



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:53 PM BST

PDB ID : 4V73
EMDB ID: : EMD-2473
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in hybrid pre-translocation state (pre5a)
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 : 15.00 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

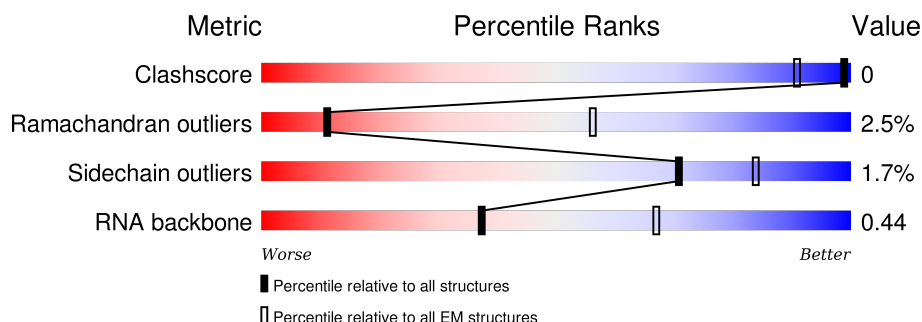
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 Å.

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













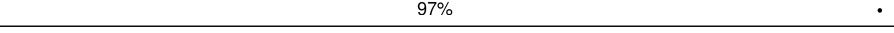
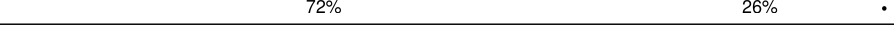
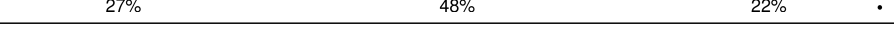


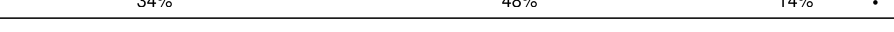


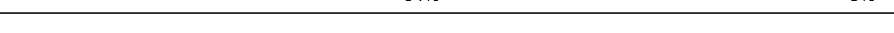






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AB	220	93% 7%
2	AC	208	90% 10%
3	AD	206	89% 10%
4	AE	152	92% 8%
5	AF	101	84% 14% .
6	AG	152	90% 9% .
7	AH	130	92% 8% .
8	AI	128	86% 13% .













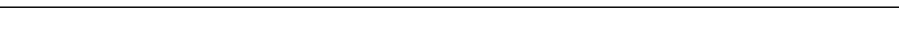



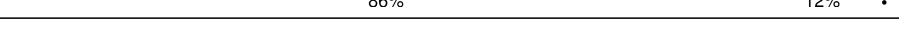




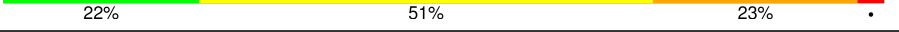
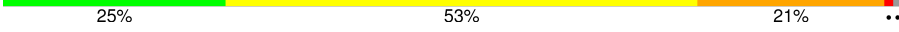
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Mol	Chain	Length	Quality of chain
9	AJ	100	 86% 13% .
10	AK	118	 92% 8%
11	AL	124	 82% 16% ..
12	AM	115	 85% 14% .
13	AN	101	 84% 13% ...
14	AO	89	 83% 16% .
15	AP	81	 86% 14%
16	AQ	82	 91% 6% .
17	AR	57	 86% 14%
18	AS	81	 88% 12%
19	AT	86	 97% .
20	AU	53	 72% 26% .
21	AA	1533	 27% 48% 22% .
22	A1	76	 32% 45% 22% .
23	A2	15	 27% 27% 47%
24	A3	77	 34% 48% 14% .
25	BC	273	 87% 12% .
26	BD	209	 90% 10%
27	BE	201	 94% 5% .
28	BF	179	 90% 9% .
29	BG	177	 91% 8% ..
30	BH	149	 93% 6% .
31	BI	142	 94% 5% .
32	BJ	142	 92% 8%
33	BK	123	 89% 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		

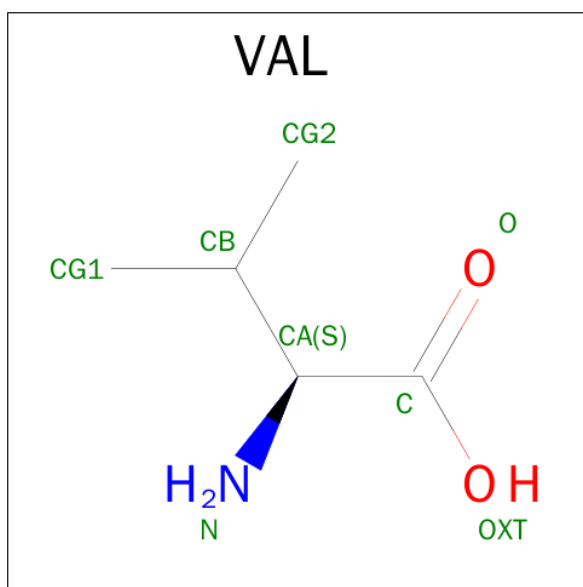
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

