



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 05:00 pm GMT

PDB ID : 8ANA
EMDB ID : EMD-15533
Title : Cryo-EM structure of the proline-rich antimicrobial peptide drosocin bound to the 50S ribosomal subunit
Authors : Koller, T.O.; Morici, M.; Wilson, D.N.
Deposited on : 2022-08-05
Resolution : 2.10 Å(reported)

This is a Full wwPDB EM Validation 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
buster-report : 1.1.7 (2018)
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

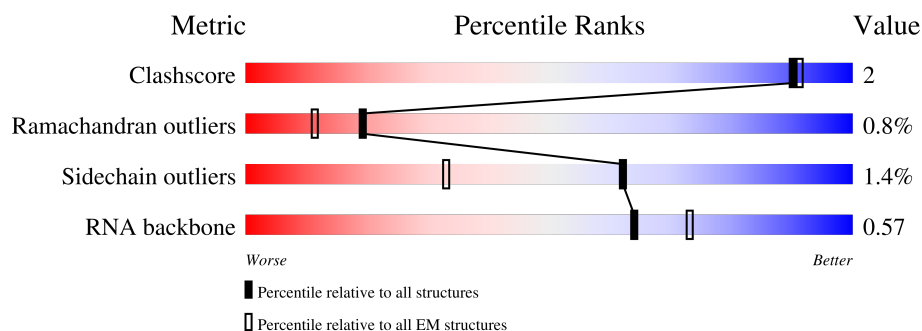
1 Overall quality at a glance

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.




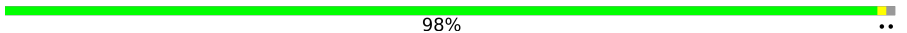
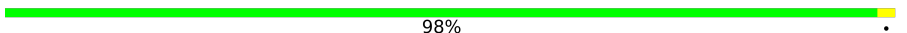
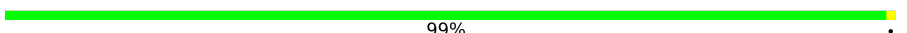

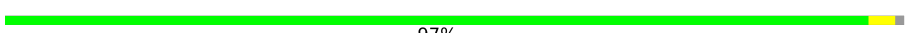









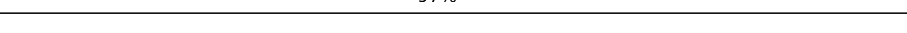
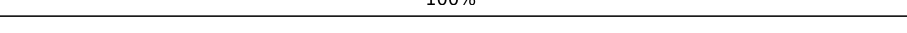
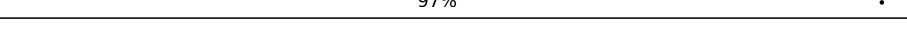


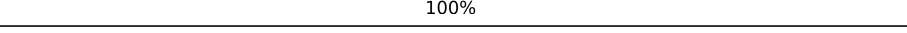

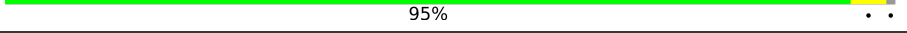
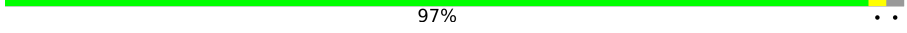
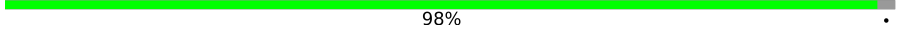
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	55	91% 7%
2	1	46	96% .
3	2	65	95% . .
4	3	38	100%
5	4	70	76% 9% . 14%
6	A	19	100%
7	a	2903	83% 11% 6%

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Mol	Chain	Length	Quality of chain
8	b	120	 88% 12%
9	c	273	 98%
10	d	209	 98%
11	e	201	 99%
12	f	179	 94%
13	g	177	 97%
14	h	149	 27% 72%
15	i	142	 99%
16	j	123	 98%
17	k	144	 98%
18	l	136	 99%
19	m	127	 93% 7%
20	n	117	 99%
21	o	115	 98%
22	p	118	 97%
23	q	103	 100%
24	r	110	 97%
25	s	100	 90% 7%
26	t	104	 92% 6%
27	u	94	 100%
28	v	85	 92% 8%
29	w	78	 95%
30	x	63	 97%
31	y	59	 98%
32	z	57	 98%

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 86461 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 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a protein called Drosocin1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	19	Total	C	N	O	0	0
			155	98	34	23		

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	2733	Total	C	N	O	P	0	0
			58702	26191	10821	18957	2733		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 9 is a protein called 50S ribosomal protein L2.

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

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 11 is a protein called 50S ribosomal protein L4.

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

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 13 is a protein called 50S ribosomal protein L6.

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

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 15 is a protein called 50S ribosomal protein L13.

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

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 18 is a protein called 50S ribosomal protein L16.

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

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 20 is a protein called 50S ribosomal protein L18.

