



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 04:31 pm GMT

PDB ID : 6HMA
EMDB ID : EMD-0243
Title : Improved model derived from cryo-EM map of Staphylococcus aureus large ribosomal subunit
Authors : Eyal, Z.; Camicata, G.; Matzov, D.; Fox, T.; de Val, N.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2018-09-12
Resolution : 2.65 Å(reported)

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

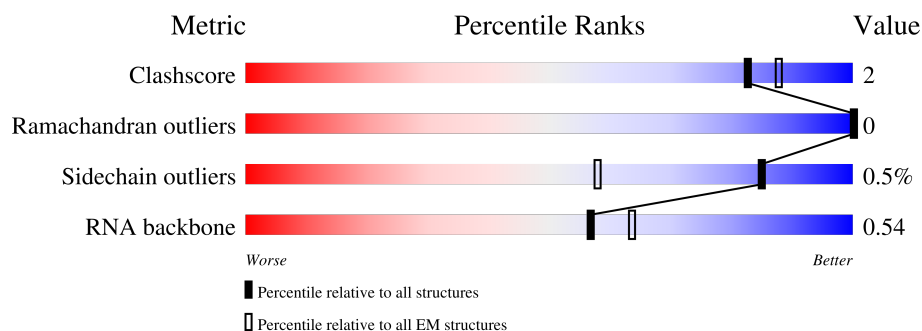
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.65 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.










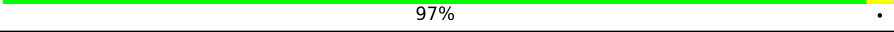

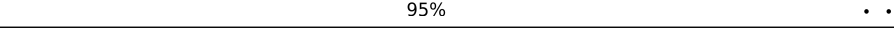
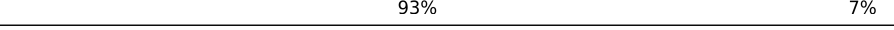
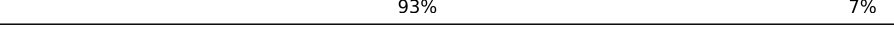
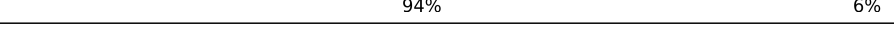

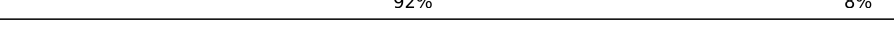
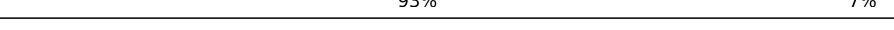
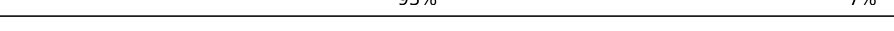


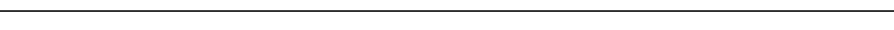

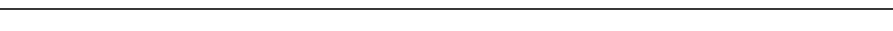
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	2923	75% 19% . .
2	B	115	83% 17%
3	C	274	92% 8%
4	D	215	90% 10%
5	E	206	92% 8%
6	F	158	97% .
7	G	175	93% 6% .

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Mol	Chain	Length	Quality of chain
8	H	145	 91% 9%
9	I	122	 80% 19% .
10	J	146	 91% 9%
11	K	137	 89% 11%
12	L	120	 93% 7%
13	M	119	 85% 15%
14	N	116	 85% 13% .
15	O	116	 97% .
16	P	102	 89% 11%
17	Q	112	 95% . .
18	R	89	 93% 7%
19	S	103	 93% 7%
20	T	94	 94% 6%
21	U	79	 90% 10%
22	V	49	 92% 8%
23	W	67	 93% 7%
24	X	58	 93% 7%
25	Z	48	 90% 10%
26	1	47	 89% 11%
27	2	43	 95% 5%
28	3	64	 95% 5%
29	4	37	 84% 14% .

