



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 04:06 pm GMT

PDB ID : 8AM9
EMDB ID : EMD-15523
Title : Cryo-EM structure of the proline-rich antimicrobial peptide drosocin bound to the elongating ribosome
Authors : Koller, T.O.; Morici, M.; Wilson, D.N.
Deposited on : 2022-08-03
Resolution : 2.80 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:

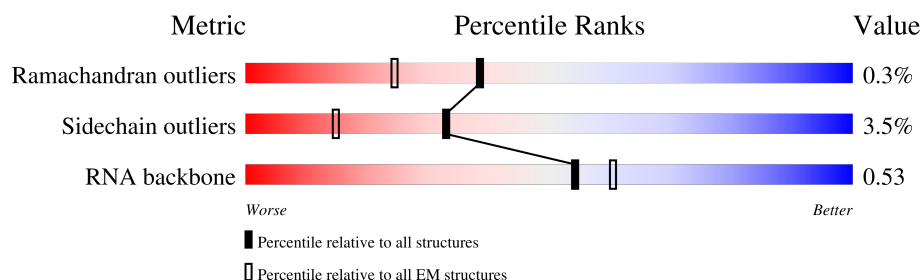
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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.






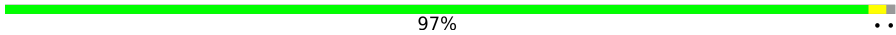
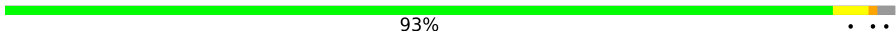




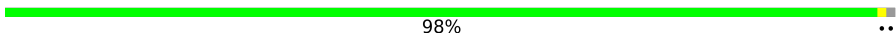
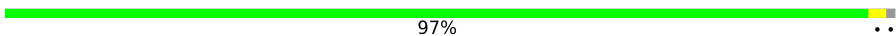
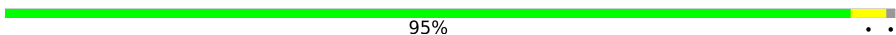







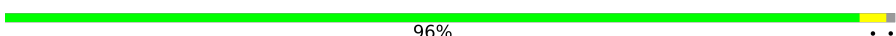
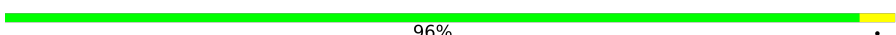
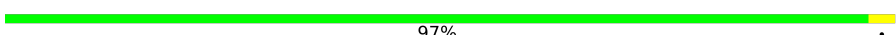
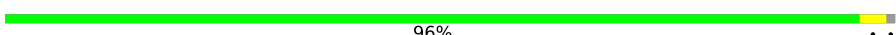


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	
2	1	46	
3	2	65	
4	3	38	
5	4	70	
6	B	1534	
7	C	241	
8	D	233	
9	E	206	

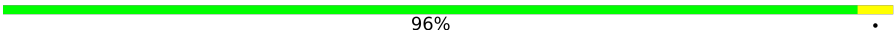
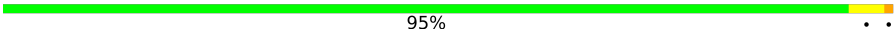
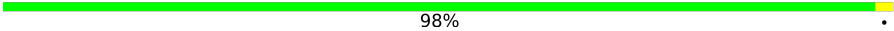
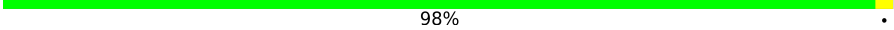

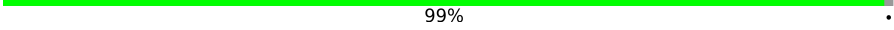
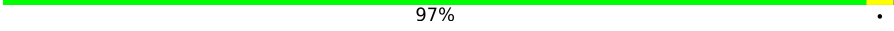
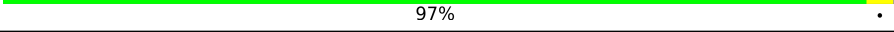
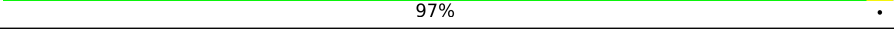
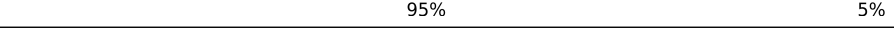

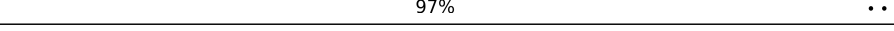
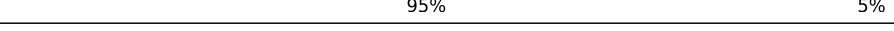

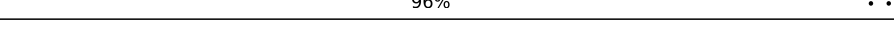
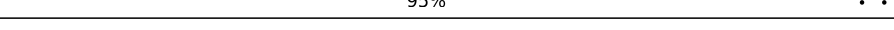
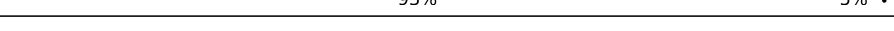
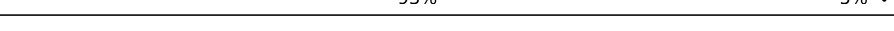

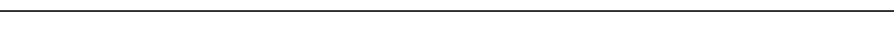

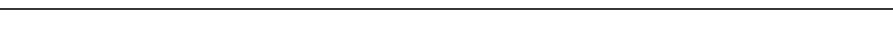
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Mol	Chain	Length	Quality of chain
10	F	167	 89% . 7%
11	G	135	 72% . 24%
12	H	179	 83% .. 15%
13	I	130	 97% ..
14	J	130	 93% . .
15	K	103	 85% 10% 5%
16	L	129	 89% . 9%
17	M	124	 91% 8% .
18	N	118	 88% 9% .
19	O	101	 98% ..
20	P	89	 97% ..
21	Q	82	 95% . .
22	R	84	 85% 8% 6%
23	S	75	 83% 5% 12%
24	T	92	 90% . 9%
25	U	87	 93% 6% .
26	V	71	 87% 11% .
27	a	2903	 81% 14% 5%
28	b	120	 82% 17% .
29	c	273	 96% ..
30	d	209	 96% .
31	e	201	 97% .
32	f	179	 96% ..
33	g	177	 94% 6% .
34	h	149	 26% . 72%

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Mol	Chain	Length	Quality of chain
35	i	142	 96% .
36	j	123	 95% . .
37	k	144	 98% .
38	l	136	 98% .
39	m	127	 89% . 7%
40	n	117	 99% .
41	o	115	 97% . .
42	p	118	 97% . .
43	q	103	 97% .
44	r	110	 95% 5%
45	s	100	 90% . 7%
46	t	104	 97% . .
47	u	94	 95% 5%
48	v	85	 88% . 8%
49	w	78	 96% . .
50	x	63	 95% . .
51	y	59	 93% 5% .
52	z	57	 93% 5% .
53	X	12	 67% 33%
54	Y	76	 76% 22% .
55	8	85	 67% 21% 12%
56	A	19	 89% 11%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 142036 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	2753	Total	C	N	O	P	1	0
			59148	26391	10899	19104	2754		

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

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

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	12	Total	C	N	O	P	0	0
			255	114	42	87	12		

- Molecule 54 is a RNA chain called Initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Y	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 55 is a RNA chain called Leucine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	75	Total	C	N	O	P	0	0
			1602	715	291	521	75		

- Molecule 56 is a protein called Drosocin1.

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

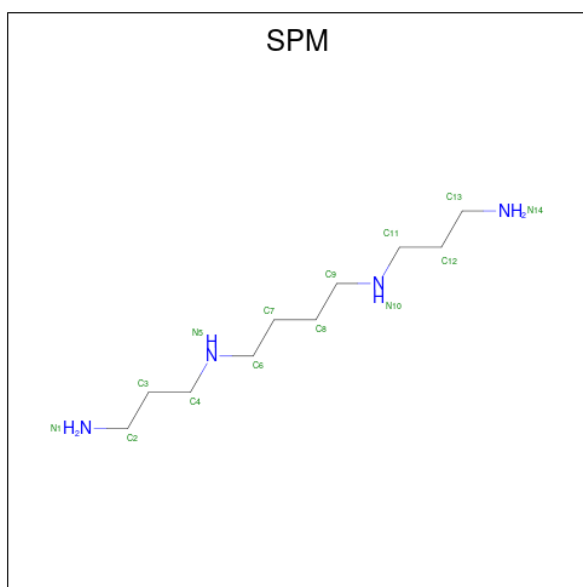
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

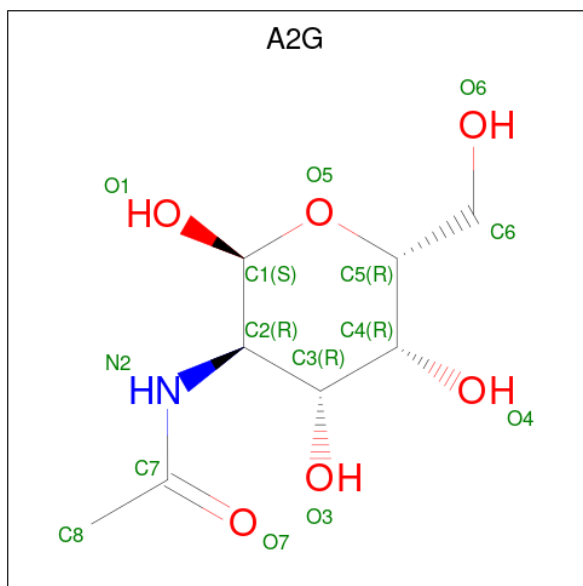
Mol	Chain	Residues	Atoms		AltConf
58	B	75	Total	Mg	0
			75	75	
58	O	1	Total	Mg	0
			1	1	
58	R	1	Total	Mg	0
			1	1	
58	a	208	Total	Mg	0
			208	208	
58	b	5	Total	Mg	0
			5	5	
58	d	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	
58	A	1	Total	Mg	0
			1	1	

- Molecule 59 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



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

- Molecule 60 is 2-acetamido-2-deoxy- α -D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	a	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.