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

- Molecule 21 is a protein called 50S ribosomal protein L19.

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

- Molecule 22 is a protein called 50S ribosomal protein L20.

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

- Molecule 23 is a protein called 50S ribosomal protein L21.

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

- Molecule 24 is a protein called 50S ribosomal protein L22.

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

- Molecule 25 is a protein called 50S ribosomal protein L23.

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

- Molecule 26 is a protein called 50S ribosomal protein L24.

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

- Molecule 27 is a protein called 50S ribosomal protein L25.

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

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 29 is a protein called 50S ribosomal protein L28.

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

- Molecule 30 is a protein called 50S ribosomal protein L29.

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

- Molecule 31 is a protein called 50S ribosomal protein L30.

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

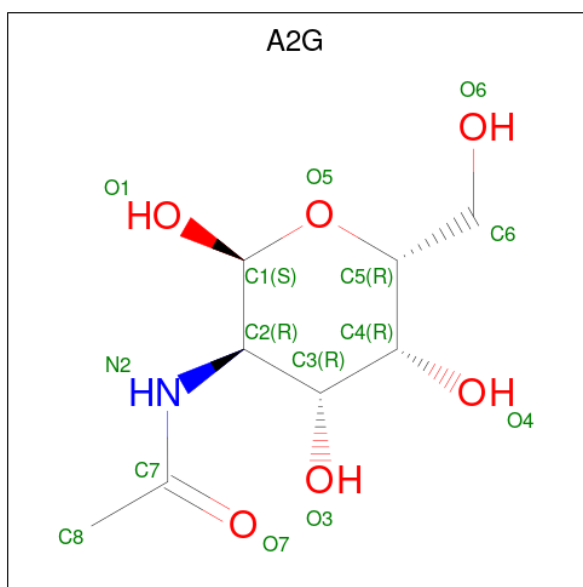
- Molecule 32 is a protein called 50S ribosomal protein L32.

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

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	3	1	Total	Zn	0
			1	1	
33	4	1	Total	Zn	0
			1	1	

- Molecule 34 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

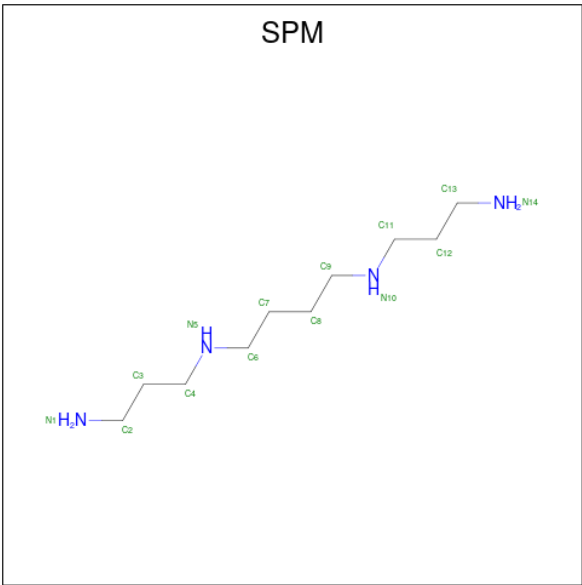


Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	a	208	Total	Mg	0
			208	208	
35	b	5	Total	Mg	0
			5	5	
35	c	1	Total	Mg	0
			1	1	
35	d	1	Total	Mg	0
			1	1	
35	z	1	Total	Mg	0
			1	1	

- Molecule 36 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	N	0
			14	10	4	


- Molecule 37 is water.

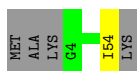
Mol	Chain	Residues	Atoms		AltConf
37	A	11	Total	O	0
			11	11	
37	a	27	Total	O	0
			27	27	
37	e	2	Total	O	0
			2	2	
37	r	2	Total	O	0
			2	2	

3 Residue-property plots [i](#)

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: 50S ribosomal protein L33

Chain 0:  91% 7%



- Molecule 2: 50S ribosomal protein L34

Chain 1:  96%



- Molecule 3: 50S ribosomal protein L35

Chain 2:  95%



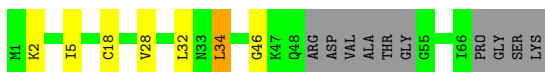
- Molecule 4: 50S ribosomal protein L36

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: 50S ribosomal protein L31

Chain 4:  76% 9% 14%



- Molecule 6: Drosocin1

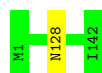
Chain A:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: 5S ribosomal RNA

Chain b: 88% 12%

Chain i:  99%



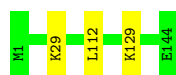
- Molecule 16: 50S ribosomal protein L14

Chain j:  98%



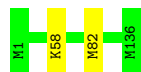
- Molecule 17: 50S ribosomal protein L15

Chain k:  98%



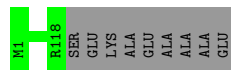
- Molecule 18: 50S ribosomal protein L16

Chain l:  99%



- Molecule 19: 50S ribosomal protein L17

Chain m:  93%  7%



- Molecule 20: 50S ribosomal protein L18

Chain n:  99%



- Molecule 21: 50S ribosomal protein L19

Chain o:  98%



- Molecule 22: 50S ribosomal protein L20

Chain p:  97% ..