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 86401 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	A	2834	Total	C	N	O	P	0	0
			60769	27128	11118	19689	2834		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	115	Total	C	N	O	P	0	0
			2448	1094	436	803	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	158	Total	C	N	O	0	0
			778	462	158	158		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1263	790	239	231	3		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	119	Total	C	N	O	0	0
			882	549	174	159		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	114	Total	C	N	O	0	0
			889	563	175	151		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	112	Total	C	N	O	S	0	0
			854	534	164	153	3		

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	94	Total	C	N	O	0	0
			722	463	130	129		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	79	Total	C	N	O	0	0
			597	369	117	111		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	49	Total	C	N	O	0	0
			379	234	82	63		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	67	Total	C	N	O	0	0
			541	333	102	106		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	58	Total	C	N	O	0	0
			449	280	85	84		

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	48	Total	C	N	O	S	0	0
			360	222	77	59	2		

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 28 is a protein called 50S ribosomal protein L35.

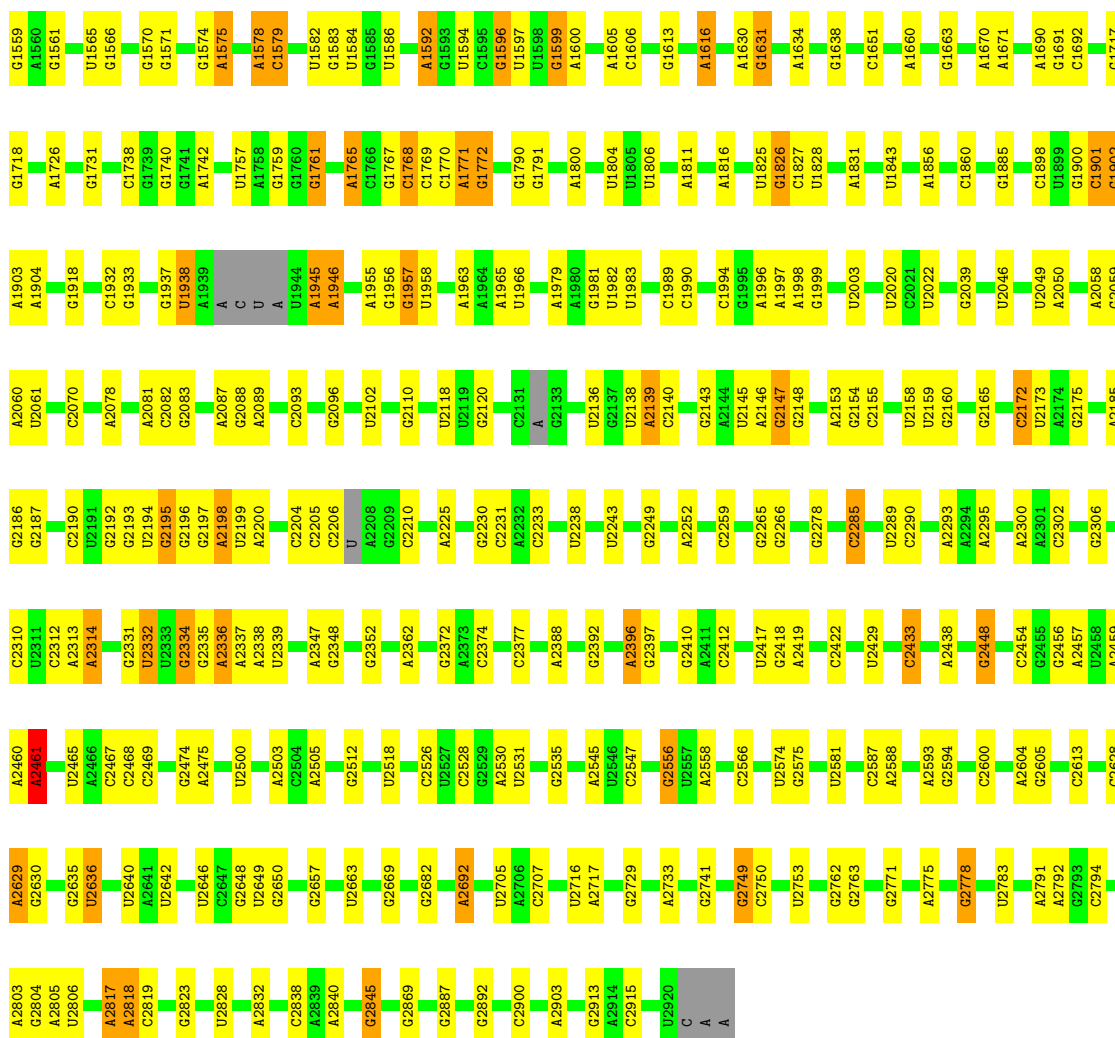
Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	37	Total	C	N	O	S	0	0
			295	186	60	44	5		

