



Full wwPDB EM Validation Report ⓘ

Mar 11, 2025 – 03:50 pm GMT

PDB ID : 6YSR
EMDB ID : EMD-10905
Title : Structure of the P+9 stalled ribosome complex
Authors : Chan, K.-H.; Petrychenko, V.; Mueller, C.; Maracci, C.; Holtkamp, W.; Wilson, D.N.; Fischer, N.; Rodnina, M.V.
Deposited on : 2020-04-23
Resolution : 3.10 Å (reported)
Based on initial models : 4RB7, 5AFI

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

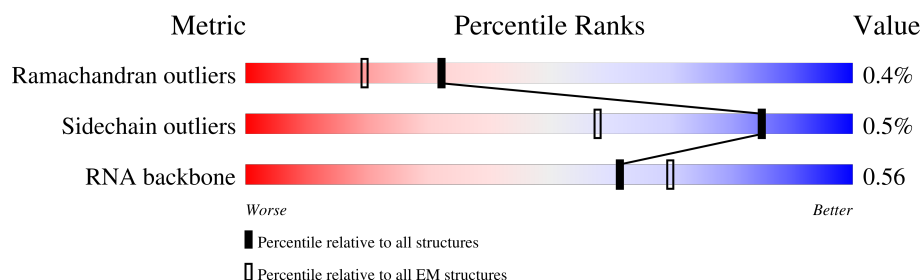
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



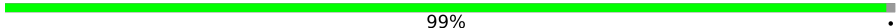
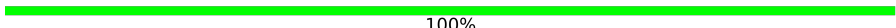

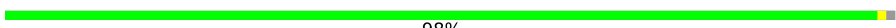
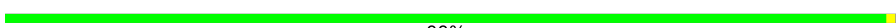








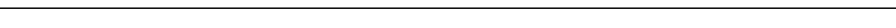

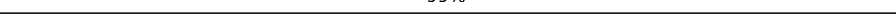
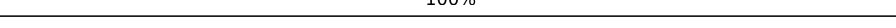
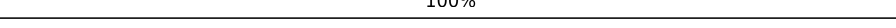

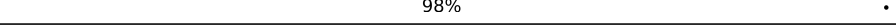
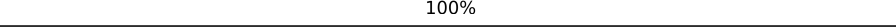

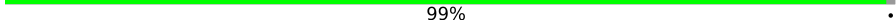
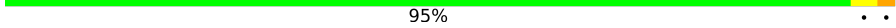
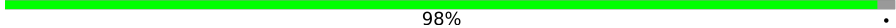
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	
9	B	120	



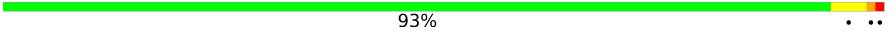
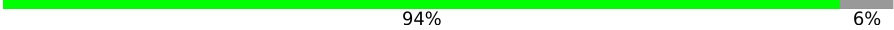


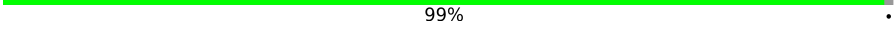
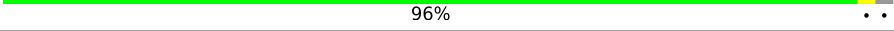


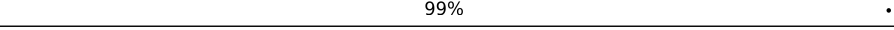
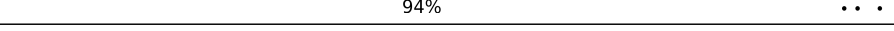
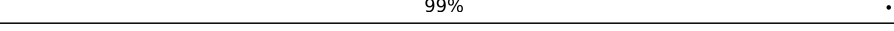
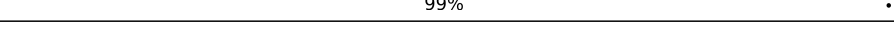
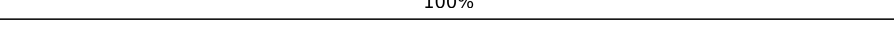



