



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 01:56 pm GMT

PDB ID : 7QQ3
EMDB ID : EMD-14121
Title : Cryo-EM structure of the E.coli 50S ribosomal subunit in complex with the antibiotic Myxovalargin A.
Authors : Koller, T.O.; Beckert, B.; Wilson, D.N.
Deposited on : 2022-01-06
Resolution : 2.10 Å(reported)
Based on initial model : 4YBB

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

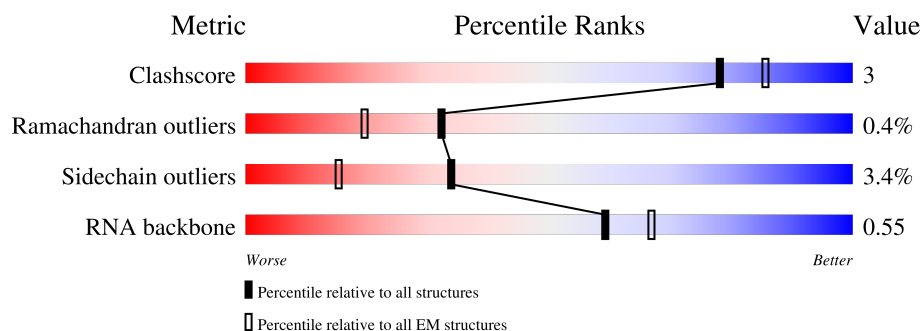
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 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.




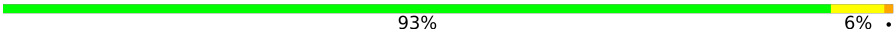
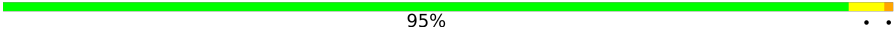


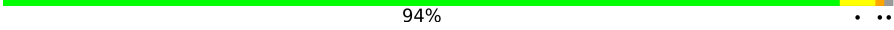
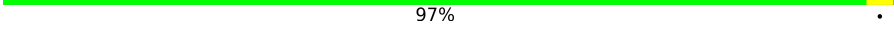

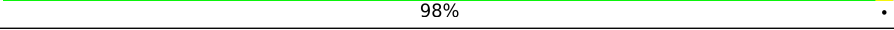


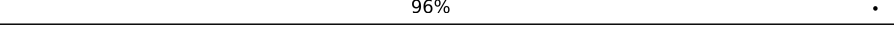

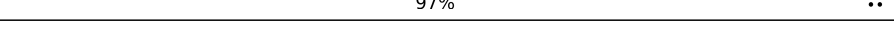
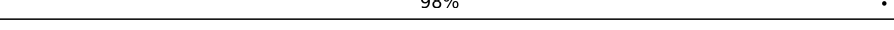
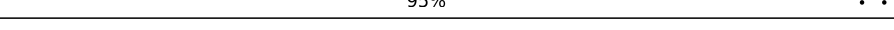


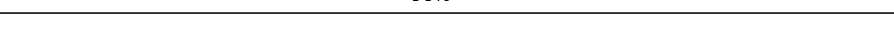
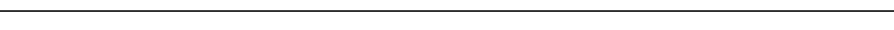

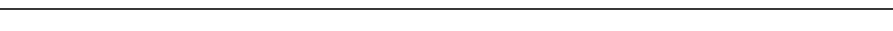
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	I	2904	80% 17% .
2	J	120	74% 22% . .
3	K	273	97% . .
4	L	209	97% .
5	M	201	98% .
6	O	177	93% 6% . .
7	R	142	94% 6%

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Mol	Chain	Length	Quality of chain
8	S	123	 90% 8% ..
9	T	143	 93% 6% .
10	U	136	 95% . .
11	V	127	 91% . 6%
12	W	117	 91% 8% .
13	X	115	 94% . .
14	Y	118	 97% . .
15	Z	103	 90% 9% .
16	a	110	 98% .
17	b	100	 87% 6% 7%
18	c	104	 91% 7% .
19	d	94	 96% .
20	e	85	 86% . 12%
21	f	78	 97% ..
22	g	63	 98% .
23	h	59	 95% . .
24	i	57	 91% 7% .
25	j	55	 91% 9%
26	k	46	 96% .
27	l	65	 95% . .
28	m	38	 100%
29	B	16	 75% 25%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 87594 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	2898	Total	C	N	O	P	0	0
			62225	27764	11448	20115	2898		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	118	Total	C	N	O	P	0	0
			2531	1127	465	821	118		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L6.