- Molecule 23: 50S ribosomal protein L21

Chain q:  100%


There are no outlier residues recorded for this chain.

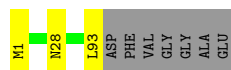
- Molecule 24: 50S ribosomal protein L22

Chain r:  97% .




- Molecule 25: 50S ribosomal protein L23

Chain s:  90% . 7%



- Molecule 26: 50S ribosomal protein L24

Chain t:  92% 6% .



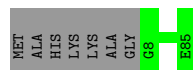
- Molecule 27: 50S ribosomal protein L25

Chain u:  100%

There are no outlier residues recorded for this chain.

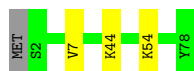
- Molecule 28: 50S ribosomal protein L27

Chain v:  92% 8%



- Molecule 29: 50S ribosomal protein L28

Chain w:  95% ..



- Molecule 30: 50S ribosomal protein L29

Chain x: 97%



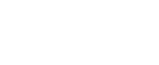
- Molecule 31: 50S ribosomal protein L30

Chain y: 98%



- Molecule 32: 50S ribosomal protein L32

Chain z: 98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159749	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: 1MG, A2G, MG, MEQ, ZN, PSU, SPM, H2U, G7M, 2MG, OMU, OMC, OMG, 5MC, 5MU, 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	0	0.24	0/424	0.47	0/565
2	1	0.27	0/380	0.48	0/498
3	2	0.28	0/513	0.50	0/676
4	3	0.26	0/303	0.51	0/397
5	4	0.27	0/488	0.45	0/649
6	A	0.36	0/162	0.61	0/221
7	a	0.58	4/65294 (0.0%)	0.91	11/101861 (0.0%)
8	b	0.98	0/2850	1.14	0/4444
9	c	0.65	0/2121	0.74	0/2852
10	d	0.65	0/1576	0.74	0/2119
11	e	0.67	0/1571	0.71	0/2113
12	f	0.69	0/1434	0.72	0/1926
13	g	0.69	0/1343	0.74	0/1816
14	h	0.71	0/306	0.75	0/413
15	i	0.63	0/1152	0.70	0/1551
16	j	0.67	0/955	0.74	0/1279
17	k	0.68	0/1062	0.73	0/1413
18	l	0.64	0/1093	0.72	0/1460
19	m	0.63	0/958	0.73	0/1281
20	n	0.69	0/902	0.73	0/1209
21	o	0.66	0/929	0.72	0/1242
22	p	0.63	0/960	0.70	0/1278
23	q	0.66	0/829	0.74	0/1107
24	r	0.66	0/864	0.73	0/1156
25	s	0.66	0/744	0.72	0/994
26	t	0.70	0/787	0.75	0/1051
27	u	0.66	0/766	0.72	0/1025
28	v	0.67	0/593	0.75	0/785
29	w	0.65	0/635	0.72	0/848
30	x	0.67	0/502	0.67	0/667
31	y	0.66	0/453	0.72	0/605
32	z	0.68	0/450	0.72	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.61	4/93399 (0.0%)	0.87	11/140100 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	2546	U	C4-C5	6.38	1.49	1.43
7	a	2546	U	N1-C2	6.05	1.44	1.38
7	a	592	A	C5-C6	5.25	1.45	1.41
7	a	2525	G	N7-C5	5.11	1.42	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	512	G	O4'-C1'-N9	7.39	114.11	108.20
7	a	1617	C	P-O3'-C3'	-6.98	111.32	119.70
7	a	2030	A	P-O3'-C3'	-6.42	112.00	119.70
7	a	781	A	O3'-P-O5'	-6.04	92.53	104.00
7	a	2447	G	C3'-C2'-C1'	-5.74	96.91	101.50
7	a	784	G	OP1-P-O3'	5.51	117.32	105.20
7	a	748	G	C1'-O4'-C4'	-5.41	105.58	109.90
7	a	2050	C	O3'-P-O5'	-5.39	93.75	104.00
7	a	512	G	C1'-O4'-C4'	-5.25	105.70	109.90
7	a	242	G	C3'-C2'-C1'	-5.08	97.44	101.50
7	a	1936	A	C1'-O4'-C4'	-5.00	105.90	109.90

There are no chirality outliers.

There are no planarity outliers.

