



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 02:23 pm GMT

PDB ID : 7ACR
EMDB ID : EMD-11718
Title : Structure of post-translocated trans-translation complex on E. coli stalled ribosome.
Authors : Guyomar, C.; D'Urso, G.; Chat, S.; Giudice, E.; Gillet, R.
Deposited on : 2020-09-11
Resolution : 3.44 Å(reported)
Based on initial model : 4YBB

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:

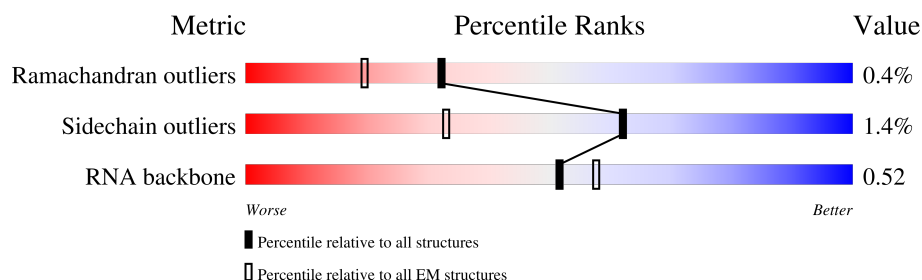
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 3.44 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.



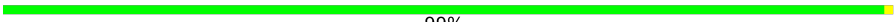
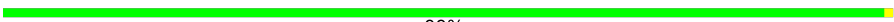












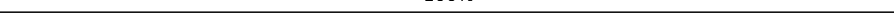
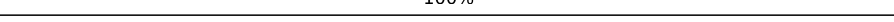
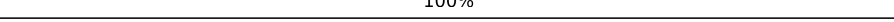
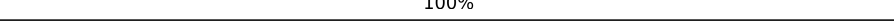
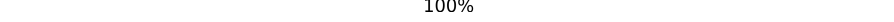
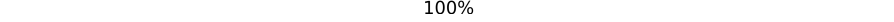
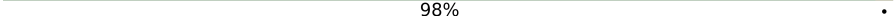


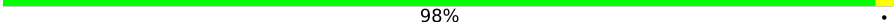
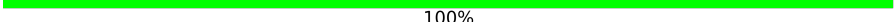

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	2903	
2	2	1534	
3	3	120	
4	4	363	
5	5	150	
6	A	76	
7	B	271	
8	C	209	
9	D	201	

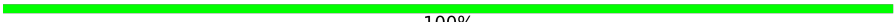
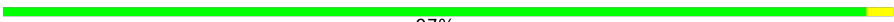










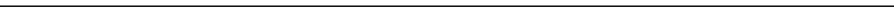


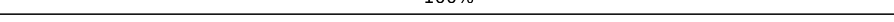
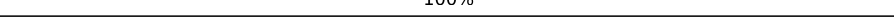
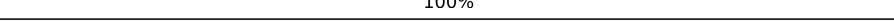
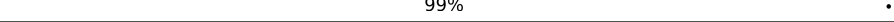
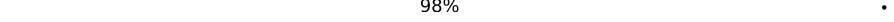
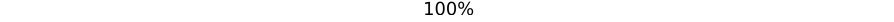
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Mol	Chain	Length	Quality of chain
10	E	177	 99% .
11	F	175	 99% .
12	G	149	 96% .
13	J	142	 99% .
14	K	123	 100%
15	L	144	 100%
16	M	136	 99% .
17	N	119	 100%
18	O	116	 100%
19	P	114	 100%
20	Q	117	 100%
21	R	103	 98% ..
22	S	110	 100%
23	T	94	 100%
24	U	103	 100%
25	V	94	 100%
26	W	2	 100%
27	X	77	 100%
28	Y	62	 100%
29	Z	58	 98% .
30	a	65	 88%  12%
31	b	56	 98% .
32	c	52	 100%
33	d	46	 100%
34	e	64	 98% .

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Mol	Chain	Length	Quality of chain
35	f	38	 100%
36	g	225	 97%
37	h	212	 99%
38	i	205	 100%
39	j	156	 100%
40	k	104	 100%
41	l	151	 100%
42	m	129	 100%
43	n	127	 54% 42%
44	o	99	 99%
45	p	117	 100%
46	q	122	 99%
47	r	112	 99%
48	s	100	 96%
49	t	88	 100%
50	u	82	 100%
51	v	80	 100%
52	w	67	 99%
53	x	83	 98%
54	y	86	 100%
55	z	70	 99%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 151668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62335	27816	11470	20147	2902		

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32927	14693	6041	10660	1533		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called transfer-messenger RNA (tmRNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	363	Total	C	N	O	P	0	0
			7755	3466	1410	2518	361		

- Molecule 5 is a protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	150	Total	C	N	O	S	0	0
			1209	763	226	216	4		

- Molecule 6 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 7 is a protein called 50S ribosomal protein L2.

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

- Molecule 8 is a protein called 50S ribosomal protein L3.

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

- Molecule 9 is a protein called 50S ribosomal protein L4.

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

- Molecule 10 is a protein called 50S ribosomal protein L5.

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

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	103	Total	C	N	O		0	0
			788	498	148	142			

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	2	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	65	Total	C	N	O	S	0	0
			514	317	98	93	6		

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

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

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

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

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	112	Total	C	N	O	S	0	0
			867	535	175	154	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

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

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	67	Total	C	N	O	S	0	0
			553	350	104	98	1		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	1	172	Total 172	Mg 172	0
56	2	31	Total 31	Mg 31	0
56	3	3	Total 3	Mg 3	0
56	C	1	Total 1	Mg 1	0
56	O	1	Total 1	Mg 1	0
56	Q	1	Total 1	Mg 1	0
56	b	1	Total 1	Mg 1	0
56	d	1	Total 1	Mg 1	0
56	h	1	Total 1	Mg 1	0

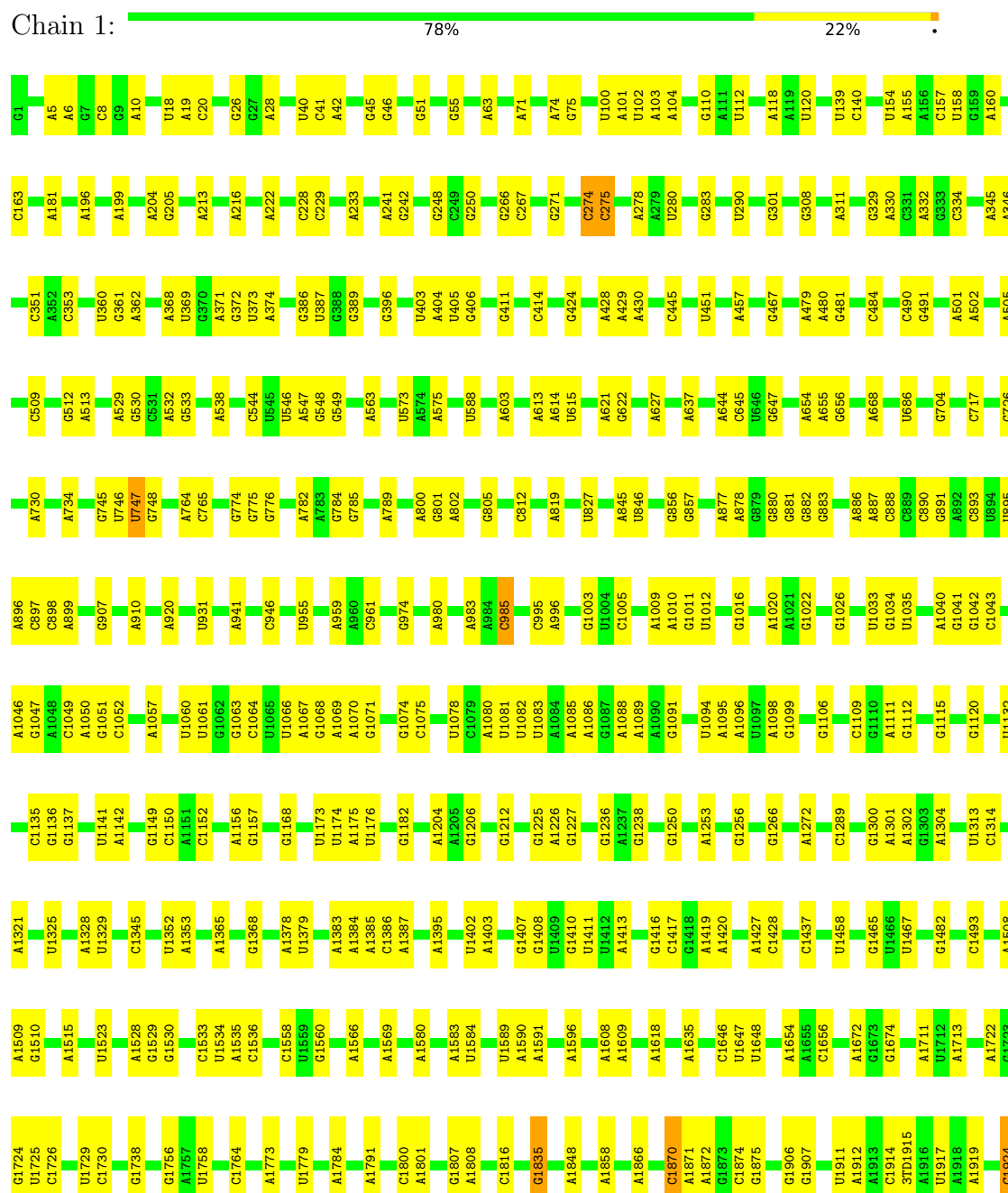
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

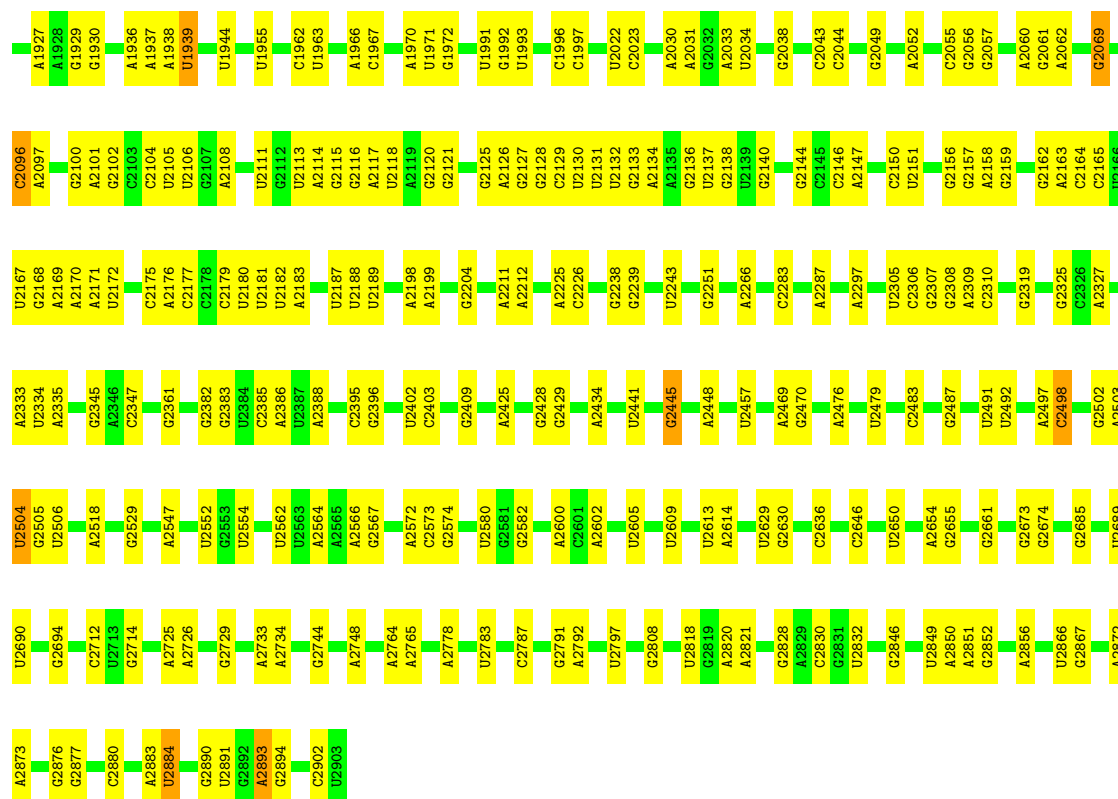
Mol	Chain	Residues	Atoms		AltConf
57	a	1	Total 1	Zn 1	0
57	f	1	Total 1	Zn 1	0