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

Mol	Chain	Residues	Atoms		AltConf
30	A	229	Total	Mg	0
			229	229	
30	B	2	Total	Mg	0
			2	2	
30	C	2	Total	Mg	0
			2	2	
30	J	1	Total	Mg	0
			1	1	
30	K	1	Total	Mg	0
			1	1	
30	U	1	Total	Mg	0
			1	1	
30	Z	1	Total	Mg	0
			1	1	



• Molecule 2: 5S ribosomal RNA

Chain B: 83% 17%



• Molecule 3: 50S ribosomal protein L2

Chain C: 92% 8%



• Molecule 4: 50S ribosomal protein L3

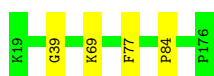
Chain D: 90% 10%



- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



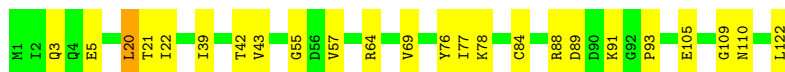
- Molecule 7: 50S ribosomal protein L6



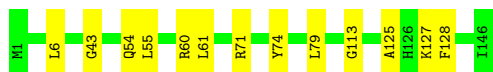
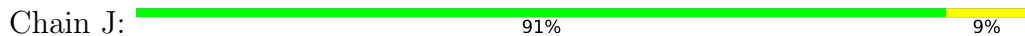
- Molecule 8: 50S ribosomal protein L13



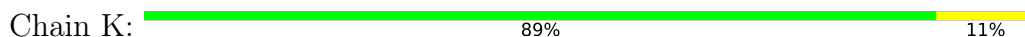
- Molecule 9: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L16





- Molecule 12: 50S ribosomal protein L17

Chain L: 93% 7%



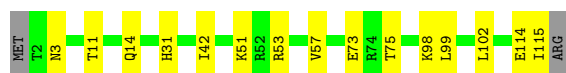
- Molecule 13: 50S ribosomal protein L18

Chain M: 85% 15%



- Molecule 14: 50S ribosomal protein L19

Chain N: 85% 13%



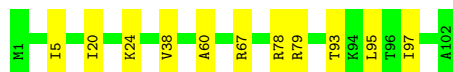
- Molecule 15: 50S ribosomal protein L20

Chain O: 97%



- Molecule 16: 50S ribosomal protein L21

Chain P: 89% 11%



- Molecule 17: 50S ribosomal protein L22

Chain Q: 95%



- Molecule 18: 50S ribosomal protein L23

Chain R: 93% 7%



- Molecule 19: 50S ribosomal protein L24

Chain S: 93% 7%



- Molecule 20: 50S ribosomal protein L25

Chain T: 94% 6%



- Molecule 21: 50S ribosomal protein L27

Chain U: 90% 10%



- Molecule 22: 50S ribosomal protein L28

Chain V: 92% 8%



- Molecule 23: 50S ribosomal protein L29

Chain W: 93% 7%



- Molecule 24: 50S ribosomal protein L30

Chain X: 93% 7%

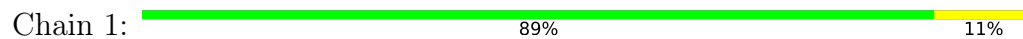


- Molecule 25: 50S ribosomal protein L32

Chain Z: 90% 10%



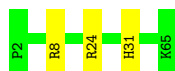
- Molecule 26: 50S ribosomal protein L33



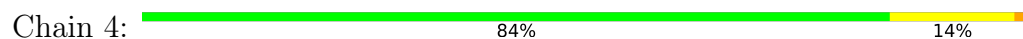
- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



- Molecule 29: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	211046	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
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: 5MU, MG, 2MA