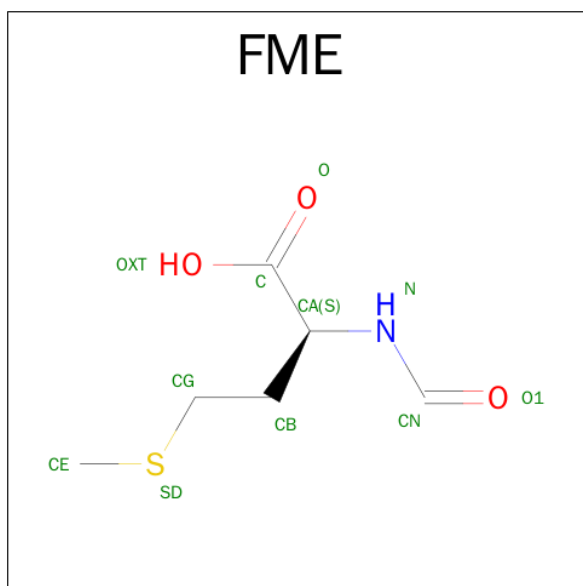
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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: $C_6H_{11}NO_3S$).

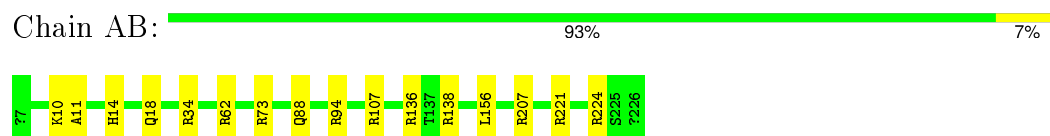


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

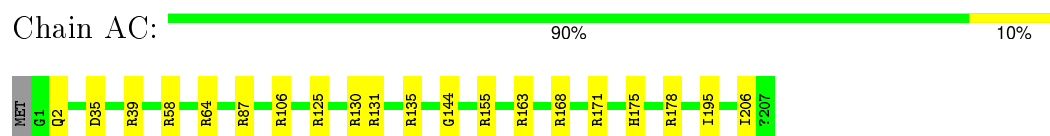
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

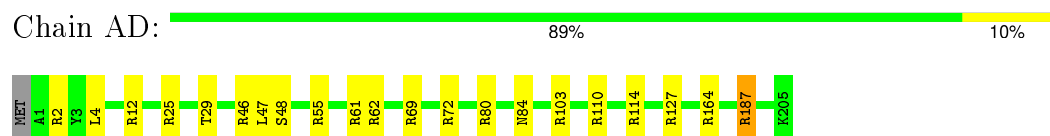
- Molecule 1: 30S ribosomal protein S2



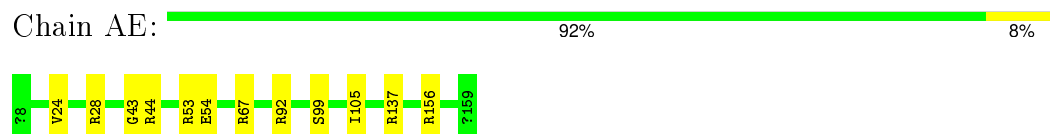
- Molecule 2: 30S ribosomal protein S3



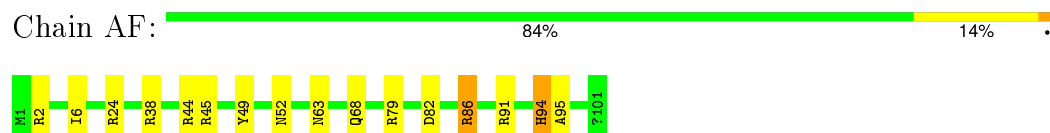
- Molecule 3: 30S ribosomal protein S4



- 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: 92% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 86% 13%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 86% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 8%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 82% 16%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%




- Molecule 13: 30S ribosomal protein S14

Chain AN: 84% 13%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  83% 16%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  86% 14%




- Molecule 16: 30S ribosomal protein S17

Chain AQ:  91% 6%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  86% 14%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  88% 12%



