



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:08 PM BST

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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

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

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

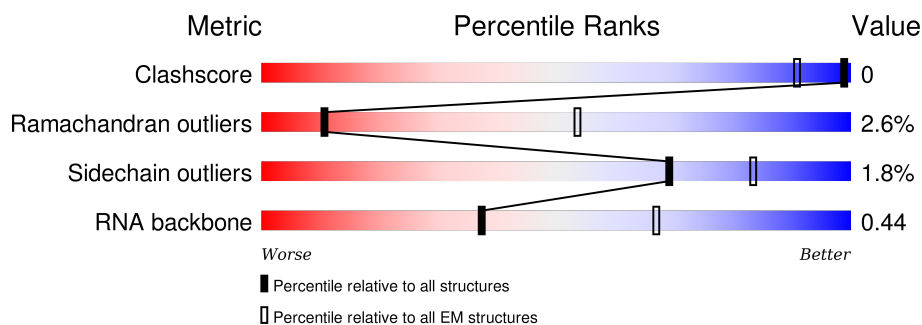
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 Å.

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















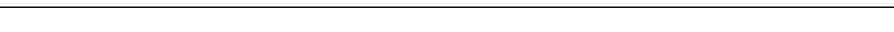

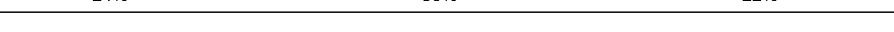
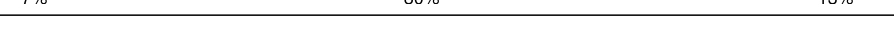
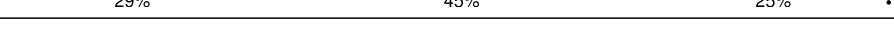





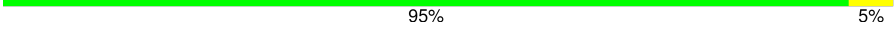


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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


















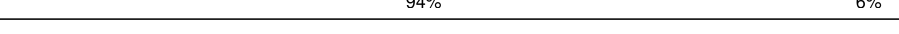



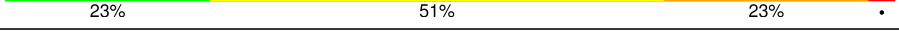
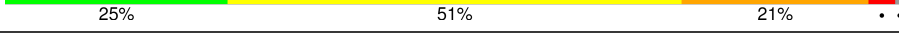
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Mol	Chain	Length	Quality of chain
9	AJ	100	 84% 15% .
10	AK	118	 92% 7% .
11	AL	124	 83% 15% ..
12	AM	115	 85% 14% .
13	AN	101	 86% 13% .
14	AO	89	 85% 13% .
15	AP	81	 84% 16%
16	AQ	82	 91% 9%
17	AR	57	 79% 21%
18	AS	81	 88% 11% .
19	AT	86	 93% 7%
20	AU	53	 79% 21%
21	AA	1533	 25% 49% 22% .
22	A1	76	 24% 50% 22% .
23	A2	15	 7% 80% 13%
24	A3	77	 29% 45% 25% .
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	
35	BM	136	
36	BN	121	
37	BO	117	
38	BP	115	
39	BQ	118	
40	BR	103	
41	BS	110	
42	BT	94	
43	BU	104	
44	BV	94	
45	BW	80	
46	BX	79	
47	BY	63	
48	BZ	59	
49	B0	57	
50	B1	52	
51	B2	46	
52	B3	65	
53	B4	38	
54	BA	2903	
55	BB	118	
56	B5	234	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	ACETYLATION	UNP P0A7V0
AB	226	NH2	-	AMIDATION	UNP P0A7V0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AC	207	Total	C	N	O	S	0	1
			1625	1028	306	288	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	207	NH2	-	AMIDATION	UNP P0A7V3

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	152	Total	C	N	O	S	0	1
			1109	689	212	202	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	ACETYLATION	UNP P0A7W1
AE	159	NH2	-	AMIDATION	UNP P0A7W1

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	101	Total	C	N	O	S	0	1
			818	515	149	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	101	NH2	-	AMIDATION	UNP P02358

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	152	Total	C	N	O	S	0	1
			1178	732	227	215	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	ACETYLATION	UNP P02359
AG	152	NH2	-	AMIDATION	UNP P02359

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AI	128	Total	C	N	O	S	0	0
			1025	636	206	180	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	2	ACE	-	ACETYLATION	UNP P0A7X3

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AJ	100	Total	C	N	O	S	0	1
			790	495	151	143	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	ACETYLATION	UNP P0A7R5
AJ	103	NH2	-	AMIDATION	UNP P0A7R5

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	118	Total	C	N	O	S	0	0
			880	542	174	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	11	ACE	-	ACETYLATION	UNP P0A7R9

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AM	114	Total	C	N	O	S	0	1
			877	541	178	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	114	NH2	-	AMIDATION	UNP P0A7S9

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AN	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	81	Total	C	N	O	S	0	1
			639	400	127	111	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP	81	NH2	-	AMIDATION	UNP P0A7T3

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	82	Total	C	N	O	S	0	1
			652	413	122	114	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	ACETYLATION	UNP P0AG63
AQ	83	NH2	-	AMIDATION	UNP P0AG63

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AR	57	Total	C	N	O	0	1
			459	290	87	82		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	18	ACE	-	ACETYLATION	UNP P0A7T7

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Chain	Residue	Modelled	Actual	Comment	Reference
AR	74	NH2	-	AMIDATION	UNP P0A7T7

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AS	81	Total	C	N	O	S	0	1
			641	410	121	108	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	ACETYLATION	UNP P0A7U3
AS	81	NH2	-	AMIDATION	UNP P0A7U3

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AT	86	Total	C	N	O	S	0	0
			668	413	137	115	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	1	ACE	-	ACETYLATION	UNP P0A7U7

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AU	53	Total	C	N	O	S	0	1
			429	267	87	74	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	ACETYLATION	UNP P68679
AU	54	NH2	-	AMIDATION	UNP P68679

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32828	14642	6024	10633	1529		

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	A1	76	Total	C	N	O	P	S	0	0
			1627	728	292	531	75	1		

- Molecule 23 is a RNA chain called 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*P*AP*UP*U)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	15	Total	C	N	O	P	0	0
			309	140	46	109	14		

- Molecule 24 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1642	734	297	534	76	1		

