



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:49 pm GMT

PDB ID : 4V74  
EMDB ID: : EMD-1720  
Title : 70S-fMetVal-tRNAVal-tRNAfMet complex in hybrid pre-translocation state (pre5b)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 17.00 Å(reported)  
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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

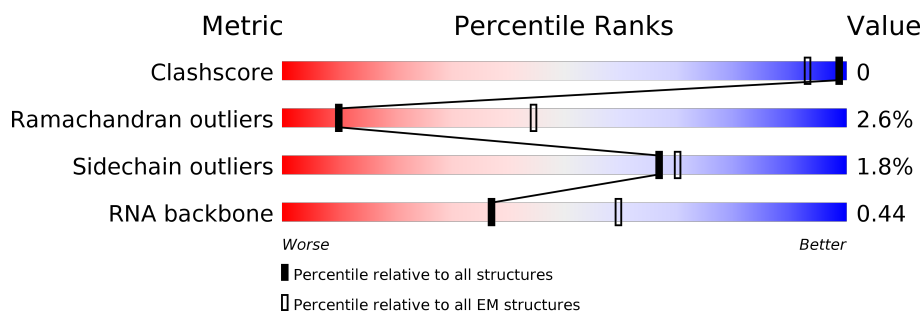
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 17.00 Å.

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















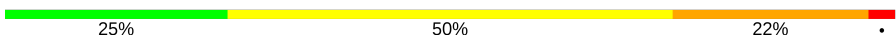
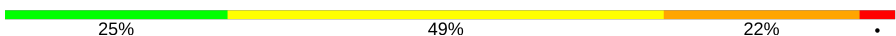
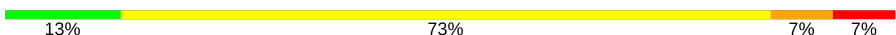










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AB	220	95% 5% •
2	AC	208	89% 10%
3	AD	206	88% 12%
4	AE	152	89% 11% •
5	AF	101	90% 9% •
6	AG	152	87% 13% •
7	AH	130	89% 10% •
8	AI	128	82% 16% •











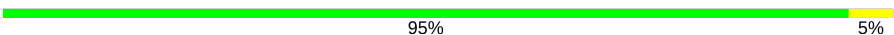





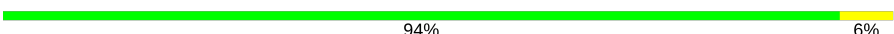



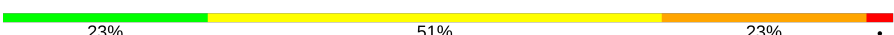
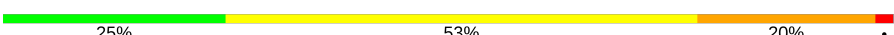

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Mol	Chain	Length	Quality of chain
9	AJ	100	 84% 15% .
10	AK	118	 92% 7% .
11	AL	124	 83% 15% ..
12	AM	115	 85% 14% .
13	AN	101	 86% 13% .
14	AO	89	 85% 13% .
15	AP	81	 84% 16%
16	AQ	82	 91% 9%
17	AR	57	 79% 21%
18	AS	81	 88% 11% .
19	AT	86	 93% 7%
20	AU	53	 79% 21%
21	AA	1533	 25% 50% 22% .
22	A1	76	 25% 49% 22% .
23	A2	15	 13% 73% 7% 7%
24	A3	77	 31% 45% 22% .
25	BC	273	 87% 12%
26	BD	209	 90% 9%
27	BE	201	 91% 9%
28	BF	179	 89% 11% .
29	BG	177	 89% 11% .
30	BH	149	 95% 5%
31	BI	142	 94% 5% .
32	BJ	142	 90% 10%
33	BK	123	 88% 11% ..

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Mol	Chain	Length	Quality of chain
34	BL	144	 85% 13% ..
35	BM	136	 85% 15%
36	BN	121	 87% 12% .
37	BO	117	 87% 11% ..
38	BP	115	 87% 12% .
39	BQ	118	 84% 15% .
40	BR	103	 90% 10%
41	BS	110	 89% 11%
42	BT	94	 85% 15%
43	BU	104	 89% 10% .
44	BV	94	 95% 5%
45	BW	80	 83% 14% ..
46	BX	79	 82% 14% ..
47	BY	63	 90% 10%
48	BZ	59	 83% 15% .
49	B0	57	 86% 12% .
50	B1	52	 94% 6%
51	B2	46	 78% 22%
52	B3	65	 85% 14% .
53	B4	38	 87% 13%
54	BA	2903	 23% 51% 23% .
55	BB	118	 25% 53% 20% ..
56	B5	234	 89% 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 L2.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

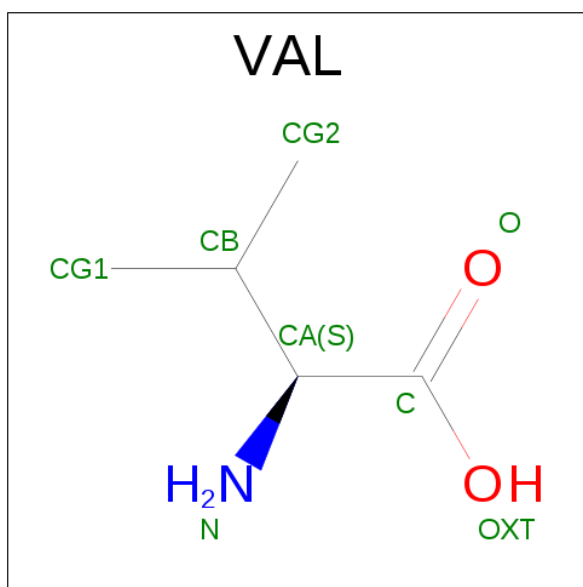
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