- Molecule 19: 30S ribosomal protein S20

Chain AT:  97%



- Molecule 20: 30S ribosomal protein S21

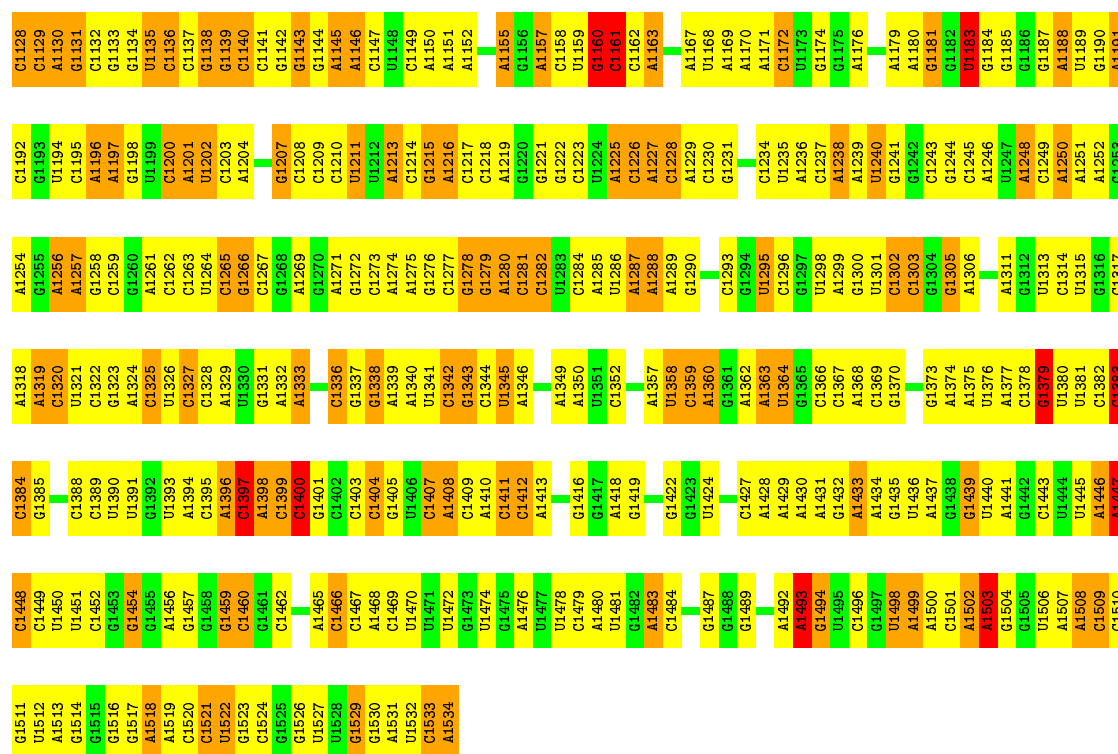
Chain AU:  72% 26%



- Molecule 21: 16S ribosomal RNA

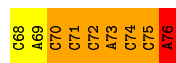
Chain AA:  27% 48% 22%



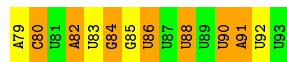
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 32% 45% 22% .



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

Chain A2: 27% 27% 47%



• Molecule 24: tRNA-fMet

Chain A3: 34% 48% 14% .



• Molecule 25: 50S ribosomal protein L2

Chain BC: 87% 12% .



- Molecule 26: 50S ribosomal protein L3

Chain BD: 90% 10%



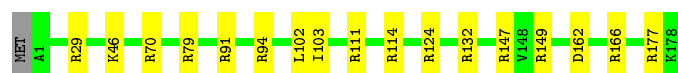
- Molecule 27: 50S ribosomal protein L4

Chain BE: 94% 5%



- Molecule 28: 50S ribosomal protein L5

Chain BF: 90% 9%



- Molecule 29: 50S ribosomal protein L6

Chain BG: 91% 8%



- Molecule 30: 50S ribosomal protein L9

Chain BH: 93% 6%



- Molecule 31: 50S ribosomal protein L11

Chain BI: 94% 5%



- Molecule 32: 50S ribosomal protein L13

Chain BJ: 92% 8%



- Molecule 33: 50S ribosomal protein L14

Chain BK: 89% 11%



- Molecule 34: 50S ribosomal protein L15

Chain BL: 85% 14%



- Molecule 35: 50S ribosomal protein L16

Chain BM: 90% 8%



- Molecule 36: 50S ribosomal protein L17

Chain BN: 83% 17%



- Molecule 37: 50S ribosomal protein L18

Chain BO: 91% 9%



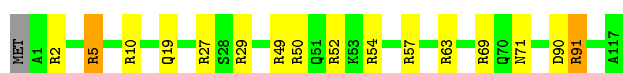
- Molecule 38: 50S ribosomal protein L19

Chain BP: 83% 15%



- Molecule 39: 50S ribosomal protein L20

Chain BQ: 86% 12%



- Molecule 40: 50S ribosomal protein L21

Chain BR:  89% 11%



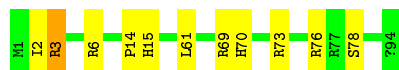
- Molecule 41: 50S ribosomal protein L22