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

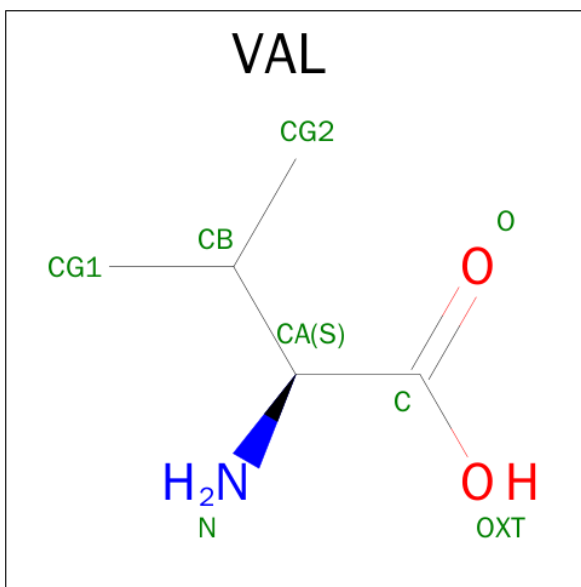
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

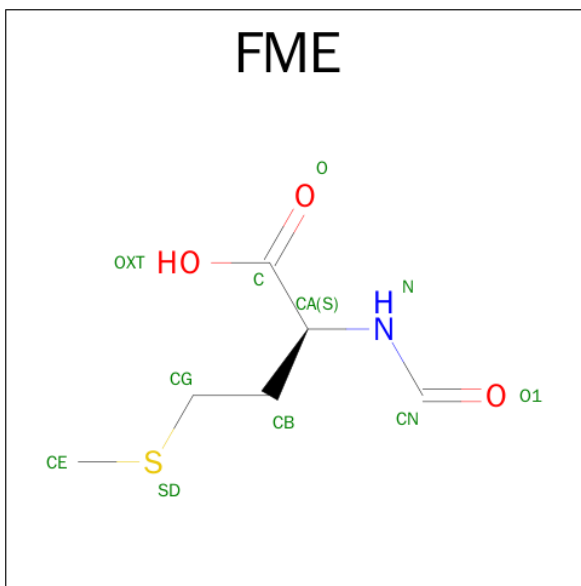
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: 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: C₆H₁₁NO₃S).

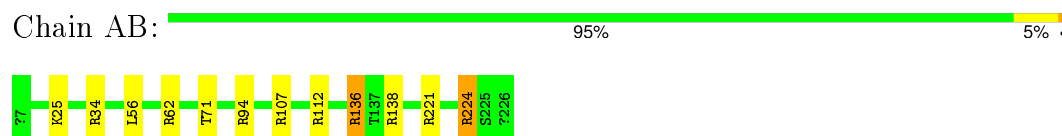


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

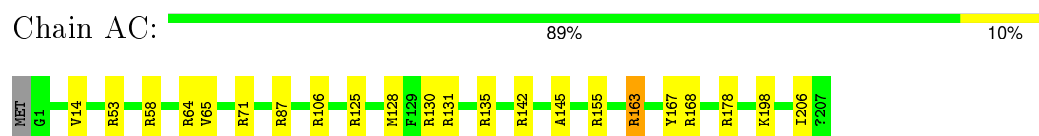
3 Residue-property plots [i](#)

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

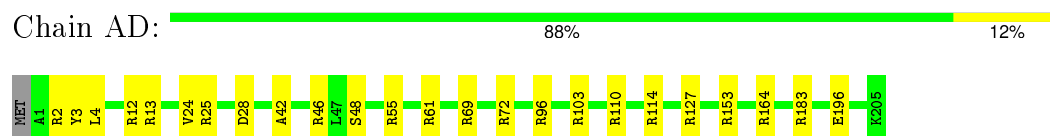
- Molecule 1: 30S ribosomal protein S2



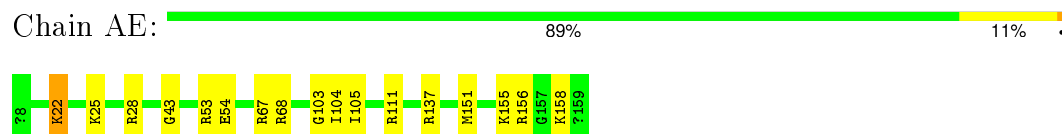
- Molecule 2: 30S ribosomal protein S3



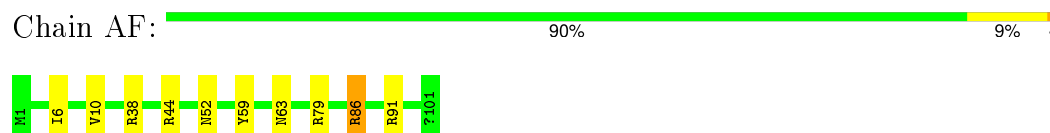
- Molecule 3: 30S ribosomal protein S4



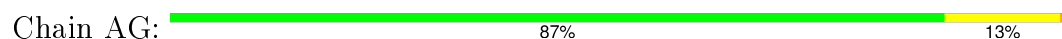
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 89% 10%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 82% 16%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 84% 15%



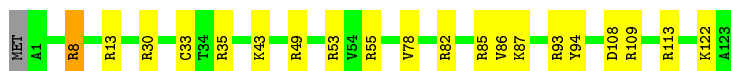
- Molecule 10: 30S ribosomal protein S11

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

Chain AO:  85% 13%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  84% 16%




- Molecule 16: 30S ribosomal protein S17

Chain AQ:  91% 9%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  79% 21%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  88% 11%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  93% 7%