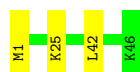
- Molecule 1: 50S ribosomal protein L33

Chain 0:  91% 7%



- Molecule 2: 50S ribosomal protein L34

Chain 1:  93% 7%



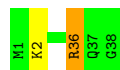
- Molecule 3: 50S ribosomal protein L35

Chain 2:  92% 6%




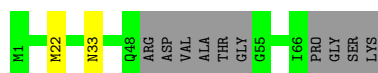
- Molecule 4: 50S ribosomal protein L36

Chain 3:  95%




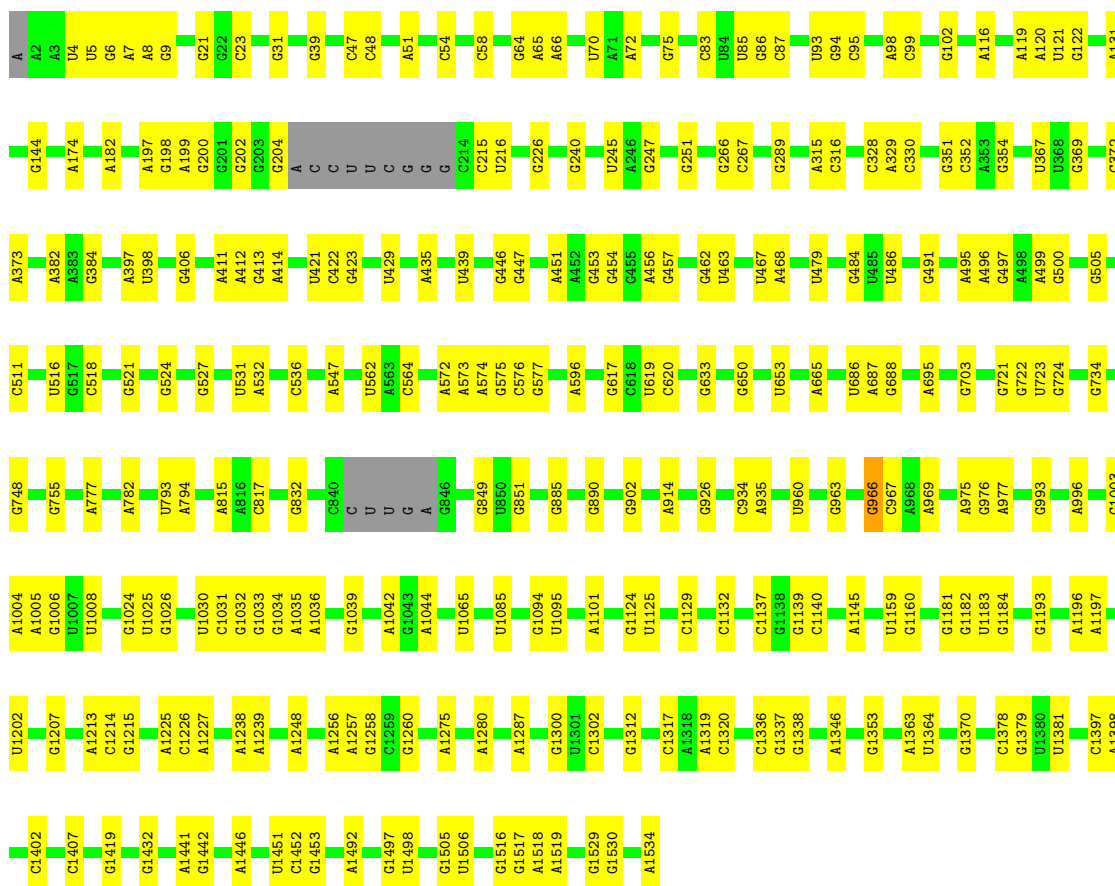
- Molecule 5: 50S ribosomal protein L31

Chain 4:  83% 14%



- Molecule 6: 16S ribosomal RNA

Chain B:  82% 17%



- Molecule 7: 30S ribosomal protein S2

Chain C: 90% 7%



- Molecule 8: 30S ribosomal protein S3

Chain D: 83% 6% 12%



- Molecule 9: 30S ribosomal protein S4

Chain E: 90% 8%



- Molecule 10: 30S ribosomal protein S5

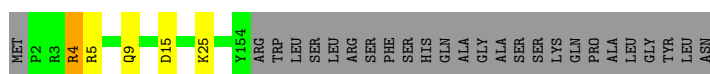
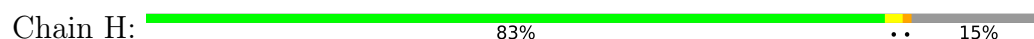
Chain F: 89% 7%



- Molecule 11: 30S ribosomal protein S6, fully modified isoform



- Molecule 12: 30S ribosomal protein S7



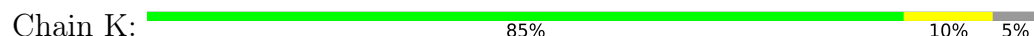
- Molecule 13: 30S ribosomal protein S8



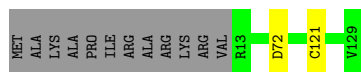
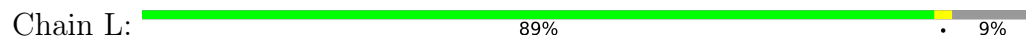
- Molecule 14: 30S ribosomal protein S9



- Molecule 15: 30S ribosomal protein S10



- Molecule 16: 30S ribosomal protein S11

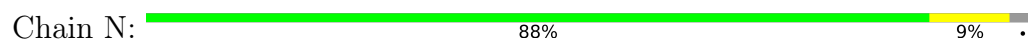


- Molecule 17: 30S ribosomal protein S12





- Molecule 18: 30S ribosomal protein S13



- Molecule 19: 30S ribosomal protein S14



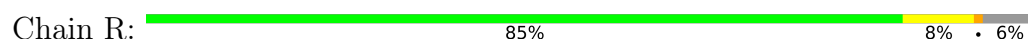
- Molecule 20: 30S ribosomal protein S15



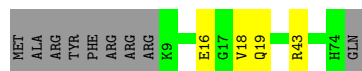
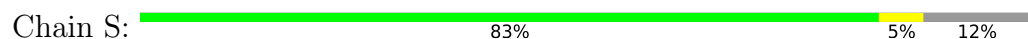
- Molecule 21: 30S ribosomal protein S16



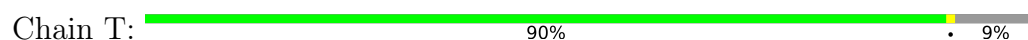
- Molecule 22: 30S ribosomal protein S17

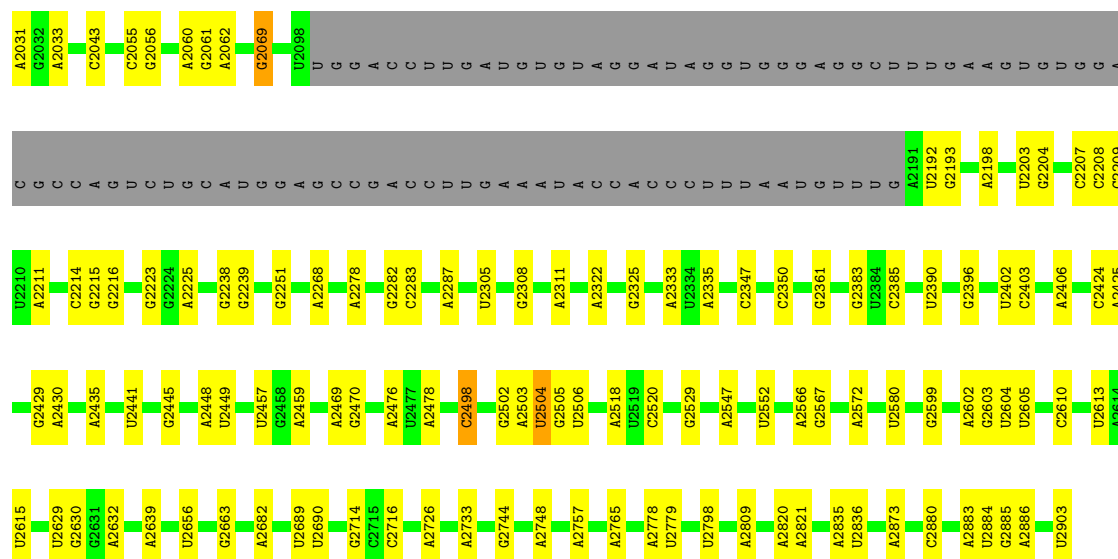


- Molecule 23: 30S ribosomal protein S18



- Molecule 24: 30S ribosomal protein S19





• Molecule 28: 5S ribosomal RNA

Chain b: 82% 17%



• Molecule 29: 50S ribosomal protein L2

Chain c: 96%



• Molecule 30: 50S ribosomal protein L3

Chain d: 96%




• Molecule 31: 50S ribosomal protein L4

Chain e: 97%



• Molecule 32: 50S ribosomal protein L5

Chain f: 96%

Chain m:  89% 7%



- Molecule 40: 50S ribosomal protein L18

Chain n:  99%



- Molecule 41: 50S ribosomal protein L19

Chain o:  97%



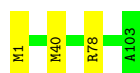
- Molecule 42: 50S ribosomal protein L20

Chain p:  97%



- Molecule 43: 50S ribosomal protein L21

Chain q:  97%




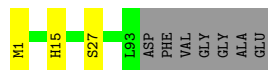
- Molecule 44: 50S ribosomal protein L22

Chain r:  95% 5%



- Molecule 45: 50S ribosomal protein L23

Chain s:  90% 7%



- Molecule 46: 50S ribosomal protein L24

Chain t:  97% ..




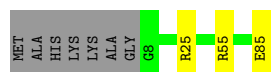
- Molecule 47: 50S ribosomal protein L25

Chain u:  95% 5%



- Molecule 48: 50S ribosomal protein L27

Chain v:  88% 8%



- Molecule 49: 50S ribosomal protein L28

Chain w:  96% ..



- Molecule 50: 50S ribosomal protein L29

Chain x:  95% ..



- Molecule 51: 50S ribosomal protein L30

Chain y:  93% 5%



- Molecule 52: 50S ribosomal protein L32

Chain z:  93% 5%



- Molecule 53: mRNA

Chain X:

67%

33%



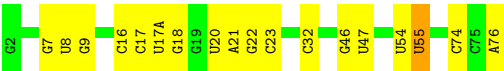
• Molecule 54: Initiator tRNA

Chain Y:

76%

22%

.



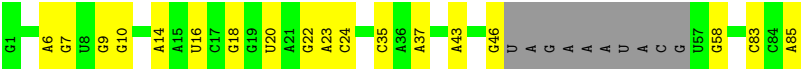
• Molecule 55: Leucine tRNA

Chain 8:

67%

21%

12%



• Molecule 56: Drosocin1

Chain A:

89%

11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84697	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: OMC, 5MC, 4SU, A2G, 6MZ, MEQ, 4OC, UR3, MG, 1MG, OMG, PSU, ZN, SPM, G7M, 5MU, H2U, 2MG, OMU, 2MA, MA6