Chain BS:  90% 9%



- Molecule 42: 50S ribosomal protein L23

Chain BT:  88% 11%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  88% 11%




- Molecule 44: 50S ribosomal protein L25

Chain BV:  91% 9%




- Molecule 45: 50S ribosomal protein L27

Chain BW:  83% 18%



- Molecule 46: 50S ribosomal protein L28

Chain BX:  85% 13%




- Molecule 47: 50S ribosomal protein L29

Chain BY:  89% 10%




- Molecule 48: 50S ribosomal protein L30

Chain BZ:  88% 8%



- Molecule 49: 50S ribosomal protein L32

Chain B0:  86% 12%




- Molecule 50: 50S ribosomal protein L33

Chain B1:  88% 12%




- Molecule 51: 50S ribosomal protein L34

Chain B2:  78% 22%




- Molecule 52: 50S ribosomal protein L35

Chain B3:  88% 11%

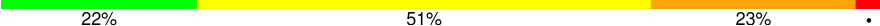


- Molecule 53: 50S ribosomal protein L36

Chain B4:  87% 13%

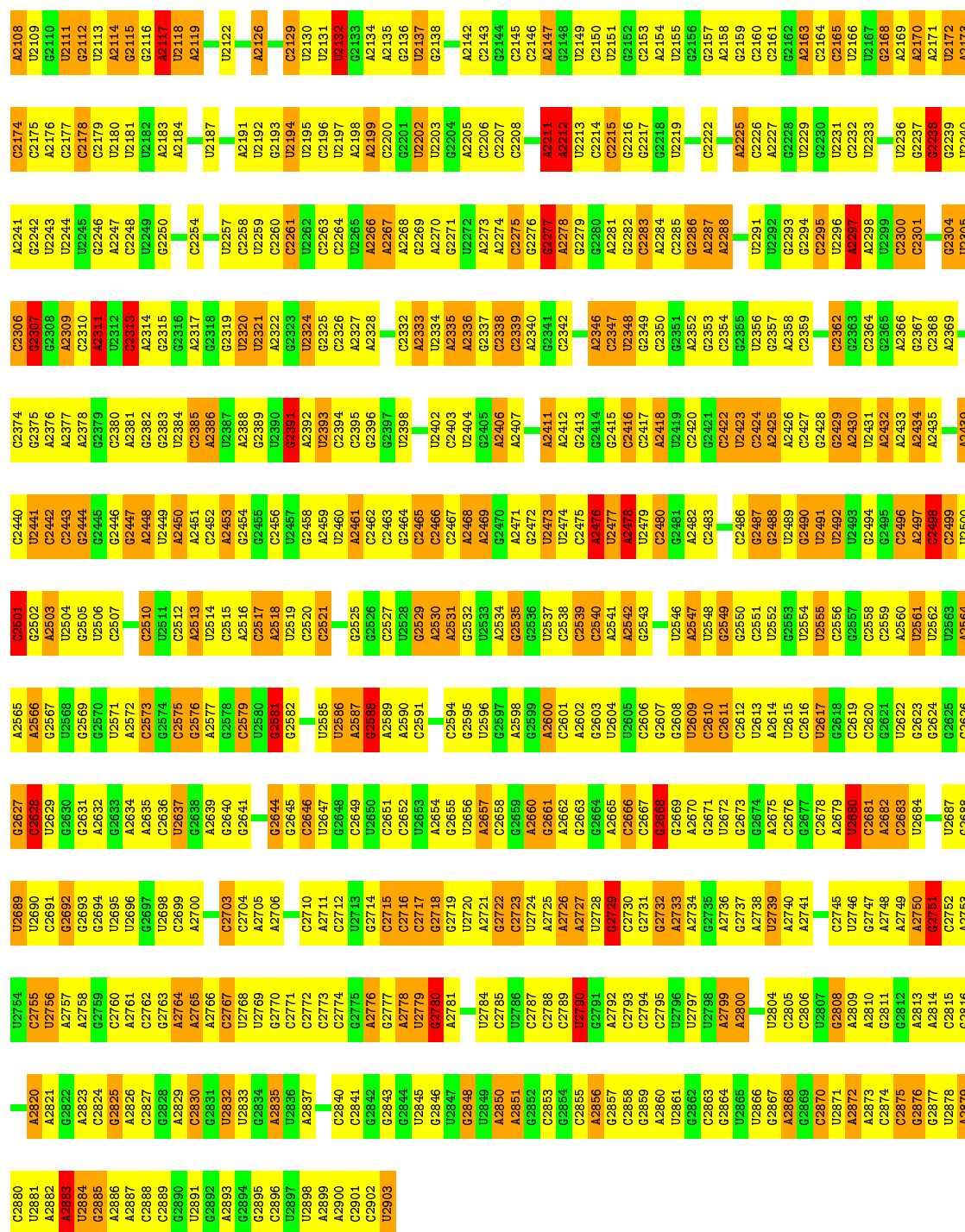


- Molecule 54: 23S ribosomal RNA

Chain BA:  22% 51% 23%

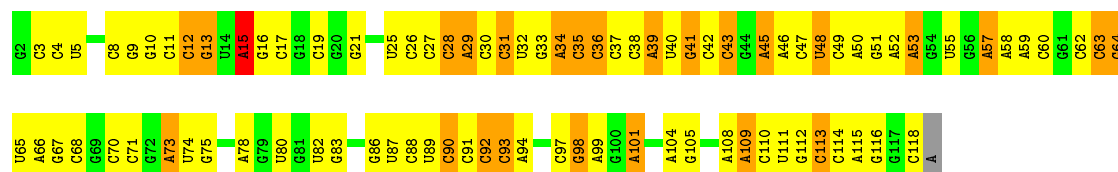
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A1040	A973	A909		U714	G651	C587		A454	G388	A320	A255	A195	C128	C66	A5
G1041	G974	A910	A781	A715	U652	U588	A522	C455	G389	U321	A256	A196	C129	U67	A6
G1042	A975	A911	A782	A716	U653	U589	C523	C456	U390	A322	C257	A197	C130	G68	A7
C1043	G976	A912	A783	C717	A654	A590	G524	A457	A391	C323	G258	C198	A131	C69	A8
C1044		C912	G784	A718	A655	U591	U525	C458	U392	A324		A199	G132	G70	A9
C1045	A979	U913	G785	C719	G656	A592	A526	U459	C393		A282	U200	U133	A71	
C1046	A980	C915	C786	U720	U657	U593	C527	A460	C394	G329	G263	C201	G134	U72	A10
A1047	A981	C916	C787	A721	U658	U594	A528	C461	U395	A330	A264	U202		A73	A11
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A1049	A983	A917	A789	G723	C660	U596	G530	U459	U397	A332	G266	A204	U138	G75	A13
C1049	A984	A918	U790	U724	A661	G597	C531	U464	C398	G333	C267	G205	U139	C76	A14
A1050	C985	U919	C791	G725	G662	U598	A532	G465		C334	C268	U206	C140	G77	A15
G1051	C986	A920	A792	G726	G663	A599	G533	A466	A401	C335	C269	A207	G141	U78	A16
C1052	C987	C921	A793	A727		G600		G467	A402	C336	A270	C208	G142	C79	A17
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C1054	G989	G923	C795	G729	U667	A602	G539	G469	A404	G338	A272	C210	A144	G81	A19
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U1060	C995		U803	A735	G673		C545	A477	C414	A344	A278	A216	U150	G89	G27
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G1074	C1011	C946	C818	A749		C624		A492	A428	G359	G295	G230	C164	U40	
C1075	U1012	A947	A819	A750	A689	G625	A563	A493	A429	U360	U296	A231	A165	A103	
G1076	C1013	C948	A820	A751	G690	A626	C564		A430	G361	G297	G232	U166	A104	C41