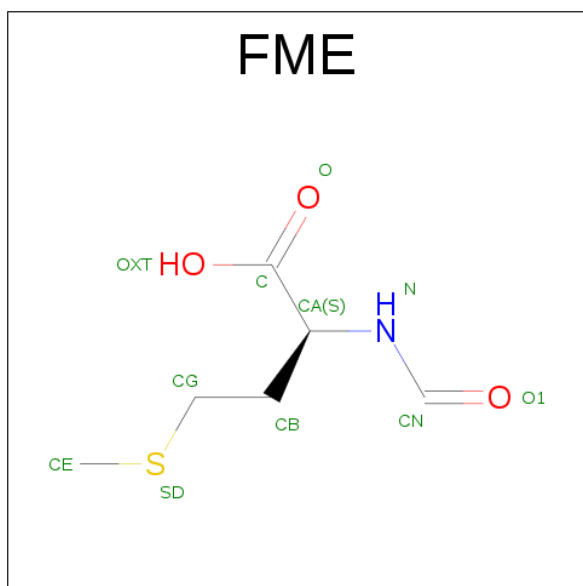
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

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



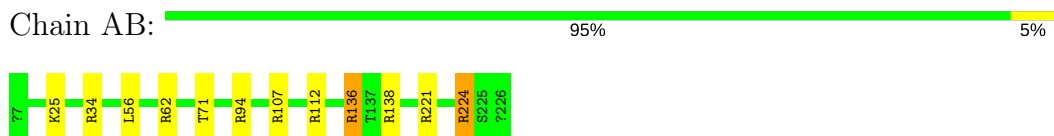
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



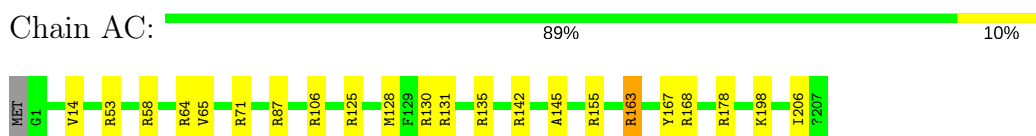
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

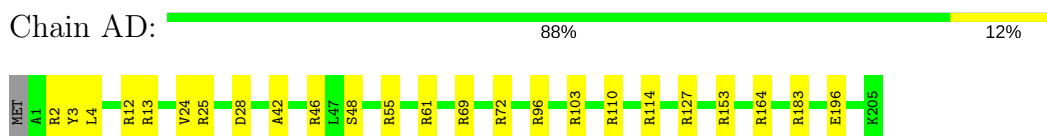
- Molecule 1: 30S ribosomal protein S2



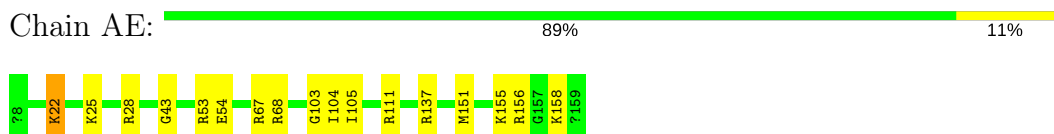
- Molecule 2: 30S ribosomal protein S3



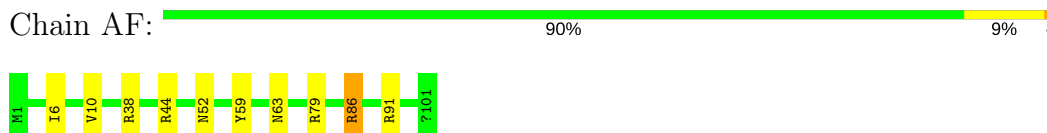
- Molecule 3: 30S ribosomal protein S4



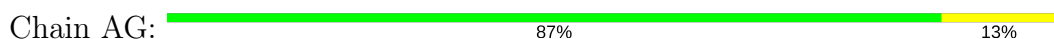
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 89% 10% .



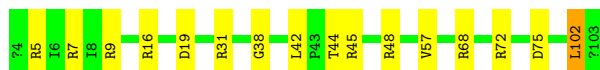
- Molecule 8: 30S ribosomal protein S9

Chain AI: 82% 16% .



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 84% 15% .



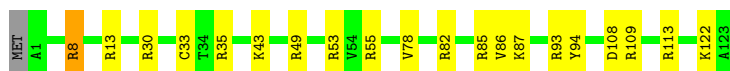
- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 7% .



- Molecule 11: 30S ribosomal protein S12

Chain AL: 83% 15% ..



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14% .

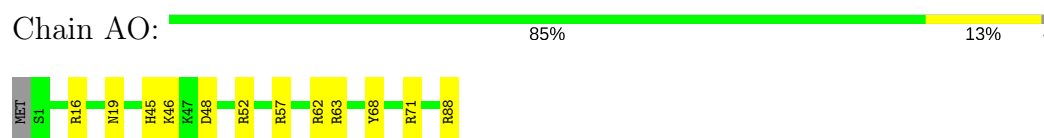


- Molecule 13: 30S ribosomal protein S14

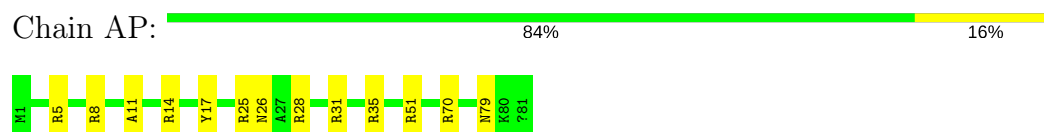
Chain AN: 86% 13% .