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	A	1.19	15/67975 (0.0%)	1.12	142/105995 (0.1%)
2	B	0.97	0/2736	1.04	11/4261 (0.3%)
3	C	0.67	0/2129	0.64	0/2858
4	D	0.70	0/1651	0.66	0/2215
5	E	0.64	0/1595	0.65	0/2154
6	F	0.25	0/777	0.48	0/1079
7	G	0.39	0/1281	0.55	0/1736
8	H	0.69	0/1165	0.67	1/1570 (0.1%)
9	I	0.67	1/925 (0.1%)	0.73	2/1242 (0.2%)
10	J	0.67	0/1100	0.71	0/1467
11	K	0.64	0/1095	0.60	0/1472
12	L	0.63	0/936	0.70	0/1253
13	M	0.43	0/891	0.62	1/1194 (0.1%)
14	N	0.65	0/901	0.63	0/1209
15	O	0.73	0/954	0.65	0/1264
16	P	0.69	0/800	0.69	0/1070
17	Q	0.66	0/862	0.68	0/1161
18	R	0.65	0/723	0.63	0/966
19	S	0.53	0/779	0.66	1/1043 (0.1%)
20	T	0.51	0/730	0.65	0/981
21	U	0.74	0/603	0.66	0/802
22	V	0.56	0/384	0.62	0/515
23	W	0.55	0/542	0.68	0/722
24	X	0.63	0/451	0.62	0/606
25	Z	0.61	0/366	0.63	0/489
26	1	0.33	0/395	0.56	0/530
27	2	0.77	0/371	0.70	0/484
28	3	0.62	0/526	0.63	0/690
29	4	0.56	0/298	0.60	0/392
All	All	1.07	16/93941 (0.0%)	1.03	158/141420 (0.1%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	792	5MU	O3'-P	-35.00	1.19	1.61
1	A	790	G	O3'-P	-22.26	1.34	1.61
1	A	1224	U	O3'-P	-11.14	1.47	1.61
1	A	1966	5MU	O3'-P	-10.64	1.48	1.61
1	A	1599	G	N3-C4	-7.42	1.30	1.35

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2397	G	O5'-P-OP1	-30.54	74.06	110.70
1	A	2397	G	OP1-P-OP2	-26.01	80.58	119.60
1	A	2397	G	O5'-P-OP2	20.15	134.88	110.70
1	A	1599	G	N3-C2-N2	-14.67	109.63	119.90
1	A	2396	A	OP2-P-O3'	-13.24	76.06	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A	60769	0	30549	154	0
2	B	2448	0	1239	1	0
3	C	2094	0	2205	15	0
4	D	1627	0	1667	14	0
5	E	1572	0	1619	22	0
6	F	778	0	348	4	0
7	G	1263	0	1225	9	0
8	H	1143	0	1134	7	0
9	I	918	0	981	19	0
10	J	1086	0	1125	14	0
11	K	1071	0	1123	10	0
12	L	932	0	983	4	0
13	M	882	0	900	9	0
14	N	889	0	937	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	942	0	1014	4	0
16	P	790	0	830	6	0
17	Q	854	0	914	6	0
18	R	715	0	748	3	0
19	S	770	0	809	4	0
20	T	722	0	766	3	0
21	U	597	0	604	5	0
22	V	379	0	400	3	0
23	W	541	0	563	3	0
24	X	449	0	491	3	0
25	Z	360	0	358	4	0
26	1	390	0	394	3	0
27	2	367	0	415	2	0
28	3	521	0	586	3	0
29	4	295	0	340	5	0
30	A	229	0	0	0	0
30	B	2	0	0	0	0
30	C	2	0	0	0	0
30	J	1	0	0	0	0
30	K	1	0	0	0	0
30	U	1	0	0	0	0
30	Z	1	0	0	0	0
All	All	86401	0	55267	287	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 2.

The worst 5 of 287 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:A:2338:A:C2	6:F:77:PHE:CB	2.50	0.95
5:E:34:PHE:CE1	10:J:6:LEU:HD13	2.08	0.88
1:A:2669:G:OP2	8:H:86:LYS:NZ	2.09	0.86
4:D:131:ILE:HD11	4:D:149:ARG:CZ	2.07	0.84
1:A:1825:U:OP2	3:C:274:ARG:NH2	2.14	0.80

