wwPDB EM Validation Summary Report

Mar 6, 2025 – 04:57 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 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:

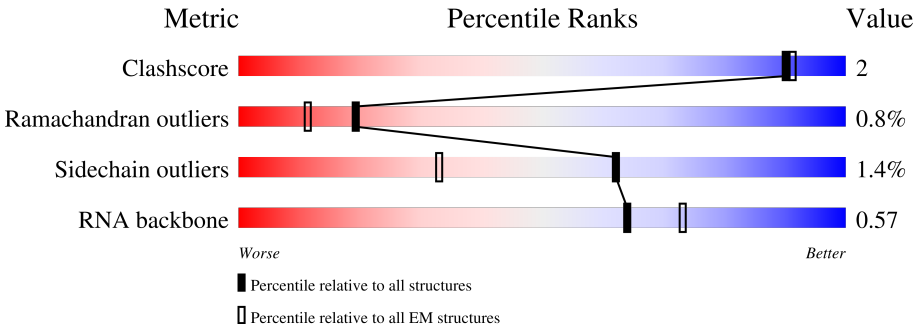
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

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 <=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 (i)

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
			Total	C	N	O		
1	0	51	417	269	76	72	0	0

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called Drosocin1.

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

- 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 917	C 574	N 179	O 163	S 1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

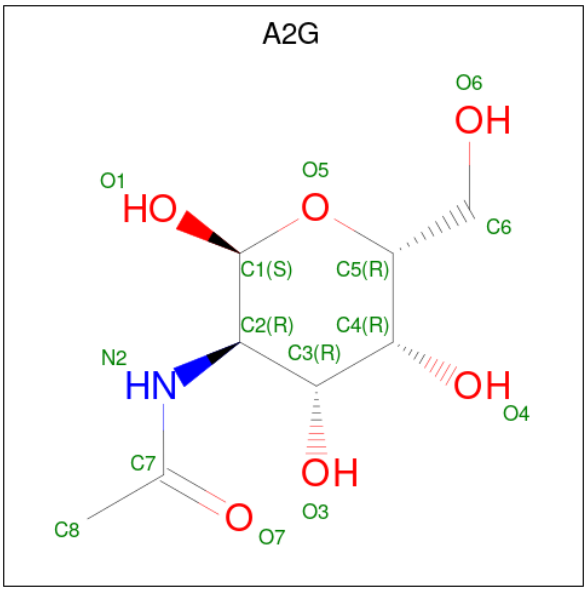
- Molecule 32 is a protein called 50S ribosomal protein L32.

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: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

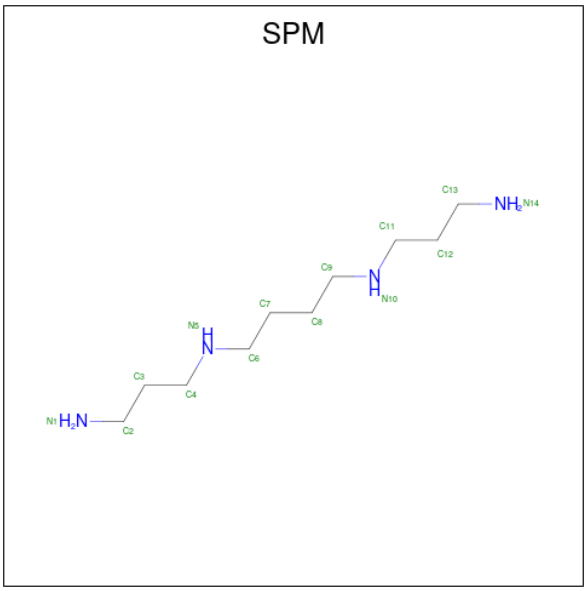


Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C N O 14 8 1 5	0

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

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

- Molecule 36 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



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

- Molecule 37 is water.