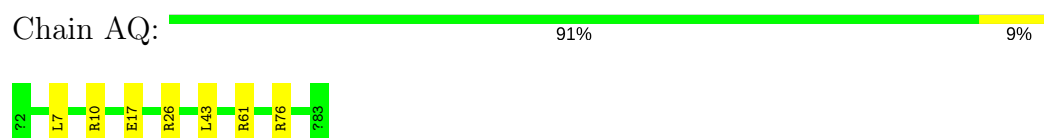
- Molecule 14: 30S ribosomal protein S15



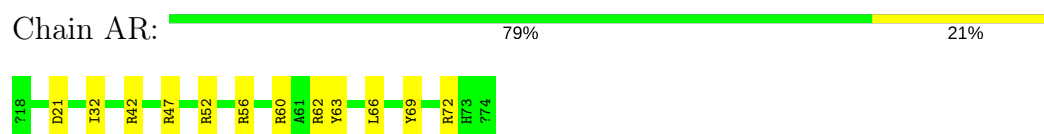
- Molecule 15: 30S ribosomal protein S16



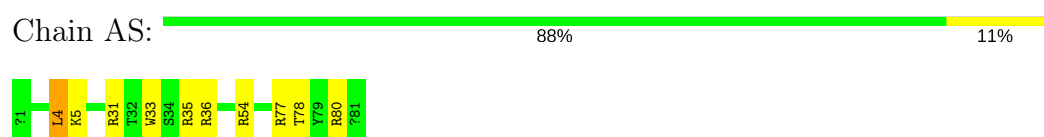
- Molecule 16: 30S ribosomal protein S17



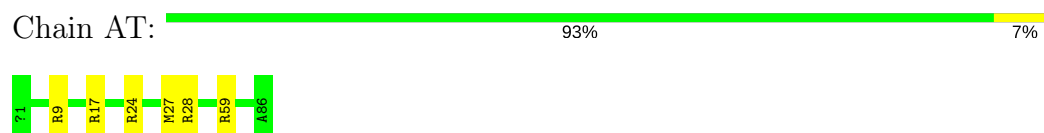
- Molecule 17: 30S ribosomal protein S18



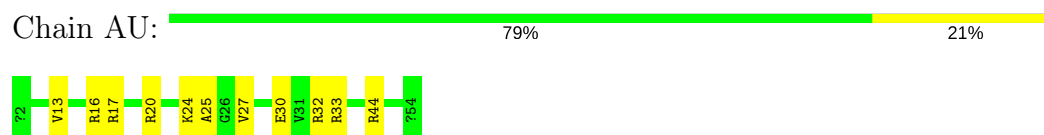
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



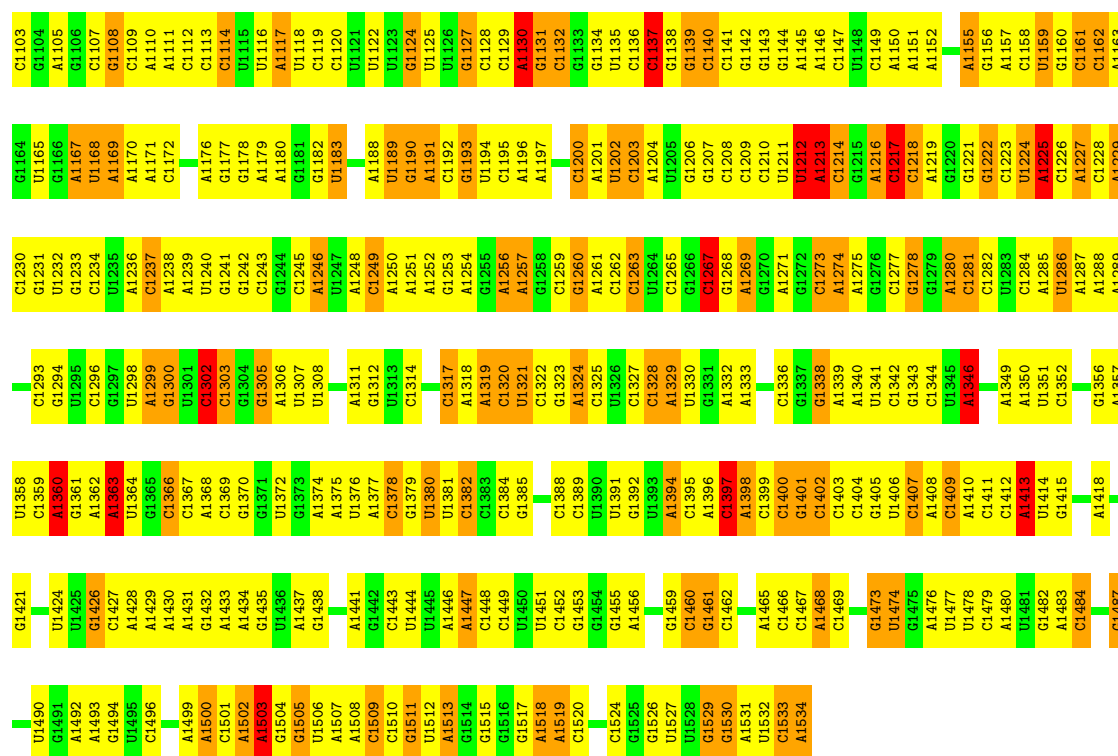
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA

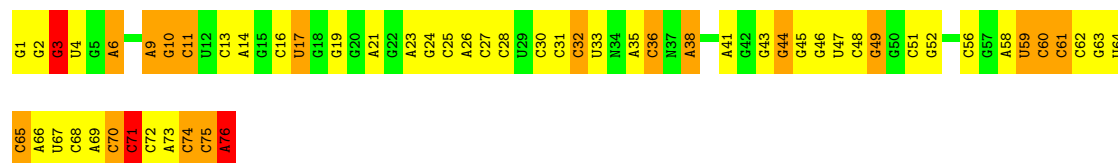




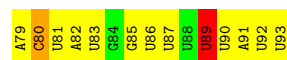
- Molecule 22: fMet-Val-tRNA-Val

Chain A1:  25% 49% 22% 4%



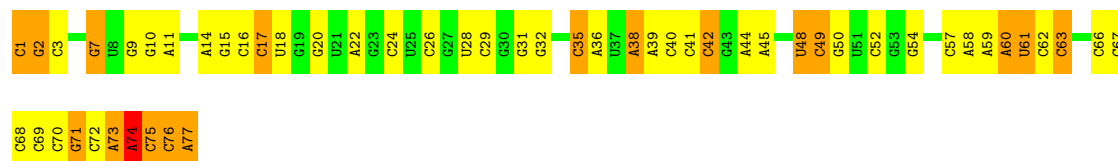
● Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

Chain A2:  13% 73% 7% 7%

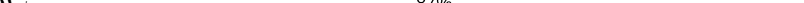


- Molecule 24: tRNA-fMet

Chain A3:  31% 45% 22%



- Molecule 25: 50S ribosomal protein L2

Chain BC:  87% 12%



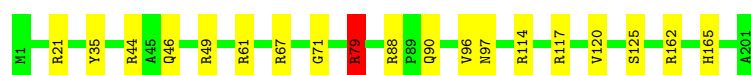
- Molecule 26: 50S ribosomal protein L3

Chain BD: 90% 9%



- Molecule 27: 50S ribosomal protein L4

Chain BE: 91% 9%



- Molecule 28: 50S ribosomal protein L5

Chain BF: 89% 11%



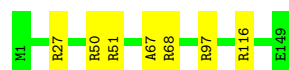
- Molecule 29: 50S ribosomal protein L6

Chain BG: 89% 11%



- Molecule 30: 50S ribosomal protein L9

Chain BH: 95% 5%



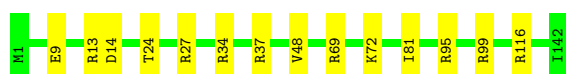
- Molecule 31: 50S ribosomal protein L11

Chain BI: 94% 5%



- Molecule 32: 50S ribosomal protein L13

Chain BJ: 90% 10%



- Molecule 33: 50S ribosomal protein L14

Chain BK: 88% 11% ..



- Molecule 34: 50S ribosomal protein L15

Chain BL: 85% 13% ..



- Molecule 35: 50S ribosomal protein L16

Chain BM: 85% 15%



- Molecule 36: 50S ribosomal protein L17

Chain BN: 87% 12% .



- Molecule 37: 50S ribosomal protein L18

Chain BO: 87% 11% ..



- Molecule 38: 50S ribosomal protein L19

Chain BP: 87% 12% .



- Molecule 39: 50S ribosomal protein L20

Chain BQ: 84% 15% .



- Molecule 40: 50S ribosomal protein L21

Chain BR:  90% 10%




- Molecule 41: 50S ribosomal protein L22

Chain BS:  89% 11%



- Molecule 42: 50S ribosomal protein L23

Chain BT:  85% 15%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  89% 10%




- Molecule 44: 50S ribosomal protein L25

Chain BV:  95% 5%




- Molecule 45: 50S ribosomal protein L27

Chain BW:  83% 14%



- Molecule 46: 50S ribosomal protein L28

Chain BX:  82% 14%




- Molecule 47: 50S ribosomal protein L29



Chain BY:  90% 10%




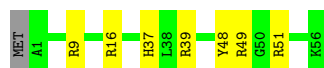
- Molecule 48: 50S ribosomal protein L30