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

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 12 is a protein called 50S ribosomal protein L18.

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

- Molecule 13 is a protein called 50S ribosomal protein L19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	b	93	Total	C	N	O	S	0
			738	466	139	131	2	0

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	102	Total	C	N	O		0
			779	492	146	141		0

- Molecule 19 is a protein called 50S ribosomal protein L25.

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

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	e	75	Total	C	N	O	S	0
			569	353	113	102	1	0

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

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

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	j	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 26 is a protein called 50S ribosomal protein L34.

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

- Molecule 27 is a protein called 50S ribosomal protein L35.

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

- Molecule 28 is a protein called 50S ribosomal protein L36.

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

- Molecule 29 is a protein called Myxovalargin A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	B	16	Total	C	N	O	0	0
			119	81	21	17		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	I	141	Total	Mg	0
			141	141	
30	J	3	Total	Mg	0
			3	3	
30	L	1	Total	Mg	0
			1	1	

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
31	m	1	Total	Zn	0
			1	1	

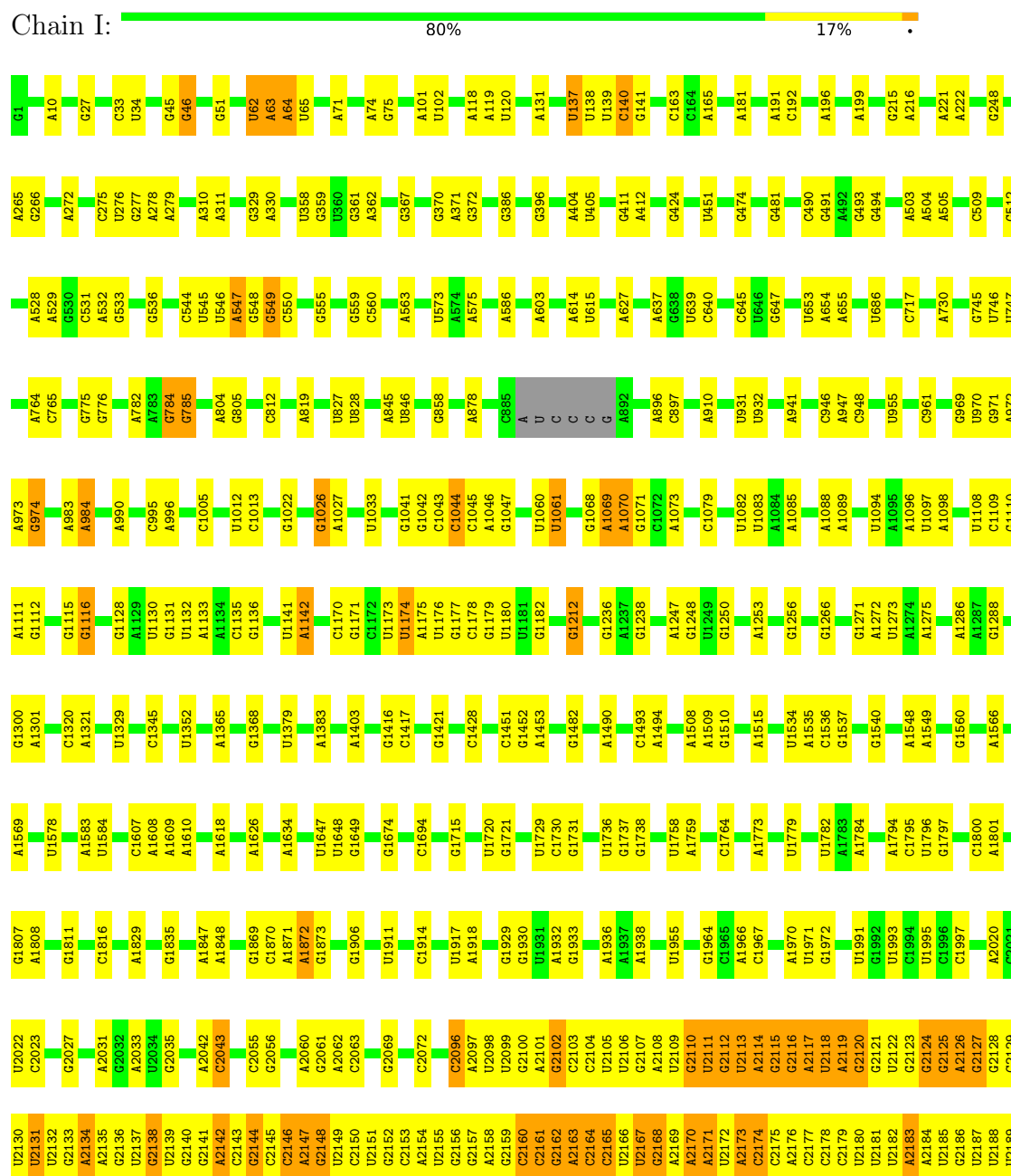
- Molecule 32 is water.