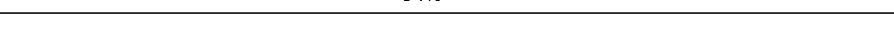


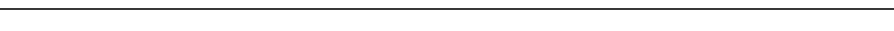

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Mol	Chain	Length	Quality of chain
10	C	273	 99%
11	D	209	 100%
12	E	201	 100%
13	F	179	 98%
14	G	177	 99%
15	H	149	 97%
16	I	142	 99%
17	J	142	 99%
18	K	123	 98%
19	L	144	 99%
20	M	136	 100%
21	N	127	 94% 6%
22	O	117	 99%
23	P	115	 99%
24	Q	118	 99%
25	R	103	 100%
26	S	110	 100%
27	T	100	 92% 7%
28	U	104	 98%
29	V	94	 100%
30	W	85	 87% 12%
31	X	78	 99%
32	Y	63	 95%
33	Z	59	 98%
34	a	1542	 81% 19%

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Mol	Chain	Length	Quality of chain
35	b	240	 90% 9%
36	c	233	 88% 12%
37	d	206	 93% ..
38	e	167	 94% 6%
39	f	135	 74% 26%
40	g	179	 84% 16%
41	h	130	 99% .
42	i	130	 96% ..
43	j	103	 92% ... 5%
44	k	129	 90% 10%
45	l	124	 99% .
46	m	118	 94% ...
47	n	102	 99% .
48	o	89	 99% .
49	p	82	 100%
50	q	84	 90% ... 5%
51	r	75	 87% 13%
52	s	92	 89% 11%
53	t	87	 94% ...
54	u	71	 89% .. 8%
55	v	2	 50% 50%
56	w	76	 75% 18% 5% .
57	x	15	 47% 53%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 145959 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 L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62336	27815	11468	20150	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1539	Total	C	N	O	P	0	0
			33028	14738	6052	10699	1539		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

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

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a protein called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	2	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace	
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	15	Total	C	N	O	P	0	0
			314	141	49	109	15		

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

Mol	Chain	Residues	Atoms		AltConf
58	0	1	Total	Mg	0
			1	1	
58	6	1	Total	Mg	0
			1	1	
58	A	236	Total	Mg	0
			236	236	
58	B	5	Total	Mg	0
			5	5	
58	O	1	Total	Mg	0
			1	1	
58	Q	1	Total	Mg	0
			1	1	
58	T	1	Total	Mg	0
			1	1	
58	a	82	Total	Mg	0
			82	82	
58	g	1	Total	Mg	0
			1	1	
58	w	3	Total	Mg	0
			3	3	

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	4	1	Total 1	Zn 1	0
59	6	1	Total 1	Zn 1	0

- Molecule 60 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
60	A	1	Total 1	Cl 1	0

- Molecule 61 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
61	A	1	Total 1	Na 1	0
61	V	1	Total 1	Na 1	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	A	1	Total 1	O 1	0
62	a	1	Total 1	O 1	0

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.

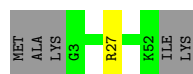
- Molecule 1: 50S ribosomal protein L32

Chain 0:  98% .



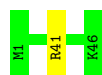
- Molecule 2: 50S ribosomal protein L33

Chain 1:  89% . 9%



- Molecule 3: 50S ribosomal protein L34

Chain 2:  98% .



- Molecule 4: 50S ribosomal protein L35

Chain 3:  97% . .




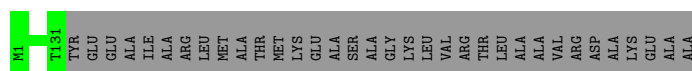
- Molecule 5: 50S ribosomal protein L36

Chain 4:  100%

There are no outlier residues recorded for this chain.