Chain BZ:  83% 15%



- Molecule 49: 50S ribosomal protein L32

Chain B0:  86% 12%




- Molecule 50: 50S ribosomal protein L33

Chain B1:  94% 6%




- Molecule 51: 50S ribosomal protein L34

Chain B2:  78% 22%




- Molecule 52: 50S ribosomal protein L35

Chain B3:  85% 14%

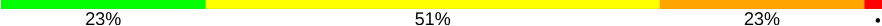


- Molecule 53: 50S ribosomal protein L36

Chain B4:  87% 13%



- Molecule 54: 23S ribosomal RNA

Chain BA:  23% 51% 23%




G2053	C1986	C1925	G1863	G1799	A1735	G1673	A1610	A1548	C1417	C1351	G1288	G1223	C1161	G1093
C2054	A1987	U1926	U1864	C1800	U1736	G1674	C1611	A1549	U1487	U1352	C1289		C1161	U1094
C2055		A1927	U1865	A1801	G1737	G1675	C1612	C1550		A1353	C1290		C1290	A1095
G2056	G1990	A1928	A1866	A1802	G1738	A1676	G1613	A1551	A1420	G1355	C1291	G1227	G1163	A1096
A2058	U1991	G1929	G1867	A1803	A1677	A1678	A1614	A1552	G1490	G1355	G1292	G1228	C1164	U1097
	G1992	C1930	C1868	C1804	G1740	A1678	C1615	A1553	G1491	G1356	C1293	C1229	A1165	A1098
A2059	U1993	A1931	G1869	A1805	C1741	A1679	A1616	A1554	G1492	C1357	U1294	A1230	G1166	G1099
A2060	G1994	A1932	C1870	C1806	U1742	U1680	C1617	G1555	C1493	G1358	C1295	A1231	C1167	C1100
G2061	U1995	G1933	A1871	G1807	G1743	G1681	A1618	C1556	A1494	A1359	G1296	G1232	G1168	U1101
A2062	C1996	C1934	A1872	A1808	A1744	G1682	G1619	C1557	A1495	G1360	C1297	G1233	A1169	C1102
C2063	C1997	G1935	G1873	A1869	A1745	U1683	G1620	C1558	A1496	G1361	C1298	C1233	C1170	A1103
C2064	A1998	A1936	C1874	A1810	A1746	G1684	U1621	U1559	U1497	C1362	G1299	G1236	G1171	C1104
C2065	U1999	A1937	G1875	G1811	U1747	C1685	G1622	G1560	C1498	C1363	G1300	A1237	G1172	
G2066	C2001	U1938	A1876	U1812	A1748	C1686	G1623	C1561	C1499	G1364	A1301	G1238	U1173	U1108
G2067	C2002	A1939	A1877	G1813	A1749		U1624	U1562	G1500	A1365	A1302	G1239	U1174	U1109
U2068	G2003	U1940	G1878	G1814		A1689	C1625	U1563	G1501	A1366	G1303	U1240	A1175	G1110
G2069	A2003	C1941	C1879	A1815	C1752	A1690	A1626	C1564	A1502	A1367	A1304	U1241	U1176	A1111
A2070	G2004	C1942	U1880	C1816	G1753	C1691	G1627	C1565	A1503		C1305	U1242	G1177	G1112
A2071	A2005	U1943	C1881			C1692	G1628			C1370	C1306	C1243	C1178	U1113
C2072	C2006	U1944	A1878	U1818	A1754	U1693	U1629	U1566	A1504	G1371	A1307	A1244	G1179	C1114
C2073	U2007	G1945	G1884	A1819	G1756	C1694	A1630	G1568	U1506	A1439	A1308	G1245	C1114	G1115
U2074	C2008	U1946	A1885	U1820	A1757	G1695	G1631	A1569	C1507	U1440	A1373	A1246	U1183	G1116
U2075	A2009	C1947	U1886	A1821	U1758	G1696	A1632	A1570	A1508	G1441		A1247	U1184	G1117
U2076		G1948	C1887	C1822	A1759	G1697	G1633	A1571	A1509	U1442			U1185	C1118
U2077	A2013	G1949	G1888	G1823	C1760	A1698	A1634	A1572		C1376	C1313		G1186	U1119
C2078	A2014	U1950	A1889	G1824	C1761	G1699	A1635	A1573	G1511	G1446	C1315	C1251	G1186	G1120
U2079	A2015	G1951	A1890	U1825	A1762	A1700	U1636	C1574	C1512	C1446	A1316	G1252	U1187	C1121
A2080	U2016	A1952	G1891	G1826	G1763	A1701	A1637	C1575	G1513	C1447		A1253	U1188	G1122
U2081	U2017	A1953	C1892	U1827	C1764	G1702	G1638	U1576	G1514		G1317	A1254	A1189	C1123
G2082	G2018	G1954	C1893	G1828	U1765	G1703	C1639	C1577	A1515		U1318	U1255	G1190	C1123
G2083	A2019	U1955	C1894	A1829	G1766	C1704	A1640	U1578		A1383	C1319	G1256	G1191	
C2084	A2020	G1956	A1895	C1830	G1767	A1705	A1641	A1579	C1518	A1384	C1320	C1257	G1192	A1126
U2085	C2021	C1957	G1896	G1831	C1768	A1706	G1642	A1580	U1519	A1385	A1321	U1258	G1193	A1127
U2086	U2022	G1958	G1897	C1832	U1769	G1707	G1643	G1581	U1520	C1386	A1322	G1259	A1194	G1128
G2087	C2023	G1959	U1898	C1833	G1770	C1708	G1644	C1582	G1521	G1456	C1323	A1260	G1195	A1129
A2088	G2024	A1960	A1899	G1834	C1771		C1645	A1583	A1522	G1388	G1324	C1261	C1196	
C2089	C2025	C1961	A1900	U1835	A1772		G1646	U1584	U1523	G1389	U1325	A1262	C1197	U1132
A2090		G1962	C1902	A1901	A1773	A1711	C1646	C1585	G1452	U1390	C1326	U1263	G1198	A1133
C2091	A2030	U1963	C1902	C1837	C1774	A1713	U1647	A1586	U1524	A1391	A1327	A1264	U1199	A1134
G2092	A2031	G1964	C1902	C1838	U1775	A1713	G1648		G1526	A1392	A1328	A1265	C1200	G1135
G2093	G2032	C1965	G1905	G1839		G1715	G1649	A1590	G1527	U1393	C1329	G1266	U1201	
A2094	A2033	A1966	G1906	G1840	A1780	G1715	G1650	A1591	A1528	A1394	U1330	U1267	G1202	G1139
C2095	U2034	G1967	C1907	U1841	U1781	U1716	G1651	A1591		A1395	G1331	A1268	U1203	C1140
G2096	G2035	U1968	G1908	C1842	U1781	A1717	A1652	C1592	C1531	U1396	G1332	A1269	U1204	U1411
A2097	C2036	A1969	C1909	C1843	A1783	G1719	G1653	A1593	U1532	U1397	G1333	C1270	A1205	A1142
U2098	U2037	U1970	G1910	C1844	A1784	G1720	A1654	U1594	A1469	C1398	G1334	G1271	G1206	A1143
G2099	G2038	C1971	U1911		A1785	G1721	A1655	C1595	C1533	A1470	C1335	A1272	C1207	A1144
C2100	U2039	G1972	A1912	A1847	A1786	G1722	U1656	A1596	U1534	G1337	G1336	U1273	C1208	C1145
A2101	G2040	U1973	A1913	A1848	A1787	G1723	U1657	A1597	A1535	G1338	G1337	A1274	U1209	C1146
C2102	U2041	C1974	C1914	U1849	C1788	G1724	C1658	A1598	C1472	C1403	A1275	A1274	U1209	A1147
C2103	A2042	G1975	U1915	U1852	A1789	G1725	G1659	U1599	U1474	G1473	A1276	A1276	G1211	U1148
C2104	C2043	U1976	A1916	A1853	C1790	C1726	A1664	C1600	G1538	U1476	G1340	G1277	G1212	G1149
U2105	C2044	A1977	U1917	A1854	A1791	C1727	A1665	G1601	U1539	U1476	G1341	C1278	A1213	C1150
	C2045	U1978	A1918	U1855	G1792	C1728	G1666	U1602	G1540	A1477	A1342		A1214	A1151
A2108			A1919	U1856	G1793	C1728	G1667	A1603	C1541	G1478	A1342	G1281	C1152	C1151
U2111	C2046	A1981	C1920	U1857	C1794	U1729	G1667	C1604	U1542	G1479	C1345	U1282	G1153	G1154
G2112	C2050	U1982	G1921	G1857	A1794	C1730	A1668	C1605	G1543	U1411	G1283	G1283	G1154	G1154
U2113	A2051	G1983	G1922	A1858	U1796	C1731	A1669	C1606	A1544	U1481	A1347	A1284	U1219	A1156
		G1984	G1922		C1795	C1732	C1670	C1607	A1545	G1482	C1348	A1285	G1220	A1156
U2114	A2052	C1985	U1923	G1861	G1797	G1733	U1671	A1608	G1546	U1415	C1349	A1286	G1221	G1157
				C1852	U1798	A1738	A1672	A1609	C1547	C1416	C1350	A1287	G1222	C1157