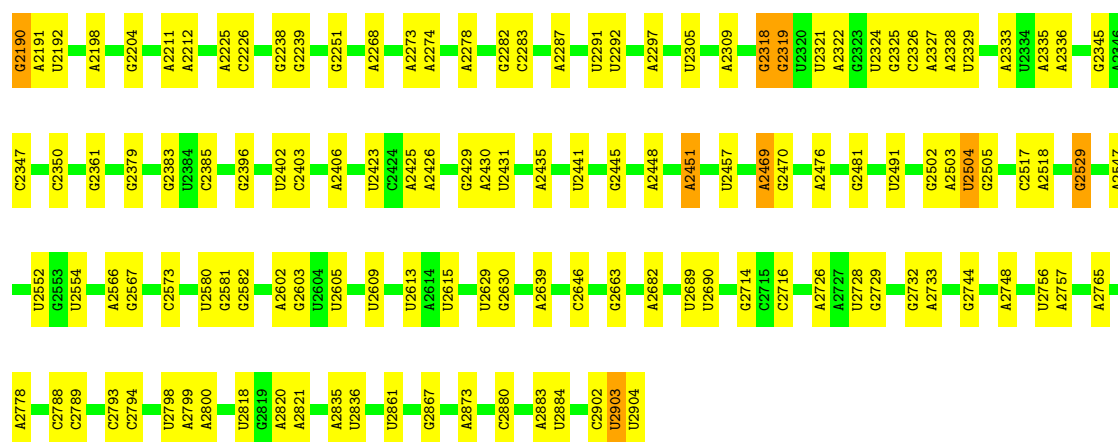
Mol	Chain	Residues	Atoms		AltConf
32	I	18	Total	O	0
			18	18	
32	B	10	Total	O	0
			10	10	

3 Residue-property plots

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

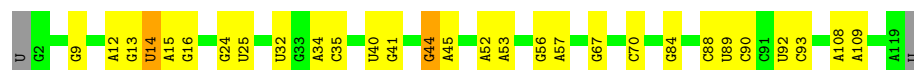
• Molecule 1: 23S ribosomal RNA





- Molecule 2: 5S ribosomal RNA

Chain J: 74% 22% ..



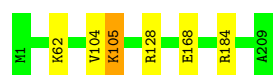
- Molecule 3: 50S ribosomal protein L2

Chain K: 97% ..



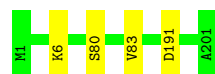
- Molecule 4: 50S ribosomal protein L3

Chain L: 97% .



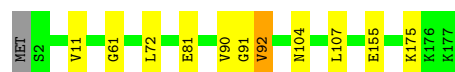
- Molecule 5: 50S ribosomal protein L4

Chain M: 98% .




- Molecule 6: 50S ribosomal protein L6

Chain O: 93% 6% ..




- Molecule 7: 50S ribosomal protein L13

Chain R:  94% 6%



- Molecule 8: 50S ribosomal protein L14

Chain S:  90% 8% ..



- Molecule 9: 50S ribosomal protein L15

Chain T:  93% 6% .



- Molecule 10: 50S ribosomal protein L16

Chain U:  95% . .



- Molecule 11: 50S ribosomal protein L17

Chain V:  91% . 6%



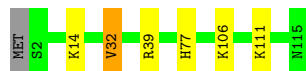
- Molecule 12: 50S ribosomal protein L18

Chain W:  91% 8% .



- Molecule 13: 50S ribosomal protein L19

Chain X:  94% . .




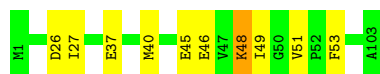
- Molecule 14: 50S ribosomal protein L20

Chain Y:  97% ..



- Molecule 15: 50S ribosomal protein L21

Chain Z:  90% 9% .