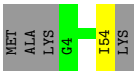
Mol	Chain	Residues	Atoms		AltConf
37	A	11	Total	O	0
			11	11	
37	a	27	Total	O	0
			27	27	
37	e	2	Total	O	0
			2	2	
37	r	2	Total	O	0
			2	2	

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.

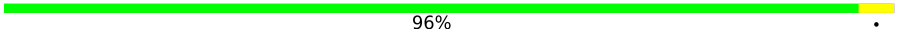
- Molecule 1: 50S ribosomal protein L33

Chain 0:



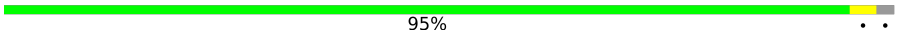
- Molecule 2: 50S ribosomal protein L34

Chain 1:



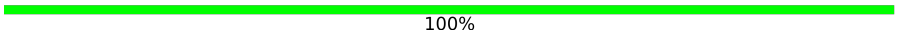
- Molecule 3: 50S ribosomal protein L35

Chain 2:



- Molecule 4: 50S ribosomal protein L36

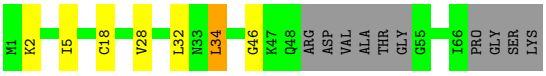
Chain 3:



There are no outlier residues recorded for this chain.

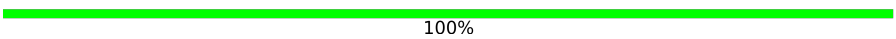
- Molecule 5: 50S ribosomal protein L31

Chain 4:



- Molecule 6: Drosocin1

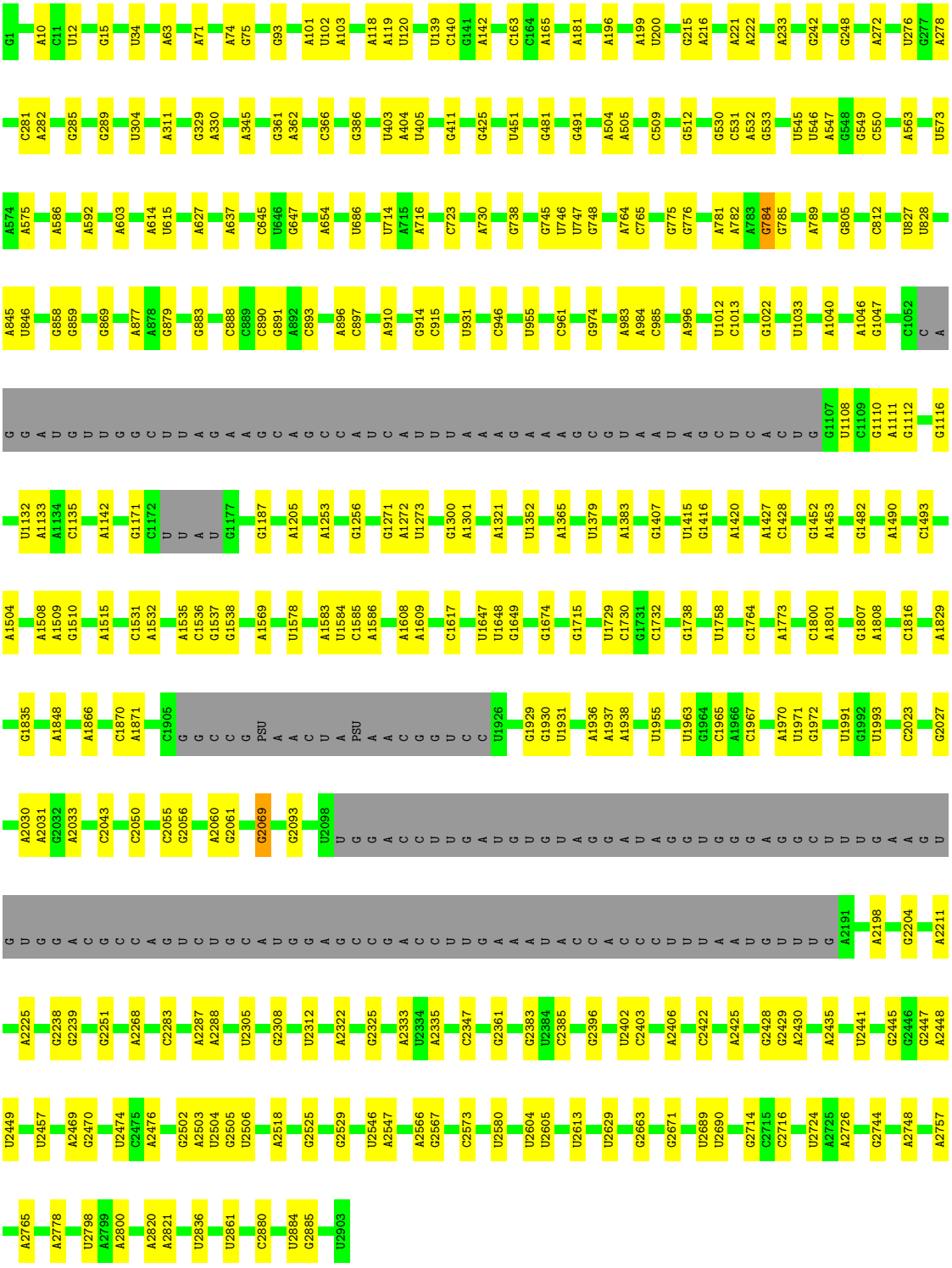
Chain A:



There are no outlier residues recorded for this chain.

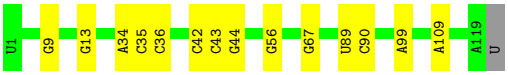
• Molecule 7: 23S ribosomal RNA

Chain a:



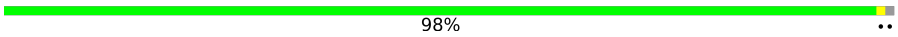
• Molecule 8: 5S ribosomal RNA

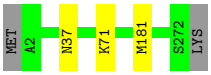
Chain b:



• Molecule 9: 50S ribosomal protein L2

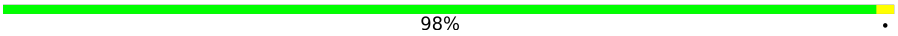
Chain c:





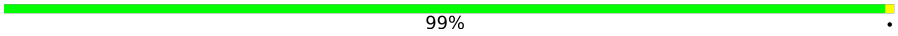
• Molecule 10: 50S ribosomal protein L3

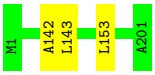
Chain d:



• Molecule 11: 50S ribosomal protein L4

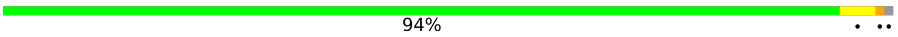
Chain e:

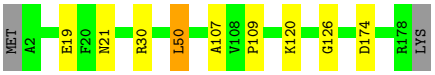




• Molecule 12: 50S ribosomal protein L5

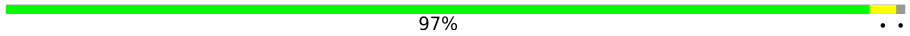
Chain f:

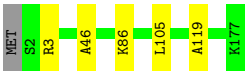




• Molecule 13: 50S ribosomal protein L6

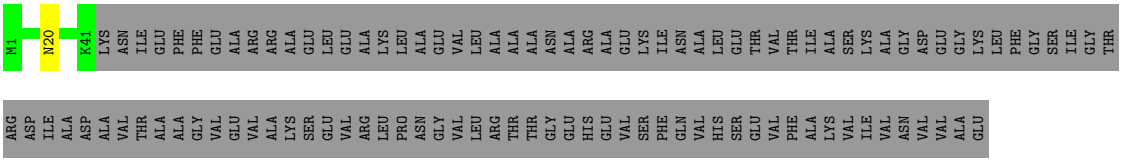
Chain g:





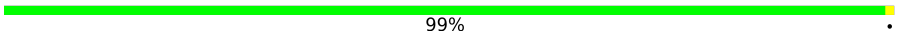
• Molecule 14: 50S ribosomal protein L9

Chain h:



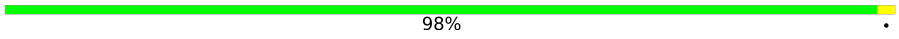
• Molecule 15: 50S ribosomal protein L13

Chain i:



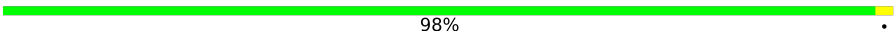
• Molecule 16: 50S ribosomal protein L14

Chain j:



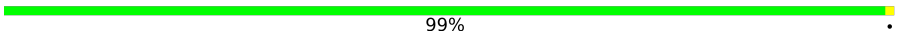
• Molecule 17: 50S ribosomal protein L15

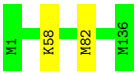
Chain k:



• Molecule 18: 50S ribosomal protein L16

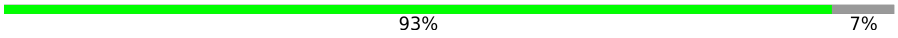
Chain l:





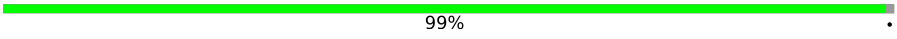
• Molecule 19: 50S ribosomal protein L17

Chain m:



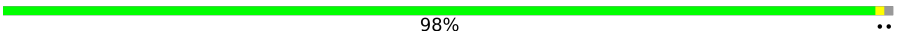
• Molecule 20: 50S ribosomal protein L18

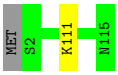
Chain n:



• Molecule 21: 50S ribosomal protein L19

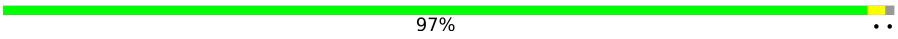
Chain o:





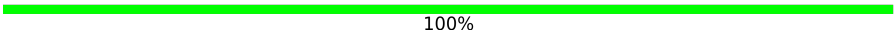
• Molecule 22: 50S ribosomal protein L20

Chain p:



• Molecule 23: 50S ribosomal protein L21

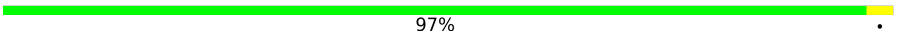
Chain q:

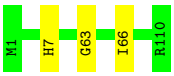


There are no outlier residues recorded for this chain.

• Molecule 24: 50S ribosomal protein L22

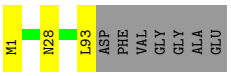
Chain r:





• Molecule 25: 50S ribosomal protein L23

Chain s:



• Molecule 26: 50S ribosomal protein L24

Chain t:

• Molecule 27: 50S ribosomal protein L25

Chain u:

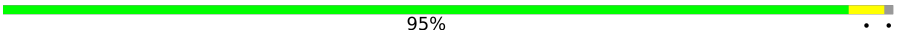
There are no outlier residues recorded for this chain.

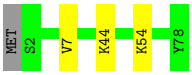
• Molecule 28: 50S ribosomal protein L27

Chain v:

• Molecule 29: 50S ribosomal protein L28

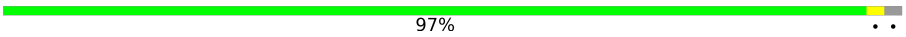
Chain w:

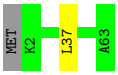




• Molecule 30: 50S ribosomal protein L29

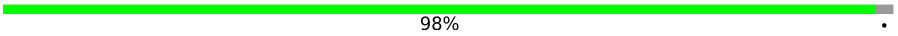
Chain x:





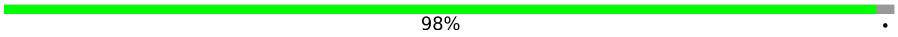
• Molecule 31: 50S ribosomal protein L30

Chain y:



• Molecule 32: 50S ribosomal protein L32

Chain z:



4 Experimental information (i)

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 ($e^-/Å^2$)	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

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

5 of 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

5.3.2 Protein sidechains (i)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	p	112	LYS
26	t	74	ASN

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Mol	Chain	Res	Type
24	r	7	HIS
25	s	93	LEU
11	e	153	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
25	s	91	GLN
32	z	6	ASN
25	s	92	ASN
30	x	15	ASN
14	h	20	ASN

5.3.3 RNA (i)

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

5 of 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

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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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'

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(^{o})	Ideal(^{o})
34	A	101	A2G	O5-C1-C2	-3.33	106.03	111.29

There are no chirality outliers.

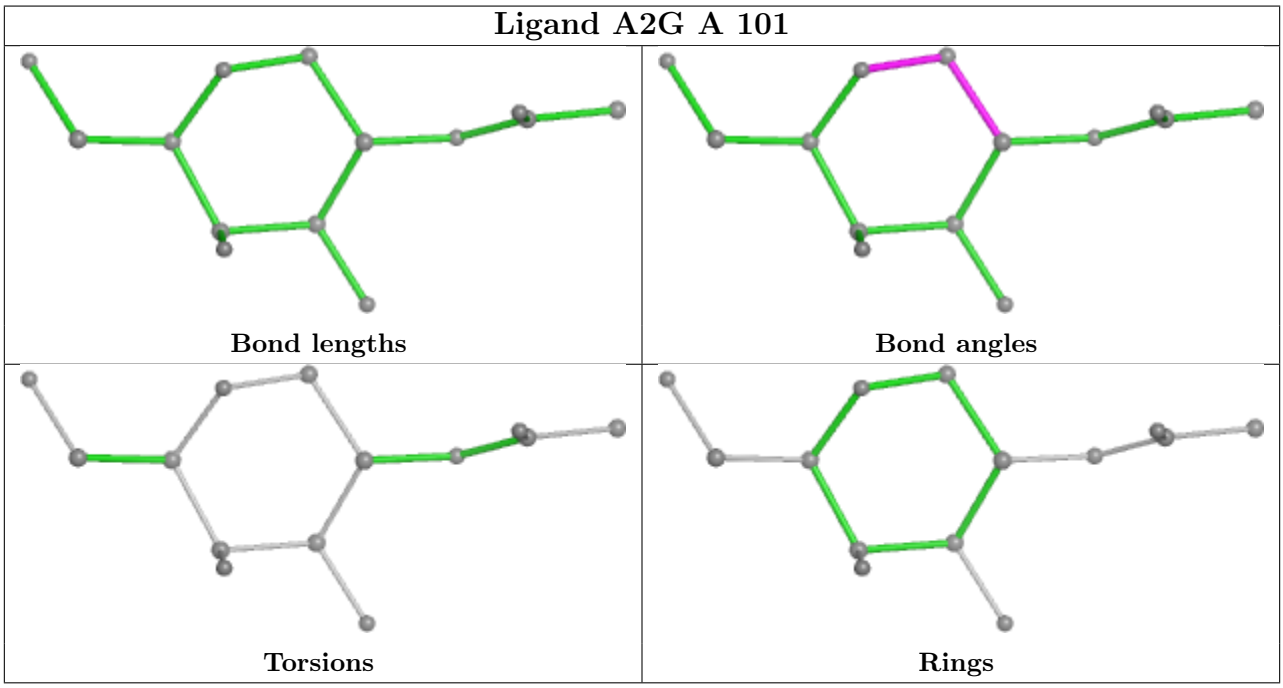
5 of 6 torsion outliers are listed below:

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
36	a	6209	SPM	C3-C4-N5-C6
36	a	6209	SPM	C7-C6-N5-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 then 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.