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	0	417	0	451	0	0
2	1	377	0	418	0	0
3	2	504	0	572	0	0
4	3	302	0	340	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	480	0	478	3	0
6	A	155	0	164	0	0
7	a	58702	0	29546	0	0
8	b	2549	0	1291	0	0
9	c	2082	0	2154	0	0
10	d	1566	0	1618	0	0
11	e	1552	0	1619	0	0
12	f	1410	0	1444	0	0
13	g	1323	0	1371	0	0
14	h	303	0	327	0	0
15	i	1129	0	1162	0	0
16	j	946	0	1023	0	0
17	k	1053	0	1129	0	0
18	l	1074	0	1157	0	0
19	m	945	0	989	0	0
20	n	892	0	923	0	0
21	o	917	0	962	0	0
22	p	947	0	1019	0	0
23	q	816	0	839	0	0
24	r	857	0	922	0	0
25	s	738	0	807	0	0
26	t	779	0	831	0	0
27	u	753	0	780	0	0
28	v	586	0	596	0	0
29	w	625	0	652	0	0
30	x	501	0	531	0	0
31	y	449	0	488	0	0
32	z	444	0	458	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
34	A	14	0	12	0	0
35	a	208	0	0	0	0
35	b	5	0	0	0	0
35	c	1	0	0	0	0
35	d	1	0	0	0	0
35	z	1	0	0	0	0
36	a	14	0	26	0	0
37	A	11	0	0	0	0
37	a	27	0	0	0	0
37	e	2	0	0	0	0
37	r	2	0	0	0	0
All	All	86461	0	57099	3	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.

All (3) 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)
5:4:34:LEU:N	5:4:34:LEU:HD23	2.21	0.56
5:4:28:VAL:HG21	5:4:32:LEU:HD21	1.91	0.52
5:4:2:LYS:HB2	5:4:5:ILE:HD11	1.98	0.45

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	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	47 (84%)	7 (12%)	2 (4%)	3	1
6	A	17/19 (90%)	17 (100%)	0	0	100	100
9	c	269/273 (98%)	256 (95%)	12 (4%)	1 (0%)	30	29
10	d	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	13	9
11	e	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	25	23
12	f	175/179 (98%)	146 (83%)	22 (13%)	7 (4%)	2	0
13	g	174/177 (98%)	158 (91%)	14 (8%)	2 (1%)	12	8
14	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
15	i	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
16	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	k	142/144 (99%)	128 (90%)	13 (9%)	1 (1%)	19	16
18	l	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	19	16
19	m	116/127 (91%)	104 (90%)	12 (10%)	0	100	100
20	n	114/117 (97%)	102 (90%)	12 (10%)	0	100	100
21	o	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
22	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
23	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
24	r	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	14	11
25	s	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	12	8
26	t	100/104 (96%)	86 (86%)	11 (11%)	3 (3%)	3	1
27	u	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
28	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
29	w	75/78 (96%)	73 (97%)	0	2 (3%)	4	1
30	x	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	7	4
31	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
32	z	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
All	All	3133/3356 (93%)	2928 (94%)	180 (6%)	25 (1%)	19	13

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	f	174	ASP
24	r	63	GLY
26	t	99	ASN
12	f	50	LEU
18	l	58	LYS
25	s	28	ASN
29	w	44	LYS
12	f	19	GLU
12	f	107	ALA
13	g	46	ALA
13	g	119	ALA
26	t	89	ASP
9	c	71	LYS
17	k	29	LYS
5	4	18	CYS

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Mol	Chain	Res	Type
10	d	94	GLN
10	d	149	ASN
12	f	21	ASN
30	x	37	LEU
11	e	142	ALA
12	f	109	PRO
12	f	126	GLY
29	w	7	VAL
5	4	46	GLY
26	t	39	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	0	46/49 (94%)	45 (98%)	1 (2%)	47	53
2	1	38/38 (100%)	36 (95%)	2 (5%)	19	18
3	2	51/52 (98%)	49 (96%)	2 (4%)	27	29
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	54 (98%)	1 (2%)	54	61
6	A	18/18 (100%)	18 (100%)	0	100	100
9	c	216/218 (99%)	214 (99%)	2 (1%)	75	82
10	d	163/163 (100%)	160 (98%)	3 (2%)	54	61
11	e	165/165 (100%)	163 (99%)	2 (1%)	67	74
12	f	148/150 (99%)	145 (98%)	3 (2%)	50	57
13	g	137/138 (99%)	134 (98%)	3 (2%)	47	53
14	h	32/114 (28%)	31 (97%)	1 (3%)	35	39
15	i	116/116 (100%)	115 (99%)	1 (1%)	75	82
16	j	104/104 (100%)	102 (98%)	2 (2%)	52	59
17	k	103/103 (100%)	101 (98%)	2 (2%)	52	59
18	l	109/109 (100%)	108 (99%)	1 (1%)	75	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	m	98/103 (95%)	98 (100%)	0	100	100
20	n	86/87 (99%)	86 (100%)	0	100	100
21	o	99/100 (99%)	98 (99%)	1 (1%)	73	79
22	p	89/90 (99%)	87 (98%)	2 (2%)	47	53
23	q	84/84 (100%)	84 (100%)	0	100	100
24	r	93/93 (100%)	91 (98%)	2 (2%)	47	53
25	s	80/84 (95%)	78 (98%)	2 (2%)	42	47
26	t	83/85 (98%)	80 (96%)	3 (4%)	30	32
27	u	78/78 (100%)	78 (100%)	0	100	100
28	v	58/63 (92%)	58 (100%)	0	100	100
29	w	67/68 (98%)	66 (98%)	1 (2%)	60	67
30	x	54/55 (98%)	54 (100%)	0	100	100
31	y	48/49 (98%)	48 (100%)	0	100	100
32	z	47/48 (98%)	47 (100%)	0	100	100
All	All	2599/2720 (96%)	2562 (99%)	37 (1%)	62	70

