chirality outliers.

5 of 1072 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	25	C	Sidechain
21	AA	26	A	Sidechain
21	AA	5	U	Sidechain
3	AD	75	TYR	Sidechain
10	AK	127	ARG	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
2	AC	1625	0	1699	1	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	1	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	1	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16457	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	839	0	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	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31205	8	0
55	BB	2504	0	1269	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99454	17	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 17 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BA:1068:G:H1'	54:BA:1069:A:C6	2.45	0.51
54:BA:1131:G:C5	54:BA:2025:C:H4'	2.50	0.46
22:A1:53:G:C8	22:A1:54:5MU:H72	2.50	0.46
18:AS:46:LEU:HD23	18:AS:46:LEU:H	1.81	0.46
3:AD:86:GLY:H	3:AD:200:VAL:HG23	1.81	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%)	200 (92%)	15 (7%)	3 (1%)	13	54
2	AC	205/208 (99%)	188 (92%)	12 (6%)	5 (2%)	7	42
3	AD	203/206 (98%)	190 (94%)	7 (3%)	6 (3%)	5	37
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	9	46
5	AF	99/101 (98%)	83 (84%)	12 (12%)	4 (4%)	3	31
6	AG	150/152 (99%)	133 (89%)	14 (9%)	3 (2%)	9	46
7	AH	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
8	AI	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	7	42
9	AJ	98/100 (98%)	87 (89%)	6 (6%)	5 (5%)	2	26
10	AK	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	11	50
11	AL	121/124 (98%)	109 (90%)	8 (7%)	4 (3%)	4	35
12	AM	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
13	AN	98/101 (97%)	86 (88%)	9 (9%)	3 (3%)	5	37
14	AO	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	7	43
15	AP	79/81 (98%)	64 (81%)	9 (11%)	6 (8%)	1	18
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	14	56
17	AR	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	10	49
18	AS	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	14	56
19	AT	84/86 (98%)	75 (89%)	5 (6%)	4 (5%)	2	28
20	AU	51/53 (96%)	34 (67%)	13 (26%)	4 (8%)	1	18
25	BC	270/273 (99%)	241 (89%)	21 (8%)	8 (3%)	5	37
26	BD	207/209 (99%)	181 (87%)	18 (9%)	8 (4%)	3	31
27	BE	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	3	29
28	BF	176/179 (98%)	151 (86%)	20 (11%)	5 (3%)	6	39
29	BG	174/177 (98%)	151 (87%)	16 (9%)	7 (4%)	3	31
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	13	54
31	BI	139/142 (98%)	128 (92%)	10 (7%)	1 (1%)	25	68
32	BJ	140/142 (99%)	123 (88%)	14 (10%)	3 (2%)	8	45
33	BK	121/123 (98%)	104 (86%)	13 (11%)	4 (3%)	4	35
34	BL	141/144 (98%)	110 (78%)	23 (16%)	8 (6%)	2	24
35	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	8	44
36	BN	119/121 (98%)	102 (86%)	16 (13%)	1 (1%)	22	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
38	BP	112/115 (97%)	96 (86%)	12 (11%)	4 (4%)	4	33
39	BQ	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	20	63
40	BR	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
41	BS	108/110 (98%)	95 (88%)	12 (11%)	1 (1%)	20	63
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	8	44
43	BU	101/104 (97%)	83 (82%)	13 (13%)	5 (5%)	2	27
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	63 (81%)	11 (14%)	4 (5%)	2	26
46	BX	75/79 (95%)	68 (91%)	5 (7%)	2 (3%)	6	40
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	50 (89%)	3 (5%)	3 (5%)	2	25
49	B0	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	4	33
50	B1	50/52 (96%)	42 (84%)	4 (8%)	4 (8%)	1	17
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	7	43
52	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	5	36
53	B4	36/38 (95%)	27 (75%)	8 (22%)	1 (3%)	6	39
56	B5	221/234 (94%)	207 (94%)	11 (5%)	3 (1%)	13	54
All	All	5876/6008 (98%)	5232 (89%)	490 (8%)	154 (3%)	10	40

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	73	ARG
2	AC	14	VAL
3	AD	82	LYS
9	AJ	77	VAL
15	AP	79	ASN