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	0.36	0/424	0.53	0/565
2	1	0.35	0/380	0.72	0/498
3	2	0.33	0/513	0.63	0/676
4	3	0.35	0/303	0.66	0/397
5	4	0.31	0/488	0.58	0/649
6	B	0.60	0/36236	0.92	1/56520 (0.0%)
7	C	0.27	0/1784	0.53	0/2403
8	D	0.30	0/1651	0.59	0/2225
9	E	0.29	0/1665	0.59	0/2227
10	F	0.32	0/1165	0.55	0/1568
11	G	0.31	0/858	0.55	0/1160
12	H	0.28	0/1219	0.58	0/1635
13	I	0.31	0/989	0.58	0/1326
14	J	0.32	0/1034	0.62	0/1375
15	K	0.31	0/796	0.60	0/1077
16	L	0.29	0/893	0.58	0/1205
17	M	0.29	0/969	0.65	0/1300
18	N	0.28	0/900	0.62	0/1204
19	O	0.32	0/817	0.61	0/1088
20	P	0.28	0/722	0.60	0/964
21	Q	0.28	0/653	0.62	0/877
22	R	0.32	0/650	0.59	0/871
23	S	0.34	0/553	0.59	0/742
24	T	0.32	0/685	0.55	0/922
25	U	0.26	0/676	0.51	0/895
26	V	0.31	0/597	0.65	0/792
27	a	0.75	0/65722	0.93	16/102528 (0.0%)
28	b	0.64	0/2850	0.91	0/4444
29	c	0.36	0/2121	0.62	0/2852
30	d	0.36	0/1576	0.56	0/2119
31	e	0.33	0/1571	0.55	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f	0.31	0/1434	0.57	0/1926
33	g	0.30	0/1343	0.57	0/1816
34	h	0.32	0/306	0.51	0/413
35	i	0.35	0/1152	0.57	0/1551
36	j	0.35	0/955	0.61	0/1279
37	k	0.33	0/1062	0.60	0/1413
38	l	0.35	0/1093	0.62	0/1460
39	m	0.34	0/958	0.65	0/1281
40	n	0.32	0/902	0.60	0/1209
41	o	0.34	0/929	0.58	0/1242
42	p	0.35	0/960	0.61	0/1278
43	q	0.34	0/829	0.59	0/1107
44	r	0.29	0/864	0.56	0/1156
45	s	0.29	0/744	0.55	0/994
46	t	0.30	0/787	0.56	0/1051
47	u	0.34	0/766	0.56	0/1025
48	v	0.36	0/593	0.58	0/785
49	w	0.31	0/635	0.65	0/848
50	x	0.27	0/502	0.58	0/667
51	y	0.30	0/453	0.62	0/605
52	z	0.34	0/450	0.62	0/599
53	X	0.64	0/284	1.01	0/440
54	Y	0.49	0/1725	0.95	1/2689 (0.0%)
55	8	0.43	0/1790	0.97	0/2786
56	A	0.42	0/162	0.68	0/221
All	All	0.61	0/153138	0.85	18/229058 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	2	0	2
4	3	0	1
7	C	0	2
8	D	0	3
9	E	0	7
10	F	0	1
12	H	0	1
14	J	0	4
15	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	M	0	5
18	N	0	5
19	O	0	1
21	Q	0	1
22	R	0	5
25	U	0	2
26	V	0	3
29	c	0	6
30	d	0	3
31	e	0	1
32	f	0	1
33	g	0	1
35	i	0	1
36	j	0	3
37	k	0	1
38	l	0	2
39	m	0	3
42	p	0	1
43	q	0	1
47	u	0	1
48	v	0	2
50	x	0	1
51	y	0	1
52	z	0	1
56	A	0	1
All	All	0	77

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	168	G	P-O3'-C3'	-10.84	106.69	119.70
27	a	160	A	P-O3'-C3'	-10.52	107.07	119.70
27	a	2216	G	P-O3'-C3'	-10.40	107.22	119.70
27	a	2208	C	P-O3'-C3'	-10.13	107.54	119.70
27	a	167	A	P-O3'-C3'	-10.12	107.56	119.70
27	a	2207	C	P-O3'-C3'	-9.45	108.37	119.70
27	a	166	U	P-O3'-C3'	-9.24	108.61	119.70
27	a	2215	G	P-O3'-C3'	-8.85	109.09	119.70
27	a	2209	C	P-O3'-C3'	-8.55	109.44	119.70
27	a	159	G	P-O3'-C3'	-8.27	109.78	119.70
27	a	2214	C	P-O3'-C3'	-7.37	110.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	165	A	P-O3'-C3'	-6.32	112.12	119.70
27	a	1565	C	C6-N1-C2	-5.51	118.10	120.30
27	a	12	U	N3-C2-O2	-5.40	118.42	122.20
6	B	1183	U	O4'-C1'-N1	5.31	112.45	108.20
27	a	2029	G	C2'-C3'-O3'	5.15	121.94	113.70
27	a	12	U	C2-N1-C1'	5.09	123.80	117.70
54	Y	74	C	C6-N1-C2	-5.03	118.29	120.30

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	30	ARG	Sidechain
3	2	40	ARG	Sidechain
4	3	36	ARG	Sidechain
56	A	9	ARG	Sidechain
7	C	7	ARG	Sidechain
7	C	95	ARG	Sidechain
8	D	107	ARG	Sidechain
8	D	11	ARG	Sidechain
8	D	59	ARG	Sidechain
9	E	111	ARG	Sidechain
9	E	13	ARG	Sidechain
9	E	184	ARG	Sidechain
9	E	188	ARG	Sidechain
9	E	3	ARG	Sidechain
9	E	44	ARG	Sidechain
9	E	70	ARG	Sidechain
10	F	112	ARG	Sidechain
12	H	4	ARG	Sidechain
14	J	12	ARG	Sidechain
14	J	45	ARG	Sidechain
14	J	85	ARG	Sidechain
14	J	95	ARG	Sidechain
15	K	5	ARG	Sidechain
15	K	62	ARG	Sidechain
15	K	72	ARG	Sidechain
17	M	114	ARG	Sidechain
17	M	12	ARG	Sidechain
17	M	14	ARG	Sidechain
17	M	56	ARG	Sidechain
17	M	94	ARG	Sidechain

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Mol	Chain	Res	Type	Group
18	N	107	ARG	Sidechain
18	N	113	ARG	Sidechain
18	N	87	ARG	Sidechain
18	N	90	ARG	Sidechain
18	N	93	ARG	Sidechain
19	O	85	ARG	Sidechain
21	Q	28	ARG	Sidechain
22	R	11	ARG	Sidechain
22	R	40	ARG	Sidechain
22	R	62	ARG	Sidechain
22	R	65	ARG	Sidechain
22	R	77	ARG	Sidechain
25	U	25	ARG	Sidechain
25	U	60	ARG	Sidechain
26	V	17	ARG	Sidechain
26	V	35	ARG	Sidechain
26	V	62	ARG	Sidechain
29	c	101	ARG	Sidechain
29	c	156	ARG	Sidechain
29	c	182	ARG	Sidechain
29	c	48	ARG	Sidechain
29	c	63	ARG	Sidechain
29	c	69	ARG	Sidechain
30	d	128	ARG	Sidechain
30	d	184	ARG	Sidechain
30	d	83	ARG	Sidechain
31	e	40	ARG	Sidechain
32	f	95	ARG	Sidechain
33	g	35	ARG	Sidechain
35	i	116	ARG	Sidechain
36	j	18	ARG	Sidechain
36	j	49	ARG	Sidechain
36	j	64	ARG	Sidechain
37	k	123	ARG	Sidechain
38	l	10	ARG	Sidechain
38	l	6	ARG	Sidechain
39	m	2	ARG	Sidechain
39	m	8	ARG	Sidechain
39	m	86	ARG	Sidechain
42	p	13	ARG	Sidechain
43	q	78	ARG	Sidechain
47	u	93	ARG	Sidechain

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Mol	Chain	Res	Type	Group
48	v	25	ARG	Sidechain
48	v	55	ARG	Sidechain
50	x	29	ARG	Sidechain
51	y	30	ARG	Sidechain
52	z	13	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
7	C	222/241 (92%)	212 (96%)	10 (4%)	0	100	100
8	D	204/233 (88%)	194 (95%)	9 (4%)	1 (0%)	25	56
9	E	203/206 (98%)	195 (96%)	7 (3%)	1 (0%)	25	56
10	F	154/167 (92%)	144 (94%)	9 (6%)	1 (1%)	22	51
11	G	101/135 (75%)	98 (97%)	2 (2%)	1 (1%)	13	39
12	H	151/179 (84%)	142 (94%)	8 (5%)	1 (1%)	19	48
13	I	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	16	44
14	J	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
15	K	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	13	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	L	115/129 (89%)	111 (96%)	3 (3%)	1 (1%)	14	42
17	M	121/124 (98%)	117 (97%)	4 (3%)	0	100	100
18	N	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
19	O	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
20	P	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	Q	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
22	R	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
23	S	64/75 (85%)	64 (100%)	0	0	100	100
24	T	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
25	U	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	V	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
29	c	269/273 (98%)	253 (94%)	16 (6%)	0	100	100
30	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
31	e	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	25	56
32	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
33	g	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	22	51
34	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
35	i	140/142 (99%)	140 (100%)	0	0	100	100
36	j	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
37	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
38	l	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
39	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
40	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
41	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
42	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
43	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
44	r	108/110 (98%)	106 (98%)	1 (1%)	1 (1%)	14	42
45	s	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	12	37
46	t	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
47	u	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	12	37
48	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
50	x	60/63 (95%)	58 (97%)	1 (2%)	1 (2%)	7	26
51	y	56/59 (95%)	56 (100%)	0	0	100	100
52	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
56	A	17/19 (90%)	17 (100%)	0	0	100	100
All	All	5503/5932 (93%)	5279 (96%)	210 (4%)	14 (0%)	38	67

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	109	GLY
11	G	33	GLU
44	r	12	SER
15	K	57	VAL
47	u	67	GLY
9	E	155	VAL
12	H	9	GLN
13	I	108	LYS
16	L	121	CYS
33	g	167	GLU
45	s	27	SER
50	x	37	LEU
8	D	17	PRO
31	e	4	VAL

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	79
2	1	38/38 (100%)	35 (92%)	3 (8%)	10	30
3	2	51/52 (98%)	49 (96%)	2 (4%)	27	61
4	3	34/34 (100%)	32 (94%)	2 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	55/62 (89%)	53 (96%)	2 (4%)	30	64
7	C	186/199 (94%)	180 (97%)	6 (3%)	34	68
8	D	170/190 (90%)	161 (95%)	9 (5%)	19	49
9	E	172/173 (99%)	159 (92%)	13 (8%)	11	32
10	F	119/126 (94%)	114 (96%)	5 (4%)	25	58
11	G	90/116 (78%)	85 (94%)	5 (6%)	17	47
12	H	126/147 (86%)	122 (97%)	4 (3%)	34	68
13	I	104/105 (99%)	102 (98%)	2 (2%)	52	82
14	J	105/107 (98%)	102 (97%)	3 (3%)	37	71
15	K	86/90 (96%)	80 (93%)	6 (7%)	12	36
16	L	90/99 (91%)	89 (99%)	1 (1%)	70	90
17	M	103/104 (99%)	98 (95%)	5 (5%)	21	52
18	N	93/96 (97%)	87 (94%)	6 (6%)	14	40
19	O	83/84 (99%)	83 (100%)	0	100	100
20	P	76/77 (99%)	74 (97%)	2 (3%)	41	75
21	Q	65/65 (100%)	63 (97%)	2 (3%)	35	69
22	R	73/78 (94%)	69 (94%)	4 (6%)	18	47
23	S	57/65 (88%)	53 (93%)	4 (7%)	12	36
24	T	72/79 (91%)	71 (99%)	1 (1%)	62	87
25	U	65/66 (98%)	62 (95%)	3 (5%)	23	55
26	V	60/61 (98%)	55 (92%)	5 (8%)	9	28
29	c	216/218 (99%)	214 (99%)	2 (1%)	75	92
30	d	163/163 (100%)	158 (97%)	5 (3%)	35	69
31	e	165/165 (100%)	161 (98%)	4 (2%)	44	77
32	f	148/150 (99%)	143 (97%)	5 (3%)	32	66
33	g	137/138 (99%)	129 (94%)	8 (6%)	17	45
34	h	32/114 (28%)	30 (94%)	2 (6%)	15	42
35	i	116/116 (100%)	112 (97%)	4 (3%)	32	66
36	j	104/104 (100%)	100 (96%)	4 (4%)	28	62
37	k	103/103 (100%)	101 (98%)	2 (2%)	52	82
38	l	109/109 (100%)	108 (99%)	1 (1%)	75	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	m	98/103 (95%)	96 (98%)	2 (2%)	50	81
40	n	86/87 (99%)	86 (100%)	0	100	100
41	o	99/100 (99%)	96 (97%)	3 (3%)	36	70
42	p	89/90 (99%)	87 (98%)	2 (2%)	47	79
43	q	84/84 (100%)	82 (98%)	2 (2%)	44	77
44	r	93/93 (100%)	89 (96%)	4 (4%)	25	57
45	s	80/84 (95%)	78 (98%)	2 (2%)	42	75
46	t	83/85 (98%)	82 (99%)	1 (1%)	67	89
47	u	78/78 (100%)	75 (96%)	3 (4%)	28	62
48	v	58/63 (92%)	57 (98%)	1 (2%)	56	84
49	w	67/68 (98%)	65 (97%)	2 (3%)	36	70
50	x	54/55 (98%)	54 (100%)	0	100	100
51	y	48/49 (98%)	46 (96%)	2 (4%)	25	58
52	z	47/48 (98%)	45 (96%)	2 (4%)	25	57
56	A	18/18 (100%)	17 (94%)	1 (6%)	17	47
All	All	4594/4847 (95%)	4434 (96%)	160 (4%)	33	65