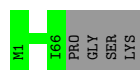
- Molecule 6: 50S ribosomal protein L10

Chain 5:  79% 21%



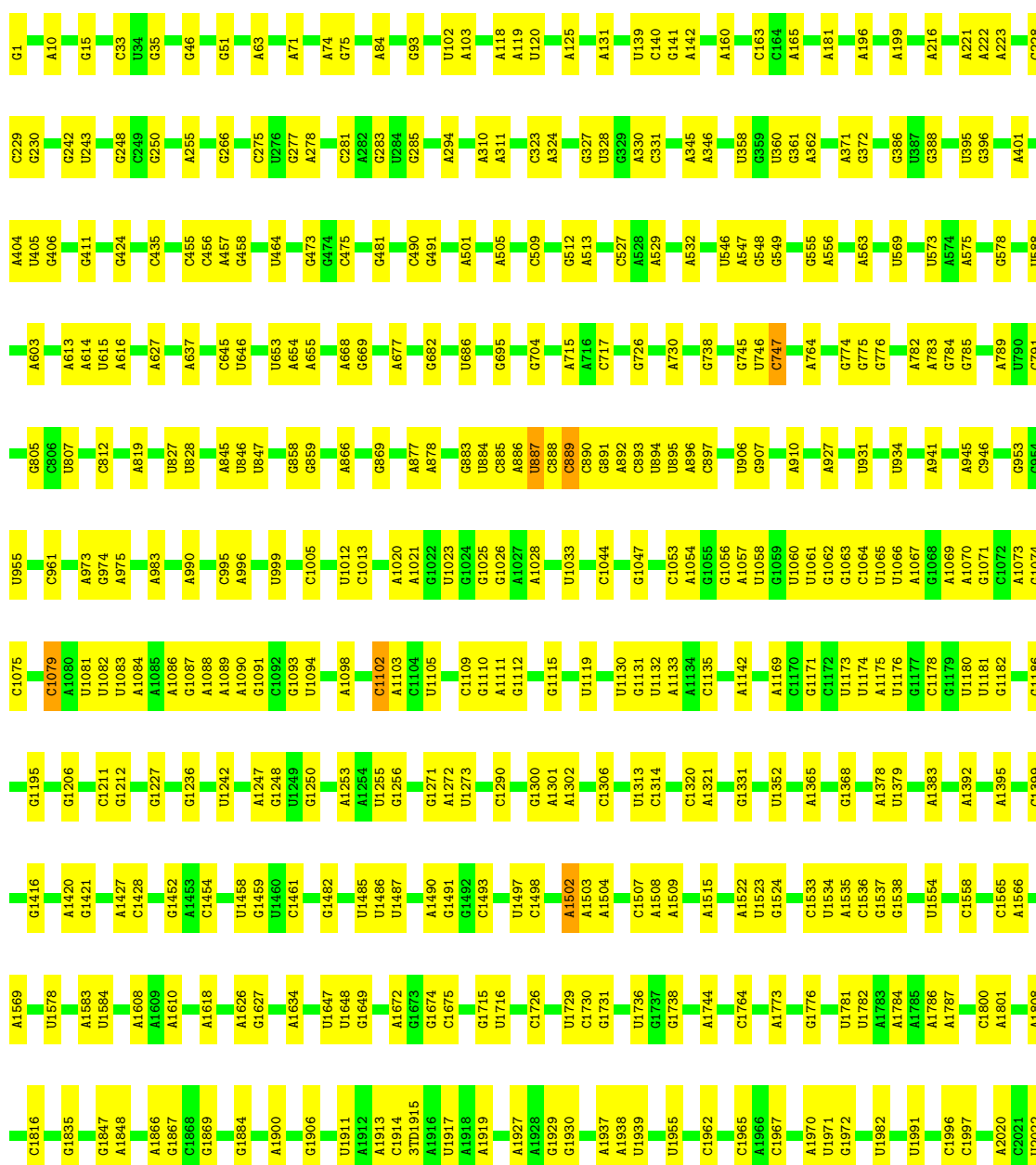
- Molecule 7: 50S ribosomal protein L31

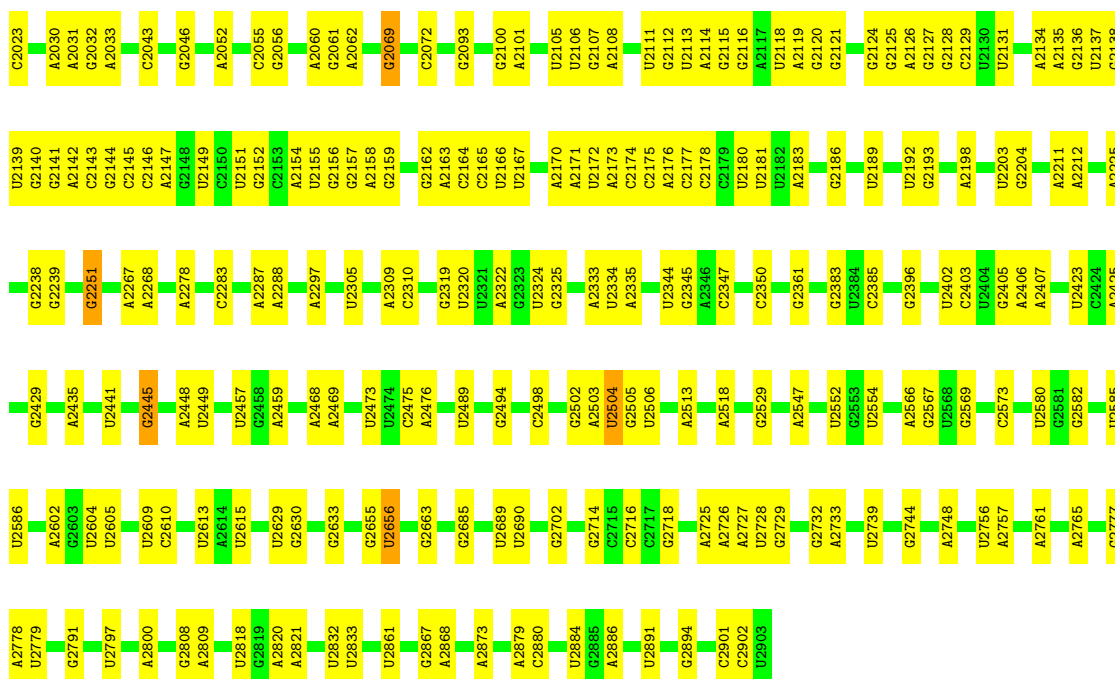
Chain 6: 94% 6%



- Molecule 8: 23S ribosomal RNA

Chain A: 78% 21%





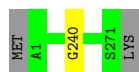
- Molecule 9: 5S ribosomal RNA

Chain B: 82% 18% .



- Molecule 10: 50S ribosomal protein L2

Chain C: 99% .



- Molecule 11: 50S ribosomal protein L3

Chain D: 100%

There are no outlier residues recorded for this chain.

- Molecule 12: 50S ribosomal protein L4

Chain E: 100%

There are no outlier residues recorded for this chain.

- Molecule 13: 50S ribosomal protein L5

Chain F: 98% ..



- Molecule 14: 50S ribosomal protein L6

Chain G:  99%



- Molecule 15: 50S ribosomal protein L9

Chain H:  97%



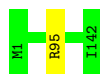
- Molecule 16: 50S ribosomal protein L11

Chain I:  99%



- Molecule 17: 50S ribosomal protein L13

Chain J:  99%



- Molecule 18: 50S ribosomal protein L14

Chain K:  98%



- Molecule 19: 50S ribosomal protein L15

Chain L:  99%



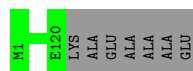
- Molecule 20: 50S ribosomal protein L16

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 50S ribosomal protein L17

Chain N:  94% 6%



- Molecule 22: 50S ribosomal protein L18

Chain O:  99% .



- Molecule 23: 50S ribosomal protein L19

Chain P:  99% .



- Molecule 24: 50S ribosomal protein L20

Chain Q:  99% .



- Molecule 25: 50S ribosomal protein L21

Chain R:  100%

There are no outlier residues recorded for this chain.

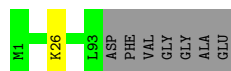
- Molecule 26: 50S ribosomal protein L22

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L23

Chain T:  92% . 7%



- Molecule 28: 50S ribosomal protein L24

Chain U:  98% .



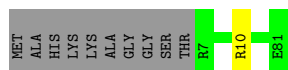
- Molecule 29: 50S ribosomal protein L25