3 Residue-property plots

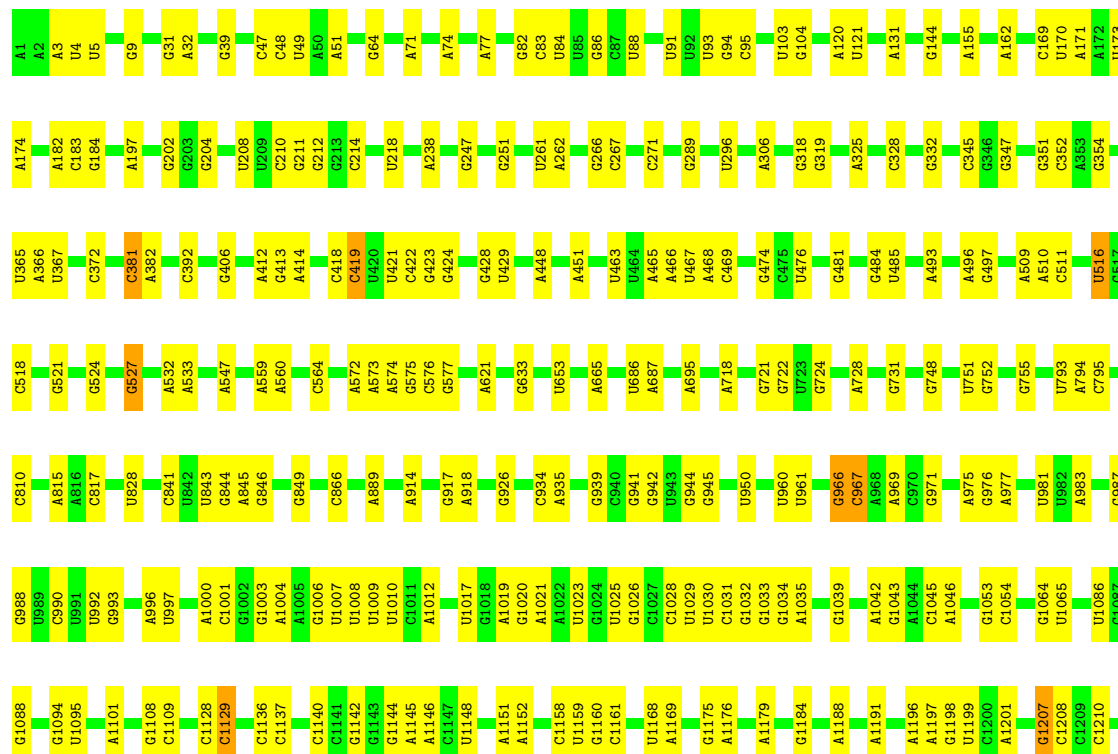
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

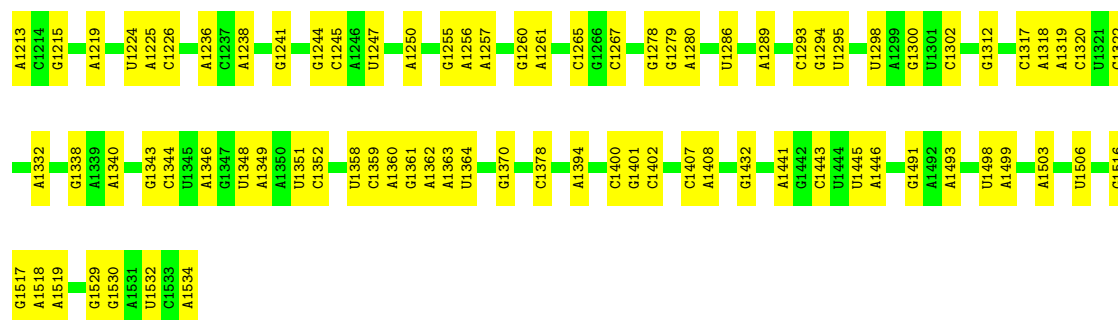
• Molecule 1: 23S ribosomal RNA



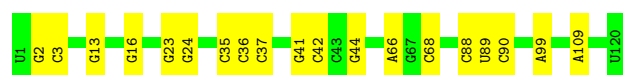
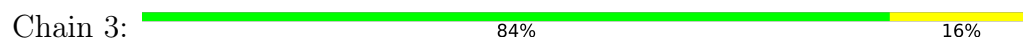


- Molecule 2: 16S ribosomal RNA

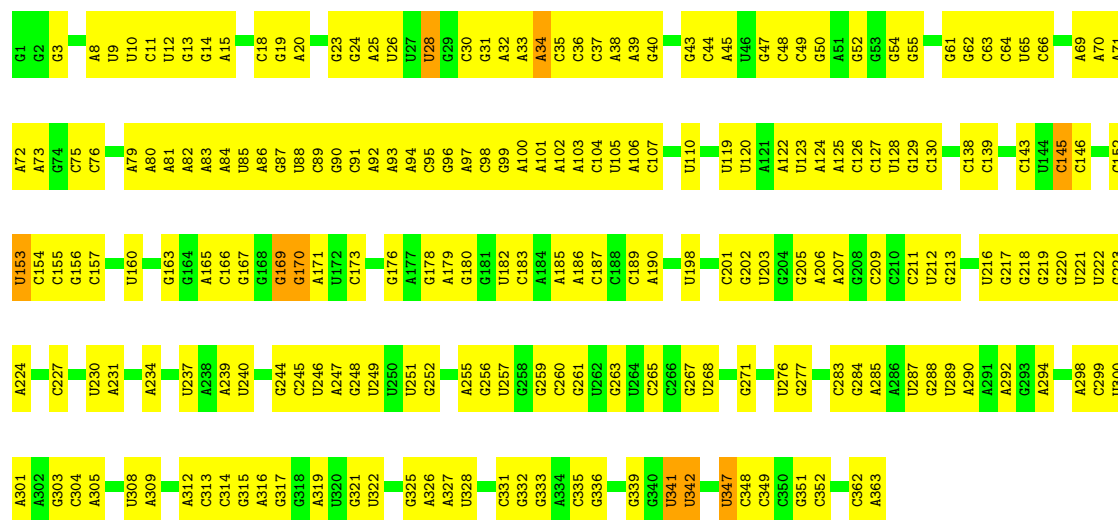




• Molecule 3: 5S ribosomal RNA



• Molecule 4: transfer-messenger RNA (tmRNA)



• Molecule 5: SsrA-binding protein

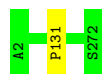


• Molecule 6: 50S ribosomal protein L27



- Molecule 7: 50S ribosomal protein L2

Chain B:  100%



- Molecule 8: 50S ribosomal protein L3

Chain C:  98%



- Molecule 9: 50S ribosomal protein L4

Chain D:  100%

There are no outlier residues recorded for this chain.

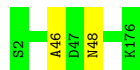
- Molecule 10: 50S ribosomal protein L5

Chain E:  99%



- Molecule 11: 50S ribosomal protein L6

Chain F:  99%



- Molecule 12: 50S ribosomal protein L9

Chain G:  96%



- Molecule 13: 50S ribosomal protein L13

Chain J:  99%



- Molecule 14: 50S ribosomal protein L14

Chain K:  100%

There are no outlier residues recorded for this chain.

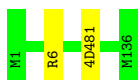
- Molecule 15: 50S ribosomal protein L15

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 50S ribosomal protein L16

Chain M:  99%



- Molecule 17: 50S ribosomal protein L17

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L18

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L19

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: 50S ribosomal protein L20

Chain Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 50S ribosomal protein L21

Chain R:  98%



- Molecule 22: 50S ribosomal protein L22

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: 50S ribosomal protein L23

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L24

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L25

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: Nascent peptide

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L28

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: 50S ribosomal protein L29

Chain Y:  100%


There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L30

Chain Z:  98%



- Molecule 30: 50S ribosomal protein L31

Chain a:  88% 12%



- Molecule 31: 50S ribosomal protein L32

Chain b:  98% .



- Molecule 32: 50S ribosomal protein L33

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L34

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 50S ribosomal protein L35

Chain e:  98% .



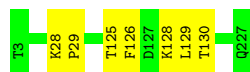
- Molecule 35: 50S ribosomal protein L36

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: 30S ribosomal protein S2

Chain g:  97% .



- Molecule 37: 30S ribosomal protein S3

Chain h:  99% .



- Molecule 38: 30S ribosomal protein S4

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 30S ribosomal protein S5

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 30S ribosomal protein S6

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: 30S ribosomal protein S7

Chain l:  100%

There are no outlier residues recorded for this chain.

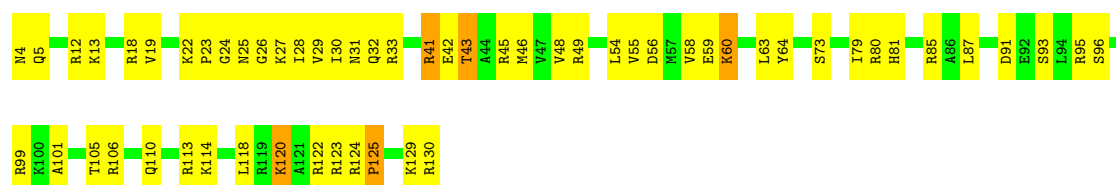
- Molecule 42: 30S ribosomal protein S8

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 30S ribosomal protein S9

Chain n:  54% 42%



- Molecule 44: 30S ribosomal protein S10

Chain o:  99%



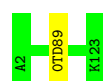
- Molecule 45: 30S ribosomal protein S11

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 30S ribosomal protein S12

Chain q:  99%



- Molecule 47: 30S ribosomal protein S13

Chain r:  99%



- Molecule 48: 30S ribosomal protein S14

Chain s:  96%



- Molecule 49: 30S ribosomal protein S15

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 30S ribosomal protein S16

Chain u:  100%

There are no outlier residues recorded for this chain.