All (160) 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
2	1	42	LEU
3	2	7	VAL
3	2	13	ARG
4	3	2	LYS
4	3	36	ARG
5	4	22	MET
5	4	33	ASN
7	C	8	ASP
7	C	117	LEU
7	C	127	ASP
7	C	128	LYS
7	C	131	LYS
7	C	184	PHE
8	D	18	TRP

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Mol	Chain	Res	Type
8	D	46	GLU
8	D	62	LYS
8	D	70	THR
8	D	80	LYS
8	D	132	ARG
8	D	178	LEU
8	D	195	VAL
8	D	201	TRP
9	E	8	LYS
9	E	10	LYS
9	E	28	ILE
9	E	57	GLU
9	E	68	LEU
9	E	70	ARG
9	E	82	LEU
9	E	97	ARG
9	E	117	LEU
9	E	128	ARG
9	E	171	LEU
9	E	183	LYS
9	E	188	ARG
10	F	26	LYS
10	F	61	GLN
10	F	97	GLN
10	F	116	GLU
10	F	152	MET
11	G	17	GLN
11	G	74	LEU
11	G	90	MET
11	G	91	ARG
11	G	102	MET
12	H	4	ARG
12	H	5	ARG
12	H	15	ASP
12	H	25	LYS
13	I	56	LYS
13	I	89	LYS
14	J	58	VAL
14	J	85	ARG
14	J	123	ARG
15	K	17	LEU
15	K	18	ILE

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Mol	Chain	Res	Type
15	K	27	GLU
15	K	28	THR
15	K	30	LYS
15	K	35	GLN
16	L	72	ASP
17	M	15	LYS
17	M	50	ARG
17	M	62	GLU
17	M	86	ARG
17	M	121	ARG
18	N	16	VAL
18	N	27	LYS
18	N	54	ASP
18	N	58	ASP
18	N	68	ASP
18	N	83	LEU
20	P	17	ARG
20	P	89	ARG
21	Q	23	ASP
21	Q	80	LYS
22	R	16	LYS
22	R	27	ARG
22	R	62	ARG
22	R	67	LEU
23	S	16	GLU
23	S	18	VAL
23	S	19	GLN
23	S	43	ARG
24	T	27	ASP
25	U	27	MET
25	U	44	LYS
25	U	59	ASP
26	V	2	PRO
26	V	39	GLU
26	V	58	LYS
26	V	63	GLU
26	V	67	ARG
29	c	132	MET
29	c	181	MET
30	d	1	MET
30	d	30	GLU
30	d	33	ARG

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Mol	Chain	Res	Type
30	d	52	THR
30	d	100	LEU
31	e	9	GLN
31	e	143	LEU
31	e	150	THR
31	e	176	ASP
32	f	30	ARG
32	f	50	LEU
32	f	51	ASP
32	f	69	LYS
32	f	120	LYS
33	g	18	LYS
33	g	29	LYS
33	g	48	ASN
33	g	52	PHE
33	g	139	GLN
33	g	141	ILE
33	g	143	GLN
33	g	155	GLU
34	h	12	LEU
34	h	17	ASP
35	i	1	MET
35	i	4	PHE
35	i	64	VAL
35	i	131	ASN
36	j	49	ARG
36	j	80	ASP
36	j	89	ASN
36	j	107	LEU
37	k	112	LEU
37	k	129	LYS
38	l	82	MET
39	m	51	LEU
39	m	96	ARG
41	o	53	ARG
41	o	68	GLU
41	o	115	ASN
42	p	11	ARG
42	p	71	GLN
43	q	1	MET
43	q	40	MET
44	r	7	HIS

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Mol	Chain	Res	Type
44	r	66	ILE
44	r	67	ASP
44	r	109	ASP
45	s	1	MET
45	s	15	HIS
46	t	52	LEU
47	u	11	GLU
47	u	20	LEU
47	u	62	THR
48	v	85	GLU
49	w	17	ASN
49	w	54	LYS
51	y	24	LEU
51	y	54	MET
52	z	12	LYS
52	z	32	LYS
56	A	19	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	39	HIS
16	L	119	ASN
32	f	5	HIS
44	r	61	ASN
49	w	34	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	a	2746/2903 (94%)	373 (13%)	0
28	b	118/120 (98%)	20 (16%)	0
53	X	11/12 (91%)	4 (36%)	0
54	Y	75/76 (98%)	12 (16%)	4 (5%)
55	8	73/85 (85%)	18 (24%)	2 (2%)
6	B	1513/1534 (98%)	244 (16%)	38 (2%)
All	All	4536/4730 (95%)	671 (14%)	44 (0%)

All (671) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	4	U
6	B	5	U
6	B	6	G
6	B	8	A
6	B	9	G
6	B	23	C
6	B	31	G
6	B	39	G
6	B	47	C
6	B	48	C
6	B	51	A
6	B	54	C
6	B	58	C
6	B	64	G
6	B	65	A
6	B	66	A
6	B	70	U
6	B	72	A
6	B	75	G
6	B	83	C
6	B	85	U
6	B	86	G
6	B	87	C
6	B	93	U
6	B	94	G
6	B	95	C
6	B	98	A
6	B	99	C
6	B	102	G
6	B	116	A
6	B	119	A
6	B	120	A
6	B	121	U
6	B	122	G
6	B	131	A
6	B	144	G
6	B	174	A
6	B	182	A
6	B	197	A
6	B	198	G
6	B	199	A
6	B	200	G
6	B	202	G

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Mol	Chain	Res	Type
6	B	204	G
6	B	215	C
6	B	216	U
6	B	226	G
6	B	240	G
6	B	245	U
6	B	247	G
6	B	251	G
6	B	266	G
6	B	267	C
6	B	289	G
6	B	316	C
6	B	328	C
6	B	329	A
6	B	330	C
6	B	351	G
6	B	352	C
6	B	354	G
6	B	367	U
6	B	369	G
6	B	372	C
6	B	373	A
6	B	382	A
6	B	384	G
6	B	397	A
6	B	398	U
6	B	406	G
6	B	411	A
6	B	412	A
6	B	413	G
6	B	414	A
6	B	421	U
6	B	422	C
6	B	423	G
6	B	429	U
6	B	435	A
6	B	439	U
6	B	446	G
6	B	447	G
6	B	451	A
6	B	453	G
6	B	454	G

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Mol	Chain	Res	Type
6	B	456	A
6	B	457	G
6	B	462	G
6	B	463	U
6	B	467	U
6	B	468	A
6	B	479	U
6	B	484	G
6	B	486	U
6	B	491	G
6	B	495	A
6	B	496	A
6	B	497	G
6	B	499	A
6	B	500	G
6	B	505	G
6	B	511	C
6	B	518	C
6	B	521	G
6	B	524	G
6	B	531	U
6	B	532	A
6	B	536	C
6	B	547	A
6	B	562	U
6	B	564	C
6	B	572	A
6	B	573	A
6	B	574	A
6	B	576	C
6	B	577	G
6	B	596	A
6	B	617	G
6	B	619	U
6	B	620	C
6	B	633	G
6	B	650	G
6	B	653	U
6	B	665	A
6	B	687	A
6	B	688	G
6	B	695	A

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Mol	Chain	Res	Type
6	B	703	G
6	B	721	G
6	B	722	G
6	B	723	U
6	B	724	G
6	B	734	G
6	B	748	G
6	B	755	G
6	B	777	A
6	B	782	A
6	B	793	U
6	B	794	A
6	B	815	A
6	B	817	C
6	B	832	G
6	B	849	G
6	B	851	G
6	B	885	G
6	B	890	G
6	B	902	G
6	B	914	A
6	B	926	G
6	B	934	C
6	B	935	A
6	B	960	U
6	B	963	G
6	B	966	2MG
6	B	969	A
6	B	975	A
6	B	976	G
6	B	977	A
6	B	993	G
6	B	996	A
6	B	1003	G
6	B	1004	A
6	B	1005	A
6	B	1006	G
6	B	1008	U
6	B	1024	G
6	B	1025	U
6	B	1026	G
6	B	1030	U

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Mol	Chain	Res	Type
6	B	1031	C
6	B	1032	G
6	B	1033	G
6	B	1034	G
6	B	1036	A
6	B	1039	G
6	B	1042	A
6	B	1044	A
6	B	1065	U
6	B	1085	U
6	B	1094	G
6	B	1095	U
6	B	1101	A
6	B	1124	G
6	B	1125	U
6	B	1129	C
6	B	1132	C
6	B	1137	C
6	B	1139	G
6	B	1140	C
6	B	1159	U
6	B	1160	G
6	B	1182	G
6	B	1184	G
6	B	1193	G
6	B	1196	A
6	B	1197	A
6	B	1202	U
6	B	1213	A
6	B	1214	C
6	B	1215	G
6	B	1226	C
6	B	1227	A
6	B	1238	A
6	B	1248	A
6	B	1256	A
6	B	1257	A
6	B	1258	G
6	B	1260	G
6	B	1275	A
6	B	1280	A
6	B	1287	A

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Mol	Chain	Res	Type
6	B	1300	G
6	B	1302	C
6	B	1312	G
6	B	1317	C
6	B	1319	A
6	B	1320	C
6	B	1336	C
6	B	1338	G
6	B	1346	A
6	B	1353	G
6	B	1363	A
6	B	1364	U
6	B	1370	G
6	B	1378	C
6	B	1379	G
6	B	1381	U
6	B	1397	C
6	B	1398	A
6	B	1419	G
6	B	1432	G
6	B	1441	A
6	B	1442	G
6	B	1446	A
6	B	1451	U
6	B	1452	C
6	B	1453	G
6	B	1492	A
6	B	1497	G
6	B	1506	U
6	B	1517	G
6	B	1529	G
6	B	1530	G
6	B	1534	A
27	a	10	A
27	a	27	G
27	a	34	U
27	a	42	A
27	a	61	C
27	a	71	A
27	a	74	A
27	a	75	G
27	a	91	A

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Mol	Chain	Res	Type
27	a	101	A
27	a	102	U
27	a	119	A
27	a	120	U
27	a	125	A
27	a	135	U
27	a	136	G
27	a	139	U
27	a	140	C
27	a	142	A
27	a	163	C
27	a	181	A
27	a	196	A
27	a	199	A
27	a	200	U
27	a	215	G
27	a	216	A
27	a	221	A
27	a	222	A
27	a	223	A
27	a	228	C
27	a	233	A
27	a	248	G
27	a	272	A
27	a	276	U
27	a	279	A
27	a	281	C
27	a	282	A
27	a	285	G
27	a	289	G
27	a	291	G
27	a	311	A
27	a	329	G
27	a	330	A
27	a	332	A
27	a	361	G
27	a	362	A
27	a	363	G
27	a	367	G
27	a	386	G
27	a	396	G
27	a	404	A