● Molecule 56: 50S ribosomal protein L1

Chain B5: 

89%

6%

5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	3052	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	162740	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	0.70	0/1736	1.07	11/2340 (0.5%)
10	AK	0.74	0/894	1.15	10/1207 (0.8%)
11	AL	0.76	0/969	1.23	15/1300 (1.2%)
12	AM	0.75	0/884	1.32	11/1181 (0.9%)
13	AN	0.77	0/817	1.26	12/1088 (1.1%)
14	AO	0.74	0/722	1.16	8/964 (0.8%)
15	AP	0.76	0/648	1.27	11/870 (1.3%)
16	AQ	0.70	0/658	1.06	4/883 (0.5%)
17	AR	0.81	0/463	1.29	10/623 (1.6%)
18	AS	0.76	0/653	1.13	7/879 (0.8%)
19	AT	0.68	0/672	1.05	5/890 (0.6%)
2	AC	0.72	0/1651	1.16	16/2225 (0.7%)
20	AU	0.83	0/431	1.44	8/572 (1.4%)
21	AA	1.53	1/36759 (0.0%)	2.22	1991/57346 (3.5%)
22	A1	1.53	0/1668	2.20	85/2595 (3.3%)
23	A2	1.47	0/343	2.25	15/531 (2.8%)
24	A3	1.53	0/1722	2.18	81/2685 (3.0%)
25	BC	0.74	0/2121	1.30	26/2852 (0.9%)
26	BD	0.68	0/1586	1.20	14/2134 (0.7%)
27	BE	0.67	0/1571	1.15	11/2113 (0.5%)
28	BF	0.74	0/1444	1.18	14/1937 (0.7%)
29	BG	0.69	0/1343	1.12	8/1816 (0.4%)
3	AD	0.77	0/1665	1.23	24/2227 (1.1%)
30	BH	0.65	0/1122	1.10	6/1515 (0.4%)
31	BI	0.65	0/1046	1.06	4/1410 (0.3%)
32	BJ	0.73	0/1152	1.16	8/1551 (0.5%)
33	BK	0.70	0/947	1.21	10/1268 (0.8%)
34	BL	0.73	0/1054	1.36	17/1403 (1.2%)
35	BM	0.74	0/1093	1.21	11/1460 (0.8%)
36	BN	0.77	0/973	1.36	15/1301 (1.2%)
37	BO	0.72	0/902	1.25	11/1209 (0.9%)
38	BP	0.75	0/929	1.27	8/1242 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.80	0/960	1.32	15/1278 (1.2%)
4	AE	0.70	0/1119	1.06	10/1506 (0.7%)
40	BR	0.70	0/829	1.22	7/1107 (0.6%)
41	BS	0.64	0/864	1.19	10/1156 (0.9%)
42	BT	0.65	0/744	1.19	7/994 (0.7%)
43	BU	0.68	0/787	1.10	4/1051 (0.4%)
44	BV	0.71	0/766	1.16	5/1025 (0.5%)
45	BW	0.77	0/604	1.36	9/799 (1.1%)
46	BX	0.75	0/635	1.28	10/848 (1.2%)
47	BY	0.65	0/510	1.17	5/677 (0.7%)
48	BZ	0.69	0/453	1.24	6/605 (1.0%)
49	B0	0.72	0/450	1.23	5/599 (0.8%)
5	AF	0.74	0/835	1.17	6/1128 (0.5%)
50	B1	0.73	0/417	1.05	2/556 (0.4%)
51	B2	0.81	0/380	1.49	11/498 (2.2%)
52	B3	0.72	0/513	1.23	5/676 (0.7%)
53	B4	0.68	0/303	1.24	4/397 (1.0%)
54	BA	1.41	2/69796 (0.0%)	2.21	4018/108888 (3.7%)
55	BB	1.42	0/2800	2.17	151/4367 (3.5%)
56	B5	0.64	0/1673	1.08	9/2255 (0.4%)
6	AG	0.74	0/1188	1.21	19/1593 (1.2%)
7	AH	0.70	0/989	1.08	5/1326 (0.4%)
8	AI	0.81	0/1035	1.34	20/1377 (1.5%)
9	AJ	0.69	0/797	1.23	13/1079 (1.2%)
All	All	1.28	3/160085 (0.0%)	2.00	6843/239402 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	1
14	AO	0	2
21	AA	0	368
22	A1	0	21
23	A2	0	4
24	A3	0	16
4	AE	0	1
43	BU	0	1
49	B0	0	1
54	BA	0	707