U1015	A1014	G949	A821	C692	C691	A627	C565	A496	U431	A362	G298	A233	A167	C105	A42
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C1079	G1016	G953	U824	A756	U694	A632	U568	G500	C434	U365	G301	G236	A172	G108	G45
A1080	U1019	G954	A825	G757	G695	A633	U569	A501	C435	C366	C302	C237	A173	C47	
U1081	A1020		C826	C758		A634		A502	C436	G367	G303	C238	U174	G48	
U1082	A1021	C957	U827		G697	C635	U571	A503	U437	A368	G175	C239	G175	U112	A49
A1083	G1022	U958	U828	A761	C698	G636	A572	A504	G438	U369	A176	C240	A176	U113	U50
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A1085	U1023	A959	G830	G763	G700	G638	A574	G506	C440	A371	G307	G242	G178	C115	A52
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G1087	G1025	C961	G831	C765	U702	C640	U576	A508	A443	U373	A309	G244	G180	G117	G54
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C2084	C2023	C1961	U1708	A1834	C1708	C1644	U1578	A1515	G1452	A1384	C1323	A1262	A1133	A1133
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G2087	U2026	C1965	U1779	G1838	U1712	U1648	C1582	U1522	C1454	A1387	A1327	A1265	U1203	G1138
A2088	G2027	A1966	A1780	U1842	A1713	G1649	A1583	U1523	U1458	U1329	U1328	G1266	A1204	G1139
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U2092	C2031	C1970	A1784	G1846	A1717	G1653	G1587	C1526	C1461	A1392	G1333	G1271	C1208	A1142
G2093	G2032	C1908	U1884	U1851	U1720	A1654	U1590	A1527	C1462	U1394	G1334	A1272	U1209	A1143
A2094	A2033	G1910	A1785	A1847	G1721	A1655	C1595	G1528	C1463	A1395	C1335	U1273	G1210	A1144
C2095	C2034	U1911	A1786	A1848	U1722	C1656	A1591	G1529	C1464	U1396	C1336	A1274	C1211	C1145
G2096	G2035	A1912	A1787	G1849	G1723	U1657	C1592	G1530	G1465	U1397	G1337	A1275	C1212	C1146
A2097	C2036	C1913	C1788	C1850	G1723	C1658	A1593	C1531	U1466	C1398	G1338	A1276	A1214	A1147
U2098	A2037	C1914	A1789	U1852	G1724	G1659	U1594	A1532	U1467	C1399	G1339	G1277	G1215	C1150
G2099	U2038	U1915	C1790	G1853	U1725	U1664	C1595	C1533	U1468	U1400	U1340	C1278	A1151	A1151
G2100	C2039	A1916	A1791	C1854	C1726	A1664	A1596	U1534	A1469	G1401	G1341	G1279	C1152	C1152
A2101	G2040	U1917	G1792	A1854	C1727	A1665	A1597	A1535	U1470	U1402	A1342	G1280	C1153	C1153
C2102	U2041	C1918	C1793	U1855	C1728	G1666	U1598	C1536	G1471	A1403	G1343	G1281	G1154	G1154
A2103	A2042	A1919	A1794	U1856	U1729	G1667	U1599	G1537	C1472	C1404	U1344	U1282	C1221	A1155
C2104	C2043	G1983	C1795	G1857	C1730	A1668	C1600	G1538	C1475	U1405	C1345	G1283	U1222	A1156
U2105	C2044	G1984	U1796	A1858	C1731	A1669	A1603	U1539	G1476	U1406	G1346	A1284	G1223	G1197
G2106	C2045	C1985	G1797	U1859	C1732	C1670	A1671	G1540	U1477	A1407	A1347	A1285	U1224	C1158
C2107	G2046	C1986	U1798	G1860	U1671	U1671	C1604	C1541	A1477	G1408	C1348	A1286	G1225	U1159