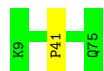
- Molecule 51: 30S ribosomal protein S17

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein S18

Chain w:  99%



- Molecule 53: 30S ribosomal protein S19

Chain x:  98%



- Molecule 54: 30S ribosomal protein S20

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 55: 30S ribosomal protein S21

Chain z:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11059	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 BASE (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: 2MG, OMG, ZN, 0TD, MA6, 4D4, OMC, 6MZ, 5MC, 5MU, 3TD, PSU, G7M, MG, OMU, 2MA, 4OC, UR3, 1MG

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	1	0.17	0/69282	0.76	28/108079 (0.0%)
2	2	0.21	0/36585	0.77	18/57064 (0.0%)
3	3	0.15	0/2872	0.73	0/4478
4	4	0.24	0/8608	0.84	10/13418 (0.1%)
5	5	0.25	0/1231	0.57	2/1655 (0.1%)
6	A	0.35	0/589	0.62	1/779 (0.1%)
7	B	0.28	1/2121 (0.0%)	0.48	0/2852
8	C	0.27	0/1586	0.58	1/2134 (0.0%)
9	D	0.24	0/1571	0.44	0/2113
10	E	0.25	0/1434	0.52	1/1926 (0.1%)
11	F	0.27	0/1333	0.56	2/1805 (0.1%)
12	G	0.32	0/1121	0.76	5/1515 (0.3%)
13	J	0.25	0/1152	0.47	0/1551
14	K	0.24	0/955	0.45	0/1279
15	L	0.25	0/1062	0.45	0/1413
16	M	0.26	0/1081	0.54	1/1443 (0.1%)
17	N	0.24	0/964	0.46	0/1289
18	O	0.24	0/902	0.44	0/1209
19	P	0.24	0/929	0.46	0/1242
20	Q	0.23	0/960	0.36	0/1278
21	R	0.27	0/829	0.48	0/1107
22	S	0.24	0/864	0.48	0/1156
23	T	0.23	0/752	0.44	0/1005
24	U	0.26	0/796	0.51	0/1062
25	V	0.25	0/766	0.46	0/1025
26	W	0.27	0/16	0.20	0/20
27	X	0.23	0/635	0.42	0/848
28	Y	0.23	0/502	0.41	0/667
29	Z	0.27	0/452	0.59	1/605 (0.2%)
30	a	0.37	0/523	0.58	0/698
31	b	0.23	0/450	0.55	1/599 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.23	0/433	0.49	0/576
33	d	0.23	0/380	0.39	0/498
34	e	0.29	0/513	0.63	0/676
35	f	0.23	0/303	0.46	0/397
36	g	0.47	1/1791 (0.1%)	0.61	3/2413 (0.1%)
37	h	0.24	0/1685	0.57	2/2270 (0.1%)
38	i	0.23	0/1665	0.38	0/2227
39	j	0.25	0/1165	0.50	0/1568
40	k	0.23	0/867	0.45	0/1171
41	l	0.24	0/1195	0.43	0/1602
42	m	0.24	0/989	0.43	0/1326
43	n	0.62	0/1034	0.94	2/1375 (0.1%)
44	o	0.23	0/800	0.56	1/1082 (0.1%)
45	p	0.24	0/893	0.45	0/1205
46	q	0.23	0/954	0.45	0/1279
47	r	0.25	0/875	0.51	1/1170 (0.1%)
48	s	0.35	0/817	0.57	0/1088
49	t	0.23	0/722	0.44	0/964
50	u	0.24	0/659	0.47	0/884
51	v	0.23	0/657	0.48	0/881
52	w	0.55	1/562 (0.2%)	0.51	2/754 (0.3%)
53	x	0.27	0/680	0.65	2/915 (0.2%)
54	y	0.23	0/675	0.37	0/895
55	z	0.24	0/597	0.54	1/792 (0.1%)
All	All	0.22	3/163834 (0.0%)	0.71	85/245322 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	g	29	PRO	N-CD	16.27	1.70	1.47
52	w	41	PRO	N-CD	11.76	1.64	1.47
7	B	131	PRO	N-CD	-6.85	1.38	1.47

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	275	C	C2-N1-C1'	8.70	128.37	118.80
36	g	29	PRO	CA-N-CD	-8.58	99.49	111.50
1	1	275	C	N1-C2-O2	8.57	124.04	118.90
2	2	1129	C	N3-C2-O2	-7.62	116.56	121.90
4	4	146	C	N3-C2-O2	-7.33	116.77	121.90
37	h	30	ALA	N-CA-CB	7.11	120.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	g	29	PRO	N-CA-CB	7.07	111.79	103.30
1	1	275	C	N3-C2-O2	-7.05	116.97	121.90
2	2	1158	C	C2-N1-C1'	7.04	126.54	118.80
1	1	1924	C	N3-C2-O2	-7.03	116.98	121.90
11	F	48	ASN	N-CA-CB	6.96	123.12	110.60
55	z	57	ALA	N-CA-CB	6.73	119.52	110.10
8	C	56	LYS	N-CA-CB	-6.72	98.50	110.60
1	1	1313	U	C2-N1-C1'	6.70	125.74	117.70
10	E	107	ALA	N-CA-CB	6.58	119.31	110.10
1	1	2884	U	C2-N1-C1'	6.49	125.48	117.70
53	x	25	SER	N-CA-CB	6.41	120.12	110.50
1	1	2884	U	N1-C2-O2	6.31	127.22	122.80
2	2	1161	C	N1-C2-O2	6.23	122.64	118.90
1	1	2902	C	N3-C2-O2	-6.22	117.54	121.90
4	4	169	G	N3-C4-N9	6.21	129.73	126.00
1	1	275	C	C6-N1-C2	-6.17	117.83	120.30
2	2	810	C	N3-C2-O2	-6.09	117.64	121.90
1	1	1313	U	N3-C2-O2	-6.03	117.98	122.20
44	o	101	SER	N-CA-CB	-6.00	101.51	110.50
4	4	145	C	N1-C2-O2	5.99	122.49	118.90
47	r	109	ARG	N-CA-CB	5.91	121.23	110.60
1	1	1313	U	N1-C2-O2	5.87	126.91	122.80
52	w	41	PRO	N-CA-CB	5.86	110.34	103.30
1	1	2884	U	N3-C2-O2	-5.86	118.10	122.20
1	1	275	C	C6-N1-C1'	-5.85	113.78	120.80
2	2	1158	C	N1-C2-O2	5.81	122.39	118.90
52	w	41	PRO	CA-N-CD	-5.80	103.38	111.50
4	4	34	A	P-O3'-C3'	5.77	126.62	119.70
2	2	1129	C	N1-C2-O2	5.77	122.36	118.90
1	1	414	C	N1-C2-O2	5.76	122.36	118.90
29	Z	11	ARG	N-CA-CB	-5.71	100.32	110.60
12	G	48	GLU	N-CA-CB	-5.65	100.43	110.60
12	G	12	LEU	N-CA-C	5.64	126.24	111.00
2	2	1175	G	N9-C1'-C2'	-5.63	105.80	112.00
1	1	274	C	N1-C2-O2	5.59	122.25	118.90
12	G	98	ASP	CB-CA-C	-5.53	99.33	110.40
11	F	46	ALA	CB-CA-C	5.52	118.38	110.10
5	5	101	TYR	CB-CA-C	-5.47	99.47	110.40
1	1	1870	C	N1-C2-O2	5.41	122.14	118.90
2	2	810	C	N1-C2-O2	5.39	122.13	118.90
2	2	1161	C	N3-C2-O2	-5.38	118.13	121.90
2	2	419	C	N3-C2-O2	-5.35	118.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	170	G	C5-C6-O6	5.35	131.81	128.60
1	1	2096	C	N1-C2-O2	5.33	122.09	118.90
6	A	14	ARG	N-CA-CB	5.32	120.18	110.60
16	M	6	ARG	N-CA-CB	-5.31	101.04	110.60
5	5	107	GLU	N-CA-C	5.30	125.32	111.00
4	4	34	A	OP2-P-O3'	5.30	116.86	105.20
4	4	23	G	P-O3'-C3'	5.30	126.06	119.70
1	1	1924	C	N1-C2-O2	5.27	122.06	118.90
2	2	381	C	N1-C2-O2	5.25	122.05	118.90
12	G	137	GLU	N-CA-C	5.25	125.17	111.00
43	n	125	PRO	N-CA-CB	-5.25	96.83	102.60
12	G	91	PHE	CB-CA-C	-5.24	99.92	110.40
31	b	34	SER	N-CA-CB	5.23	118.35	110.50
36	g	28	LYS	C-N-CD	5.21	139.33	128.40
1	1	2096	C	C2-N1-C1'	5.20	124.52	118.80
43	n	43	THR	CB-CA-C	-5.18	97.62	111.60
1	1	414	C	N3-C2-O2	-5.15	118.29	121.90
4	4	153	U	O5'-P-OP1	-5.15	101.06	105.70
2	2	1144	G	C5-C6-O6	5.14	131.68	128.60
4	4	203	U	C2-N1-C1'	5.13	123.86	117.70
2	2	1267	C	N1-C2-O2	5.11	121.97	118.90
1	1	985	C	N1-C2-O2	5.11	121.96	118.90
1	1	274	C	OP1-P-O3'	5.10	116.43	105.20
37	h	152	GLU	N-CA-CB	-5.09	101.43	110.60
1	1	445	C	N1-C2-O2	5.09	121.95	118.90
2	2	381	C	C2-N1-C1'	5.09	124.40	118.80
1	1	2902	C	N1-C2-O2	5.08	121.95	118.90
1	1	2830	C	N1-C2-O2	5.07	121.94	118.90
1	1	274	C	N3-C2-O2	-5.04	118.37	121.90
4	4	28	U	C5-C4-O4	5.04	128.92	125.90
1	1	2830	C	C2-N1-C1'	5.03	124.33	118.80
2	2	418	C	N1-C2-O2	5.03	121.92	118.90
1	1	2893	A	OP2-P-O3'	5.01	116.23	105.20
2	2	1289	A	O5'-P-OP2	5.01	116.72	110.70
2	2	1267	C	C2-N1-C1'	5.01	124.31	118.80
2	2	1144	G	N1-C2-N2	-5.00	111.70	116.20
53	x	14	HIS	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	148/150 (99%)	131 (88%)	17 (12%)	0	100	100
6	A	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	B	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
8	C	207/209 (99%)	196 (95%)	8 (4%)	3 (1%)	9	37
9	D	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
10	E	175/177 (99%)	158 (90%)	17 (10%)	0	100	100
11	F	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
12	G	147/149 (99%)	121 (82%)	25 (17%)	1 (1%)	19	52
13	J	140/142 (99%)	125 (89%)	15 (11%)	0	100	100
14	K	121/123 (98%)	121 (100%)	0	0	100	100
15	L	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	M	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
17	N	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
18	O	114/116 (98%)	110 (96%)	4 (4%)	0	100	100
19	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
20	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
21	R	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	13	44
22	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
23	T	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	U	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
25	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
28	Y	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
29	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
30	a	63/65 (97%)	49 (78%)	14 (22%)	0	100	100
31	b	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
32	c	50/52 (96%)	50 (100%)	0	0	100	100
33	d	44/46 (96%)	44 (100%)	0	0	100	100
34	e	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	8	34
35	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
36	g	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
37	h	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
38	i	203/205 (99%)	195 (96%)	8 (4%)	0	100	100
39	j	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
40	k	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
41	l	149/151 (99%)	141 (95%)	8 (5%)	0	100	100
42	m	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
43	n	125/127 (98%)	73 (58%)	36 (29%)	16 (13%)	0	3
44	o	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
45	p	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
46	q	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
47	r	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
48	s	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	13	44
49	t	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
50	u	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
51	v	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
52	w	65/67 (97%)	65 (100%)	0	0	100	100
53	x	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
54	y	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
55	z	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
All	All	5754/5856 (98%)	5423 (94%)	308 (5%)	23 (0%)	32	63