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	C	272/274 (99%)	259 (95%)	13 (5%)	0	100	100
4	D	213/215 (99%)	195 (92%)	18 (8%)	0	100	100
5	E	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
6	F	156/158 (99%)	140 (90%)	16 (10%)	0	100	100
7	G	173/175 (99%)	159 (92%)	14 (8%)	0	100	100
8	H	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
9	I	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	J	144/146 (99%)	134 (93%)	10 (7%)	0	100	100
11	K	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
12	L	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
13	M	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
14	N	112/116 (97%)	103 (92%)	9 (8%)	0	100	100
15	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
16	P	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
17	Q	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
18	R	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
19	S	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
20	T	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
21	U	77/79 (98%)	72 (94%)	5 (6%)	0	100	100
22	V	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
23	W	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
24	X	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
25	Z	46/48 (96%)	39 (85%)	7 (15%)	0	100	100
26	1	45/47 (96%)	45 (100%)	0	0	100	100
27	2	41/43 (95%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	3	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
29	4	35/37 (95%)	35 (100%)	0	0	100	100
All	All	2985/3041 (98%)	2766 (93%)	219 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	C	221/221 (100%)	221 (100%)	0	100	100
4	D	173/173 (100%)	173 (100%)	0	100	100
5	E	168/168 (100%)	168 (100%)	0	100	100
7	G	124/153 (81%)	123 (99%)	1 (1%)	79	89
8	H	122/123 (99%)	121 (99%)	1 (1%)	79	89
9	I	100/100 (100%)	100 (100%)	0	100	100
10	J	109/112 (97%)	109 (100%)	0	100	100
11	K	108/114 (95%)	108 (100%)	0	100	100
12	L	96/101 (95%)	95 (99%)	1 (1%)	73	85
13	M	83/95 (87%)	81 (98%)	2 (2%)	44	65
14	N	93/102 (91%)	91 (98%)	2 (2%)	47	68
15	O	96/96 (100%)	96 (100%)	0	100	100
16	P	84/86 (98%)	84 (100%)	0	100	100
17	Q	89/91 (98%)	88 (99%)	1 (1%)	70	84
18	R	78/80 (98%)	78 (100%)	0	100	100
19	S	81/88 (92%)	81 (100%)	0	100	100
20	T	78/82 (95%)	78 (100%)	0	100	100
21	U	59/62 (95%)	57 (97%)	2 (3%)	32	51
22	V	39/41 (95%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	58/60 (97%)	58 (100%)	0	100	100
24	X	52/52 (100%)	52 (100%)	0	100	100
25	Z	35/44 (80%)	35 (100%)	0	100	100
26	1	44/45 (98%)	44 (100%)	0	100	100
27	2	39/39 (100%)	39 (100%)	0	100	100
28	3	55/55 (100%)	55 (100%)	0	100	100
29	4	35/35 (100%)	34 (97%)	1 (3%)	37	58
All	All	2319/2418 (96%)	2308 (100%)	11 (0%)	85	94

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	98	LYS
21	U	22	ARG
29	4	35	ARG
21	U	61	ARG
13	M	87	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	4	HIS
10	J	54	GLN
14	N	3	ASN
3	C	232	HIS
3	C	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2820/2923 (96%)	450 (15%)	6 (0%)
2	B	114/115 (99%)	12 (10%)	0
All	All	2934/3038 (96%)	462 (15%)	6 (0%)

5 of 462 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	10	A
1	A	28	A
1	A	34	U
1	A	36	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1670	A
1	A	1957	G
1	A	2749	G
1	A	577	A
1	A	576	U

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

3 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	5MU	A	1966	1	19,22,23	4.61	7 (36%)	28,32,35	3.83	10 (35%)
1	2MA	A	2530	30,1	19,25,26	0.90	0	21,37,40	2.26	6 (28%)
1	5MU	A	792	1	19,22,23	4.51	7 (36%)	28,32,35	3.85	10 (35%)

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	5MU	A	1966	1	-	0/7/25/26	0/2/2/2
1	2MA	A	2530	30,1	-	2/3/25/26	0/3/3/3
1	5MU	A	792	1	-	2/7/25/26	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1966	5MU	C2-N1	9.99	1.54	1.38
1	A	792	5MU	C2-N1	9.89	1.54	1.38
1	A	1966	5MU	C6-N1	9.73	1.54	1.38
1	A	792	5MU	C6-N1	9.39	1.54	1.38
1	A	1966	5MU	C4-C5	9.18	1.60	1.44

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	792	5MU	C5-C4-N3	12.99	126.40	115.31
1	A	1966	5MU	C5-C4-N3	12.45	125.94	115.31
1	A	1966	5MU	C5-C6-N1	-11.06	111.96	123.34
1	A	792	5MU	C5-C6-N1	-10.44	112.59	123.34
1	A	2530	2MA	C2-N3-C4	7.69	121.77	115.52

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	792	5MU	O4'-C4'-C5'-O5'
1	A	792	5MU	C3'-C4'-C5'-O5'
1	A	2530	2MA	O4'-C4'-C5'-O5'
1	A	2530	2MA	C3'-C4'-C5'-O5'

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 237 ligands modelled in this entry, 237 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1299:U	O3'	1300:G	P	3.08
1	A	1232:G	O3'	1233:A	P	3.01
1	A	1294:G	O3'	1295:C	P	2.95
1	A	790:G	O3'	791:U	P	1.34
1	A	792:5MU	O3'	793:G	P	1.19