- Molecule 55: 5S ribosomal RNA

Chain BB: 



● Molecule 56: 50S ribosomal protein L1

Chain B5:

91%

5%

5%



4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	AB	0.72	0/1736	1.05	13/2340 (0.6%)
10	AK	0.76	0/894	1.14	8/1207 (0.7%)
11	AL	0.77	0/969	1.28	13/1300 (1.0%)
12	AM	0.75	0/884	1.29	16/1181 (1.4%)
13	AN	0.76	0/817	1.24	12/1088 (1.1%)
14	AO	0.75	0/722	1.17	10/964 (1.0%)
15	AP	0.79	0/648	1.28	12/870 (1.4%)
16	AQ	0.70	0/658	1.15	6/883 (0.7%)
17	AR	0.82	0/463	1.19	6/623 (1.0%)
18	AS	0.76	0/653	1.18	9/879 (1.0%)
19	AT	0.68	0/672	0.97	3/890 (0.3%)
2	AC	0.74	0/1651	1.07	13/2225 (0.6%)
20	AU	0.86	0/431	1.43	7/572 (1.2%)
21	AA	1.52	1/36759 (0.0%)	2.22	1955/57346 (3.4%)
22	A1	1.55	0/1668	2.27	88/2595 (3.4%)
23	A2	1.50	0/343	2.33	19/531 (3.6%)
24	A3	1.55	0/1722	2.18	90/2685 (3.4%)
25	BC	0.75	0/2121	1.29	30/2852 (1.1%)
26	BD	0.68	0/1586	1.13	9/2134 (0.4%)
27	BE	0.68	0/1571	1.15	10/2113 (0.5%)
28	BF	0.75	0/1444	1.21	16/1937 (0.8%)
29	BG	0.69	0/1343	1.10	9/1816 (0.5%)
3	AD	0.77	0/1665	1.13	16/2227 (0.7%)
30	BH	0.66	0/1122	1.10	7/1515 (0.5%)
31	BI	0.68	0/1046	1.08	5/1410 (0.4%)
32	BJ	0.74	0/1152	1.17	12/1551 (0.8%)
33	BK	0.71	0/947	1.23	11/1268 (0.9%)
34	BL	0.74	0/1054	1.33	11/1403 (0.8%)
35	BM	0.75	0/1093	1.28	12/1460 (0.8%)
36	BN	0.76	0/973	1.31	13/1301 (1.0%)
37	BO	0.73	0/902	1.24	10/1209 (0.8%)
38	BP	0.76	0/929	1.33	13/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.80	0/960	1.31	12/1278 (0.9%)
4	AE	0.71	0/1119	1.06	7/1506 (0.5%)
40	BR	0.73	0/829	1.10	5/1107 (0.5%)
41	BS	0.65	0/864	1.15	6/1156 (0.5%)
42	BT	0.67	0/744	1.19	6/994 (0.6%)
43	BU	0.69	0/787	1.12	6/1051 (0.6%)
44	BV	0.73	0/766	1.16	6/1025 (0.6%)
45	BW	0.77	0/604	1.27	8/799 (1.0%)
46	BX	0.76	0/635	1.22	6/848 (0.7%)
47	BY	0.67	0/510	1.17	6/677 (0.9%)
48	BZ	0.69	0/453	1.20	3/605 (0.5%)
49	B0	0.75	0/450	1.24	5/599 (0.8%)
5	AF	0.74	0/835	1.14	8/1128 (0.7%)
50	B1	0.73	0/417	1.16	3/556 (0.5%)
51	B2	0.80	0/380	1.50	10/498 (2.0%)
52	B3	0.75	0/513	1.23	6/676 (0.9%)
53	B4	0.69	0/303	1.32	5/397 (1.3%)
54	BA	1.40	0/69796	2.21	4028/108888 (3.7%)
55	BB	1.41	0/2800	2.20	152/4367 (3.5%)
56	B5	0.66	0/1673	1.07	10/2255 (0.4%)
6	AG	0.76	0/1188	1.24	14/1593 (0.9%)
7	AH	0.72	0/989	1.07	6/1326 (0.5%)
8	AI	0.81	0/1035	1.27	14/1377 (1.0%)
9	AJ	0.72	0/797	1.12	9/1079 (0.8%)
All	All	1.28	1/160085 (0.0%)	1.99	6805/239402 (2.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AK	0	1
21	AA	0	358
22	A1	0	15
23	A2	0	5
24	A3	0	9
26	BD	0	1
41	BS	0	1
50	B1	0	1
54	BA	0	709
55	BB	0	21
All	All	0	1121

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	348	G	C4'-O4'	-5.47	1.38	1.45

The worst 5 of 6805 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	76	A	N1-C6-N6	-15.19	109.49	118.60
54	BA	1714	U	O4'-C1'-N1	14.33	119.66	108.20
54	BA	546	U	O4'-C1'-N1	13.75	119.20	108.20
54	BA	218	A	N1-C6-N6	-12.03	111.39	118.60
21	AA	152	A	N1-C6-N6	-11.78	111.53	118.60

There are no chirality outliers.