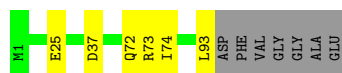
- Molecule 16: 50S ribosomal protein L22

Chain a:  98% .



- Molecule 17: 50S ribosomal protein L23

Chain b:  87% 6% 7%



- Molecule 18: 50S ribosomal protein L24

Chain c:  91% 7% .




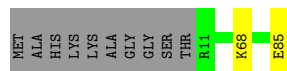
- Molecule 19: 50S ribosomal protein L25

Chain d:  96% .



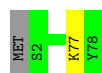
- Molecule 20: 50S ribosomal protein L27

Chain e:  86% . 12%



- Molecule 21: 50S ribosomal protein L28

Chain f:  97% ..



- Molecule 22: 50S ribosomal protein L29

Chain g:  98% .




- Molecule 23: 50S ribosomal protein L30

Chain h:  95% ..




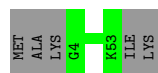
- Molecule 24: 50S ribosomal protein L32

Chain i:  91% 7% .



- Molecule 25: 50S ribosomal protein L33

Chain j:  91% 9%



- Molecule 26: 50S ribosomal protein L34

Chain k:  96% .



- Molecule 27: 50S ribosomal protein L35

Chain l:  95% ..



- Molecule 28: 50S ribosomal protein L36

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: Myxovalargin A

Chain B:  75% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	580425	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAA, IVA, IB9, DHV, OMU, MG, DVA, 1MG, PSU, RXL, ZN, 2MA, RX9, 2MG, DAR, AG2, 5MU, DAL, OMG, 5MC, OMC

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 > 5$	RMSZ	# $ Z > 5$
1	I	0.79	0/69266	0.76	0/108061
2	J	0.56	0/2831	0.73	0/4415
3	K	0.42	0/2121	0.61	0/2852
4	L	0.33	0/1586	0.55	0/2134
5	M	0.32	0/1571	0.52	0/2113
6	O	0.30	0/1343	0.54	0/1816
7	R	0.37	0/1152	0.55	0/1551
8	S	0.33	0/947	0.61	0/1268
9	T	0.33	0/1052	0.61	0/1401
10	U	0.34	0/1093	0.59	0/1460
11	V	0.34	0/973	0.61	0/1301
12	W	0.29	0/902	0.57	0/1209
13	X	0.34	0/929	0.56	0/1242
14	Y	0.34	0/960	0.58	0/1278
15	Z	0.34	0/829	0.55	0/1107
16	a	0.29	0/864	0.56	0/1156
17	b	0.31	0/744	0.56	0/994
18	c	0.31	0/787	0.53	0/1051
19	d	0.33	0/766	0.49	0/1025
20	e	0.34	0/576	0.57	0/762
21	f	0.31	0/635	0.60	0/848
22	g	0.27	0/502	0.55	0/667
23	h	0.28	0/453	0.56	0/605
24	i	0.33	0/450	0.62	0/599
25	j	0.36	0/416	0.51	0/554
26	k	0.32	0/380	0.71	0/498
27	l	0.31	0/513	0.57	0/676
28	m	0.34	0/303	0.62	0/397
29	B	0.17	0/10	0.63	0/11
All	All	0.70	0/94954	0.72	0/143051

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
29	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	B	15	DHV	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	I	62225	0	31309	327	0
2	J	2531	0	1280	6	0
3	K	2082	0	2154	2	0
4	L	1565	0	1616	2	0
5	M	1552	0	1619	0	0
6	O	1323	0	1371	2	0
7	R	1129	0	1162	2	0
8	S	938	0	1012	3	0
9	T	1043	0	1122	4	0
10	U	1074	0	1157	1	0
11	V	960	0	1000	2	0
12	W	892	0	923	2	0
13	X	917	0	962	2	0
14	Y	947	0	1019	2	0
15	Z	816	0	839	2	0
16	a	857	0	922	0	0
17	b	738	0	807	0	0
18	c	779	0	831	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	d	753	0	780	0	0
20	e	569	0	581	0	0
21	f	625	0	652	0	0
22	g	501	0	531	0	0
23	h	449	0	488	0	0
24	i	444	0	458	0	0
25	j	409	0	440	0	0
26	k	377	0	418	0	0
27	l	504	0	572	0	0
28	m	302	0	340	0	0
29	B	119	0	102	0	0
30	I	141	0	0	0	0
30	J	3	0	0	0	0
30	L	1	0	0	0	0
31	m	1	0	0	0	0
32	B	10	0	0	0	0
32	I	18	0	0	0	0
All	All	87594	0	56467	357	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 3.