- Molecule 20: 30S ribosomal protein S21

Chain AU:  79% 21%



- Molecule 21: 16S ribosomal RNA

Chain AA:  25% 49% 22%

A1036	A1037	C1038	G1039	A1042	G1043	A1044	C1045	G1046	A1047	G1048	C1049	A1050	G1051	C1052	G1053	C1054	A1055	G1056	C1057	G1058	C1059	A1060	G1061	C1062	G1063	C1064	A1065	G1066	C1067	G1068	C1069	G1070	C1071	G1075	C1076	G1077	C1078	G1079	A1080	C1081	A1082	G1083	C1084	G1085	C1086	A1092	C1093	G1094	C1095	G1096	C1097	G1098	C1099	A1100	G1101	C1102	A1103	G1104	C1105	A1106	G1107	C1108	A1109	G1110	C1111	A1114	C1115	A1116	G1117	C1118	A1119	C1120	G1121	C1122	A1123	G1124	C1125	A1126	G1127	C1128	A1129	G1130	C1131	A1132	G1133	C1134	A1135	G1136	C1137	A1138	G1139	C1140	A1141	G1142	C1143	A1144	G1145	C1146	A1147	G1148	C1149	A1150	G1151	C1152	A1153	G1154	C1155	A1156	G1157	C1158	A1159	G1160	C1161	A1162	G1163	C1164	A1165	G1166	C1167	A1168	G1169	C1170	A1171	G1172	C1173	A1174	G1175	C1176	A1177	G1178	C1179	A1180	G1181	C1182	A1183	G1184	C1185	A1186	G1187	C1188	A1189	G1190	C1191	A1192	G1193	C1194	A1195	G1196	C1197	A1198	G1199	C1200	A1201	G1202	C1203	A1204	G1205	C1206	A1207	G1208	C1209	A1210	G1211	C1212	A1213	G1214	C1215	A1216	G1217	C1218	A1219	G1220	C1221	A1222	G1223	C1224	A1225	G1226	C1227	A1228	G1229	C1230	A1231	G1232	C1233	A1234	G1235	C1236	A1237	G1238	C1239	A1240	G1241	C1242	A1243	G1244	C1245	A1246	G1247	C1248	A1249	G1250	C1251	A1252	G1253	C1254	A1255	G1256	C1257	A1258	G1259	C1260	A1261	G1262	C1263	A1264	G1265	C1266	A1267	G1268	C1269	A1270	G1271	C1272	A1273	G1274	C1275	A1276	G1277	C1278	A1279	G1280	C1281	A1282	G1283	C1284	A1285	G1286	C1287	A1288	G1289	C1290	A1291	G1292	C1293	A1294	G1295	C1296	A1297	G1298	C1299	A1300	G1301	C1302	A1303	G1304	C1305	A1306	G1307	C1308	A1309	G1310	C1311	A1312	G1313	C1314	A1315	G1316	C1317	A1318	G1319	C1320	A1321	G1322	C1323	A1324	G1325	C1326	A1327	G1328	C1329	A1330	G1331	C1332	A1333	G1334	C1335	A1336	G1337	C1338	A1339	G1340	C1341	A1342	G1343	C1344	A1345	G1346	C1347	A1348	G1349	C1350	A1351	G1352	C1353	A1354	G1355	C1356	A1357	G1358	C1359	A1360	G1361	C1362	A1363	G1364	C1365	A1366	G1367	C1368	A1369	G1370	C1371	A1372	G1373	C1374	A1375	G1376	C1377	A1378	G1379	C1380	A1381	G1382	C1383	A1384	G1385	C1386	A1387	G1388	C1389	A1390	G1391	C1392	A1393	G1394	C1395	A1396	G1397	C1398	A1399	G1400	C1401	A1402	G1403	C1404	A1405	G1406	C1407	A1408	G1409	C1410	A1411	G1412	C1413	A1414	G1415	C1416	A1417	G1418	C1419	A1420	G1421	C1422	A1423	G1424	C1425	A1426	G1427	C1428	A1429	G1430	C1431	A1432	G1433	C1434	A1435	G1436	C1437	A1438	G1439	C1440	A1441	G1442	C1443	A1444	G1445	C1446	A1447	G1448	C1449	A1450	G1451	C1452	A1453	G1454	C1455	A1456	G1457	C1458	A1459	G1460	C1461	A1462	G1463	C1464	A1465	G1466	C1467	A1468	G1469	C1470	A1471	G1472	C1473	A1474	G1475	C1476	A1477	G1478	C1479	A1480	G1481	C1482	A1483	G1484	C1485	A1486	G1487	C1488	A1489	G1490	C1491	A1492	G1493	C1494	A1495	G1496	C1497	A1498	G1499	C1500	A1501	G1502	C1503	A1504	G1505	C1506	A1507	G1508	C1509	A1510	G1511	C1512	A1513	G1514	C1515	A1516	G1517	C1518	A1519	G1520	C1521	A1522	G1523	C1524	A1525	G1526	C1527	A1528	G1529	C1530	A1531	G1532	C1533	A1534	G1535	C1536	A1537	G1538	C1539	A1540	G1541	C1542	A1543	G1544	C1545	A1546	G1547	C1548	A1549	G1550	C1551	A1552	G1553	C1554	A1555	G1556	C1557	A1558	G1559	C1560	A1561	G1562	C1563	A1564	G1565	C1566	A1567	G1568	C1569	A1570	G1571	C1572	A1573	G1574	C1575	A1576	G1577	C1578	A1579	G1580	C1581	A1582	G1583	C1584	A1585	G1586	C1587	A1588	G1589	C1590	A1591	G1592	C1593	A1594	G1595	C1596	A1597	G1598	C1599	A1600	G1601	C1602	A1603	G1604	C1605	A1606	G1607	C1608	A1609	G1610	C1611	A1612	G1613	C1614	A1615	G1616	C1617	A1618	G1619	C1620	A1621	G1622	A1623	C1624	A1625	G1626	C1627	A1628	G1629	C1630	A1631	G1632	C1633	A1634	G1635	C1636	A1637	G1638	C1639	A1640	G1641	C1642	A1643	G1644	C1645	A1646	G1647	C1648	A1649	G1650	C1651	A1652	G1653	C1654	A1655	G1656	C1657	A1658	G1659	C1660	A1661	G1662	C1663	A1664	G1665	C1666	A1667	G1668	C1669	A1670	G1671	C1672	A1673	G1674	C1675	A1676	G1677	C1678	A1679	G1680	C1681	A1682	G1683	C1684	A1685	G1686	C1687	A1688	G1689	C1690	A1691	G1692	C1693	A1694	G1695	C1696	A1697	G1698	C1699	A1700	G1701	C1702	A1703	G1704	C1705	A1706	G1707	C1708	A1709	G1710	C1711	A1712	G1713	C1714	A1715	G1716	C1717	A1718	G1719	C1720	A1721	G1722	C1723	A1724	G1725	C1726	A1727	G1728	C1729	A1730	G1731	C1732	A1733	G1734	C1735	A1736	G1737	C1738	A1739	G1740	C1741	A1742	G1743	C1744	A1745	G1746	C1747	A1748	G1749	C1750	A1751	G1752	A1753	C1754	A1755	G1756	C1757	A1758	C1759	A1760	G1761	C1762	A1763	G1764	C1765	A1766	G1767	C1768	A1769	G1770	C1771	A1772	G1773	C1774	A1775	G1776	C1777	A1778	G1779	C1780	A1781	G1782	C1783	A1784	G1785	C1786	A1787	G1788	C1789	A1790	G1791	C1792	A1793	G1794	C1795	A1796	G1797	C1798	A1799	G1800	C1801	A1802	G1803	C1804	A1805	G1806	C1807	A1808	G1809	C1810	A1811	G1812	C1813	A1814	G1815	C1816	A1817	G1818	C1819	A1820	G1821	C1822	A1823	G1824	C1825	A1826	G1827	C1828	A1829	G1830	C1831	A1832	G1833	C1834	A1835	G1836	C1837	A1838	G1839	C1840	A1841	G1842	C1843	A1844	G1845	C1846	A1847	G1848	C1849	A1850	G1851	C1852	A1853	G1854	C1855	A1856	G1857	C1858	A1859	G1860	C1861	A1862	G1863	C1864	A1865	G1866	C1867	A1868	G1869	C1870	A1871	G1872	C1873	A1874	G1875	C1876	A1877	G1878	C1879	A1880	G1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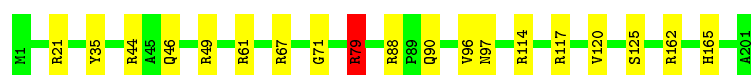
- Molecule 26: 50S ribosomal protein L3