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	25
All	All	0	1147

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	6	G	C2-N2	-5.63	1.28	1.34
54	BA	1568	G	C2-N2	-5.08	1.29	1.34
54	BA	2627	G	C2-N2	-5.01	1.29	1.34

The worst 5 of 6843 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1301	A	O4'-C1'-N9	17.59	122.27	108.20
54	BA	2126	A	O4'-C1'-N9	13.48	118.98	108.20
21	AA	547	A	N1-C6-N6	-12.92	110.85	118.60
54	BA	323	C	O4'-C1'-N1	12.84	118.47	108.20
54	BA	2199	A	N1-C6-N6	-12.76	110.94	118.60

There are no chirality outliers.

5 of 1147 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	5	U	Sidechain
1	AB	224	ARG	Sidechain
4	AE	22	LYS	Peptide
14	AO	48	ASP	Peptide
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
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AE	1109	0	1152	1	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	2	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	0	0
21	AA	32828	0	16520	3	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	1	0
24	A3	1642	0	843	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	3	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	2	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	1	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31341	4	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99659	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)
34:BL:30:THR:HG21	34:BL:36:LYS:H	1.72	0.54
54:BA:388:G:H2'	54:BA:389:G:H3'	1.91	0.52
42:BT:15:HIS:CG	42:BT:16:VAL:H	2.29	0.50
21:AA:1054:C:C6	23:A2:89:U:H1'	2.48	0.48
37:BO:53:THR:HG21	37:BO:70:ALA:HB1	1.98	0.46

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	17 (8%)	1 (0%)	32	74
2	AC	205/208 (99%)	184 (90%)	15 (7%)	6 (3%)	5	38
3	AD	203/206 (98%)	185 (91%)	14 (7%)	4 (2%)	9	46
4	AE	150/152 (99%)	134 (89%)	10 (7%)	6 (4%)	3	31
5	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	2	22
6	AG	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	6	40
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	7	42
8	AI	126/128 (98%)	107 (85%)	15 (12%)	4 (3%)	5	36
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	26
10	AK	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	11	50
11	AL	121/124 (98%)	107 (88%)	8 (7%)	6 (5%)	2	27
12	AM	112/115 (97%)	94 (84%)	13 (12%)	5 (4%)	3	29
13	AN	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
14	AO	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	15	57
15	AP	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	4	32
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	10	49
18	AS	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	4	32
19	AT	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
20	AU	51/53 (96%)	32 (63%)	15 (29%)	4 (8%)	1	18
25	BC	270/273 (99%)	238 (88%)	25 (9%)	7 (3%)	6	40
26	BD	207/209 (99%)	185 (89%)	17 (8%)	5 (2%)	7	42
27	BE	199/201 (99%)	171 (86%)	20 (10%)	8 (4%)	3	31
28	BF	176/179 (98%)	155 (88%)	17 (10%)	4 (2%)	7	43
29	BG	174/177 (98%)	155 (89%)	12 (7%)	7 (4%)	3	31
30	BH	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	25	68
31	BI	139/142 (98%)	125 (90%)	12 (9%)	2 (1%)	13	54
32	BJ	140/142 (99%)	126 (90%)	11 (8%)	3 (2%)	8	45
33	BK	121/123 (98%)	107 (88%)	10 (8%)	4 (3%)	4	35
34	BL	141/144 (98%)	124 (88%)	11 (8%)	6 (4%)	3	29
35	BM	134/136 (98%)	115 (86%)	14 (10%)	5 (4%)	4	33
36	BN	119/121 (98%)	105 (88%)	11 (9%)	3 (2%)	6	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	108 (95%)	3 (3%)	3 (3%)	6	40
38	BP	112/115 (97%)	92 (82%)	17 (15%)	3 (3%)	6	40
39	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	11	50
40	BR	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	5	37
41	BS	108/110 (98%)	105 (97%)	2 (2%)	1 (1%)	20	63
42	BT	92/94 (98%)	80 (87%)	6 (6%)	6 (6%)	1	22
43	BU	101/104 (97%)	83 (82%)	14 (14%)	4 (4%)	3	31
44	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
45	BW	78/80 (98%)	59 (76%)	17 (22%)	2 (3%)	6	40
46	BX	75/79 (95%)	68 (91%)	3 (4%)	4 (5%)	2	26
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	49 (88%)	4 (7%)	3 (5%)	2	25
49	B0	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
52	B3	62/65 (95%)	54 (87%)	5 (8%)	3 (5%)	2	28
53	B4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6	39
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	32	74
All	All	5876/6008 (98%)	5245 (89%)	476 (8%)	155 (3%)	10	40