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	54	ILE
2	1	1	MET
2	1	25	LYS
3	2	31	HIS
3	2	47	LYS
5	4	34	LEU
9	c	37	ASN
9	c	181	MET
10	d	1	MET
10	d	33	ARG
10	d	110	THR
11	e	143	LEU
11	e	153	LEU
12	f	30	ARG
12	f	50	LEU
12	f	120	LYS
13	g	3	ARG
13	g	86	LYS

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Mol	Chain	Res	Type
13	g	105	LEU
14	h	20	ASN
15	i	128	ASN
16	j	49	ARG
16	j	113	MET
17	k	112	LEU
17	k	129	LYS
18	l	82	MET
21	o	111	LYS
22	p	51	ARG
22	p	112	LYS
24	r	7	HIS
24	r	66	ILE
25	s	1	MET
25	s	93	LEU
26	t	15	THR
26	t	52	LEU
26	t	74	ASN
29	w	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	31	HIS
5	4	61	ASN
6	A	13	HIS
9	c	37	ASN
9	c	115	GLN
9	c	142	HIS
9	c	243	HIS
11	e	115	GLN
12	f	63	GLN
13	g	116	GLN
13	g	128	GLN
14	h	2	GLN
14	h	20	ASN
15	i	128	ASN
15	i	131	ASN
15	i	138	GLN
17	k	104	GLN
19	m	18	GLN
20	n	61	GLN

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Mol	Chain	Res	Type
20	n	98	GLN
20	n	116	GLN
21	o	10	GLN
21	o	12	GLN
22	p	37	GLN
22	p	52	GLN
22	p	71	GLN
24	r	31	GLN
25	s	72	GLN
25	s	91	GLN
25	s	92	ASN
27	u	5	ASN
29	w	6	GLN
30	x	15	ASN
30	x	27	ASN
30	x	31	GLN
32	z	6	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	a	2727/2903 (93%)	300 (11%)	0
8	b	118/120 (98%)	14 (11%)	0
All	All	2845/3023 (94%)	314 (11%)	0

All (314) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	a	10	A
7	a	12	U
7	a	15	G
7	a	34	U
7	a	63	A
7	a	71	A
7	a	74	A
7	a	75	G
7	a	93	G
7	a	101	A
7	a	102	U
7	a	103	A
7	a	118	A

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Mol	Chain	Res	Type
7	a	119	A
7	a	120	U
7	a	139	U
7	a	140	C
7	a	142	A
7	a	163	C
7	a	165	A
7	a	181	A
7	a	196	A
7	a	199	A
7	a	200	U
7	a	215	G
7	a	216	A
7	a	221	A
7	a	222	A
7	a	233	A
7	a	248	G
7	a	272	A
7	a	276	U
7	a	278	A
7	a	281	C
7	a	282	A
7	a	285	G
7	a	289	G
7	a	304	U
7	a	311	A
7	a	329	G
7	a	330	A
7	a	345	A
7	a	361	G
7	a	362	A
7	a	366	C
7	a	386	G
7	a	403	U
7	a	404	A
7	a	405	U
7	a	411	G
7	a	425	G
7	a	451	U
7	a	481	G
7	a	491	G
7	a	504	A

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Mol	Chain	Res	Type
7	a	505	A
7	a	509	C
7	a	530	G
7	a	531	C
7	a	532	A
7	a	533	G
7	a	545	U
7	a	546	U
7	a	547	A
7	a	549	G
7	a	550	C
7	a	563	A
7	a	573	U
7	a	575	A
7	a	586	A
7	a	603	A
7	a	614	A
7	a	615	U
7	a	627	A
7	a	637	A
7	a	645	C
7	a	647	G
7	a	654	A
7	a	686	U
7	a	714	U
7	a	716	A
7	a	723	C
7	a	730	A
7	a	738	G
7	a	747	5MU
7	a	764	A
7	a	765	C
7	a	775	G
7	a	776	G
7	a	782	A
7	a	784	G
7	a	785	G
7	a	789	A
7	a	805	G
7	a	812	C
7	a	827	U
7	a	828	U