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% ..



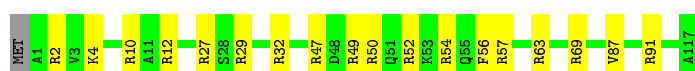
- Molecule 38: 50S ribosomal protein L19

Chain BP: 87% 12% .

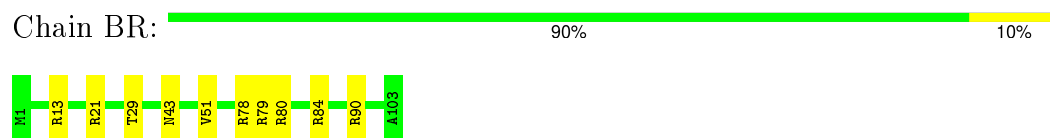


- Molecule 39: 50S ribosomal protein L20

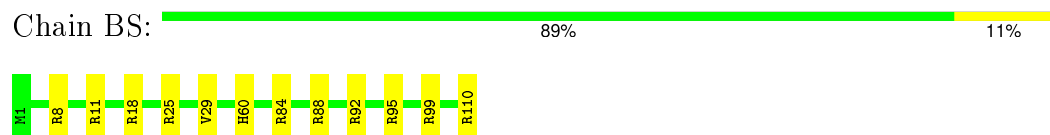
Chain BQ: 84% 15%



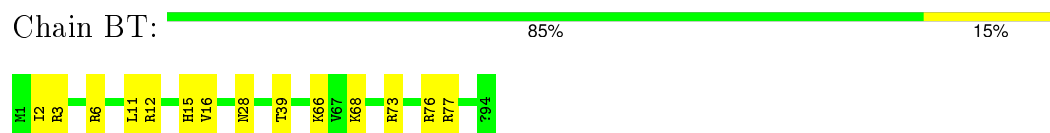
- Molecule 40: 50S ribosomal protein L21



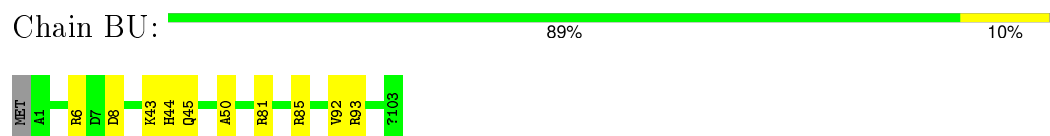
- Molecule 41: 50S ribosomal protein L22



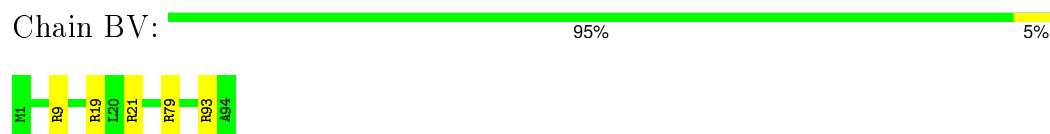
- Molecule 42: 50S ribosomal protein L23



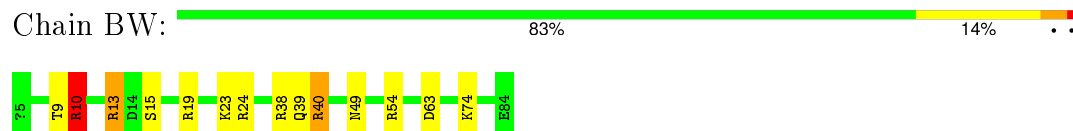
- Molecule 43: 50S ribosomal protein L24



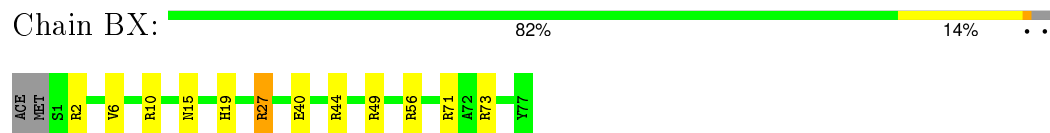
- Molecule 44: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28




- Molecule 47: 50S ribosomal protein L29

Chain BY:  90% 10%




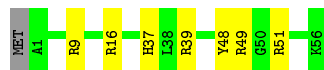
- Molecule 48: 50S ribosomal protein L30