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	224	ARG
2	AC	14	VAL
5	AF	86	ARG
15	AP	11	ALA
15	AP	17	TYR

### 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%)	66	84
2	AC	170/171 (99%)	168 (99%)	2 (1%)	75	88
3	AD	172/173 (99%)	171 (99%)	1 (1%)	89	94
4	AE	113/113 (100%)	112 (99%)	1 (1%)	82	91
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	85	92
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%)	83 (96%)	3 (4%)	41	69
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	80	90
12	AM	91/92 (99%)	90 (99%)	1 (1%)	78	89
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%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	35	65
17	AR	48/48 (100%)	45 (94%)	3 (6%)	21	53
18	AS	70/70 (100%)	69 (99%)	1 (1%)	71	86
19	AT	65/65 (100%)	64 (98%)	1 (2%)	70	85
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	49	74
26	BD	164/164 (100%)	160 (98%)	4 (2%)	54	78
27	BE	165/165 (100%)	162 (98%)	3 (2%)	64	84
28	BF	149/150 (99%)	147 (99%)	2 (1%)	73	87
29	BG	137/138 (99%)	133 (97%)	4 (3%)	48	73
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	82	91
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	51	75
33	BK	103/103 (100%)	102 (99%)	1 (1%)	80	90
34	BL	102/103 (99%)	100 (98%)	2 (2%)	60	82
35	BM	109/109 (100%)	107 (98%)	2 (2%)	64	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	80	90
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	60	82
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	57	79
40	BR	84/84 (100%)	84 (100%)	0	100	100
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%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	53 (90%)	6 (10%)	8	33
46	BX	67/68 (98%)	66 (98%)	1 (2%)	70	85
47	BY	55/55 (100%)	54 (98%)	1 (2%)	64	84
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	59	80
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%)	48 (94%)	3 (6%)	23	55
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	169 (98%)	4 (2%)	56	79
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	67	84

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

Mol	Chain	Res	Type
26	BD	15	PHE
29	BG	148	ARG
52	B3	37	THR
26	BD	33	ARG
27	BE	79	ARG

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

Mol	Chain	Res	Type
12	AM	104	ASN

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Mol	Chain	Res	Type
44	BV	88	HIS
46	BX	15	ASN
49	B0	41	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	248 (16%)	0
22	A1	73/76 (96%)	15 (20%)	0
23	A2	14/15 (93%)	5 (35%)	0
24	A3	76/77 (98%)	13 (17%)	0
54	BA	2902/2903 (99%)	464 (15%)	0
55	BB	116/118 (98%)	15 (12%)	0
All	All	4710/4722 (99%)	760 (16%)	0

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	16	A

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	21,22	16,26,27	1.90	3 (18%)	14,37,40	3.35	3 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	6MZ	A1	37	22	18,25,26	1.05	1 (5%)	16,36,39	1.68	2 (12%)
22	7MG	A1	46	22	20,26,27	2.19	3 (15%)	22,39,42	1.92	2 (9%)
22	5MU	A1	54	22	14,22,23	1.29	2 (14%)	16,32,35	4.09	2 (12%)
22	PSU	A1	55	22	16,21,22	1.11	1 (6%)	20,30,33	5.31	7 (35%)
22	4SU	A1	7	22	14,21,22	1.19	1 (7%)	15,30,33	2.77	4 (26%)
24	H2U	A3	21	24	17,21,22	1.51	2 (11%)	21,30,33	1.32	4 (19%)
24	OMC	A3	33	24	15,22,23	1.24	0	19,31,34	1.05	1 (5%)
24	5MU	A3	55	24	14,22,23	1.09	1 (7%)	16,32,35	3.86	3 (18%)
24	PSU	A3	56	24	16,21,22	1.36	2 (12%)	20,30,33	5.54	7 (35%)
24	4SU	A3	8	24	14,21,22	1.32	3 (21%)	15,30,33	2.80	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	21,22	-	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 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.13	1.33	1.45
22	A1	34	CM0	O5-C5	-6.13	1.25	1.37
24	A3	21	H2U	C4-N3	-3.60	1.31	1.37
24	A3	21	H2U	C2-N3	-3.45	1.31	1.38
22	A1	46	7MG	C8-N7	-2.76	1.31	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	56	PSU	N1-C2-N3	-16.31	116.67	128.40
22	A1	55	PSU	N1-C2-N3	-15.43	117.30	128.40
24	A3	56	PSU	C5-C4-N3	-12.61	115.08	125.43
22	A1	55	PSU	C5-C4-N3	-12.19	115.43	125.43
22	A1	54	5MU	C5-C4-N3	-9.96	114.26	125.24

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	6,6,7	1.45	1 (16%)	6,7,9	2.30	2 (33%)
58	FME	BA	3001	57	9,9,10	1.31	1 (11%)	7,9,11	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	58,22	-	0/5/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A1	101	VAL	CA-C	3.21	1.54	1.50
58	BA	3001	FME	CA-C	3.54	1.54	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-4.27	115.18	125.15
57	A1	101	VAL	C-CA-N	3.62	117.17	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.