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	n	56	ASP
43	n	122	ARG
43	n	5	GLN
43	n	18	ARG
43	n	26	GLY
43	n	41	ARG
43	n	55	VAL
43	n	64	TYR
43	n	73	SER
34	e	32	ILE
43	n	60	LYS
48	s	94	PRO
43	n	96	SER
43	n	120	LYS
8	C	32	ASN
8	C	55	LYS
43	n	101	ALA
43	n	48	VAL
21	R	101	ILE
43	n	23	PRO
43	n	24	GLY
8	C	34	VAL
12	G	44	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	5	125/125 (100%)	125 (100%)	0	100	100
6	A	58/58 (100%)	58 (100%)	0	100	100
7	B	216/216 (100%)	216 (100%)	0	100	100
8	C	164/164 (100%)	164 (100%)	0	100	100
9	D	165/165 (100%)	165 (100%)	0	100	100
10	E	148/148 (100%)	148 (100%)	0	100	100
11	F	136/136 (100%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	G	114/114 (100%)	114 (100%)	0	100	100
13	J	116/116 (100%)	114 (98%)	2 (2%)	56	75
14	K	104/104 (100%)	104 (100%)	0	100	100
15	L	103/103 (100%)	103 (100%)	0	100	100
16	M	108/108 (100%)	108 (100%)	0	100	100
17	N	99/99 (100%)	99 (100%)	0	100	100
18	O	86/86 (100%)	86 (100%)	0	100	100
19	P	99/99 (100%)	99 (100%)	0	100	100
20	Q	89/89 (100%)	89 (100%)	0	100	100
21	R	84/84 (100%)	82 (98%)	2 (2%)	44	68
22	S	93/93 (100%)	93 (100%)	0	100	100
23	T	81/81 (100%)	81 (100%)	0	100	100
24	U	84/84 (100%)	84 (100%)	0	100	100
25	V	78/78 (100%)	78 (100%)	0	100	100
26	W	1/1 (100%)	1 (100%)	0	100	100
27	X	67/67 (100%)	67 (100%)	0	100	100
28	Y	54/54 (100%)	54 (100%)	0	100	100
29	Z	48/48 (100%)	48 (100%)	0	100	100
30	a	58/58 (100%)	50 (86%)	8 (14%)	3	15
31	b	47/47 (100%)	47 (100%)	0	100	100
32	c	47/47 (100%)	47 (100%)	0	100	100
33	d	38/38 (100%)	38 (100%)	0	100	100
34	e	51/51 (100%)	51 (100%)	0	100	100
35	f	34/34 (100%)	34 (100%)	0	100	100
36	g	187/187 (100%)	182 (97%)	5 (3%)	40	66
37	h	172/172 (100%)	172 (100%)	0	100	100
38	i	172/172 (100%)	172 (100%)	0	100	100
39	j	119/119 (100%)	119 (100%)	0	100	100
40	k	91/91 (100%)	91 (100%)	0	100	100
41	l	124/124 (100%)	124 (100%)	0	100	100
42	m	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	n	105/105 (100%)	60 (57%)	45 (43%)	0	0
44	o	86/86 (100%)	86 (100%)	0	100	100
45	p	90/90 (100%)	90 (100%)	0	100	100
46	q	102/102 (100%)	102 (100%)	0	100	100
47	r	90/90 (100%)	90 (100%)	0	100	100
48	s	83/83 (100%)	80 (96%)	3 (4%)	30	58
49	t	76/76 (100%)	76 (100%)	0	100	100
50	u	65/65 (100%)	65 (100%)	0	100	100
51	v	74/74 (100%)	74 (100%)	0	100	100
52	w	58/58 (100%)	58 (100%)	0	100	100
53	x	72/72 (100%)	72 (100%)	0	100	100
54	y	65/65 (100%)	65 (100%)	0	100	100
55	z	60/60 (100%)	60 (100%)	0	100	100
All	All	4790/4790 (100%)	4725 (99%)	65 (1%)	62	79

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	J	141	ASP
13	J	142	ILE
21	R	51	VAL
21	R	101	ILE
30	a	48	GLN
30	a	50	ASP
30	a	51	VAL
30	a	53	THR
30	a	56	ARG
30	a	57	VAL
30	a	59	ARG
30	a	60	PHE
36	g	125	THR
36	g	126	PHE
36	g	128	LYS
36	g	129	LEU
36	g	130	THR
43	n	4	ASN
43	n	12	ARG

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Mol	Chain	Res	Type
43	n	13	LYS
43	n	19	VAL
43	n	22	LYS
43	n	25	ASN
43	n	27	LYS
43	n	28	ILE
43	n	29	VAL
43	n	30	ILE
43	n	31	ASN
43	n	32	GLN
43	n	33	ARG
43	n	41	ARG
43	n	42	GLU
43	n	43	THR
43	n	45	ARG
43	n	46	MET
43	n	49	ARG
43	n	54	LEU
43	n	58	VAL
43	n	59	GLU
43	n	60	LYS
43	n	63	LEU
43	n	79	ILE
43	n	80	ARG
43	n	81	HIS
43	n	85	ARG
43	n	87	LEU
43	n	91	ASP
43	n	93	SER
43	n	95	ARG
43	n	99	ARG
43	n	105	THR
43	n	106	ARG
43	n	110	GLN
43	n	113	ARG
43	n	114	LYS
43	n	118	LEU
43	n	120	LYS
43	n	123	ARG
43	n	124	ARG
43	n	125	PRO
43	n	129	LYS

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Mol	Chain	Res	Type
43	n	130	ARG
48	s	97	LYS
48	s	98	LYS
48	s	101	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
8	C	32	ASN
12	G	18	GLN
12	G	133	GLN
13	J	58	ASN
14	K	3	GLN
17	N	16	HIS
20	Q	52	GLN
30	a	61	ASN
37	h	32	ASN
42	m	16	ASN
42	m	18	GLN
43	n	4	ASN
43	n	31	ASN
43	n	126	GLN
44	o	64	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2897/2903 (99%)	614 (21%)	24 (0%)
2	2	1528/1534 (99%)	318 (20%)	14 (0%)
3	3	119/120 (99%)	18 (15%)	1 (0%)
4	4	361/363 (99%)	212 (58%)	13 (3%)
All	All	4905/4920 (99%)	1162 (23%)	52 (1%)

All (1162) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	6	A
1	1	8	C
1	1	10	A
1	1	19	A

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Mol	Chain	Res	Type
1	1	20	C
1	1	26	G
1	1	28	A
1	1	41	C
1	1	42	A
1	1	45	G
1	1	46	G
1	1	51	G
1	1	55	G
1	1	63	A
1	1	71	A
1	1	74	A
1	1	75	G
1	1	100	U
1	1	101	A
1	1	102	U
1	1	103	A
1	1	104	A
1	1	110	G
1	1	112	U
1	1	118	A
1	1	120	U
1	1	139	U
1	1	140	C
1	1	155	A
1	1	158	U
1	1	160	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	204	A
1	1	205	G
1	1	213	A
1	1	216	A
1	1	222	A
1	1	228	C
1	1	229	C
1	1	233	A
1	1	241	A
1	1	242	G
1	1	248	G

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Mol	Chain	Res	Type
1	1	250	G
1	1	266	G
1	1	267	C
1	1	271	G
1	1	275	C
1	1	278	A
1	1	280	U
1	1	283	G
1	1	290	U
1	1	301	G
1	1	308	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	332	A
1	1	334	C
1	1	345	A
1	1	346	A
1	1	351	C
1	1	353	C
1	1	360	U
1	1	361	G
1	1	362	A
1	1	368	A
1	1	369	U
1	1	371	A
1	1	372	G
1	1	373	U
1	1	374	A
1	1	386	G
1	1	387	U
1	1	389	G
1	1	396	G
1	1	403	U
1	1	404	A
1	1	405	U
1	1	406	G
1	1	411	G
1	1	424	G
1	1	428	A
1	1	429	A
1	1	430	A

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Mol	Chain	Res	Type
1	1	451	U
1	1	457	A
1	1	467	G
1	1	480	A
1	1	481	G
1	1	484	C
1	1	490	C
1	1	491	G
1	1	502	A
1	1	505	A
1	1	509	C
1	1	513	A
1	1	529	A
1	1	530	G
1	1	532	A
1	1	533	G
1	1	538	A
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	588	U
1	1	603	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	621	A
1	1	622	G
1	1	627	A
1	1	637	A
1	1	644	A
1	1	645	C
1	1	647	G
1	1	654	A
1	1	655	A
1	1	656	G
1	1	668	A
1	1	686	U

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Mol	Chain	Res	Type
1	1	704	G
1	1	717	C
1	1	726	G
1	1	730	A
1	1	734	A
1	1	747	5MU
1	1	748	G
1	1	764	A
1	1	765	C
1	1	774	G
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	789	A
1	1	801	G
1	1	802	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	845	A
1	1	846	U
1	1	856	G
1	1	857	G
1	1	877	A
1	1	878	A
1	1	880	G
1	1	881	G
1	1	882	G
1	1	883	G
1	1	886	A
1	1	887	A
1	1	888	C
1	1	890	C
1	1	891	G
1	1	893	C
1	1	895	U
1	1	896	A
1	1	897	C
1	1	898	C

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Mol	Chain	Res	Type
1	1	899	A
1	1	907	G
1	1	910	A
1	1	920	A
1	1	931	U
1	1	941	A
1	1	946	C
1	1	959	A
1	1	961	C
1	1	974	G
1	1	980	A
1	1	983	A
1	1	985	C
1	1	995	C
1	1	996	A
1	1	1003	G
1	1	1005	C
1	1	1009	A
1	1	1010	A
1	1	1011	G
1	1	1012	U
1	1	1016	G
1	1	1020	A
1	1	1022	G
1	1	1026	G
1	1	1033	U
1	1	1034	G
1	1	1035	U
1	1	1040	A
1	1	1041	G
1	1	1042	G
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1049	C
1	1	1050	A
1	1	1051	G
1	1	1052	C
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1063	G

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Mol	Chain	Res	Type
1	1	1064	C
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1071	G
1	1	1074	G
1	1	1075	C
1	1	1078	U
1	1	1080	A
1	1	1081	U
1	1	1082	U
1	1	1083	U
1	1	1085	A
1	1	1086	A
1	1	1088	A
1	1	1089	A
1	1	1091	G
1	1	1094	U
1	1	1095	A
1	1	1096	A
1	1	1098	A
1	1	1099	G
1	1	1106	G
1	1	1109	C
1	1	1111	A
1	1	1112	G
1	1	1115	G
1	1	1120	G
1	1	1132	U
1	1	1135	C
1	1	1136	G
1	1	1137	G
1	1	1141	U
1	1	1142	A
1	1	1149	G
1	1	1150	C
1	1	1152	C
1	1	1156	A
1	1	1157	G
1	1	1168	G

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Mol	Chain	Res	Type
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1182	G
1	1	1204	A
1	1	1206	G
1	1	1212	G
1	1	1225	G
1	1	1226	A
1	1	1227	G
1	1	1236	G
1	1	1238	G
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G
1	1	1272	A
1	1	1289	C
1	1	1300	G
1	1	1301	A
1	1	1302	A
1	1	1304	A
1	1	1314	C
1	1	1321	A
1	1	1325	U
1	1	1328	A
1	1	1329	U
1	1	1345	C
1	1	1352	U
1	1	1353	A
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1383	A
1	1	1384	A
1	1	1385	A
1	1	1387	A
1	1	1395	A
1	1	1402	U
1	1	1403	A

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Mol	Chain	Res	Type
1	1	1407	G
1	1	1408	G
1	1	1410	G
1	1	1411	U
1	1	1413	A
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1458	U
1	1	1465	G
1	1	1467	U
1	1	1482	G
1	1	1493	C
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1523	U
1	1	1528	A
1	1	1529	G
1	1	1530	G
1	1	1533	C
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1558	C
1	1	1560	G
1	1	1566	A
1	1	1569	A
1	1	1580	A
1	1	1583	A
1	1	1584	U
1	1	1589	U
1	1	1590	A
1	1	1591	A
1	1	1596	A
1	1	1608	A
1	1	1609	A