5 of 1121 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	AA	10	A	Sidechain
21	AA	5	U	Sidechain
21	AA	6	G	Sidechain
21	AA	8	A	Sidechain
10	AK	115	ILE	Peptide

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
4	AE	1109	0	1152	0	0
5	AF	818	0	808	3	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	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	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	16522	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	1	0
25	BC	2083	0	2157	1	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	1	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BA	62317	0	31345	6	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	99665	15	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 15 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)
30:BH:143:ILE:H	30:BH:143:ILE:HD13	1.72	0.54
24:A3:72:C:C5	24:A3:73:A:C8	2.98	0.51
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.33	0.47
35:BM:80:VAL:H	35:BM:81:ARG:HA	1.81	0.46
22:A1:76:A:H62	54:BA:2600:A:H3'	1.82	0.44

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AB	218/220 (99%)	202 (93%)	13 (6%)	3 (1%)	14 58
2	AC	205/208 (99%)	189 (92%)	13 (6%)	3 (2%)	13 57
3	AD	203/206 (98%)	192 (95%)	6 (3%)	5 (2%)	7 46
4	AE	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	6 45
5	AF	99/101 (98%)	85 (86%)	8 (8%)	6 (6%)	2 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AG	150/152 (99%)	139 (93%)	9 (6%)	2 (1%)	15	60
7	AH	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AI	126/128 (98%)	112 (89%)	10 (8%)	4 (3%)	5	41
9	AJ	98/100 (98%)	90 (92%)	4 (4%)	4 (4%)	3	35
10	AK	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
11	AL	121/124 (98%)	109 (90%)	7 (6%)	5 (4%)	3	35
12	AM	112/115 (97%)	93 (83%)	17 (15%)	2 (2%)	11	53
13	AN	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	3	35
14	AO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	8	48
15	AP	79/81 (98%)	67 (85%)	10 (13%)	2 (2%)	7	46
16	AQ	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	15	60
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	11	53
18	AS	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	15	60
19	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	AU	51/53 (96%)	34 (67%)	9 (18%)	8 (16%)	0	5
25	BC	270/273 (99%)	245 (91%)	21 (8%)	4 (2%)	13	57
26	BD	207/209 (99%)	182 (88%)	17 (8%)	8 (4%)	4	36
27	BE	199/201 (99%)	183 (92%)	11 (6%)	5 (2%)	7	46
28	BF	176/179 (98%)	156 (89%)	17 (10%)	3 (2%)	11	55
29	BG	174/177 (98%)	156 (90%)	14 (8%)	4 (2%)	8	48
30	BH	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	26	71
31	BI	139/142 (98%)	125 (90%)	11 (8%)	3 (2%)	8	49
32	BJ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
33	BK	121/123 (98%)	109 (90%)	9 (7%)	3 (2%)	7	46
34	BL	141/144 (98%)	124 (88%)	10 (7%)	7 (5%)	3	31
35	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	13	57
36	BN	119/121 (98%)	101 (85%)	13 (11%)	5 (4%)	3	34
37	BO	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
38	BP	112/115 (97%)	98 (88%)	9 (8%)	5 (4%)	3	33
39	BQ	115/118 (98%)	103 (90%)	8 (7%)	4 (4%)	4	39
40	BR	101/103 (98%)	95 (94%)	3 (3%)	3 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BS	108/110 (98%)	95 (88%)	11 (10%)	2 (2%)	10	52
42	BT	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	1	20
43	BU	101/104 (97%)	85 (84%)	11 (11%)	5 (5%)	3	31
44	BV	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	17	63
45	BW	78/80 (98%)	58 (74%)	17 (22%)	3 (4%)	4	37
46	BX	75/79 (95%)	60 (80%)	11 (15%)	4 (5%)	2	29
47	BY	61/63 (97%)	57 (93%)	2 (3%)	2 (3%)	5	40
48	BZ	56/59 (95%)	49 (88%)	6 (11%)	1 (2%)	11	53
49	B0	54/57 (95%)	50 (93%)	3 (6%)	1 (2%)	10	52
50	B1	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	4	35
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	48
52	B3	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	12	56
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	210 (95%)	11 (5%)	0	100	100
All	All	5876/6008 (98%)	5290 (90%)	442 (8%)	144 (2%)	11	46

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AF	86	ARG
8	AI	124	PRO
12	AM	42	VAL
13	AN	56	SER
17	AR	20	ILE