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%)	178 (99%)	2 (1%)	78	89
2	AC	170/171 (99%)	169 (99%)	1 (1%)	89	94
3	AD	172/173 (99%)	167 (97%)	5 (3%)	48	73
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	78	89
6	AG	123/123 (100%)	121 (98%)	2 (2%)	68	85
7	AH	104/105 (99%)	101 (97%)	3 (3%)	48	73
8	AI	105/105 (100%)	101 (96%)	4 (4%)	38	67
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	56	79
10	AK	90/90 (100%)	89 (99%)	1 (1%)	78	89
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	54	78
14	AO	76/77 (99%)	74 (97%)	2 (3%)	51	75
15	AP	65/65 (100%)	62 (95%)	3 (5%)	31	62
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	50	74
17	AR	48/48 (100%)	46 (96%)	2 (4%)	34	64
18	AS	70/70 (100%)	69 (99%)	1 (1%)	71	86
19	AT	65/65 (100%)	62 (95%)	3 (5%)	31	62
20	AU	44/44 (100%)	42 (96%)	2 (4%)	32	63
25	BC	216/217 (100%)	211 (98%)	5 (2%)	56	79
26	BD	164/164 (100%)	162 (99%)	2 (1%)	75	88
27	BE	165/165 (100%)	160 (97%)	5 (3%)	46	72
28	BF	149/150 (99%)	146 (98%)	3 (2%)	60	82
29	BG	137/138 (99%)	134 (98%)	3 (2%)	57	79
30	BH	114/114 (100%)	113 (99%)	1 (1%)	82	91
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	51	75
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	60	82
35	BM	109/109 (100%)	108 (99%)	1 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	97 (97%)	3 (3%)	46	72
37	BO	86/87 (99%)	82 (95%)	4 (5%)	30	62
38	BP	99/100 (99%)	95 (96%)	4 (4%)	36	65
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	57	79
40	BR	84/84 (100%)	83 (99%)	1 (1%)	75	88
41	BS	93/93 (100%)	92 (99%)	1 (1%)	78	89
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	54	78
44	BV	78/78 (100%)	77 (99%)	1 (1%)	73	87
45	BW	59/59 (100%)	58 (98%)	1 (2%)	66	84
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%)	46 (96%)	2 (4%)	34	64
49	B0	47/48 (98%)	43 (92%)	4 (8%)	12	42
50	B1	45/45 (100%)	44 (98%)	1 (2%)	57	79
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	50 (98%)	1 (2%)	60	82
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	75	88
All	All	4842/4870 (99%)	4750 (98%)	92 (2%)	65	82

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	BC	190	THR
28	BF	142	TYR
49	B0	32	THR
25	BC	191	LEU
27	BE	67	ARG

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

Mol	Chain	Res	Type
2	AC	184	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	254 (16%)	0
22	A1	73/76 (96%)	10 (13%)	0
23	A2	14/15 (93%)	8 (57%)	0
24	A3	76/77 (98%)	15 (19%)	0
54	BA	2902/2903 (99%)	474 (16%)	0
55	BB	116/118 (98%)	18 (15%)	0
All	All	4710/4722 (99%)	779 (16%)	0

5 of 779 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	15	G
21	AA	16	A
21	AA	22	G

There are no RNA pucker outliers to report.

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	16,26,27	1.79	3 (18%)	14,37,40	3.39	2 (14%)
22	6MZ	A1	37	22	18,25,26	1.12	2 (11%)	16,36,39	1.56	2 (12%)
22	7MG	A1	46	22	20,26,27	2.31	4 (20%)	22,39,42	1.92	2 (9%)
22	5MU	A1	54	22	14,22,23	1.13	1 (7%)	16,32,35	4.11	2 (12%)
22	PSU	A1	55	22	16,21,22	1.09	1 (6%)	20,30,33	5.37	7 (35%)
22	4SU	A1	7	22	14,21,22	1.13	1 (7%)	15,30,33	2.72	2 (13%)
24	H2U	A3	21	24	17,21,22	1.46	3 (17%)	21,30,33	1.28	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	OMC	A3	33	24	15,22,23	1.21	1 (6%)	19,31,34	0.81	0
24	5MU	A3	55	24	14,22,23	1.18	1 (7%)	16,32,35	4.02	2 (12%)
24	PSU	A3	56	24	16,21,22	1.37	3 (18%)	20,30,33	5.17	7 (35%)
24	4SU	A3	8	24	14,21,22	1.12	0	15,30,33	2.88	3 (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
22	CM0	A1	34	22	-	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	-8.64	1.32	1.45
22	A1	34	CM0	O5-C5	-5.44	1.26	1.37
24	A3	21	H2U	C4-N3	-3.53	1.32	1.37
24	A3	21	H2U	C2-N3	-3.41	1.31	1.38
22	A1	46	7MG	O5'-C5'	-3.00	1.40	1.44

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	55	PSU	N1-C2-N3	-15.74	117.08	128.40
24	A3	56	PSU	N1-C2-N3	-14.88	117.70	128.40
22	A1	55	PSU	C5-C4-N3	-12.52	115.16	125.43
24	A3	56	PSU	C5-C4-N3	-12.09	115.51	125.43
22	A1	54	5MU	C5-C4-N3	-9.68	114.56	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	54	5MU	1	0

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	6,6,7	0.71	0	6,7,9	1.82	2 (33%)
58	FME	BA	3001	57	9,9,10	1.32	1 (11%)	7,9,11	1.05	1 (14%)

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	-	0/5/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3001	FME	CA-C	3.60	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-3.89	116.07	125.15
58	BA	3001	FME	O-C-CA	-2.18	120.06	125.15
57	A1	101	VAL	C-CA-N	2.06	114.01	109.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.