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Mol	Chain	Res	Type
1	1	1635	A
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1654	A
1	1	1656	C
1	1	1672	A
1	1	1674	G
1	1	1711	A
1	1	1713	A
1	1	1722	A
1	1	1724	G
1	1	1725	U
1	1	1726	C
1	1	1729	U
1	1	1730	C
1	1	1738	G
1	1	1756	G
1	1	1758	U
1	1	1764	C
1	1	1773	A
1	1	1779	U
1	1	1784	A
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1807	G
1	1	1808	A
1	1	1816	C
1	1	1835	2MG
1	1	1848	A
1	1	1858	A
1	1	1866	A
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1874	C
1	1	1875	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C

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Mol	Chain	Res	Type
1	1	1919	A
1	1	1924	C
1	1	1927	A
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1939	5MU
1	1	1944	U
1	1	1955	U
1	1	1963	U
1	1	1966	A
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1996	C
1	1	1997	C
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2034	U
1	1	2038	G
1	1	2043	C
1	1	2044	C
1	1	2049	G
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2057	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2096	C
1	1	2097	A
1	1	2100	G

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Mol	Chain	Res	Type
1	1	2101	A
1	1	2102	G
1	1	2104	C
1	1	2105	U
1	1	2106	U
1	1	2108	A
1	1	2111	U
1	1	2113	U
1	1	2114	A
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2120	G
1	1	2121	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2129	C
1	1	2130	U
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2136	G
1	1	2137	U
1	1	2138	G
1	1	2140	G
1	1	2144	G
1	1	2146	C
1	1	2147	A
1	1	2150	C
1	1	2151	U
1	1	2156	G
1	1	2157	G
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C

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Mol	Chain	Res	Type
1	1	2167	U
1	1	2168	G
1	1	2169	A
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2175	C
1	1	2176	A
1	1	2177	C
1	1	2179	C
1	1	2180	U
1	1	2181	U
1	1	2182	U
1	1	2183	A
1	1	2187	U
1	1	2188	U
1	1	2189	U
1	1	2198	A
1	1	2199	A
1	1	2204	G
1	1	2211	A
1	1	2212	A
1	1	2225	A
1	1	2226	C
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2266	A
1	1	2283	C
1	1	2287	A
1	1	2297	A
1	1	2305	U
1	1	2306	C
1	1	2307	G
1	1	2309	A
1	1	2310	C
1	1	2319	G
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2335	A

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Mol	Chain	Res	Type
1	1	2345	G
1	1	2347	C
1	1	2361	G
1	1	2382	G
1	1	2383	G
1	1	2385	C
1	1	2386	A
1	1	2388	A
1	1	2395	C
1	1	2396	G
1	1	2402	U
1	1	2403	C
1	1	2409	G
1	1	2425	A
1	1	2428	G
1	1	2429	G
1	1	2434	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2469	A
1	1	2470	G
1	1	2476	A
1	1	2479	U
1	1	2483	C
1	1	2487	G
1	1	2491	U
1	1	2492	U
1	1	2497	A
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2518	A
1	1	2529	G
1	1	2547	A
1	1	2554	U
1	1	2562	U
1	1	2564	A
1	1	2566	A
1	1	2567	G

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Mol	Chain	Res	Type
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2582	G
1	1	2600	A
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2614	A
1	1	2629	U
1	1	2630	G
1	1	2636	C
1	1	2646	C
1	1	2650	U
1	1	2654	A
1	1	2655	G
1	1	2661	G
1	1	2673	G
1	1	2674	G
1	1	2685	G
1	1	2689	U
1	1	2690	U
1	1	2694	G
1	1	2712	C
1	1	2714	G
1	1	2725	A
1	1	2726	A
1	1	2729	G
1	1	2733	A
1	1	2734	A
1	1	2744	G
1	1	2748	A
1	1	2764	A
1	1	2765	A
1	1	2778	A
1	1	2783	U
1	1	2787	C
1	1	2791	G
1	1	2792	A
1	1	2797	U
1	1	2808	G
1	1	2818	U

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Mol	Chain	Res	Type
1	1	2820	A
1	1	2821	A
1	1	2828	G
1	1	2832	U
1	1	2846	G
1	1	2849	U
1	1	2850	A
1	1	2852	G
1	1	2856	A
1	1	2866	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2876	G
1	1	2877	G
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2890	G
1	1	2891	U
1	1	2893	A
1	1	2894	G
2	2	3	A
2	2	4	U
2	2	5	U
2	2	9	G
2	2	31	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	49	U
2	2	51	A
2	2	64	G
2	2	71	A
2	2	74	A
2	2	77	A
2	2	82	G
2	2	83	C
2	2	84	U
2	2	86	G
2	2	88	U

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Mol	Chain	Res	Type
2	2	91	U
2	2	93	U
2	2	94	G
2	2	95	C
2	2	104	G
2	2	120	A
2	2	121	U
2	2	131	A
2	2	144	G
2	2	155	A
2	2	162	A
2	2	169	C
2	2	171	A
2	2	173	U
2	2	174	A
2	2	182	A
2	2	183	C
2	2	184	G
2	2	197	A
2	2	202	G
2	2	204	G
2	2	208	U
2	2	210	C
2	2	211	G
2	2	212	G
2	2	214	C
2	2	218	U
2	2	238	A
2	2	247	G
2	2	251	G
2	2	261	U
2	2	262	A
2	2	266	G
2	2	267	C
2	2	271	C
2	2	289	G
2	2	296	U
2	2	306	A
2	2	319	G
2	2	325	A
2	2	328	C
2	2	332	G

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Mol	Chain	Res	Type
2	2	345	C
2	2	347	G
2	2	351	G
2	2	352	C
2	2	354	G
2	2	365	U
2	2	366	A
2	2	367	U
2	2	372	C
2	2	382	A
2	2	392	C
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	419	C
2	2	421	U
2	2	422	C
2	2	423	G
2	2	424	G
2	2	428	G
2	2	429	U
2	2	448	A
2	2	451	A
2	2	463	U
2	2	465	A
2	2	466	A
2	2	467	U
2	2	468	A
2	2	469	C
2	2	474	G
2	2	476	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	493	A
2	2	496	A
2	2	497	G
2	2	509	A
2	2	510	A
2	2	511	C
2	2	516	PSU

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Mol	Chain	Res	Type
2	2	518	C
2	2	521	G
2	2	524	G
2	2	527	G7M
2	2	532	A
2	2	533	A
2	2	547	A
2	2	559	A
2	2	560	A
2	2	564	C
2	2	572	A
2	2	573	A
2	2	574	A
2	2	575	G
2	2	576	C
2	2	577	G
2	2	621	A
2	2	633	G
2	2	653	U
2	2	665	A
2	2	686	U
2	2	687	A
2	2	695	A
2	2	718	A
2	2	721	G
2	2	722	G
2	2	724	G
2	2	728	A
2	2	731	G
2	2	748	G
2	2	752	G
2	2	755	G
2	2	793	U
2	2	794	A
2	2	795	C
2	2	815	A
2	2	817	C
2	2	828	U
2	2	841	C
2	2	843	U
2	2	844	G
2	2	845	A

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Mol	Chain	Res	Type
2	2	846	G
2	2	849	G
2	2	866	C
2	2	889	A
2	2	914	A
2	2	918	A
2	2	926	G
2	2	934	C
2	2	935	A
2	2	939	G
2	2	941	G
2	2	942	G
2	2	944	G
2	2	945	G
2	2	950	U
2	2	960	U
2	2	961	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	975	A
2	2	976	G
2	2	977	A
2	2	981	U
2	2	983	A
2	2	987	G
2	2	988	G
2	2	990	C
2	2	992	U
2	2	993	G
2	2	996	A
2	2	997	U
2	2	1000	A
2	2	1001	C
2	2	1003	G
2	2	1004	A
2	2	1006	G
2	2	1007	U
2	2	1008	U
2	2	1009	U
2	2	1010	U

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Mol	Chain	Res	Type
2	2	1012	A
2	2	1017	U
2	2	1019	A
2	2	1020	G
2	2	1021	A
2	2	1023	U
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1029	U
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1033	G
2	2	1034	G
2	2	1035	A
2	2	1039	G
2	2	1042	A
2	2	1043	G
2	2	1045	C
2	2	1046	A
2	2	1053	G
2	2	1054	C
2	2	1064	G
2	2	1065	U
2	2	1086	U
2	2	1088	G
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1108	G
2	2	1128	C
2	2	1129	C
2	2	1136	C
2	2	1137	C
2	2	1140	C
2	2	1142	G
2	2	1145	A
2	2	1146	A
2	2	1148	U
2	2	1151	A
2	2	1152	A

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Mol	Chain	Res	Type
2	2	1159	U
2	2	1160	G
2	2	1168	U
2	2	1169	A
2	2	1176	A
2	2	1179	A
2	2	1184	G
2	2	1188	A
2	2	1191	A
2	2	1196	A
2	2	1197	A
2	2	1198	G
2	2	1199	U
2	2	1201	A
2	2	1207	2MG
2	2	1208	C
2	2	1210	C
2	2	1213	A
2	2	1215	G
2	2	1219	A
2	2	1224	U
2	2	1225	A
2	2	1226	C
2	2	1236	A
2	2	1238	A
2	2	1241	G
2	2	1244	G
2	2	1245	C
2	2	1247	U
2	2	1250	A
2	2	1256	A
2	2	1257	A
2	2	1260	G
2	2	1261	A
2	2	1265	C
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1293	C
2	2	1294	G
2	2	1295	U

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Mol	Chain	Res	Type
2	2	1298	U
2	2	1300	G
2	2	1302	C
2	2	1312	G
2	2	1317	C
2	2	1318	A
2	2	1319	A
2	2	1320	C
2	2	1322	C
2	2	1332	A
2	2	1338	G
2	2	1340	A
2	2	1343	G
2	2	1344	C
2	2	1346	A
2	2	1348	U
2	2	1349	A
2	2	1351	U
2	2	1352	C
2	2	1359	C
2	2	1360	A
2	2	1361	G
2	2	1362	A
2	2	1363	A
2	2	1364	U
2	2	1370	G
2	2	1378	C
2	2	1394	A
2	2	1400	C
2	2	1401	G
2	2	1408	A
2	2	1432	G
2	2	1441	A
2	2	1443	C
2	2	1445	U
2	2	1446	A
2	2	1491	G
2	2	1493	A
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G

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Mol	Chain	Res	Type
2	2	1529	G
2	2	1530	G
2	2	1532	U
2	2	1534	A
3	3	2	G
3	3	3	C
3	3	13	G
3	3	16	G
3	3	23	G
3	3	24	G
3	3	35	C
3	3	37	C
3	3	41	G
3	3	42	C
3	3	44	G
3	3	66	A
3	3	68	C
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A
3	3	109	A
4	4	3	G
4	4	8	A
4	4	9	U
4	4	10	U
4	4	11	C
4	4	12	U
4	4	13	G
4	4	14	G
4	4	15	A
4	4	18	C
4	4	19	G
4	4	20	A
4	4	24	G
4	4	25	A
4	4	26	U
4	4	28	U
4	4	30	C
4	4	31	G
4	4	32	A
4	4	33	A

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Mol	Chain	Res	Type
4	4	34	A
4	4	35	C
4	4	36	C
4	4	37	C
4	4	38	A
4	4	39	A
4	4	40	G
4	4	43	G
4	4	44	C
4	4	45	A
4	4	47	G
4	4	48	C
4	4	49	C
4	4	50	G
4	4	52	G
4	4	54	G
4	4	55	G
4	4	61	G
4	4	62	G
4	4	63	C
4	4	64	C
4	4	65	U
4	4	66	C
4	4	69	A
4	4	70	A
4	4	71	A
4	4	72	A
4	4	73	A
4	4	75	C
4	4	76	C
4	4	79	A
4	4	80	A
4	4	81	A
4	4	82	A
4	4	83	A
4	4	84	A
4	4	85	U
4	4	86	A
4	4	87	G
4	4	88	U
4	4	89	C
4	4	90	G