The worst 5 of 357 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)
1:I:2119:A:H61	1:I:2167:U:H1'	1.29	0.97
1:I:2124:G:H3'	1:I:2125:G:H8	1.29	0.96
1:I:2133:G:H2'	1:I:2157:G:H22	1.32	0.93
1:I:2159:G:H2'	1:I:2160:C:C6	2.05	0.90
1:I:2111:U:H1'	1:I:2118:U:H4'	1.53	0.90

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	
3	K	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
4	L	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
5	M	199/201 (99%)	192 (96%)	5 (2%)	2 (1%)	13	9
6	O	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	12	8
7	R	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
8	S	120/123 (98%)	108 (90%)	10 (8%)	2 (2%)	7	4
9	T	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	19	16
10	U	134/136 (98%)	129 (96%)	4 (3%)	1 (1%)	19	16
11	V	118/127 (93%)	114 (97%)	4 (3%)	0	100	100
12	W	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
13	X	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
14	Y	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
15	Z	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	13	9
16	a	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
17	b	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
18	c	100/104 (96%)	88 (88%)	10 (10%)	2 (2%)	6	3
19	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
20	e	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
21	f	75/78 (96%)	75 (100%)	0	0	100	100
22	g	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
23	h	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
24	i	54/57 (95%)	52 (96%)	1 (2%)	1 (2%)	6	3
25	j	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
26	k	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
27	l	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
28	m	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
29	B	2/16 (12%)	1 (50%)	1 (50%)	0	100	100
All	All	2845/2954 (96%)	2731 (96%)	102 (4%)	12 (0%)	32	29

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	O	61	GLY
8	S	35	VAL
10	U	69	PRO
24	i	55	ILE
18	c	17	LYS

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	
3	K	216/218 (99%)	213 (99%)	3 (1%)	62	70
4	L	164/164 (100%)	160 (98%)	4 (2%)	44	49
5	M	165/165 (100%)	163 (99%)	2 (1%)	67	74
6	O	137/138 (99%)	130 (95%)	7 (5%)	20	19
7	R	116/116 (100%)	111 (96%)	5 (4%)	25	25
8	S	103/104 (99%)	98 (95%)	5 (5%)	21	20
9	T	102/102 (100%)	100 (98%)	2 (2%)	50	57
10	U	109/109 (100%)	104 (95%)	5 (5%)	23	23
11	V	100/103 (97%)	100 (100%)	0	100	100
12	W	86/87 (99%)	79 (92%)	7 (8%)	9	7
13	X	99/100 (99%)	96 (97%)	3 (3%)	36	40
14	Y	89/90 (99%)	88 (99%)	1 (1%)	70	77
15	Z	84/84 (100%)	77 (92%)	7 (8%)	9	6
16	a	93/93 (100%)	91 (98%)	2 (2%)	47	53
17	b	80/84 (95%)	74 (92%)	6 (8%)	11	9
18	c	83/85 (98%)	78 (94%)	5 (6%)	16	14
19	d	78/78 (100%)	74 (95%)	4 (5%)	20	19
20	e	56/63 (89%)	54 (96%)	2 (4%)	30	32
21	f	67/68 (98%)	66 (98%)	1 (2%)	60	67
22	g	54/55 (98%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	h	48/49 (98%)	46 (96%)	2 (4%)	25	26
24	i	47/48 (98%)	44 (94%)	3 (6%)	14	12
25	j	45/49 (92%)	45 (100%)	0	100	100
26	k	38/38 (100%)	36 (95%)	2 (5%)	19	18
27	l	51/52 (98%)	49 (96%)	2 (4%)	27	29
28	m	34/34 (100%)	34 (100%)	0	100	100
29	B	1/1 (100%)	1 (100%)	0	100	100
All	All	2345/2377 (99%)	2265 (97%)	80 (3%)	34	35

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	b	74	ILE
23	h	4	THR
18	c	18	ASP
19	d	8	VAL
24	i	54	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2895/2904 (99%)	410 (14%)	50 (1%)
2	J	117/120 (97%)	23 (19%)	4 (3%)
All	All	3012/3024 (99%)	433 (14%)	54 (1%)

5 of 433 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	10	A
1	I	34	U
1	I	46	G
1	I	51	G
1	I	63	A

5 of 54 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	1536	C
1	I	2160	C
1	I	2903	U
1	I	1608	A
1	I	1918	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