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Mol	Chain	Res	Type
7	a	845	A
7	a	846	U
7	a	858	G
7	a	859	G
7	a	869	G
7	a	877	A
7	a	879	G
7	a	883	G
7	a	888	C
7	a	890	C
7	a	891	G
7	a	893	C
7	a	896	A
7	a	897	C
7	a	910	A
7	a	914	G
7	a	915	C
7	a	931	U
7	a	946	C
7	a	961	C
7	a	974	G
7	a	983	A
7	a	984	A
7	a	985	C
7	a	996	A
7	a	1012	U
7	a	1013	C
7	a	1022	G
7	a	1033	U
7	a	1040	A
7	a	1046	A
7	a	1047	G
7	a	1108	U
7	a	1110	G
7	a	1111	A
7	a	1112	G
7	a	1116	G
7	a	1132	U
7	a	1133	A
7	a	1135	C
7	a	1142	A
7	a	1171	G

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Mol	Chain	Res	Type
7	a	1187	G
7	a	1205	A
7	a	1253	A
7	a	1256	G
7	a	1271	G
7	a	1272	A
7	a	1273	U
7	a	1300	G
7	a	1301	A
7	a	1321	A
7	a	1352	U
7	a	1365	A
7	a	1379	U
7	a	1383	A
7	a	1407	G
7	a	1415	U
7	a	1416	G
7	a	1420	A
7	a	1427	A
7	a	1428	C
7	a	1452	G
7	a	1453	A
7	a	1482	G
7	a	1490	A
7	a	1493	C
7	a	1504	A
7	a	1508	A
7	a	1509	A
7	a	1510	G
7	a	1515	A
7	a	1531	C
7	a	1532	A
7	a	1535	A
7	a	1536	C
7	a	1537	G
7	a	1538	G
7	a	1569	A
7	a	1578	U
7	a	1583	A
7	a	1584	U
7	a	1585	C
7	a	1586	A

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Mol	Chain	Res	Type
7	a	1608	A
7	a	1609	A
7	a	1647	U
7	a	1648	U
7	a	1649	G
7	a	1674	G
7	a	1715	G
7	a	1729	U
7	a	1730	C
7	a	1732	C
7	a	1738	G
7	a	1758	U
7	a	1764	C
7	a	1773	A
7	a	1800	C
7	a	1801	A
7	a	1807	G
7	a	1808	A
7	a	1816	C
7	a	1829	A
7	a	1848	A
7	a	1866	A
7	a	1870	C
7	a	1871	A
7	a	1929	G
7	a	1930	G
7	a	1931	U
7	a	1937	A
7	a	1938	A
7	a	1955	U
7	a	1963	U
7	a	1965	C
7	a	1967	C
7	a	1970	A
7	a	1971	U
7	a	1972	G
7	a	1991	U
7	a	1993	U
7	a	2023	C
7	a	2027	G
7	a	2031	A
7	a	2033	A

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Mol	Chain	Res	Type
7	a	2043	C
7	a	2055	C
7	a	2056	G
7	a	2060	A
7	a	2061	G
7	a	2069	G7M
7	a	2093	G
7	a	2198	A
7	a	2204	G
7	a	2211	A
7	a	2225	A
7	a	2238	G
7	a	2239	G
7	a	2268	A
7	a	2283	C
7	a	2287	A
7	a	2288	A
7	a	2305	U
7	a	2308	G
7	a	2312	U
7	a	2322	A
7	a	2325	G
7	a	2333	A
7	a	2335	A
7	a	2347	C
7	a	2361	G
7	a	2383	G
7	a	2385	C
7	a	2396	G
7	a	2402	U
7	a	2403	C
7	a	2406	A
7	a	2422	C
7	a	2425	A
7	a	2428	G
7	a	2429	G
7	a	2430	A
7	a	2435	A
7	a	2441	U
7	a	2448	A
7	a	2469	A
7	a	2470	G

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Mol	Chain	Res	Type
7	a	2474	U
7	a	2476	A
7	a	2502	G
7	a	2505	G
7	a	2506	U
7	a	2518	A
7	a	2529	G
7	a	2547	A
7	a	2566	A
7	a	2567	G
7	a	2573	C
7	a	2613	U
7	a	2629	U
7	a	2663	G
7	a	2671	G
7	a	2689	U
7	a	2690	U
7	a	2714	G
7	a	2716	C
7	a	2724	U
7	a	2726	A
7	a	2744	G
7	a	2748	A
7	a	2757	A
7	a	2765	A
7	a	2778	A
7	a	2798	U
7	a	2800	A
7	a	2820	A
7	a	2821	A
7	a	2836	U
7	a	2861	U
7	a	2880	C
7	a	2884	U
7	a	2885	G
8	b	9	G
8	b	13	G
8	b	34	A
8	b	35	C
8	b	36	C
8	b	42	C
8	b	43	C

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Mol	Chain	Res	Type
8	b	44	G
8	b	56	G
8	b	67	G
8	b	89	U
8	b	90	C
8	b	99	A
8	b	109	A

There are no RNA pucker outliers to report.