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Mol	Chain	Res	Type
4	4	91	C
4	4	92	A
4	4	93	A
4	4	94	A
4	4	95	C
4	4	96	G
4	4	97	A
4	4	98	C
4	4	99	G
4	4	100	A
4	4	101	A
4	4	102	A
4	4	103	A
4	4	104	C
4	4	105	U
4	4	106	A
4	4	107	C
4	4	110	U
4	4	119	U
4	4	120	U
4	4	122	A
4	4	123	U
4	4	124	A
4	4	125	A
4	4	126	C
4	4	127	C
4	4	128	U
4	4	129	G
4	4	130	C
4	4	138	C
4	4	139	C
4	4	143	C
4	4	145	C
4	4	152	C
4	4	153	U
4	4	154	C
4	4	155	C
4	4	156	G
4	4	157	C
4	4	160	U
4	4	163	G
4	4	165	A

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Mol	Chain	Res	Type
4	4	166	C
4	4	167	G
4	4	169	G
4	4	170	G
4	4	171	A
4	4	173	C
4	4	176	G
4	4	178	G
4	4	179	A
4	4	180	G
4	4	182	U
4	4	183	C
4	4	185	A
4	4	186	A
4	4	187	C
4	4	189	C
4	4	190	A
4	4	198	U
4	4	201	C
4	4	202	G
4	4	205	G
4	4	206	A
4	4	207	A
4	4	209	C
4	4	211	C
4	4	212	U
4	4	213	G
4	4	216	U
4	4	217	G
4	4	218	G
4	4	219	G
4	4	220	G
4	4	221	U
4	4	222	U
4	4	223	G
4	4	224	A
4	4	227	C
4	4	230	U
4	4	231	A
4	4	234	A
4	4	237	U
4	4	239	A

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Mol	Chain	Res	Type
4	4	240	U
4	4	244	G
4	4	245	C
4	4	246	U
4	4	247	A
4	4	248	G
4	4	249	U
4	4	251	U
4	4	252	G
4	4	255	A
4	4	256	G
4	4	257	U
4	4	259	G
4	4	260	C
4	4	261	G
4	4	263	G
4	4	265	C
4	4	267	G
4	4	268	U
4	4	271	G
4	4	276	U
4	4	277	G
4	4	283	C
4	4	284	G
4	4	285	A
4	4	287	U
4	4	288	G
4	4	289	U
4	4	290	A
4	4	292	A
4	4	294	A
4	4	298	A
4	4	299	C
4	4	300	U
4	4	301	A
4	4	303	G
4	4	304	C
4	4	305	A
4	4	308	U
4	4	309	A
4	4	312	A
4	4	313	C

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Mol	Chain	Res	Type
4	4	315	G
4	4	316	A
4	4	317	G
4	4	319	A
4	4	321	G
4	4	322	U
4	4	325	G
4	4	326	A
4	4	327	A
4	4	328	U
4	4	331	C
4	4	332	G
4	4	333	G
4	4	335	C
4	4	336	G
4	4	339	G
4	4	341	5MU
4	4	342	PSU
4	4	347	PSU
4	4	349	C
4	4	351	G
4	4	352	C
4	4	362	C
4	4	363	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	5	A
1	1	18	U
1	1	40	U
1	1	154	U
1	1	157	C
1	1	274	C
1	1	428	A
1	1	479	A
1	1	501	A
1	1	512	G
1	1	548	G
1	1	613	A
1	1	784	G
1	1	800	A

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Mol	Chain	Res	Type
1	1	1009	A
1	1	1051	G
1	1	1069	A
1	1	1384	A
1	1	1386	C
1	1	2308	G
1	1	2402	U
1	1	2505	G
1	1	2851	A
1	1	2893	A
2	2	103	U
2	2	170	U
2	2	318	G
2	2	381	C
2	2	751	U
2	2	845	A
2	2	917	G
2	2	960	U
2	2	1042	A
2	2	1109	C
2	2	1207	2MG
2	2	1255	G
2	2	1358	U
2	2	1361	G
3	3	36	C
4	4	18	C
4	4	34	A
4	4	43	G
4	4	44	C
4	4	81	A
4	4	87	G
4	4	126	C
4	4	152	C
4	4	221	U
4	4	308	U
4	4	314	C
4	4	348	C
4	4	351	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
46	0TD	q	89	46	7,9,10	1.47	0	6,11,13	2.26	2 (33%)
1	3TD	1	1915	1	18,22,23	4.20	6 (33%)	22,32,35	1.60	2 (9%)
1	5MU	1	1939	1	19,22,23	5.27	5 (26%)	28,32,35	3.60	9 (32%)
1	2MA	1	2503	1	19,25,26	3.43	5 (26%)	21,37,40	3.55	4 (19%)
2	4OC	2	1402	2	20,23,24	3.22	8 (40%)	26,32,35	0.88	1 (3%)
2	2MG	2	966	2	18,26,27	2.72	6 (33%)	16,38,41	1.45	3 (18%)
2	G7M	2	527	2	20,26,27	2.50	7 (35%)	17,39,42	1.04	1 (5%)
1	2MG	1	1835	1	18,26,27	2.73	6 (33%)	16,38,41	1.48	3 (18%)
2	MA6	2	1518	2	18,26,27	1.44	2 (11%)	19,38,41	4.24	3 (15%)
1	OMC	1	2498	1	19,22,23	3.39	8 (42%)	26,31,34	0.69	0
2	MA6	2	1519	2	18,26,27	1.46	3 (16%)	19,38,41	4.23	3 (15%)
2	5MC	2	1407	2	18,22,23	3.74	7 (38%)	26,32,35	1.00	2 (7%)
1	2MG	1	2445	1	18,26,27	2.70	6 (33%)	16,38,41	1.44	4 (25%)
2	2MG	2	1516	2	18,26,27	2.71	6 (33%)	16,38,41	1.41	3 (18%)
1	5MU	1	747	1	19,22,23	5.25	5 (26%)	28,32,35	3.63	9 (32%)
1	PSU	1	1911	1	18,21,22	1.10	1 (5%)	22,30,33	1.77	4 (18%)
16	4D4	M	81	16	9,11,12	2.05	2 (22%)	8,13,15	1.85	3 (37%)
1	PSU	1	955	1	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
2	2MG	2	1207	2	18,26,27	2.74	6 (33%)	16,38,41	1.40	3 (18%)
1	PSU	1	2580	1	18,21,22	1.10	2 (11%)	22,30,33	1.88	5 (22%)
4	5MU	4	341	4	19,22,23	5.32	5 (26%)	28,32,35	3.52	10 (35%)
1	PSU	1	1917	1	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
2	5MC	2	967	2	18,22,23	3.76	7 (38%)	26,32,35	1.01	2 (7%)
1	PSU	1	2457	1	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
1	1MG	1	745	1	18,26,27	2.61	5 (27%)	19,39,42	1.41	3 (15%)
1	5MC	1	1962	1	18,22,23	3.73	7 (38%)	26,32,35	1.06	2 (7%)
4	PSU	4	347	4	18,21,22	1.10	1 (5%)	22,30,33	1.78	5 (22%)
1	PSU	1	746	1,56	18,21,22	1.09	1 (5%)	22,30,33	1.75	5 (22%)
1	G7M	1	2069	1	20,26,27	2.50	7 (35%)	17,39,42	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	2504	1	18,21,22	1.14	1 (5%)	22,30,33	1.68	4 (18%)
2	UR3	2	1498	2	19,22,23	3.01	8 (42%)	26,32,35	1.29	1 (3%)
1	6MZ	1	2030	1	18,25,26	1.98	3 (16%)	16,36,39	2.21	5 (31%)
4	PSU	4	342	4	18,21,22	1.12	1 (5%)	22,30,33	1.74	3 (13%)
1	OMU	1	2552	1	19,22,23	2.98	8 (42%)	26,31,34	1.69	5 (19%)
2	PSU	2	516	2	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
1	PSU	1	2605	1	18,21,22	1.11	1 (5%)	22,30,33	1.76	4 (18%)
1	OMG	1	2251	4,1	18,26,27	2.91	7 (38%)	19,38,41	1.51	4 (21%)
1	6MZ	1	1618	1	18,25,26	1.98	3 (16%)	16,36,39	2.08	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
46	0TD	q	89	46	-	1/7/12/14	-
1	3TD	1	1915	1	-	3/7/25/26	0/2/2/2
1	5MU	1	1939	1	-	2/7/25/26	0/2/2/2
1	2MA	1	2503	1	-	1/3/25/26	0/3/3/3
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3
2	G7M	2	527	2	-	2/3/25/26	0/3/3/3
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	MA6	2	1518	2	-	1/7/29/30	0/3/3/3
1	OMC	1	2498	1	-	2/9/27/28	0/2/2/2
2	MA6	2	1519	2	-	2/7/29/30	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	3/5/27/28	0/3/3/3
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
16	4D4	M	81	16	-	4/11/12/14	-
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	3/5/27/28	0/3/3/3
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2
4	5MU	4	341	4	-	5/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	2	967	2	-	1/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
1	5MC	1	1962	1	-	4/7/25/26	0/2/2/2
4	PSU	4	347	4	-	3/7/25/26	0/2/2/2
1	PSU	1	746	1,56	-	1/7/25/26	0/2/2/2
1	G7M	1	2069	1	-	2/3/25/26	0/3/3/3
1	PSU	1	2504	1	-	4/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	2/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3
4	PSU	4	342	4	-	3/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	1/9/27/28	0/2/2/2
2	PSU	2	516	2	-	6/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2251	4,1	-	2/5/27/28	0/3/3/3
1	6MZ	1	1618	1	-	2/5/27/28	0/3/3/3