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Mol	Chain	Res	Type
27	a	405	U
27	a	406	G
27	a	411	G
27	a	412	A
27	a	480	A
27	a	481	G
27	a	490	C
27	a	491	G
27	a	504	A
27	a	505	A
27	a	509	C
27	a	513	A
27	a	530	G
27	a	531	C
27	a	532	A
27	a	545	U
27	a	546	U
27	a	547	A
27	a	548	G
27	a	549	G
27	a	555	G
27	a	556	A
27	a	563	A
27	a	568	U
27	a	573	U
27	a	575	A
27	a	586	A
27	a	588	U
27	a	603	A
27	a	613	A
27	a	614	A
27	a	615	U
27	a	627	A
27	a	637	A
27	a	645	C
27	a	651	G
27	a	654	A
27	a	655	A
27	a	656	G
27	a	686	U
27	a	717	C
27	a	730	A

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Mol	Chain	Res	Type
27	a	738	G
27	a	747	5MU
27	a	764	A
27	a	765	C
27	a	775	G
27	a	776	G
27	a	782	A
27	a	784	G
27	a	785	G
27	a	792	A
27	a	805	G
27	a	812	C
27	a	827	U
27	a	828	U
27	a	845	A
27	a	846	U
27	a	847	U
27	a	856	G
27	a	859	G
27	a	866	A
27	a	869	G
27	a	879	G
27	a	881	G
27	a	883	G
27	a	884	U
27	a	890	C
27	a	891	G
27	a	894	U
27	a	895	U
27	a	896	A
27	a	897	C
27	a	910	A
27	a	915	C
27	a	931	U
27	a	941	A
27	a	946	C
27	a	961	C
27	a	974	G
27	a	983	A
27	a	996	A
27	a	999	U
27	a	1005	C

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Mol	Chain	Res	Type
27	a	1012	U
27	a	1013	C
27	a	1022	G
27	a	1025	G
27	a	1026	G
27	a	1033	U
27	a	1047	G
27	a	1048	A
27	a	1108	U
27	a	1109	C
27	a	1110	G
27	a	1111	A
27	a	1112	G
27	a	1116	G
27	a	1130	U
27	a	1132	U
27	a	1133	A
27	a	1134	A
27	a	1135	C
27	a	1136	G
27	a	1141	U
27	a	1142	A
27	a	1143	A
27	a	1169	A
27	a	1171	G
27	a	1187	G
27	a	1188	U
27	a	1205	A
27	a	1250	G
27	a	1253	A
27	a	1256	G
27	a	1271	G
27	a	1272	A
27	a	1276	A
27	a	1300	G
27	a	1301	A
27	a	1302	A
27	a	1321	A
27	a	1329	U
27	a	1345	C
27	a	1352	U
27	a	1359	A

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Mol	Chain	Res	Type
27	a	1365	A
27	a	1376	C
27	a	1378	A
27	a	1379	U
27	a	1383	A
27	a	1395	A
27	a	1416	G
27	a	1420	A
27	a	1427	A
27	a	1428	C
27	a	1452	G
27	a	1460	U
27	a	1482	G
27	a	1490	A
27	a	1497	U
27	a	1508	A
27	a	1515	A
27	a	1529	G
27	a	1530	G
27	a	1534	U
27	a	1535	A
27	a	1536	C
27	a	1537	G
27	a	1538	G
27	a	1558	C
27	a	1560	G
27	a	1566	A
27	a	1569	A
27	a	1578	U
27	a	1583	A
27	a	1585	C
27	a	1587	G
27	a	1608	A
27	a	1610	A
27	a	1634	A
27	a	1635	A
27	a	1647	U
27	a	1648	U
27	a	1663	G
27	a	1674	G
27	a	1675	C
27	a	1696	G

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Mol	Chain	Res	Type
27	a	1700	A
27	a	1701	A
27	a	1713	A
27	a	1715	G
27	a	1716	U
27	a	1729	U
27	a	1730	C
27	a	1732	C
27	a	1733	G
27	a	1738	G
27	a	1739	A
27	a	1758	U
27	a	1764	C
27	a	1773	A
27	a	1791	A
27	a	1800	C
27	a	1801	A
27	a	1802	A
27	a	1808	A
27	a	1811	G
27	a	1816	C
27	a	1829	A
27	a	1847	A
27	a	1848	A
27	a	1858	A
27	a	1871	A
27	a	1872	A
27	a	1873	G
27	a	1874	C
27	a	1906	G
27	a	1907	G
27	a	1913	A
27	a	1929	G
27	a	1930	G
27	a	1936	A
27	a	1937	A
27	a	1938	A
27	a	1939	5MU
27	a	1955	U
27	a	1967	C
27	a	1970	A
27	a	1971	U

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Mol	Chain	Res	Type
27	a	1972	G
27	a	1991	U
27	a	1993	U
27	a	1996	C
27	a	2020	A
27	a	2022	U
27	a	2023	C
27	a	2029	G
27	a	2030	A
27	a	2031	A
27	a	2033	A
27	a	2043	C
27	a	2055	C
27	a	2056	G
27	a	2060	A
27	a	2061	G
27	a	2062	A
27	a	2069	G7M
27	a	2192	U
27	a	2193	G
27	a	2198	A
27	a	2203	U
27	a	2204	G
27	a	2211	A
27	a	2223	G
27	a	2225	A
27	a	2238	G
27	a	2239	G
27	a	2268	A
27	a	2278	A
27	a	2282	G
27	a	2283	C
27	a	2287	A
27	a	2305	U
27	a	2308	G
27	a	2311	A
27	a	2322	A
27	a	2325	G
27	a	2333	A
27	a	2335	A
27	a	2347	C
27	a	2350	C

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Mol	Chain	Res	Type
27	a	2361	G
27	a	2383	G
27	a	2385	C
27	a	2390	U
27	a	2396	G
27	a	2402	U
27	a	2403	C
27	a	2406	A
27	a	2424	C
27	a	2425	A
27	a	2429	G
27	a	2430	A
27	a	2435	A
27	a	2441	U
27	a	2448	A
27	a	2459	A
27	a	2469	A
27	a	2470	G
27	a	2476	A
27	a	2478	A
27	a	2498	OMC
27	a	2502	G
27	a	2504	PSU
27	a	2505	G
27	a	2506	U
27	a	2518	A
27	a	2520	C
27	a	2529	G
27	a	2547	A
27	a	2566	A
27	a	2567	G
27	a	2572	A
27	a	2599	G
27	a	2602	A
27	a	2603	G
27	a	2610	C
27	a	2613	U
27	a	2615	U
27	a	2629	U
27	a	2630	G
27	a	2632	A
27	a	2639	A

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Mol	Chain	Res	Type
27	a	2656	U
27	a	2663	G
27	a	2682	A
27	a	2689	U
27	a	2690	U
27	a	2714	G
27	a	2716	C
27	a	2726	A
27	a	2733	A
27	a	2744	G
27	a	2748	A
27	a	2757	A
27	a	2765	A
27	a	2778	A
27	a	2779	U
27	a	2798	U
27	a	2809	A
27	a	2820	A
27	a	2821	A
27	a	2835	A
27	a	2836	U
27	a	2873	A
27	a	2880	C
27	a	2883	A
27	a	2884	U
27	a	2885	G
27	a	2886	A
27	a	2903	U
28	b	9	G
28	b	21	G
28	b	25	U
28	b	33	G
28	b	34	A
28	b	35	C
28	b	36	C
28	b	44	G
28	b	45	A
28	b	51	G
28	b	56	G
28	b	57	A
28	b	67	G
28	b	87	U

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Mol	Chain	Res	Type
28	b	89	U
28	b	90	C
28	b	99	A
28	b	105	G
28	b	108	A
28	b	109	A
53	X	12	U
53	X	19	A
53	X	20	U
53	X	21	A
54	Y	7	G
54	Y	9	G
54	Y	17	C
54	Y	17(A)	U
54	Y	18	G
54	Y	20	U
54	Y	21	A
54	Y	22	G
54	Y	23	C
54	Y	46	G
54	Y	55	PSU
54	Y	76	A
55	8	6	A
55	8	7	G
55	8	9	G
55	8	10	G
55	8	14	A
55	8	16	U
55	8	18	G
55	8	20	U
55	8	22	G
55	8	23	A
55	8	24	C
55	8	35	C
55	8	37	A
55	8	43	A
55	8	46	G
55	8	58	G
55	8	83	C
55	8	85	A

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	B	7	A
6	B	21	G
6	B	95	C
6	B	98	A
6	B	119	A
6	B	198	G
6	B	315	A
6	B	351	G
6	B	384	G
6	B	446	G
6	B	453	G
6	B	462	G
6	B	468	A
6	B	491	G
6	B	496	A
6	B	499	A
6	B	573	A
6	B	575	G
6	B	619	U
6	B	686	U
6	B	722	G
6	B	1005	A
6	B	1006	G
6	B	1024	G
6	B	1035	A
6	B	1039	G
6	B	1094	G
6	B	1129	C
6	B	1145	A
6	B	1181	G
6	B	1214	C
6	B	1225	A
6	B	1239	A
6	B	1319	A
6	B	1337	G
6	B	1397	C
6	B	1441	A
6	B	1505	G
54	Y	16	C
54	Y	17	C
54	Y	22	G
54	Y	47	U
55	8	6	A

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Mol	Chain	Res	Type
55	8	23	A