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

20 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	$\# Z > 2$
7	PSU	a	2457	7	18,21,22	1.02	1 (5%)	22,30,33	0.67	0
7	PSU	a	746	35,7	18,21,22	0.92	1 (5%)	22,30,33	0.64	0
7	PSU	a	2604	7	18,21,22	0.96	1 (5%)	22,30,33	0.75	1 (4%)
7	5MC	a	1962	7	18,22,23	0.35	0	26,32,35	0.48	0
7	OMC	a	2498	35,7	19,22,23	0.28	0	26,31,34	0.53	0
7	PSU	a	2605	7	18,21,22	1.04	1 (5%)	22,30,33	0.72	0
7	OMG	a	2251	35,7	18,26,27	0.97	1 (5%)	19,38,41	0.72	0
7	2MG	a	1835	7	18,26,27	1.32	1 (5%)	16,38,41	0.76	0
7	5MU	a	1939	7	19,22,23	0.29	0	28,32,35	0.36	0
7	G7M	a	2069	7	20,26,27	1.15	3 (15%)	17,39,42	0.49	0
7	H2U	a	2449	7	18,21,22	0.63	0	21,30,33	0.70	1 (4%)
7	2MG	a	2445	7	18,26,27	1.03	1 (5%)	16,38,41	0.81	0
7	5MU	a	747	7	19,22,23	0.26	0	28,32,35	0.34	0
10	MEQ	d	150	10	8,9,10	0.47	0	5,10,12	0.58	0
7	2MA	a	2503	35,7	19,25,26	0.95	1 (5%)	21,37,40	1.89	5 (23%)
7	OMU	a	2552	7	19,22,23	0.20	0	26,31,34	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PSU	a	955	7	18,21,22	0.92	1 (5%)	22,30,33	0.64	0
7	1MG	a	745	7	18,26,27	0.97	2 (11%)	19,39,42	0.70	0
7	PSU	a	2504	7	18,21,22	0.93	1 (5%)	22,30,33	0.71	0
7	PSU	a	2580	35,7	18,21,22	1.01	1 (5%)	22,30,33	0.69	1 (4%)

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
7	PSU	a	2457	7	-	0/7/25/26	0/2/2/2
7	PSU	a	746	35,7	-	2/7/25/26	0/2/2/2
7	PSU	a	2604	7	-	0/7/25/26	0/2/2/2
7	5MC	a	1962	7	-	0/7/25/26	0/2/2/2
7	OMC	a	2498	35,7	-	0/9/27/28	0/2/2/2
7	PSU	a	2605	7	-	0/7/25/26	0/2/2/2
7	OMG	a	2251	35,7	-	0/5/27/28	0/3/3/3
7	2MG	a	1835	7	-	0/5/27/28	0/3/3/3
7	5MU	a	1939	7	-	0/7/25/26	0/2/2/2
7	G7M	a	2069	7	-	2/3/25/26	0/3/3/3
7	H2U	a	2449	7	-	0/7/38/39	0/2/2/2
7	2MG	a	2445	7	-	1/5/27/28	0/3/3/3
7	5MU	a	747	7	-	1/7/25/26	0/2/2/2
10	MEQ	d	150	10	-	2/8/9/11	-
7	2MA	a	2503	35,7	-	2/3/25/26	0/3/3/3
7	OMU	a	2552	7	-	0/9/27/28	0/2/2/2
7	PSU	a	955	7	-	0/7/25/26	0/2/2/2
7	1MG	a	745	7	-	0/3/25/26	0/3/3/3
7	PSU	a	2504	7	-	0/7/25/26	0/2/2/2
7	PSU	a	2580	35,7	-	0/7/25/26	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	1835	2MG	CM2-N2	4.28	1.53	1.45
7	a	2605	PSU	C6-C5	4.07	1.40	1.35
7	a	2580	PSU	C6-C5	3.89	1.39	1.35
7	a	2604	PSU	C6-C5	3.75	1.39	1.35
7	a	2457	PSU	C6-C5	3.74	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	2504	PSU	C6-C5	3.64	1.39	1.35
7	a	746	PSU	C6-C5	3.60	1.39	1.35
7	a	955	PSU	C6-C5	3.57	1.39	1.35
7	a	2069	G7M	C8-N9	3.57	1.39	1.33
7	a	2251	OMG	C5-C6	-2.50	1.42	1.47
7	a	2445	2MG	C5-C6	-2.46	1.42	1.47
7	a	2069	G7M	C8-N7	2.30	1.37	1.33
7	a	2069	G7M	C5-C6	-2.20	1.39	1.45
7	a	745	1MG	C6-N1	2.16	1.43	1.39
7	a	745	1MG	C5-C4	-2.05	1.37	1.43
7	a	2503	2MA	C6-N1	2.04	1.37	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	2503	2MA	C5-C6-N1	-6.09	117.01	121.01
7	a	2503	2MA	C5-C6-N6	4.38	127.01	120.35
7	a	2449	H2U	C4-N3-C2	-2.57	123.66	125.79
7	a	2503	2MA	CM2-C2-N1	2.52	121.09	117.15
7	a	2503	2MA	C2-N1-C6	2.30	121.67	118.08
7	a	2604	PSU	C2'-C3'-C4'	-2.27	98.23	102.64
7	a	2503	2MA	N3-C2-N1	-2.24	121.65	125.73
7	a	2580	PSU	C3'-C2'-C1'	2.08	104.06	101.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	a	746	PSU	C2'-C1'-C5-C4
10	d	150	MEQ	NE2-CD-CG-CB
10	d	150	MEQ	OE1-CD-CG-CB
7	a	2069	G7M	C4'-C5'-O5'-P
7	a	2503	2MA	O4'-C4'-C5'-O5'
7	a	2445	2MG	C3'-C4'-C5'-O5'
7	a	747	5MU	C3'-C4'-C5'-O5'
7	a	746	PSU	O4'-C1'-C5-C6
7	a	2069	G7M	O4'-C4'-C5'-O5'
7	a	2503	2MA	C4'-C5'-O5'-P