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	341	5MU	C6-N1	12.80	1.59	1.38
1	1	1939	5MU	C6-N1	12.70	1.59	1.38
1	1	747	5MU	C6-N1	12.70	1.59	1.38
4	4	341	5MU	C2-N1	12.56	1.58	1.38
1	1	1915	3TD	C6-C5	12.41	1.49	1.35
1	1	1939	5MU	C4-C5	12.07	1.64	1.44
1	1	1939	5MU	C2-N1	12.05	1.57	1.38
1	1	747	5MU	C2-N1	12.00	1.57	1.38
1	1	747	5MU	C4-C5	12.00	1.64	1.44
4	4	341	5MU	C4-C5	11.91	1.64	1.44
2	2	967	5MC	C6-C5	9.69	1.50	1.34
2	2	1407	5MC	C6-C5	9.57	1.50	1.34
1	1	1962	5MC	C6-C5	9.49	1.50	1.34
1	1	1915	3TD	C2-N1	9.25	1.49	1.37
1	1	2503	2MA	C4-N3	8.73	1.49	1.35
2	2	1498	UR3	C2-N1	7.66	1.49	1.38
1	1	2503	2MA	C2-N3	7.66	1.47	1.34
2	2	1402	4OC	C4-N3	7.27	1.45	1.32
1	1	1618	6MZ	C6-N6	7.18	1.46	1.35
1	1	2030	6MZ	C6-N6	7.08	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	745	1MG	C2-N3	6.91	1.47	1.34
1	1	2251	OMG	C2-N2	6.75	1.50	1.34
1	1	2498	OMC	C2-N3	6.75	1.50	1.36
1	1	2498	OMC	C6-C5	6.70	1.50	1.35
1	1	1962	5MC	C4-N3	6.69	1.45	1.34
2	2	1407	5MC	C4-N3	6.66	1.45	1.34
2	2	967	5MC	C2-N3	6.62	1.49	1.36
1	1	1962	5MC	C2-N3	6.60	1.49	1.36
2	2	967	5MC	C4-N3	6.59	1.45	1.34
2	2	1407	5MC	C2-N3	6.58	1.49	1.36
1	1	2552	OMU	C2-N1	6.51	1.48	1.38
1	1	2498	OMC	C4-N4	6.39	1.49	1.33
1	1	2503	2MA	C2-N1	6.37	1.45	1.34
2	2	1402	4OC	C6-C5	6.31	1.49	1.35
1	1	2552	OMU	C2-N3	6.29	1.49	1.38
2	2	1402	4OC	C2-N3	6.29	1.49	1.36
4	4	341	5MU	C4-N3	-6.26	1.27	1.38
1	1	747	5MU	C4-N3	-6.23	1.27	1.38
1	1	1939	5MU	C4-N3	-6.18	1.27	1.38
2	2	1498	UR3	C6-C5	6.13	1.49	1.35
1	1	1835	2MG	C2-N1	6.06	1.46	1.36
2	2	1207	2MG	C2-N1	6.04	1.46	1.36
2	2	1516	2MG	C2-N1	6.03	1.46	1.36
2	2	966	2MG	C2-N1	6.03	1.46	1.36
1	1	2445	2MG	C2-N1	6.03	1.46	1.36
1	1	1835	2MG	C2-N2	5.99	1.46	1.33
1	1	745	1MG	C4-N3	5.97	1.51	1.37
2	2	1207	2MG	C2-N2	5.97	1.46	1.33
2	2	966	2MG	C2-N2	5.96	1.46	1.33
2	2	1516	2MG	C2-N2	5.92	1.46	1.33
1	1	2445	2MG	C2-N2	5.88	1.46	1.33
1	1	1915	3TD	C6-N1	5.86	1.46	1.36
2	2	1498	UR3	C2-N3	5.84	1.50	1.39
1	1	1939	5MU	C6-C5	5.71	1.44	1.34
1	1	747	5MU	C6-C5	5.67	1.43	1.34
4	4	341	5MU	C6-C5	5.61	1.43	1.34
1	1	2069	G7M	C2-N3	5.57	1.46	1.33
1	1	2498	OMC	C4-N3	5.57	1.45	1.34
2	2	527	G7M	C2-N3	5.52	1.46	1.33
1	1	2251	OMG	C4-N3	5.33	1.50	1.37
16	M	81	4D4	CZ-NE	5.27	1.43	1.33
1	1	2069	G7M	C4-N3	5.25	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2251	OMG	C2-N3	5.18	1.45	1.33
1	1	2503	2MA	C6-N1	5.10	1.43	1.33
2	2	527	G7M	C4-N3	5.09	1.49	1.37
1	1	2552	OMU	C6-C5	4.97	1.46	1.35
1	1	2498	OMC	C2-N1	4.97	1.50	1.40
2	2	967	5MC	C6-N1	4.97	1.46	1.38
1	1	1835	2MG	C4-N3	4.94	1.49	1.37
2	2	1407	5MC	C6-N1	4.92	1.46	1.38
2	2	1207	2MG	C4-N3	4.91	1.49	1.37
2	2	527	G7M	C2-N2	4.89	1.45	1.34
2	2	966	2MG	C4-N3	4.87	1.49	1.37
1	1	2069	G7M	C2-N2	4.86	1.45	1.34
1	1	1962	5MC	C6-N1	4.85	1.46	1.38
2	2	1516	2MG	C4-N3	4.84	1.49	1.37
1	1	2445	2MG	C4-N3	4.77	1.48	1.37
2	2	1402	4OC	C4-N4	4.68	1.45	1.35
2	2	967	5MC	C4-N4	4.58	1.46	1.34
1	1	1915	3TD	C2-N3	4.57	1.48	1.38
2	2	1407	5MC	C4-N4	4.56	1.46	1.34
1	1	1962	5MC	C4-N4	4.56	1.46	1.34
1	1	2552	OMU	O2-C2	-4.44	1.14	1.23
2	2	1516	2MG	C5-C6	4.41	1.56	1.47
1	1	2445	2MG	C5-C6	4.39	1.56	1.47
1	1	1835	2MG	C5-C6	4.38	1.56	1.47
2	2	966	2MG	C5-C6	4.38	1.56	1.47
2	2	1207	2MG	C5-C6	4.36	1.56	1.47
2	2	1402	4OC	C2-N1	4.34	1.49	1.40
2	2	967	5MC	C2-N1	4.30	1.49	1.40
2	2	1407	5MC	C2-N1	4.29	1.49	1.40
2	2	1518	MA6	C9-N6	4.28	1.55	1.45
2	2	1519	MA6	C9-N6	4.27	1.55	1.45
1	1	1962	5MC	C2-N1	4.26	1.49	1.40
1	1	2251	OMG	C2-N1	4.20	1.48	1.37
2	2	1402	4OC	C5-C4	4.02	1.49	1.40
1	1	745	1MG	C2-N2	3.95	1.41	1.34
1	1	2504	PSU	C6-C5	3.85	1.39	1.35
2	2	527	G7M	C6-N1	3.83	1.43	1.37
2	2	1498	UR3	C6-N1	3.78	1.47	1.38
4	4	342	PSU	C6-C5	3.71	1.39	1.35
1	1	2251	OMG	C5-C6	3.70	1.54	1.47
1	1	2552	OMU	C4-N3	3.66	1.45	1.38
1	1	2069	G7M	C6-N1	3.65	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2605	PSU	C6-C5	3.63	1.39	1.35
1	1	1911	PSU	C6-C5	3.62	1.39	1.35
2	2	516	PSU	C6-C5	3.58	1.39	1.35
1	1	2498	OMC	C6-N1	3.56	1.46	1.38
4	4	347	PSU	C6-C5	3.56	1.39	1.35
1	1	955	PSU	C6-C5	3.56	1.39	1.35
1	1	746	PSU	C6-C5	3.52	1.39	1.35
1	1	1917	PSU	C6-C5	3.51	1.39	1.35
1	1	2552	OMU	O4-C4	-3.49	1.17	1.24
1	1	2503	2MA	C6-C5	3.44	1.56	1.43
1	1	2445	2MG	C6-N1	3.41	1.42	1.37
1	1	2069	G7M	C5-C6	3.39	1.54	1.45
1	1	2580	PSU	C6-C5	3.38	1.39	1.35
2	2	1516	2MG	C6-N1	3.34	1.42	1.37
2	2	966	2MG	C6-N1	3.34	1.42	1.37
1	1	1835	2MG	C6-N1	3.33	1.42	1.37
2	2	527	G7M	C5-C6	3.33	1.54	1.45
2	2	1207	2MG	C6-N1	3.33	1.42	1.37
1	1	2457	PSU	C6-C5	3.32	1.39	1.35
2	2	1402	4OC	C6-N1	3.20	1.45	1.38
1	1	745	1MG	C5-C6	2.96	1.56	1.47
1	1	2552	OMU	C6-N1	2.95	1.45	1.38
2	2	1498	UR3	C5-C4	2.93	1.51	1.43
1	1	2498	OMC	O2-C2	-2.93	1.18	1.23
1	1	2251	OMG	C6-N1	2.88	1.42	1.37
1	1	1915	3TD	C4-N3	2.87	1.46	1.40
1	1	2498	OMC	C5-C4	2.84	1.49	1.42
2	2	527	G7M	C2-N1	2.81	1.44	1.37
1	1	2069	G7M	C2-N1	2.70	1.44	1.37
1	1	745	1MG	C5-C4	-2.70	1.36	1.43
1	1	1962	5MC	O2-C2	-2.68	1.18	1.23
2	2	967	5MC	O2-C2	-2.66	1.18	1.23
2	2	1407	5MC	O2-C2	-2.66	1.18	1.23
2	2	1402	4OC	O2-C2	-2.61	1.18	1.23
1	1	1915	3TD	O4-C4	-2.52	1.17	1.23
1	1	2030	6MZ	C5-C4	-2.51	1.34	1.40
2	2	1519	MA6	C5-C4	-2.51	1.34	1.40
2	2	1518	MA6	C5-C4	-2.49	1.34	1.40
1	1	1618	6MZ	C2-N3	2.46	1.36	1.32
2	2	1498	UR3	O4-C4	-2.45	1.18	1.23
1	1	1618	6MZ	C5-C4	-2.44	1.34	1.40
16	M	81	4D4	CZ-NH1	2.42	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1498	UR3	C4-N3	2.40	1.46	1.40
1	1	2030	6MZ	C2-N3	2.40	1.36	1.32
2	2	1498	UR3	O2-C2	-2.37	1.18	1.22
1	1	2552	OMU	C5-C4	2.31	1.48	1.43
1	1	1835	2MG	C5-C4	-2.25	1.37	1.43
2	2	1207	2MG	C5-C4	-2.23	1.37	1.43
2	2	1516	2MG	C5-C4	-2.20	1.37	1.43
1	1	2445	2MG	C5-C4	-2.20	1.37	1.43
2	2	966	2MG	C5-C4	-2.18	1.37	1.43
1	1	2069	G7M	O6-C6	-2.17	1.18	1.23
1	1	2251	OMG	C5-C4	-2.14	1.37	1.43
2	2	527	G7M	O6-C6	-2.11	1.19	1.23
1	1	2580	PSU	O4'-C1'	-2.03	1.41	1.43
2	2	1519	MA6	C2-N3	2.03	1.35	1.32