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

38 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
27	PSU	a	1917	27	18,21,22	1.16	2 (11%)	22,30,33	1.84	4 (18%)
54	PSU	Y	55	54	18,21,22	1.17	2 (11%)	22,30,33	1.63	3 (13%)
27	5MU	a	747	27	19,22,23	7.49	7 (36%)	28,32,35	3.17	10 (35%)
27	PSU	a	2504	27	18,21,22	1.14	2 (11%)	22,30,33	1.79	3 (13%)
54	4SU	Y	8	54	18,21,22	3.54	8 (44%)	26,30,33	2.06	4 (15%)
6	2MG	B	1516	6	18,26,27	2.41	7 (38%)	16,38,41	1.51	4 (25%)
27	OMU	a	2552	27	19,22,23	2.92	8 (42%)	26,31,34	1.80	5 (19%)
6	2MG	B	966	6	18,26,27	2.45	7 (38%)	16,38,41	1.40	3 (18%)
6	G7M	B	527	6	20,26,27	2.41	7 (35%)	17,39,42	1.12	2 (11%)
6	UR3	B	1498	6	19,22,23	2.88	8 (42%)	26,32,35	1.46	2 (7%)
6	4OC	B	1402	6	20,23,24	2.96	8 (40%)	26,32,35	1.02	2 (7%)
30	MEQ	d	150	30	8,9,10	0.93	0	5,10,12	1.28	1 (20%)
27	PSU	a	955	27	18,21,22	1.05	1 (5%)	22,30,33	1.86	3 (13%)
27	OMC	a	2498	27,58	19,22,23	2.79	8 (42%)	26,31,34	0.76	0
27	PSU	a	2580	27	18,21,22	1.23	2 (11%)	22,30,33	2.00	6 (27%)
27	H2U	a	2449	27	18,21,22	3.25	6 (33%)	21,30,33	2.23	5 (23%)
27	2MA	a	2503	27,58	19,25,26	3.49	7 (36%)	21,37,40	1.82	4 (19%)
6	MA6	B	1518	6	18,26,27	1.20	1 (5%)	19,38,41	2.81	2 (10%)
6	5MC	B	967	6	18,22,23	3.60	7 (38%)	26,32,35	0.95	1 (3%)
6	5MC	B	1407	6	18,22,23	3.56	7 (38%)	26,32,35	1.03	3 (11%)
27	PSU	a	2604	27	18,21,22	1.11	2 (11%)	22,30,33	1.96	4 (18%)
27	6MZ	a	1618	27	18,25,26	2.53	2 (11%)	16,36,39	1.98	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	2MG	B	1207	6	18,26,27	2.49	7 (38%)	16,38,41	1.37	3 (18%)
27	5MC	a	1962	27	18,22,23	3.59	7 (38%)	26,32,35	1.12	3 (11%)
27	5MU	a	1939	27	19,22,23	7.52	7 (36%)	28,32,35	3.12	9 (32%)
6	PSU	B	516	6	18,21,22	1.09	2 (11%)	22,30,33	1.77	4 (18%)
27	1MG	a	745	27	18,26,27	2.72	6 (33%)	19,39,42	1.63	5 (26%)
6	MA6	B	1519	6	18,26,27	1.22	1 (5%)	19,38,41	2.86	2 (10%)
27	PSU	a	746	27,58	18,21,22	1.14	2 (11%)	22,30,33	1.71	3 (13%)
27	PSU	a	2457	27	18,21,22	1.17	1 (5%)	22,30,33	1.81	4 (18%)
54	5MC	Y	32	54	18,22,23	3.59	7 (38%)	26,32,35	0.97	1 (3%)
27	G7M	a	2069	27	20,26,27	2.31	7 (35%)	17,39,42	1.12	2 (11%)
27	OMG	a	2251	27,54,58	18,26,27	2.62	7 (38%)	19,38,41	1.47	4 (21%)
27	PSU	a	2605	27	18,21,22	1.07	2 (11%)	22,30,33	1.83	4 (18%)
27	2MG	a	2445	27	18,26,27	2.38	7 (38%)	16,38,41	1.48	4 (25%)
27	PSU	a	1911	27	18,21,22	1.09	2 (11%)	22,30,33	1.75	3 (13%)
54	5MU	Y	54	54	19,22,23	7.47	7 (36%)	28,32,35	3.05	9 (32%)
27	2MG	a	1835	27	18,26,27	2.39	7 (38%)	16,38,41	1.36	4 (25%)

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
27	PSU	a	1917	27	-	0/7/25/26	0/2/2/2
54	PSU	Y	55	54	-	2/7/25/26	0/2/2/2
27	5MU	a	747	27	-	0/7/25/26	0/2/2/2
27	PSU	a	2504	27	-	0/7/25/26	0/2/2/2
54	4SU	Y	8	54	-	0/7/25/26	0/2/2/2
6	2MG	B	1516	6	-	0/5/27/28	0/3/3/3
27	OMU	a	2552	27	-	0/9/27/28	0/2/2/2
6	2MG	B	966	6	-	2/5/27/28	0/3/3/3
6	G7M	B	527	6	-	1/3/25/26	0/3/3/3
6	UR3	B	1498	6	-	0/7/25/26	0/2/2/2
6	4OC	B	1402	6	-	0/9/29/30	0/2/2/2
30	MEQ	d	150	30	-	2/8/9/11	-
27	PSU	a	955	27	-	0/7/25/26	0/2/2/2
27	OMC	a	2498	27,58	-	0/9/27/28	0/2/2/2
27	PSU	a	2580	27	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	H2U	a	2449	27	-	0/7/38/39	0/2/2/2
27	2MA	a	2503	27,58	-	2/3/25/26	0/3/3/3
6	MA6	B	1518	6	-	0/7/29/30	0/3/3/3
6	5MC	B	967	6	-	0/7/25/26	0/2/2/2
6	5MC	B	1407	6	-	0/7/25/26	0/2/2/2
27	PSU	a	2604	27	-	0/7/25/26	0/2/2/2
27	6MZ	a	1618	27	-	1/5/27/28	0/3/3/3
6	2MG	B	1207	6	-	0/5/27/28	0/3/3/3
27	5MC	a	1962	27	-	4/7/25/26	0/2/2/2
27	5MU	a	1939	27	-	0/7/25/26	0/2/2/2
6	PSU	B	516	6	-	0/7/25/26	0/2/2/2
27	1MG	a	745	27	-	0/3/25/26	0/3/3/3
6	MA6	B	1519	6	-	0/7/29/30	0/3/3/3
27	PSU	a	746	27,58	-	3/7/25/26	0/2/2/2
27	PSU	a	2457	27	-	0/7/25/26	0/2/2/2
54	5MC	Y	32	54	-	0/7/25/26	0/2/2/2
27	G7M	a	2069	27	-	1/3/25/26	0/3/3/3
27	OMG	a	2251	27,54,58	-	1/5/27/28	0/3/3/3
27	PSU	a	2605	27	-	0/7/25/26	0/2/2/2
27	2MG	a	2445	27	-	0/5/27/28	0/3/3/3
27	PSU	a	1911	27	-	0/7/25/26	0/2/2/2
54	5MU	Y	54	54	-	2/7/25/26	0/2/2/2
27	2MG	a	1835	27	-	0/5/27/28	0/3/3/3