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%

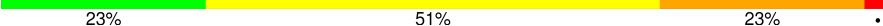


- Molecule 53: 50S ribosomal protein L36

Chain B4:  87% 13%

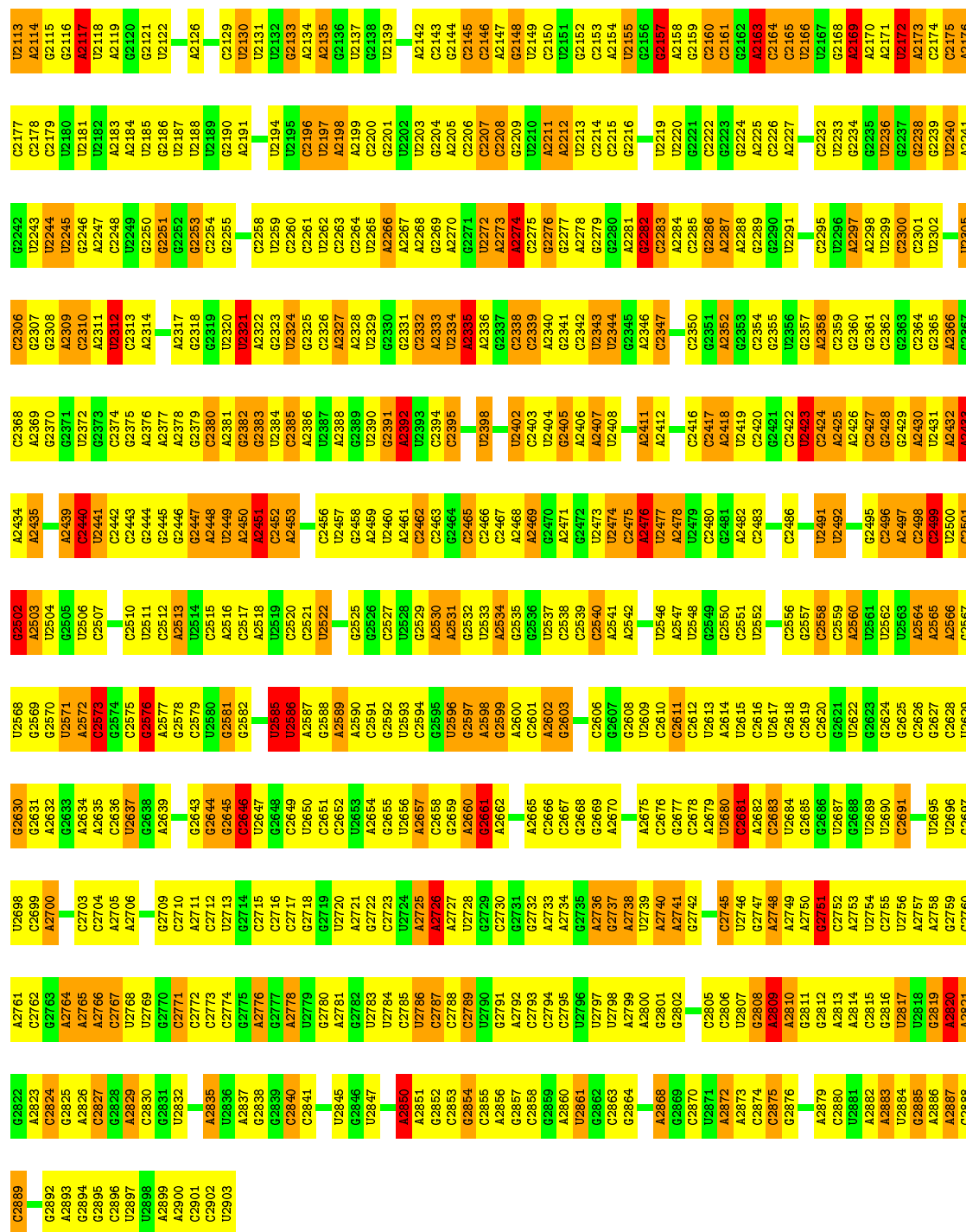


- Molecule 54: 23S ribosomal RNA

Chain BA:  23% 51% 23%

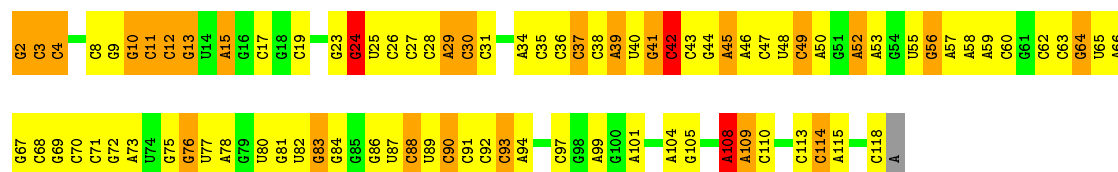
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A1028	U967	A905	A843			A843	C581	G518	A452	G389	G266	U202		G69	U3
A1029	G968	U906	A844	U779	A715	A644	A582		A453	U390	C267	A203		G70	U4
G1030	G969	G907	A845	G780	A716	U645	G583	A521	A454	A391	C268	A204		A71	A5
G1031	U970	C908	A846	U781	C717	U646	C584	A522	A455	U392	C269	G205		U72	A6
A1032	G971	A909	U846	A782	A718	G647	G585	C523	A456	U393	A270	U206		A73	G7
A1033	A972	A910	U847	A783	C719		A586	G524	A457	C394	G271	A207		A74	C8
G1034	A973	A911	C848	G784	U720	C850	C587	G525	U458	U395	A272	C208		G75	G9
U1035	A974	G912	A849	C785	A721	U651	U588	A526	U459	C396	C273	C209		A76	C10
	A975	U913	U850	C786	A722	U652	U589	C527	A460	C397	C274	C210		A77	C11
		G914	C851	C787	G723	U653	U590	A528	C461	U398	C275	C211		U78	U12
A1039	G978	C915	U852	A788	U724	A654	U591	A529	C462	G400	U276	G212		C79	U13
A1040	A979	G916	C853	A789	G725	A655	A592	G530	G463	A401	G277	A213		G80	A14
C1043	A980	A917	C854	U790	G726	A656	U593	C531		A402	A278	G214		G81	G15
C1044	A981	A918	U855	C791	A727	U657	U594	A532	A466	U403	C279	G215		U82	C16
C1045	C982	U919	G856	U792	A727		C595	G533		U404	C280	A216		A83	A19
A1046	A983	A920	C857	A793	A730	C660	U596		A470	A405	C281	A217		A84	C20
G1047	A984	C921	C858	A794	C731	A661		G537	A471	G406	A282	A218			C21
A1048	C985	G922	U859	C795	C732		A599	A538	A472	G407	G283	A219		A89	A22
C1049	C986	G923	C860	C796	G733	G664	G600	G539	G473	G408	G284	G220		U90	C22
A1050	C987	G924	A861		A734	U665	C601	C540	A474	G409	G285	A221		A91	
G1051	A988	A925	G862		A735	A666	A602	A541	C475	G410		A222		U92	A28
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C1056	G993	G930	C867	A804	C740	C671	A608	U546	A480	G415		A227		C97	C33