30 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
1	OMG	I	2251	1	18,26,27	1.26	3 (16%)	19,38,41	0.86	1 (5%)
1	5MU	I	1939	1	19,22,23	0.69	0	28,32,35	0.61	0
1	PSU	I	955	1	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
1	PSU	I	2580	1	18,21,22	1.11	2 (11%)	22,30,33	1.98	6 (27%)
29	IB9	B	7	29	12,12,13	0.28	0	12,15,17	0.56	0
1	PSU	I	2504	1	18,21,22	1.11	3 (16%)	22,30,33	1.92	6 (27%)
1	5MC	I	1962	1	18,22,23	0.68	0	26,32,35	0.59	0
1	PSU	I	746	30,1	18,21,22	1.04	1 (5%)	22,30,33	1.79	3 (13%)
1	2MA	I	2503	30,1	19,25,26	3.29	8 (42%)	21,37,40	1.88	3 (14%)
29	MAA	B	4	29	4,5,6	0.47	0	1,5,7	0.19	0
29	RXL	B	2	29	5,6,7	1.47	1 (20%)	5,7,9	1.81	2 (40%)
1	1MG	I	745	1	18,26,27	2.78	6 (33%)	19,39,42	1.61	4 (21%)
29	DHV	B	15	29	5,7,8	0.60	0	4,10,12	0.68	0
29	RXL	B	9	29	5,6,7	1.27	1 (20%)	5,7,9	2.58	2 (40%)
1	PSU	I	1917	1	18,21,22	1.05	1 (5%)	22,30,33	1.89	6 (27%)
1	PSU	I	1911	1	18,21,22	1.05	1 (5%)	22,30,33	1.85	5 (22%)
1	PSU	I	2457	1	18,21,22	1.08	1 (5%)	22,30,33	1.84	5 (22%)
1	OMC	I	2498	30,1	19,22,23	0.77	0	26,31,34	0.59	0
1	OMU	I	2552	1	19,22,23	2.85	8 (42%)	26,31,34	1.79	5 (19%)
29	RX9	B	13	29	5,7,8	1.45	1 (20%)	2,8,10	2.93	2 (100%)
1	5MU	I	747	1	19,22,23	0.67	0	28,32,35	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	I	1835	1	18,26,27	1.28	3 (16%)	16,38,41	0.86	1 (6%)
1	2MG	I	2445	1	18,26,27	1.38	3 (16%)	16,38,41	0.97	1 (6%)
1	PSU	I	2605	1	18,21,22	1.06	1 (5%)	22,30,33	1.85	3 (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
1	OMG	I	2251	1	-	0/5/27/28	0/3/3/3
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
29	IB9	B	7	29	-	0/7/7/8	0/1/1/1
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	I	746	30,1	-	2/7/25/26	0/2/2/2
1	2MA	I	2503	30,1	-	1/3/25/26	0/3/3/3
29	MAA	B	4	29	-	0/1/4/6	-
29	RXL	B	2	29	-	0/0/6/8	-
1	1MG	I	745	1	-	0/3/25/26	0/3/3/3
29	DHV	B	15	29	-	0/4/8/10	-
29	RXL	B	9	29	-	0/0/6/8	-
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	I	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	I	2498	30,1	-	0/9/27/28	0/2/2/2
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
29	RX9	B	13	29	-	2/2/8/10	-
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	2MG	I	1835	1	-	0/5/27/28	0/3/3/3
1	2MG	I	2445	1	-	1/5/27/28	0/3/3/3
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C4-N3	9.07	1.49	1.35
1	I	745	1MG	C2-N3	6.69	1.46	1.34
1	I	2552	OMU	C2-N1	6.37	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C2-N1	6.37	1.45	1.34
1	I	2503	2MA	C2-N3	6.30	1.45	1.34

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2503	2MA	C2-N3-C4	6.33	120.67	115.52
1	I	2552	OMU	C4-N3-C2	-5.59	119.21	126.58
1	I	2605	PSU	C4-N3-C2	-4.97	119.19	126.34
1	I	2580	PSU	N1-C2-N3	4.94	120.73	115.13
1	I	2504	PSU	N1-C2-N3	4.91	120.69	115.13

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	746	PSU	C2'-C1'-C5-C6
29	B	13	RX9	CG2-CB-CG1-CD1
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	2504	PSU	C3'-C4'-C5'-O5'
29	B	13	RX9	CA-CB-CG1-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 146 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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.