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%)	166 (98%)	4 (2%)	57	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	121 (98%)	2 (2%)	70	88
7	AH	104/105 (99%)	100 (96%)	4 (4%)	40	73
8	AI	105/105 (100%)	103 (98%)	2 (2%)	65	86
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	58	83
10	AK	90/90 (100%)	89 (99%)	1 (1%)	80	91
11	AL	103/104 (99%)	101 (98%)	2 (2%)	65	86
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%)	72 (97%)	2 (3%)	52	79
17	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
18	AS	70/70 (100%)	69 (99%)	1 (1%)	74	89
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	42 (96%)	2 (4%)	34	69
25	BC	216/217 (100%)	211 (98%)	5 (2%)	58	83
26	BD	164/164 (100%)	162 (99%)	2 (1%)	78	90
27	BE	165/165 (100%)	164 (99%)	1 (1%)	90	95
28	BF	149/150 (99%)	148 (99%)	1 (1%)	88	94
29	BG	137/138 (99%)	133 (97%)	4 (3%)	50	78
30	BH	114/114 (100%)	111 (97%)	3 (3%)	54	80
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	101 (99%)	1 (1%)	82	92
35	BM	109/109 (100%)	106 (97%)	3 (3%)	51	78
36	BN	100/100 (100%)	97 (97%)	3 (3%)	48	77
37	BO	86/87 (99%)	85 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BP	99/100 (99%)	98 (99%)	1 (1%)	82	92
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	60	83
40	BR	84/84 (100%)	81 (96%)	3 (4%)	42	74
41	BS	93/93 (100%)	90 (97%)	3 (3%)	46	76
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	83 (100%)	0	100	100
44	BV	78/78 (100%)	77 (99%)	1 (1%)	76	89
45	BW	59/59 (100%)	56 (95%)	3 (5%)	29	66
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	45 (94%)	3 (6%)	22	59
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%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	78	90
All	All	4842/4870 (99%)	4759 (98%)	83 (2%)	71	87

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	BC	212	TRP
29	BG	176	LYS
48	BZ	40	THR
25	BC	218	THR
28	BF	162	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
19	AT	69	ASN
34	BL	35	HIS
36	BN	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	255 (16%)	88 (5%)
22	A1	73/76 (96%)	12 (16%)	7 (9%)
23	A2	14/15 (93%)	4 (28%)	1 (7%)
24	A3	76/77 (98%)	11 (14%)	4 (5%)
54	BA	2902/2903 (99%)	485 (16%)	125 (4%)
55	BB	116/118 (98%)	14 (12%)	5 (4%)
All	All	4711/4722 (99%)	781 (16%)	230 (4%)

5 of 781 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	16	A

5 of 230 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	BA	249	C
54	BA	847	U
54	BA	2518	A
54	BA	278	A
54	BA	506	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CM0	A1	34	22	15,26,27	1.83	3 (20%)	18,37,40	3.38	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	6MZ	A1	37	22	17,25,26	0.82	0	15,36,39	1.32	1 (6%)
22	7MG	A1	46	22	20,26,27	2.20	4 (20%)	23,39,42	2.24	2 (8%)
22	5MU	A1	54	22	13,22,23	1.06	1 (7%)	16,32,35	4.60	2 (12%)
22	PSU	A1	55	22	15,21,22	1.07	1 (6%)	16,30,33	3.46	5 (31%)
22	4SU	A1	7	22	12,21,22	0.94	0	15,30,33	2.22	3 (20%)
24	H2U	A3	21	24	17,21,22	1.46	2 (11%)	23,30,33	1.45	4 (17%)
24	OMC	A3	33	24	15,22,23	1.03	0	20,31,34	0.74	0
24	5MU	A3	55	24	13,22,23	1.15	1 (7%)	16,32,35	4.57	2 (12%)
24	PSU	A3	56	24	15,21,22	1.08	1 (6%)	16,30,33	3.71	5 (31%)
24	4SU	A3	8	24	12,21,22	1.25	2 (16%)	15,30,33	2.22	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	22	-	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 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.11	1.33	1.45
22	A1	34	CM0	O5-C5	-5.53	1.26	1.37
24	A3	21	H2U	C4-N3	-3.69	1.31	1.37
24	A3	21	H2U	C2-N3	-3.35	1.31	1.38
22	A1	46	7MG	C8-N7	-2.76	1.30	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
22	A1	54	5MU	C5-C4-N3	-12.58	114.79	125.35
24	A3	55	5MU	C5-C4-N3	-12.39	114.95	125.35
24	A3	8	4SU	C5-C4-N3	-7.72	115.37	123.56
22	A1	7	4SU	C5-C4-N3	-7.43	115.68	123.56
22	A1	46	7MG	C5-C6-N1	-6.98	113.00	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	0.68	0	5,7,9	1.29	1 (20%)
58	FME	BA	3001	57	8,9,10	0.83	0	5,9,11	1.23	1 (20%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
57	A1	101	VAL	O-C-CA	-2.57	118.68	125.69
58	BA	3001	FME	O-C-CA	-2.53	118.78	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.