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	747	5MU	C4-C5	21.48	1.80	1.44
27	a	1939	5MU	C4-C5	21.40	1.80	1.44
54	Y	54	5MU	C4-C5	21.18	1.79	1.44
54	Y	54	5MU	C6-N1	16.00	1.65	1.38
27	a	1939	5MU	C6-N1	15.68	1.64	1.38
27	a	747	5MU	C6-N1	15.54	1.64	1.38
27	a	747	5MU	C6-C5	-12.75	1.13	1.34
27	a	1939	5MU	C6-C5	-12.66	1.13	1.34
54	Y	54	5MU	C6-C5	-12.54	1.14	1.34
27	a	1939	5MU	C4-N3	-11.94	1.16	1.38
27	a	747	5MU	C4-N3	-11.87	1.16	1.38
54	Y	54	5MU	C4-N3	-11.67	1.17	1.38
27	a	2449	H2U	C2-N1	9.83	1.49	1.35
27	a	2503	2MA	C4-N3	9.79	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	1618	6MZ	C6-N6	9.44	1.50	1.35
6	B	1407	5MC	C6-C5	9.24	1.49	1.34
27	a	1962	5MC	C6-C5	9.14	1.49	1.34
6	B	967	5MC	C6-C5	9.06	1.49	1.34
54	Y	32	5MC	C6-C5	9.04	1.49	1.34
6	B	1498	UR3	C2-N1	7.76	1.49	1.38
54	Y	8	4SU	C4-N3	7.21	1.45	1.37
54	Y	32	5MC	C4-N3	7.19	1.46	1.34
6	B	967	5MC	C4-N3	7.03	1.46	1.34
27	a	1962	5MC	C4-N3	6.85	1.45	1.34
6	B	1407	5MC	C4-N3	6.65	1.45	1.34
27	a	2503	2MA	C2-N3	6.63	1.45	1.34
27	a	2503	2MA	C2-N1	6.63	1.45	1.34
27	a	2552	OMU	C2-N1	6.59	1.49	1.38
6	B	1402	4OC	C4-N3	6.57	1.44	1.32
27	a	745	1MG	C2-N3	6.56	1.46	1.34
54	Y	8	4SU	C2-N3	6.53	1.49	1.38
54	Y	8	4SU	C2-N1	6.50	1.48	1.38
27	a	2552	OMU	C2-N3	6.34	1.49	1.38
27	a	2449	H2U	C2-N3	6.29	1.49	1.38
27	a	1939	5MU	O2-C2	-6.23	1.11	1.23
6	B	1402	4OC	C6-C5	6.05	1.49	1.35
27	a	747	5MU	O2-C2	-5.97	1.12	1.23
27	a	2498	OMC	C2-N3	5.91	1.48	1.36
27	a	2251	OMG	C2-N3	5.82	1.47	1.33
6	B	1498	UR3	C6-C5	5.77	1.48	1.35
27	a	2498	OMC	C6-C5	5.74	1.48	1.35
54	Y	54	5MU	O2-C2	-5.58	1.12	1.23
6	B	967	5MC	C2-N3	5.57	1.47	1.36
27	a	2552	OMU	C6-C5	5.57	1.48	1.35
54	Y	8	4SU	C6-C5	5.55	1.48	1.35
27	a	745	1MG	C2-N2	5.53	1.44	1.34
6	B	966	2MG	C2-N2	5.46	1.45	1.33
54	Y	32	5MC	C2-N3	5.43	1.47	1.36
6	B	1207	2MG	C2-N2	5.42	1.45	1.33
27	a	2251	OMG	C4-N3	5.40	1.50	1.37
27	a	1962	5MC	C2-N3	5.34	1.47	1.36
6	B	1407	5MC	C2-N3	5.34	1.47	1.36
6	B	527	G7M	C2-N3	5.27	1.46	1.33
27	a	1835	2MG	C2-N2	5.26	1.45	1.33
6	B	1498	UR3	C2-N3	5.24	1.49	1.39
27	a	1962	5MC	C6-N1	5.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1402	4OC	C2-N3	5.20	1.46	1.36
6	B	967	5MC	C6-N1	5.20	1.46	1.38
6	B	1516	2MG	C2-N2	5.18	1.44	1.33
27	a	2445	2MG	C2-N2	5.12	1.44	1.33
27	a	2069	G7M	C2-N3	5.08	1.45	1.33
6	B	1407	5MC	C6-N1	5.03	1.46	1.38
27	a	1962	5MC	C2-N1	5.02	1.50	1.40
6	B	966	2MG	C4-N3	5.00	1.49	1.37
6	B	1516	2MG	C4-N3	4.87	1.49	1.37
27	a	2449	H2U	C4-N3	4.87	1.45	1.37
6	B	1207	2MG	C4-N3	4.85	1.49	1.37
54	Y	32	5MC	C6-N1	4.82	1.46	1.38
6	B	1407	5MC	C2-N1	4.77	1.50	1.40
54	Y	32	5MC	C2-N1	4.77	1.50	1.40
6	B	967	5MC	C2-N1	4.74	1.50	1.40
27	a	1835	2MG	C4-N3	4.72	1.48	1.37
6	B	527	G7M	C2-N2	4.70	1.45	1.34
27	a	2503	2MA	C6-N1	4.68	1.42	1.33
27	a	2251	OMG	C2-N2	4.66	1.45	1.34
54	Y	8	4SU	C5-C4	4.66	1.48	1.42
27	a	2069	G7M	C4-N3	4.66	1.48	1.37
6	B	527	G7M	C4-N3	4.63	1.48	1.37
27	a	2498	OMC	C4-N3	4.56	1.43	1.34
27	a	2445	2MG	C4-N3	4.54	1.48	1.37
27	a	2069	G7M	C2-N2	4.51	1.44	1.34
6	B	1207	2MG	C2-N1	4.49	1.43	1.36
27	a	2498	OMC	C4-N4	4.47	1.44	1.33
54	Y	8	4SU	C4-S4	-4.46	1.59	1.68
6	B	966	2MG	C2-N1	4.37	1.43	1.36
6	B	1402	4OC	C4-N4	4.36	1.44	1.35
27	a	1835	2MG	C2-N1	4.31	1.43	1.36
27	a	745	1MG	C4-N3	4.31	1.47	1.37
27	a	745	1MG	O6-C6	-4.30	1.14	1.22
6	B	1516	2MG	C2-N1	4.28	1.43	1.36
6	B	527	G7M	C6-N1	4.12	1.44	1.37
27	a	2445	2MG	C2-N1	4.11	1.43	1.36
6	B	1402	4OC	C5-C4	3.85	1.49	1.40
6	B	1402	4OC	C2-N1	3.82	1.48	1.40
27	a	2498	OMC	C2-N1	3.81	1.48	1.40
27	a	2069	G7M	C6-N1	3.73	1.43	1.37
54	Y	54	5MU	C2-N1	3.71	1.44	1.38
27	a	2552	OMU	O4-C4	-3.57	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	2457	PSU	C6-C5	3.57	1.39	1.35
27	a	745	1MG	C5-C4	-3.49	1.34	1.43
27	a	2580	PSU	C6-C5	3.44	1.39	1.35
6	B	1207	2MG	C5-C6	3.41	1.54	1.47
27	a	2449	H2U	O2-C2	-3.40	1.16	1.23
27	a	2552	OMU	C4-N3	3.37	1.44	1.38
54	Y	55	PSU	C6-C5	3.37	1.39	1.35
27	a	2251	OMG	C5-C6	3.35	1.54	1.47
27	a	2251	OMG	C6-N1	3.35	1.42	1.37
54	Y	54	5MU	C2-N3	3.32	1.43	1.38
27	a	1917	PSU	C6-C5	3.30	1.39	1.35
27	a	746	PSU	C6-C5	3.30	1.39	1.35
6	B	1207	2MG	C6-N1	3.27	1.42	1.37
27	a	1939	5MU	C2-N3	3.25	1.43	1.38
27	a	747	5MU	C2-N3	3.25	1.43	1.38
27	a	1939	5MU	C2-N1	3.24	1.43	1.38
6	B	966	2MG	C6-N1	3.22	1.42	1.37
6	B	967	5MC	C4-N4	3.21	1.42	1.34
27	a	1835	2MG	C6-N1	3.18	1.42	1.37
6	B	1407	5MC	C4-N4	3.14	1.42	1.34
27	a	1962	5MC	O2-C2	-3.14	1.17	1.23
27	a	2504	PSU	C6-C5	3.13	1.39	1.35
6	B	1516	2MG	C5-C6	3.13	1.53	1.47
54	Y	32	5MC	C4-N4	3.11	1.42	1.34
54	Y	32	5MC	O2-C2	-3.10	1.18	1.23
6	B	1402	4OC	O2-C2	-3.07	1.18	1.23
27	a	2604	PSU	C6-C5	3.06	1.38	1.35
6	B	1402	4OC	C6-N1	3.06	1.45	1.38
6	B	516	PSU	C6-C5	3.04	1.38	1.35
6	B	966	2MG	C5-C6	3.02	1.53	1.47
27	a	2498	OMC	O2-C2	-2.99	1.18	1.23
27	a	2445	2MG	C5-C4	-2.98	1.35	1.43
6	B	1498	UR3	O2-C2	-2.97	1.17	1.22
27	a	1962	5MC	C4-N4	2.97	1.41	1.34
6	B	1407	5MC	O2-C2	-2.96	1.18	1.23
6	B	1516	2MG	C5-C4	-2.94	1.35	1.43
27	a	1618	6MZ	C5-C4	-2.93	1.33	1.40
27	a	2552	OMU	C6-N1	2.91	1.45	1.38
27	a	2445	2MG	C6-N1	2.90	1.42	1.37
27	a	2445	2MG	O6-C6	-2.89	1.17	1.23
27	a	2498	OMC	C6-N1	2.88	1.45	1.38
6	B	967	5MC	O2-C2	-2.88	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	2605	PSU	C6-C5	2.88	1.38	1.35
6	B	1519	MA6	C5-C4	-2.88	1.33	1.40
6	B	1516	2MG	C6-N1	2.86	1.42	1.37
27	a	1911	PSU	C6-C5	2.85	1.38	1.35
27	a	2449	H2U	O4-C4	-2.82	1.17	1.23
27	a	2552	OMU	O2-C2	-2.80	1.17	1.23
6	B	1518	MA6	C5-C4	-2.80	1.33	1.40
54	Y	8	4SU	C6-N1	2.80	1.44	1.38
27	a	747	5MU	C2-N1	2.80	1.42	1.38
6	B	1498	UR3	C6-N1	2.79	1.44	1.38
27	a	2503	2MA	C6-C5	2.79	1.53	1.43
27	a	1835	2MG	C5-C4	-2.78	1.36	1.43
27	a	2445	2MG	C5-C6	2.76	1.53	1.47
6	B	527	G7M	C5-C6	2.76	1.52	1.45
6	B	1207	2MG	C5-C4	-2.73	1.36	1.43
6	B	1498	UR3	O4-C4	-2.73	1.17	1.23
27	a	955	PSU	C6-C5	2.73	1.38	1.35
27	a	2251	OMG	C5-C4	-2.68	1.36	1.43
27	a	1835	2MG	C5-C6	2.67	1.52	1.47
27	a	2580	PSU	O4'-C1'	-2.66	1.40	1.43
27	a	745	1MG	C5-C6	2.65	1.55	1.47
6	B	966	2MG	C5-C4	-2.62	1.36	1.43
27	a	2069	G7M	C5-C6	2.59	1.52	1.45
27	a	2503	2MA	C5-N7	-2.58	1.30	1.39
27	a	1835	2MG	O6-C6	-2.58	1.18	1.23
6	B	1516	2MG	O6-C6	-2.56	1.18	1.23
6	B	527	G7M	O6-C6	-2.51	1.18	1.23
54	Y	8	4SU	O2-C2	-2.48	1.18	1.23
27	a	2069	G7M	O6-C6	-2.41	1.18	1.23
6	B	966	2MG	O6-C6	-2.37	1.18	1.23
6	B	1498	UR3	C5-C4	2.35	1.49	1.43
6	B	1207	2MG	O6-C6	-2.30	1.18	1.23
6	B	527	G7M	C2-N1	2.29	1.43	1.37
54	Y	55	PSU	O4'-C1'	-2.29	1.40	1.43
27	a	2251	OMG	C2-N1	2.28	1.43	1.37
27	a	2552	OMU	C5-C4	2.28	1.48	1.43
27	a	2069	G7M	C2-N1	2.13	1.42	1.37
6	B	516	PSU	O4'-C1'	-2.12	1.40	1.43
27	a	2503	2MA	C6-N6	-2.11	1.26	1.34
6	B	1498	UR3	C4-N3	2.07	1.45	1.40
27	a	2604	PSU	C4-C5	-2.07	1.38	1.44
27	a	2449	H2U	C6-C5	-2.06	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	2504	PSU	C4-C5	-2.06	1.38	1.44
27	a	1911	PSU	C4-C5	-2.05	1.38	1.44
27	a	2498	OMC	C5-C4	2.05	1.47	1.42
27	a	746	PSU	O4'-C1'	-2.03	1.41	1.43
27	a	1917	PSU	C4-C5	-2.02	1.38	1.44
27	a	2605	PSU	C4-C5	-2.01	1.38	1.44