A1057	C994	U931	U868	G905	U741	C672	A609	A547	C481	U416	A294	G228		G98	U34
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G1062	U999	A936	C874	U810	U747	C678	A613	U552	C486	C421	A299	A233		A103	G39
C1063	A1000	C937	G875	U811	G748	A679	A614	G553	C487	A422	A300			A104	U40
C1064		G938	C876	C812	A749	C679	U615	U554		A423				C105	C41
A1067	G1002	G939	A877	U813	A750	C680	A616	G555	C490					C106	A42
G1003	U1004	G940	A878	C814	A751	G681	G617	A556	C491	C426				G107	G43
C1005	C1006	A941		C815	A752			C557	A492	U427	U304	C236		G108	A44
A1070	G1007	G942	G881	C816	A753	U686	G620	U558	A493	A428	C305	C240		G109	G45
G1071	C1008	A943	G882	C817	U754	C887	A621	G559	A494	A430	U306	A241		G110	G46
A1072	A1009	G944	U883	C818	U755	C888	G622	C560	G495	A431	G307	G242		G111	C47
C1073	C1009	A945	U884	A819	G756	U688	C623	G561	A496	U432	G308	U243		C179	A48
G1074	A1010	G946	C885	A820	G757	A689	C624	U562	A497	A432	A309	A244		U114	A49
C1075	U1011	C948	A886	A821	C758	G900	G625	A563		C433	A310	G245		C115	U50
U1076	U1012		U887	G822	G759	C691	A626	C564	G500	G372	G312	G246		G117	A52
A1077	C1013		C888	U823	G760	C692	A627	C565	A501	U373	G313	G247		C184	G51
C1079	A1014	C951	C889	U824	A761	A693	G628	U566	A502	A374	G314	G248		A118	A53
U1080	U1015		C890	A825	U762	U694	G629	U567	A503	G375	C314	C249		A119	
	G1016	G954	A891		G763	G695	G630	U568	A504	G376	G315	G250		U120	A56
	G1017	U955	A892	U828	A764		A631	U569	A505	G377	C316	A251		G121	C57
U1083	U1018	C956	C893	A829	C765		A632	G570	G506	C378	G317	G252		G122	G58
A1084	U1019	U958		G830	U766		A633	A571	A507	G442	C318	C253		G123	U59
A1085	A1020	A959	C897	G831	U767		C634	A508	A443	G443	G319	G254		G124	G60
A1086	A1021	A960	C898	U832		U703	G635	C509	C444	C444	A320	A255		G194	C61
G1087	G1022	C961	A899	A833		G704	G636	A574	C510	C445	U321	A256		A126	U62
A1088	U1023	G962	A900	G834	G771		A637	A575		G383	A322	C257		A127	A63
A1089	G1024	U963	A706	C772	C772		G638	U576	A513	A384	C323			C128	U64
A1090	G1025	C964	G707	U773	G774		U639	G577	A514	U447	C324	A262		C129	A65
							C640	G578	A515	A449	G325	G263		C130	C66