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1518	MA6	N1-C6-N6	-15.62	100.62	117.06
2	2	1519	MA6	N1-C6-N6	-15.62	100.62	117.06
1	1	2503	2MA	C1'-N9-C4	14.45	152.03	126.64
1	1	747	5MU	C5-C4-N3	11.95	125.52	115.31
1	1	1939	5MU	C5-C4-N3	11.93	125.49	115.31
4	4	341	5MU	C5-C4-N3	11.74	125.33	115.31
1	1	747	5MU	C5-C6-N1	-10.14	112.91	123.34
1	1	1939	5MU	C5-C6-N1	-10.01	113.04	123.34
4	4	341	5MU	C5-C6-N1	-9.20	113.87	123.34
2	2	1518	MA6	C1'-N9-C4	7.86	140.45	126.64
2	2	1519	MA6	C1'-N9-C4	7.64	140.06	126.64
2	2	1519	MA6	N3-C2-N1	-5.60	119.93	128.68
1	1	1618	6MZ	N3-C2-N1	-5.49	120.09	128.68
1	1	2503	2MA	C2-N3-C4	5.40	119.91	115.52
2	2	1518	MA6	N3-C2-N1	-5.40	120.25	128.68
1	1	2030	6MZ	N3-C2-N1	-5.35	120.32	128.68
1	1	2552	OMU	C4-N3-C2	-5.14	119.81	126.58
1	1	1915	3TD	N1-C2-N3	5.04	120.12	116.14
1	1	747	5MU	C4-N3-C2	-4.93	120.97	127.35
1	1	1939	5MU	C4-N3-C2	-4.84	121.09	127.35
1	1	747	5MU	O4-C4-C5	-4.83	119.31	124.90
1	1	1939	5MU	O4-C4-C5	-4.80	119.34	124.90
2	2	1498	UR3	C4-N3-C2	-4.77	120.07	124.56
4	4	341	5MU	O4-C4-C5	-4.77	119.38	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	342	PSU	C4-N3-C2	-4.59	119.72	126.34
1	1	746	PSU	C4-N3-C2	-4.58	119.75	126.34
4	4	347	PSU	C4-N3-C2	-4.57	119.76	126.34
1	1	1911	PSU	C4-N3-C2	-4.56	119.77	126.34
1	1	2605	PSU	C4-N3-C2	-4.54	119.80	126.34
1	1	2580	PSU	N1-C2-N3	4.53	120.27	115.13
1	1	2580	PSU	C4-N3-C2	-4.52	119.83	126.34
2	2	516	PSU	C4-N3-C2	-4.51	119.84	126.34
1	1	955	PSU	C4-N3-C2	-4.51	119.84	126.34
1	1	747	5MU	N3-C2-N1	4.49	120.84	114.89
1	1	2457	PSU	C4-N3-C2	-4.48	119.88	126.34
1	1	746	PSU	N1-C2-N3	4.47	120.19	115.13
2	2	516	PSU	N1-C2-N3	4.44	120.16	115.13
1	1	2605	PSU	N1-C2-N3	4.43	120.15	115.13
1	1	1911	PSU	N1-C2-N3	4.43	120.15	115.13
1	1	1917	PSU	C4-N3-C2	-4.41	119.98	126.34
1	1	955	PSU	N1-C2-N3	4.41	120.12	115.13
4	4	347	PSU	N1-C2-N3	4.40	120.12	115.13
1	1	1917	PSU	N1-C2-N3	4.40	120.11	115.13
1	1	1939	5MU	N3-C2-N1	4.40	120.73	114.89
4	4	342	PSU	N1-C2-N3	4.38	120.09	115.13
4	4	341	5MU	C4-N3-C2	-4.37	121.69	127.35
1	1	2504	PSU	N1-C2-N3	4.35	120.06	115.13
1	1	2457	PSU	N1-C2-N3	4.32	120.03	115.13
4	4	341	5MU	N3-C2-N1	4.23	120.51	114.89
1	1	2504	PSU	C4-N3-C2	-4.23	120.24	126.34
46	q	89	0TD	OD2-CG-CB	4.13	122.08	113.15
1	1	745	1MG	C5-C6-N1	4.12	120.10	113.90
1	1	747	5MU	C5M-C5-C6	-4.10	117.37	122.85
1	1	1939	5MU	C5M-C5-C6	-4.06	117.43	122.85
4	4	341	5MU	C5M-C5-C4	4.03	123.20	118.77
1	1	2030	6MZ	C9-N6-C6	-4.02	119.41	122.87
1	1	1939	5MU	C5M-C5-C4	3.99	123.16	118.77
1	1	747	5MU	C5M-C5-C4	3.93	123.09	118.77
4	4	341	5MU	C5M-C5-C6	-3.88	117.67	122.85
1	1	1915	3TD	C4-N3-C2	-3.83	120.46	124.61
1	1	2552	OMU	N3-C2-N1	3.80	119.93	114.89
1	1	1618	6MZ	C2-N1-C6	3.79	119.84	116.59
1	1	2030	6MZ	C2-N1-C6	3.72	119.78	116.59
1	1	1618	6MZ	C9-N6-C6	-3.53	119.83	122.87
1	1	1835	2MG	C5-C6-N1	3.47	120.07	113.95
1	1	2251	OMG	C5-C6-N1	3.45	120.05	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	81	4D4	NE-CZ-NH2	3.44	126.75	120.70
1	1	1962	5MC	C5-C6-N1	-3.42	119.82	123.34
1	1	2445	2MG	C5-C6-N1	3.38	119.93	113.95
2	2	966	2MG	C5-C6-N1	3.32	119.81	113.95
1	1	2552	OMU	C5-C4-N3	3.30	119.77	114.84
1	1	2030	6MZ	C1'-N9-C4	-3.29	120.85	126.64
2	2	967	5MC	C5-C6-N1	-3.29	119.96	123.34
2	2	1407	5MC	C5-C6-N1	-3.29	119.96	123.34
2	2	1516	2MG	C5-C6-N1	3.28	119.74	113.95
2	2	1207	2MG	C5-C6-N1	3.27	119.73	113.95
1	1	2503	2MA	N3-C2-N1	-3.15	119.98	125.73
1	1	1835	2MG	C8-N7-C5	3.12	108.94	102.99
1	1	2580	PSU	O2-C2-N1	-3.09	119.39	122.79
2	2	1207	2MG	C8-N7-C5	3.06	108.81	102.99
2	2	966	2MG	C8-N7-C5	3.05	108.80	102.99
1	1	2445	2MG	C8-N7-C5	3.02	108.75	102.99
4	4	341	5MU	C1'-N1-C2	3.02	123.03	117.57
2	2	1516	2MG	C8-N7-C5	3.00	108.70	102.99
1	1	2069	G7M	C2-N1-C6	-2.99	119.59	125.10
1	1	2251	OMG	C2-N1-C6	-2.94	119.69	125.10
2	2	527	G7M	C2-N1-C6	-2.85	119.85	125.10
1	1	2552	OMU	O4-C4-C5	-2.84	120.17	125.16
1	1	1618	6MZ	C1'-N9-C4	-2.73	121.85	126.64
1	1	745	1MG	C8-N7-C5	2.70	108.13	102.99
1	1	2457	PSU	O2-C2-N1	-2.68	119.84	122.79
1	1	746	PSU	O2-C2-N1	-2.65	119.87	122.79
1	1	2580	PSU	O4'-C1'-C2'	2.63	108.86	105.14
1	1	1911	PSU	O2-C2-N1	-2.62	119.90	122.79
1	1	2605	PSU	O2-C2-N1	-2.62	119.90	122.79
1	1	1917	PSU	O2-C2-N1	-2.62	119.91	122.79
1	1	2251	OMG	C8-N7-C5	2.62	107.97	102.99
4	4	347	PSU	O2-C2-N1	-2.61	119.92	122.79
46	q	89	0TD	OD1-CG-CB	-2.61	116.98	122.44
1	1	955	PSU	O2-C2-N1	-2.58	119.94	122.79
1	1	1939	5MU	O4-C4-N3	-2.58	115.17	120.12
1	1	747	5MU	O4-C4-N3	-2.58	115.18	120.12
4	4	342	PSU	O2-C2-N1	-2.54	119.99	122.79
1	1	2504	PSU	O2-C2-N1	-2.54	120.00	122.79
4	4	341	5MU	O4-C4-N3	-2.52	115.29	120.12
1	1	747	5MU	O2-C2-N1	-2.49	119.47	122.79
1	1	2504	PSU	C6-N1-C2	-2.46	120.17	122.68
1	1	1939	5MU	O2-C2-N1	-2.44	119.54	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	516	PSU	O2-C2-N1	-2.42	120.13	122.79
1	1	2580	PSU	C6-N1-C2	-2.39	120.24	122.68
1	1	745	1MG	O6-C6-C5	-2.33	120.07	124.19
16	M	81	4D4	CB-CA-C	-2.32	108.07	111.77
1	1	1962	5MC	CM5-C5-C6	-2.31	119.76	122.85
2	2	1402	4OC	C6-C5-C4	2.29	119.77	116.96
1	1	1917	PSU	C6-N1-C2	-2.25	120.38	122.68
1	1	2251	OMG	O6-C6-C5	-2.24	120.00	124.37
1	1	1835	2MG	O6-C6-C5	-2.23	120.02	124.37
1	1	955	PSU	C6-N1-C2	-2.22	120.41	122.68
1	1	2445	2MG	CM2-N2-C2	-2.20	119.00	123.86
1	1	2445	2MG	O6-C6-C5	-2.20	120.07	124.37
1	1	2503	2MA	CM2-C2-N1	2.20	120.59	117.15
1	1	2605	PSU	C6-N1-C2	-2.20	120.44	122.68
4	4	341	5MU	C1'-N1-C6	-2.19	117.48	121.12
2	2	516	PSU	C6-N1-C2	-2.19	120.44	122.68
16	M	81	4D4	O-C-CA	-2.19	119.04	124.78
1	1	746	PSU	C6-C5-C4	2.18	119.72	118.20
4	4	347	PSU	C6-C5-C4	2.17	119.71	118.20
1	1	746	PSU	C6-N1-C2	-2.16	120.47	122.68
2	2	966	2MG	O6-C6-C5	-2.13	120.21	124.37
1	1	1911	PSU	C6-N1-C2	-2.13	120.50	122.68
2	2	1516	2MG	O6-C6-C5	-2.13	120.22	124.37
2	2	1207	2MG	O6-C6-C5	-2.10	120.28	124.37
1	1	2030	6MZ	C3'-C2'-C1'	2.08	104.11	100.98
1	1	2457	PSU	C6-N1-C2	-2.03	120.61	122.68
2	2	1407	5MC	CM5-C5-C6	-2.02	120.14	122.85
4	4	347	PSU	C6-N1-C2	-2.02	120.62	122.68
1	1	2552	OMU	O2-C2-N1	-2.01	120.11	122.79
2	2	967	5MC	CM5-C5-C6	-2.01	120.17	122.85

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	M	81	4D4	C-CA-CB-OB
16	M	81	4D4	C-CA-CB-CG
16	M	81	4D4	N-CA-CB-OB
16	M	81	4D4	N-CA-CB-CG
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	C2'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	1939	5MU	O4'-C4'-C5'-O5'
1	1	2504	PSU	C2'-C1'-C5-C4
1	1	2504	PSU	O4'-C1'-C5-C4
1	1	2504	PSU	C2'-C1'-C5-C6
1	1	2504	PSU	O4'-C1'-C5-C6
1	1	2552	OMU	C1'-C2'-O2'-CM2
2	2	516	PSU	C2'-C1'-C5-C6
2	2	516	PSU	O4'-C1'-C5-C6
2	2	516	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	966	2MG	O4'-C4'-C5'-O5'
2	2	966	2MG	C3'-C4'-C5'-O5'
2	2	1207	2MG	O4'-C4'-C5'-O5'
2	2	1207	2MG	C3'-C4'-C5'-O5'
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
4	4	341	5MU	O4'-C4'-C5'-O5'
4	4	342	PSU	C3'-C4'-C5'-O5'
4	4	342	PSU	C4'-C5'-O5'-P
4	4	347	PSU	C3'-C4'-C5'-O5'
4	4	347	PSU	O4'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	2069	G7M	C3'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2498	OMC	C3'-C4'-C5'-O5'
1	1	2498	OMC	O4'-C4'-C5'-O5'
4	4	341	5MU	C3'-C4'-C5'-O5'
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	1939	5MU	C3'-C4'-C5'-O5'
4	4	342	PSU	O4'-C4'-C5'-O5'
1	1	1962	5MC	C2'-C1'-N1-C6
1	1	2251	OMG	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C10
1	1	1962	5MC	C2'-C1'-N1-C2
1	1	1962	5MC	O4'-C1'-N1-C6
1	1	2030	6MZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
46	q	89	0TD	CG-CB-SB-CSB
2	2	1207	2MG	C4'-C5'-O5'-P
2	2	1498	UR3	C3'-C4'-C5'-O5'
2	2	516	PSU	C4'-C5'-O5'-P
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	1962	5MC	O4'-C1'-N1-C2
4	4	347	PSU	C4'-C5'-O5'-P
4	4	341	5MU	C2'-C1'-N1-C2
4	4	341	5MU	C2'-C1'-N1-C6
2	2	967	5MC	C4'-C5'-O5'-P
4	4	341	5MU	C4'-C5'-O5'-P
1	1	746	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C4
1	1	1618	6MZ	C5-C6-N6-C9
1	1	2251	OMG	C3'-C4'-C5'-O5'
1	1	2445	2MG	C4'-C5'-O5'-P
1	1	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 214 ligands modelled in this entry, 214 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.