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1519	MA6	N1-C6-N6	-10.99	105.49	117.06
6	B	1518	MA6	N1-C6-N6	-10.40	106.11	117.06
54	Y	54	5MU	C5-C4-N3	9.89	123.75	115.31
27	a	1939	5MU	C5-C4-N3	9.82	123.69	115.31
27	a	747	5MU	C5-C4-N3	9.48	123.40	115.31
27	a	747	5MU	C5-C6-N1	-7.92	115.19	123.34
54	Y	54	5MU	C5-C6-N1	-7.37	115.75	123.34
27	a	1939	5MU	C5-C6-N1	-7.31	115.82	123.34
54	Y	8	4SU	C4-N3-C2	-7.17	120.37	127.34
27	a	2449	H2U	C4-N3-C2	-6.56	120.35	125.79
27	a	747	5MU	C4-N3-C2	-6.30	119.20	127.35
27	a	1939	5MU	C4-N3-C2	-6.10	119.45	127.35
54	Y	54	5MU	C4-N3-C2	-6.02	119.55	127.35
27	a	2503	2MA	C2-N3-C4	6.02	120.41	115.52
6	B	1518	MA6	N3-C2-N1	-5.76	119.68	128.68
27	a	1618	6MZ	N3-C2-N1	-5.57	119.98	128.68
27	a	2552	OMU	C4-N3-C2	-5.49	119.34	126.58
6	B	1519	MA6	N3-C2-N1	-5.28	120.42	128.68
27	a	2449	H2U	N3-C2-N1	5.28	122.24	116.65
27	a	2604	PSU	C4-N3-C2	-5.26	118.76	126.34
54	Y	8	4SU	C5-C4-N3	5.15	119.46	114.69
27	a	955	PSU	C4-N3-C2	-5.05	119.06	126.34
27	a	2580	PSU	N1-C2-N3	4.97	120.76	115.13
27	a	2457	PSU	N1-C2-N3	4.96	120.75	115.13
27	a	1917	PSU	C4-N3-C2	-4.94	119.23	126.34
6	B	1498	UR3	C4-N3-C2	-4.90	119.95	124.56
27	a	2604	PSU	N1-C2-N3	4.90	120.68	115.13
27	a	2605	PSU	C4-N3-C2	-4.89	119.29	126.34
27	a	955	PSU	N1-C2-N3	4.84	120.61	115.13
27	a	2504	PSU	C4-N3-C2	-4.83	119.38	126.34
27	a	745	1MG	C5-C6-N1	4.79	121.10	113.90
6	B	516	PSU	C4-N3-C2	-4.72	119.54	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Y	55	PSU	C4-N3-C2	-4.71	119.56	126.34
27	a	2605	PSU	N1-C2-N3	4.69	120.45	115.13
27	a	746	PSU	C4-N3-C2	-4.64	119.66	126.34
27	a	1911	PSU	C4-N3-C2	-4.63	119.66	126.34
27	a	1917	PSU	N1-C2-N3	4.62	120.37	115.13
27	a	2504	PSU	N1-C2-N3	4.55	120.28	115.13
27	a	2580	PSU	C4-N3-C2	-4.50	119.86	126.34
27	a	747	5MU	N3-C2-N1	4.49	120.85	114.89
27	a	2457	PSU	C4-N3-C2	-4.45	119.93	126.34
6	B	516	PSU	N1-C2-N3	4.45	120.17	115.13
27	a	1939	5MU	C5M-C5-C6	-4.42	116.95	122.85
27	a	1911	PSU	N1-C2-N3	4.40	120.12	115.13
27	a	746	PSU	N1-C2-N3	4.39	120.11	115.13
27	a	1939	5MU	N3-C2-N1	4.32	120.63	114.89
27	a	2552	OMU	N3-C2-N1	4.30	120.60	114.89
27	a	747	5MU	C5M-C5-C6	-4.24	117.18	122.85
54	Y	54	5MU	N3-C2-N1	4.18	120.44	114.89
27	a	1939	5MU	C5M-C5-C4	4.12	123.30	118.77
54	Y	55	PSU	N1-C2-N3	4.10	119.78	115.13
54	Y	54	5MU	O4-C4-C5	-4.08	120.17	124.90
27	a	2449	H2U	O2-C2-N1	-4.01	118.07	123.11
6	B	1516	2MG	C5-C6-N1	3.77	120.62	113.95
27	a	2445	2MG	C5-C6-N1	3.74	120.55	113.95
27	a	2552	OMU	C5-C4-N3	3.60	120.23	114.84
6	B	966	2MG	C5-C6-N1	3.59	120.30	113.95
27	a	747	5MU	O4-C4-C5	-3.52	120.82	124.90
54	Y	8	4SU	N3-C2-N1	3.51	119.55	114.89
27	a	747	5MU	C5M-C5-C4	3.41	122.52	118.77
6	B	1498	UR3	C1'-N1-C2	3.37	122.67	116.99
6	B	967	5MC	C5-C6-N1	-3.33	119.91	123.34
27	a	2251	OMG	C5-C6-N1	3.31	119.80	113.95
54	Y	54	5MU	C5M-C5-C6	-3.27	118.48	122.85
6	B	1207	2MG	C5-C6-N1	3.26	119.71	113.95
27	a	1835	2MG	C5-C6-N1	3.24	119.67	113.95
27	a	1618	6MZ	C2-N1-C6	3.22	119.35	116.59
54	Y	8	4SU	C5-C4-S4	-3.20	120.34	124.47
27	a	747	5MU	O2-C2-N1	-3.08	118.70	122.79
27	a	2503	2MA	N3-C2-N1	-3.05	120.16	125.73
27	a	2251	OMG	C2-N1-C6	-3.05	119.48	125.10
6	B	1407	5MC	C5-C6-N1	-3.01	120.24	123.34
27	a	1618	6MZ	C9-N6-C6	-2.89	120.38	122.87
27	a	2580	PSU	O2-C2-N1	-2.88	119.62	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	1939	5MU	O4-C4-N3	-2.88	114.60	120.12
27	a	2503	2MA	C1'-N9-C4	-2.82	121.68	126.64
54	Y	32	5MC	C5-C6-N1	-2.82	120.44	123.34
27	a	1962	5MC	C5-C6-N1	-2.81	120.44	123.34
27	a	2251	OMG	C8-N7-C5	2.77	108.27	102.99
6	B	527	G7M	C2-N1-C6	-2.77	120.00	125.10
27	a	1939	5MU	O4-C4-C5	-2.75	121.71	124.90
27	a	747	5MU	C6-C5-C4	2.71	120.30	118.03
6	B	1516	2MG	C8-N7-C5	2.71	108.15	102.99
27	a	2580	PSU	C3'-C2'-C1'	2.70	104.78	101.64
27	a	746	PSU	O2-C2-N1	-2.68	119.84	122.79
6	B	966	2MG	C8-N7-C5	2.68	108.09	102.99
27	a	2445	2MG	C8-N7-C5	2.64	108.02	102.99
27	a	2457	PSU	C6-N1-C2	-2.62	120.00	122.68
27	a	2605	PSU	O2-C2-N1	-2.61	119.91	122.79
6	B	516	PSU	O2-C2-N1	-2.60	119.93	122.79
27	a	2580	PSU	C6-N1-C2	-2.58	120.04	122.68
30	d	150	MEQ	CG-CD-NE2	2.57	119.86	116.29
27	a	2069	G7M	C2-N1-C6	-2.57	120.36	125.10
54	Y	54	5MU	C5M-C5-C4	2.55	121.58	118.77
27	a	2580	PSU	O4'-C1'-C2'	2.52	108.70	105.14
27	a	2445	2MG	CM2-N2-C2	-2.51	118.31	123.86
27	a	2552	OMU	O4-C4-C5	-2.51	120.75	125.16
27	a	2604	PSU	O2-C2-N1	-2.50	120.04	122.79
27	a	1835	2MG	O6-C6-C5	-2.50	119.50	124.37
27	a	745	1MG	CM1-N1-C2	2.48	123.29	120.72
27	a	745	1MG	C2-N1-C6	-2.46	118.95	120.95
6	B	1207	2MG	C8-N7-C5	2.45	107.66	102.99
27	a	1618	6MZ	O5'-C5'-C4'	2.45	117.32	108.99
27	a	1962	5MC	O2-C2-N3	-2.43	118.37	122.33
27	a	745	1MG	O6-C6-C5	-2.43	119.88	124.19
27	a	745	1MG	C8-N7-C5	2.43	107.62	102.99
27	a	2604	PSU	C6-C5-C4	2.42	119.89	118.20
27	a	1962	5MC	CM5-C5-C6	-2.37	119.69	122.85
27	a	2445	2MG	O6-C6-C5	-2.36	119.77	124.37
27	a	1835	2MG	C8-N7-C5	2.34	107.45	102.99
54	Y	55	PSU	O2-C2-N1	-2.33	120.22	122.79
6	B	966	2MG	O6-C6-C5	-2.32	119.85	124.37
27	a	2251	OMG	O6-C6-C5	-2.30	119.87	124.37
27	a	2449	H2U	O4-C4-N3	2.30	123.93	120.28
6	B	1516	2MG	CM2-N2-C2	-2.29	118.80	123.86
54	Y	54	5MU	C6-C5-C4	2.29	119.94	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	747	5MU	O4-C4-N3	-2.26	115.78	120.12
27	a	2457	PSU	O2-C2-N1	-2.25	120.31	122.79
27	a	2504	PSU	O2-C2-N1	-2.23	120.33	122.79
27	a	2069	G7M	N1-C2-N3	-2.23	119.16	123.32
6	B	1516	2MG	O6-C6-C5	-2.21	120.05	124.37
27	a	1835	2MG	CM2-N2-C2	-2.18	119.04	123.86
6	B	1402	4OC	C6-C5-C4	2.18	119.63	116.96
27	a	2449	H2U	C5-C4-N3	-2.17	114.21	116.65
27	a	2552	OMU	O2-C2-N1	-2.16	119.91	122.79
6	B	1407	5MC	CM5-C5-C6	-2.16	119.97	122.85
27	a	1911	PSU	O2-C2-N1	-2.13	120.44	122.79
27	a	2503	2MA	CM2-C2-N3	2.12	120.45	117.16
27	a	2605	PSU	C6-N1-C2	-2.11	120.53	122.68
54	Y	54	5MU	O4-C4-N3	-2.11	116.08	120.12
6	B	516	PSU	C6-N1-C2	-2.10	120.54	122.68
6	B	1407	5MC	C5-C4-N3	-2.10	119.41	121.67
6	B	1207	2MG	O6-C6-C5	-2.09	120.29	124.37
6	B	1402	4OC	O2-C2-N3	-2.05	118.99	122.33
27	a	1939	5MU	C6-C5-C4	2.05	119.75	118.03
27	a	955	PSU	C6-N1-C2	-2.02	120.62	122.68
27	a	1917	PSU	O2-C2-N1	-2.00	120.59	122.79
6	B	527	G7M	N1-C2-N3	-2.00	119.58	123.32
27	a	1917	PSU	C6-N1-C2	-2.00	120.64	122.68

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	a	746	PSU	C2'-C1'-C5-C4
27	a	746	PSU	O4'-C1'-C5-C6
27	a	1618	6MZ	C4'-C5'-O5'-P
30	d	150	MEQ	NE2-CD-CG-CB
30	d	150	MEQ	OE1-CD-CG-CB
54	Y	54	5MU	O4'-C4'-C5'-O5'
54	Y	54	5MU	C3'-C4'-C5'-O5'
27	a	1962	5MC	C2'-C1'-N1-C6
6	B	527	G7M	C4'-C5'-O5'-P
27	a	2503	2MA	C4'-C5'-O5'-P
6	B	966	2MG	C3'-C4'-C5'-O5'
27	a	1962	5MC	O4'-C1'-N1-C6
27	a	2069	G7M	O4'-C4'-C5'-O5'
27	a	746	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
6	B	966	2MG	O4'-C4'-C5'-O5'
27	a	1962	5MC	O4'-C1'-N1-C2
27	a	2251	OMG	C1'-C2'-O2'-CM2
54	Y	55	PSU	C4'-C5'-O5'-P
27	a	2503	2MA	O4'-C4'-C5'-O5'
54	Y	55	PSU	C3'-C4'-C5'-O5'
27	a	1962	5MC	C2'-C1'-N1-C2

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 297 ligands modelled in this entry, 295 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	$\# Z > 2$
60	A2G	A	101	56	14,14,15	0.47	0	17,19,21	0.58	0
59	SPM	a	3209	-	13,13,13	0.31	0	12,12,12	0.86	0

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	A2G	A	101	56	-	0/6/23/26	0/1/1/1
59	SPM	a	3209	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

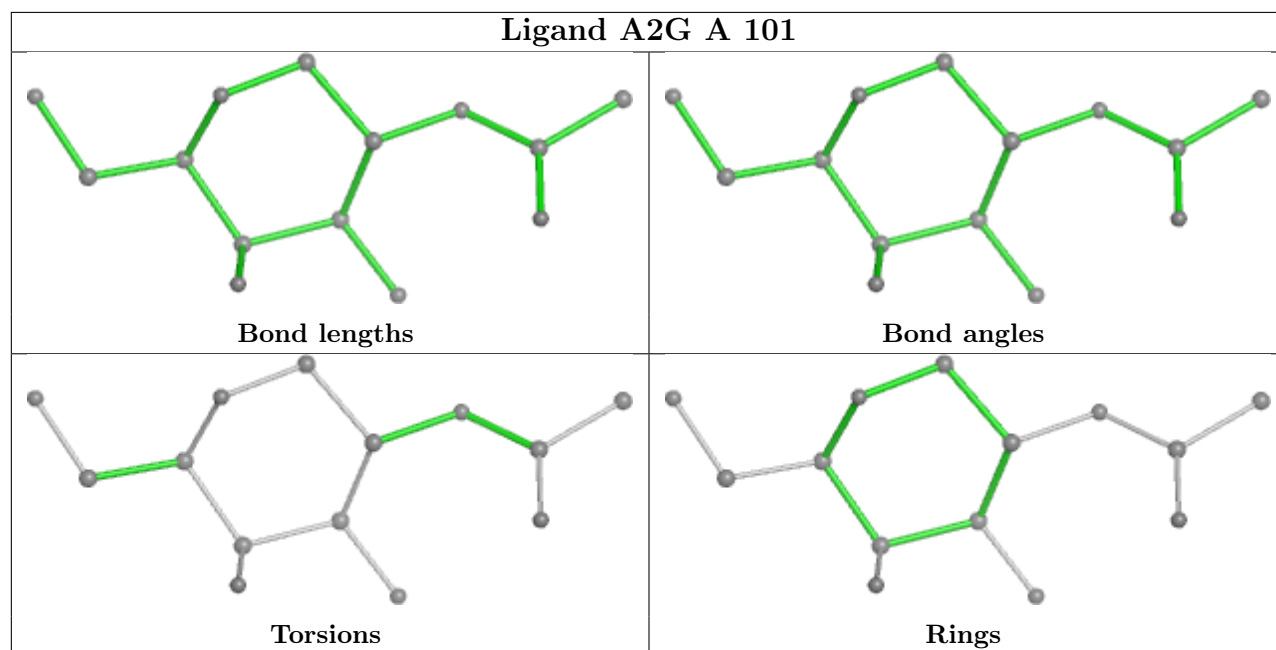
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	a	3209	SPM	C12-C11-N10-C9
59	a	3209	SPM	C3-C4-N5-C6

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.