A2051	G1984	G1993	G1861	G1797	G1733	G1671	A1608	G1546	G1483	U1415	C1349	A1286	C1221	G1157	G1091
A2052	C1985	C1924	G1862	U1798	G1734	A1672	A1609	C1547	U1484	G1416	C1350	A1287	U1222	C1158	C1092
G2053	C1986	G1925	G1863	G1799	A1735	G1673	A1610	A1548		C1417	C1351	G1288	G1223		U1093
A2054	A1987	U1926	U1864	C1800	G1736	G1674	C1611	A1549	U1487	G1418	U1352	C1289		C1161	U1094
C2055	A1927	U1926	U1865	A1801	G1737	C1675	G1612	C1550	C1489	A1419	A1353	C1291	A1226	G1163	A1095
G2056	A1928	A1802	A1866	A1802	G1738	C1676	G1613	A1551	C1489	A1420	A1354	C1291	G1227	G1164	A1096
G2057	G1929	A1803	G1867	A1803	A1739	A1677	A1614	A1552	A1490	G1421	G1355	G1292	G1228		U1097
A2058	G1930	C1804	C1868	C1804	A1739	A1678	C1615	A1553	G1491		G1356	C1293	C1229	A1165	A1098
A2059	U1931	A1805	G1869	A1805	C1741	A1679	A1616	U1554	G1492		C1357	U1294	A1230	G1166	G1099
A2060	C1806	C1806	G1870	C1806	U1742	G1680	C1617	G1555	C1493	A1427	G1358	C1295	U1231	C1167	C1100
G2061	G1807	G1807	C1871	G1807	G1743	G1681	A1618	C1556	A1494	A1428	G1359	G1296	G1232	G1168	U1101
C1986	A1744	A1744	A1872	A1808	A1745	G1682	G1619	C1557	A1495	C1428	G1360	C1297	G1233		U1102
C2063	G1873	G1873	G1873	A1809	A1745	G1683	G1620	C1558	A1496	G1429	G1361	C1298	C1233		A1103
C2064	C1874	A1746	C1874	A1810	A1746	G1684	U1621	U1559	U1497	G1430	C1362	G1299	G1236	G1171	C1104
	G1875	U1747	G1875	G1811	U1747	C1685	G1622	G1560	C1498	A1431	C1363	G1300	A1237		
C2066	U1812	C1748	C1686	G1812	C1748	C1686	G1623	C1561	C1499	G1432	G1364	A1301	G1238	U1172	U1108
G2067	G1813	A1749		G1813	A1749		U1624	U1562	G1500	A1433	A1365	A1302	G1239	U1173	C1109
G2068	G1814			G1814			C1625	U1563	G1501	A1434	A1366	G1303	U1240	A1174	C1110
G2069	A1815	C1752	A1689	A1815	C1752	A1689	A1626	C1564	A1502	G1435	A1367	A1304	A1241	U1176	A1111
G2070	C1816	G1753	C1691	C1816	G1753	C1691	G1627	C1565	A1503	G1436		C1305	U1242	G1177	G1112
A2071	C1817	A1754	G1692	C1817	A1754	G1692	G1628	C1566	A1504	A1437	C1370	C1306	U1243	C1178	U1113
C2072	U1818	A1755	U1693	U1818	A1755	U1693	U1629	G1567	A1505	U1438	G1371	A1307	A1244	G1179	C1114
C2073	A1819	G1756	C1694	A1819	G1756	C1694	A1630	G1568	U1506	A1439	U1372	A1308	G1245		G1115
U2074	G1820	A1757	G1695	G1820	A1757	G1695	G1631	A1569	C1507	U1440	A1373		A1246	U1183	G1116
U2075	U1821	U1758	G1696	U1821	U1758	G1696	A1632	A1570	A1508	G1441		U1312	A1247	U1184	G1117
U2076	C1822	A1759	G1697	C1822	A1759	G1697	G1633	A1571	A1509	U1442	C1376	U1313	A1247	G1185	C1118
	G1823	C1760	A1698	G1823	C1760	A1698	A1634	A1572	G1510		G1377	C1314		G1186	U1119
A2013	G1824	C1761	G1699	G1824	C1761	G1699	A1635	A1573	G1511	G1445	G1378	C1315	G1251	G1187	U1120
A2014	U1951	A1754	G1700	U1951	A1754	G1700	U1636	A1580	C1512	C1446	U1379	C1316	G1252	G1188	G1121
A2015	G1826	G1763	A1701	G1826	G1763	A1701	A1637	G1575	U1513	C1447		G1317	A1253	U1189	C1122
A2016	U1827	C1764	G1702	U1827	C1764	G1702	C1638	C1582	G1521	G1456	G1388	C1323	A1260	G1195	A1129
U2017	G1828	U1765	G1703	G1828	U1765	G1703	C1639	A1583	A1522	U1457	G1389	G1324	C1261	C1196	U1132
A2082	C1829	G1766	C1704	C1829	G1766	C1704	A1640	U1578			U1390	U1325	A1262	G1197	U1132
A2019	U1955	U1766	A1705	U1955	U1766	A1705	A1641	C1584	U1523	U1460	U1391	U1326	U1263	U1198	A1133
C2084	C1830	C1767	G1706	C1830	C1767	G1706	G1642	U1585	G1524	C1461	A1392	A1328	A1265	U1199	A1134
C2021	G1831	C1768	C1707	G1831	C1768	C1707	G1643	A1586	C1526	C1462	A1393	U1329	G1266	U1201	C1135
U2022	C1832	U1769	G1707	C1832	U1769	G1707	G1644	C1587	G1527	C1463	U1394	G1330	U1267	G1202	G1139
C2023	G1833	G1770	C1708	G1833	G1770	C1708	G1645	A1583	U1527	G1464	U1395	G1331	U1268	U1203	G1140
G2024	U1834	C1771		U1834	C1771		G1646	U1584	A1528	G1465	U1396	G1332	A1269	A1204	U1141
A2030	G1835	A1772	U1711	G1835	A1772	U1711	U1646	U1585			U1397	G1333	C1270	A1205	A1142
A2031	C1836	A1773	U1712	C1836	A1773	U1712	G1647	A1586	C1531	A1469	U1398	G1334	G1271	G1206	A1143
G2032	U1837	U1775	G1715	U1837	U1775	G1715	G1649	A1590	U1537	G1474	U1399	G1335	A1272	C1207	A1144
A2033	G1840	A1780	U1716	G1840	A1780	U1716	G1651	A1591	C1532		U1400	G1336	U1273	C1208	C1145
A2095	U1841	U1781	G1717	U1841	U1781	G1717	A1652	C1592	U1533	A1477	C1399	A1336	U1274	U1209	C1146
C2096	C1842	U1782	G1718	C1842	U1782	G1718	A1653	A1593	C1533	G1471		G1337	A1275	G1210	A1147
A2097	C1843	A1783	G1719	C1843	A1783	G1719	A1654	U1594	C1534	U1476	G1408	U1340	G1277	G1212	U1148
U2098	C1844	A1784	U1720	C1844	A1784	U1720	C1656	A1595	U1534	C1472	U1409	G1341	C1278	G1213	C1150
G2038		A1785	G1721		A1785	G1721	U1657	A1597	A1535	C1472	A1403	A1342		A1151	A1151
U2039		A1786	A1722		A1786	A1722	C1658	A1598	C1536	G1473	C1404			C1152	C1152
A2101	A1847	A1787	G1723	A1847	A1787	G1723	G1659	U1599	U1537	U1474				U1217	C1153
G2040	A1848	C1788	G1724	A1848	C1788	G1724		U1599	G1537	U1475				G1218	G1154
U2041		C1788	U1725		C1788	U1725	A1664	C1600	G1538	G1475	G1407			G1219	A1155
A2042	U1852	A1789	G1726	U1852	A1789	G1726	A1665	G1601	U1539	U1476	G1408			G1220	A1156
C2043	A1853	C1790	C1726	A1853	C1790	C1726	A1666	U1602	G1540	A1477	U1409				
C2044	A1854	A1791	C1727	A1854	A1791	C1727	G1667	A1603	C1541	G1478	G1410				
U2105	U1855	G1792	C1728	U1855	G1792	C1728	G1667	C1604	U1542	G1479	U1411				
	U1856	C1793	U1729	U1856	C1793	U1729	G1667	C1605	U1543	G1480	U1412				
	U1857	A1794	C1730	U1857	A1794	C1730	A1668	C1606	G1544	U1481	U1413				
	A1858	C1795	G1731	A1858	C1795	G1731	A1669	C1607	A1544	U1482	C1414				
		U1796	C1732		U1796	C1732	C1670		A1545						