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 220 ligands modelled in this entry, 218 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
36	SPM	a	6209	-	13,13,13	0.22	0	12,12,12	0.31	0
34	A2G	A	101	6	14,14,15	0.46	0	17,19,21	0.98	1 (5%)

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
36	SPM	a	6209	-	-	6/11/11/11	-
34	A2G	A	101	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	101	A2G	O5-C1-C2	-3.33	106.03	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	a	6209	SPM	N10-C11-C12-C13
36	a	6209	SPM	C8-C9-N10-C11
36	a	6209	SPM	C6-C7-C8-C9

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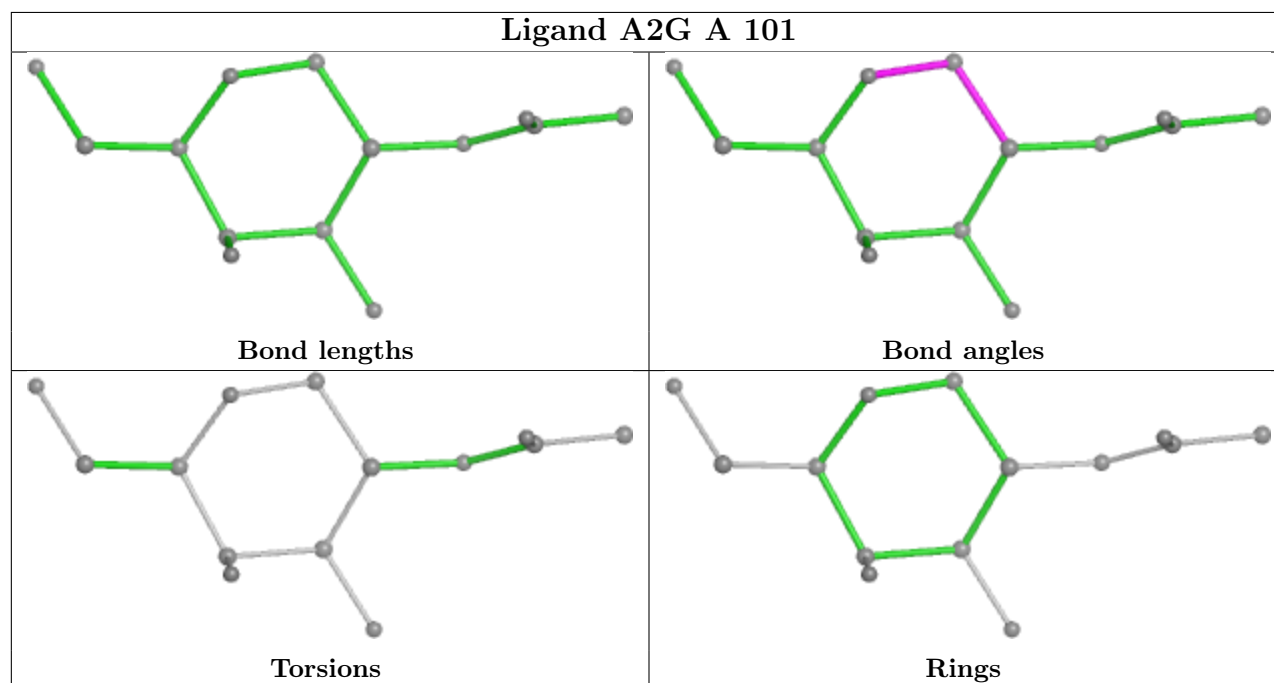
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Mol	Chain	Res	Type	Atoms
36	a	6209	SPM	C3-C4-N5-C6
36	a	6209	SPM	C7-C6-N5-C4
36	a	6209	SPM	N1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.