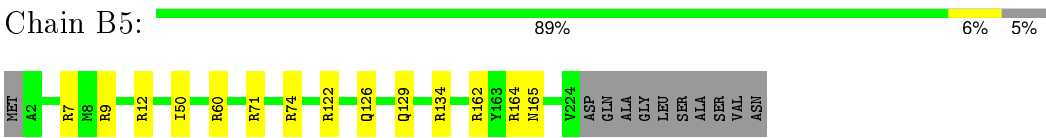


• Molecule 55: 5S ribosomal RNA

Chain BB: 25% 51% 21%



- Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	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	161000	Depositor
Image detector	4k CCD camera (TVIPS)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	AB	0.70	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%)	34	77
2	AC	205/208 (99%)	184 (90%)	15 (7%)	6 (3%)	6	43
3	AD	203/206 (98%)	185 (91%)	14 (7%)	4 (2%)	9	51
4	AE	150/152 (99%)	134 (89%)	10 (7%)	6 (4%)	4	35
5	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	2	26
6	AG	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	6	45
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	7	47
8	AI	126/128 (98%)	107 (85%)	15 (12%)	4 (3%)	5	41
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	30
10	AK	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	11	55
11	AL	121/124 (98%)	107 (88%)	8 (7%)	6 (5%)	3	31
12	AM	112/115 (97%)	94 (84%)	13 (12%)	5 (4%)	3	33
13	AN	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
14	AO	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	16	61
15	AP	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	4	37
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	11	53
18	AS	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	4	37
19	AT	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
20	AU	51/53 (96%)	32 (63%)	15 (29%)	4 (8%)	1	20
25	BC	270/273 (99%)	238 (88%)	25 (9%)	7 (3%)	7	45
26	BD	207/209 (99%)	185 (89%)	17 (8%)	5 (2%)	7	47
27	BE	199/201 (99%)	171 (86%)	20 (10%)	8 (4%)	4	35
28	BF	176/179 (98%)	155 (88%)	17 (10%)	4 (2%)	8	48
29	BG	174/177 (98%)	155 (89%)	12 (7%)	7 (4%)	4	35
30	BH	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	26	71
31	BI	139/142 (98%)	125 (90%)	12 (9%)	2 (1%)	14	58
32	BJ	140/142 (99%)	126 (90%)	11 (8%)	3 (2%)	9	50
33	BK	121/123 (98%)	107 (88%)	10 (8%)	4 (3%)	5	40
34	BL	141/144 (98%)	124 (88%)	11 (8%)	6 (4%)	3	34
35	BM	134/136 (98%)	115 (86%)	14 (10%)	5 (4%)	4	38
36	BN	119/121 (98%)	105 (88%)	11 (9%)	3 (2%)	7	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	108 (95%)	3 (3%)	3 (3%)	7	45
38	BP	112/115 (97%)	92 (82%)	17 (15%)	3 (3%)	6	45
39	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	11	55
40	BR	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	5	42
41	BS	108/110 (98%)	105 (97%)	2 (2%)	1 (1%)	21	67
42	BT	92/94 (98%)	80 (87%)	6 (6%)	6 (6%)	1	25
43	BU	101/104 (97%)	83 (82%)	14 (14%)	4 (4%)	4	35
44	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
45	BW	78/80 (98%)	59 (76%)	17 (22%)	2 (3%)	7	45
46	BX	75/79 (95%)	68 (91%)	3 (4%)	4 (5%)	2	29
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	49 (88%)	4 (7%)	3 (5%)	2	29
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%)	3	32
53	B4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6	44
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	34	77
All	All	5876/6008 (98%)	5245 (89%)	476 (8%)	155 (3%)	11	45

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%)	68	87
2	AC	170/171 (99%)	168 (99%)	2 (1%)	78	90
3	AD	172/173 (99%)	171 (99%)	1 (1%)	90	95
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	86	94
7	AH	104/105 (99%)	101 (97%)	3 (3%)	50	78
8	AI	105/105 (100%)	101 (96%)	4 (4%)	40	73
9	AJ	86/86 (100%)	83 (96%)	3 (4%)	43	74
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	90 (99%)	1 (1%)	80	91
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	37	71
17	AR	48/48 (100%)	45 (94%)	3 (6%)	22	59
18	AS	70/70 (100%)	69 (99%)	1 (1%)	74	89
19	AT	65/65 (100%)	64 (98%)	1 (2%)	72	88
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	51	78
26	BD	164/164 (100%)	160 (98%)	4 (2%)	57	82
27	BE	165/165 (100%)	162 (98%)	3 (2%)	66	87
28	BF	149/150 (99%)	147 (99%)	2 (1%)	76	89
29	BG	137/138 (99%)	133 (97%)	4 (3%)	50	78
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	84	93
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	54	80
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	100 (98%)	2 (2%)	63	85
35	BM	109/109 (100%)	107 (98%)	2 (2%)	66	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BN	100/100 (100%)	99 (99%)	1 (1%)	82	92
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	60	83
40	BR	84/84 (100%)	84 (100%)	0	100	100
41	BS	93/93 (100%)	92 (99%)	1 (1%)	80	91
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	53 (90%)	6 (10%)	9	37
46	BX	67/68 (98%)	66 (98%)	1 (2%)	72	88
47	BY	55/55 (100%)	54 (98%)	1 (2%)	66	87
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	61	84
50	B1	45/45 (100%)	44 (98%)	1 (2%)	60	83
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	48 (94%)	3 (6%)	24	61
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	169 (98%)	4 (2%)	58	83
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	69	87

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

Mol	Chain	Res	Type
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	1530/1533 (99%)	248 (16%)	86 (5%)
22	A1	73/76 (96%)	15 (20%)	7 (9%)
23	A2	14/15 (93%)	5 (35%)	3 (21%)
24	A3	76/77 (98%)	13 (17%)	5 (6%)
54	BA	2902/2903 (99%)	464 (15%)	110 (3%)
55	BB	117/118 (99%)	15 (12%)	4 (3%)
All	All	4712/4722 (99%)	760 (16%)	215 (4%)

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

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A3	19	G
54	BA	531	C
54	BA	2423	U
24	A3	62	C
54	BA	222	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CM0	A1	34	21,22	15,26,27	1.92	3 (20%)	18,37,40	3.16	4 (22%)
22	6MZ	A1	37	22	17,25,26	0.99	1 (5%)	15,36,39	1.09	1 (6%)
22	7MG	A1	46	22	20,26,27	2.19	3 (15%)	23,39,42	2.14	2 (8%)
22	5MU	A1	54	22	13,22,23	1.21	2 (15%)	16,32,35	4.75	2 (12%)
22	PSU	A1	55	22	15,21,22	1.03	1 (6%)	16,30,33	3.32	5 (31%)
22	4SU	A1	7	22	12,21,22	1.10	1 (8%)	15,30,33	2.24	3 (20%)
24	H2U	A3	21	24	17,21,22	1.45	2 (11%)	23,30,33	1.29	4 (17%)
24	OMC	A3	33	24	15,22,23	1.13	0	20,31,34	1.07	1 (5%)
24	5MU	A3	55	24	13,22,23	1.06	1 (7%)	16,32,35	4.45	2 (12%)
24	PSU	A3	56	24	15,21,22	1.35	2 (13%)	16,30,33	3.44	4 (25%)
24	4SU	A3	8	24	12,21,22	1.19	2 (16%)	15,30,33	2.20	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	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 18 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	-6.17	1.25	1.37
24	A3	21	H2U	C4-N3	-3.55	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C2-N3	-3.36	1.31	1.38
22	A1	46	7MG	C8-N7	-2.68	1.31	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-13.21	114.26	125.35
24	A3	55	5MU	C5-C4-N3	-12.35	114.98	125.35
24	A3	8	4SU	C5-C4-N3	-7.81	115.28	123.56
22	A1	7	4SU	C5-C4-N3	-7.11	116.02	123.56
22	A1	46	7MG	C5-C6-N1	-6.89	113.14	123.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	VAL	A1	101	58,22	5,6,7	0.63	0	5,7,9	2.26	2 (40%)
58	FME	BA	3001	57	8,9,10	0.61	0	5,9,11	1.37	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	58,22	-	0/4/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-3.85	115.18	125.69
58	BA	3001	FME	O1-CN-N	-2.29	121.30	124.80
57	A1	101	VAL	C-CA-N	3.27	117.17	109.95

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.