Chain V: 100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L27

Chain W: 87% 12%



- Molecule 31: 50S ribosomal protein L28

Chain X: 99%



- Molecule 32: 50S ribosomal protein L29

Chain Y: 95%



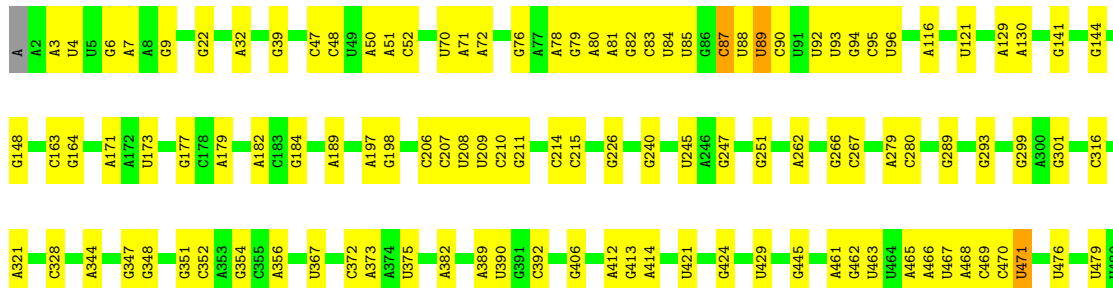
- Molecule 33: 50S ribosomal protein L30

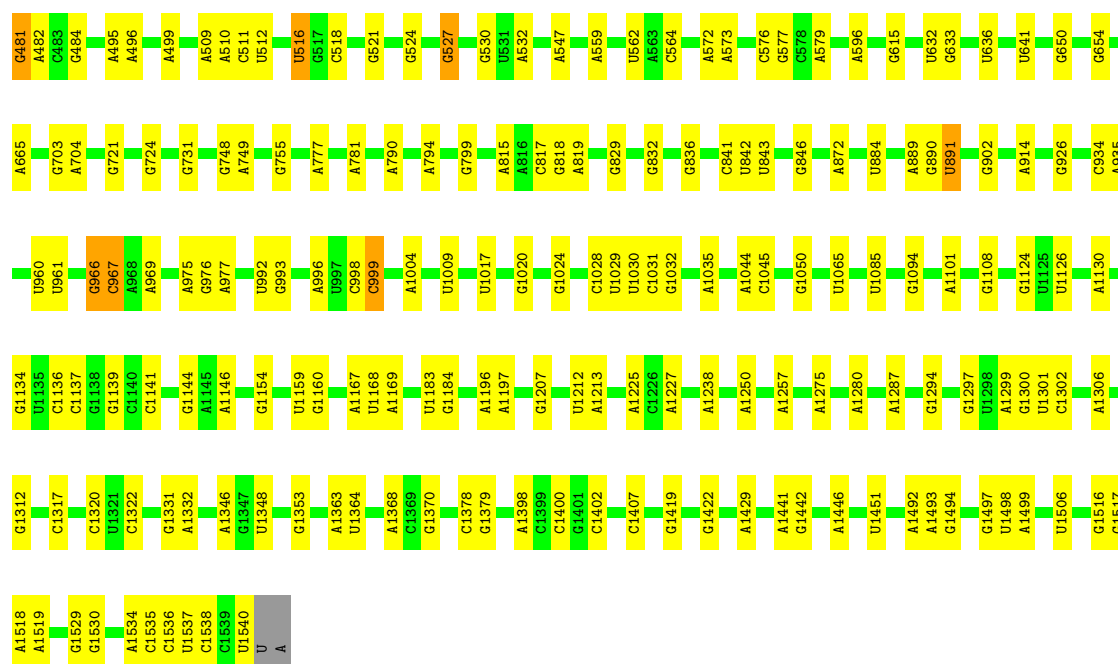
Chain Z: 98%



- Molecule 34: 16S ribosomal RNA

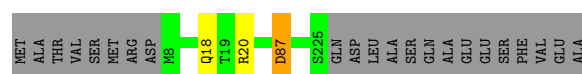
Chain a: 81% 19%





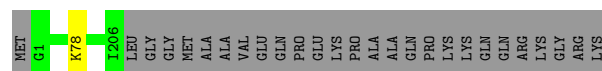
- Molecule 35: 30S ribosomal protein S2

Chain b: 90% 9%



- Molecule 36: 30S ribosomal protein S3

Chain c: 88% 12%



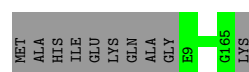
- Molecule 37: 30S ribosomal protein S4

Chain d: 93% 6%



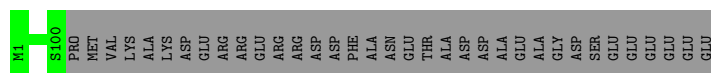
- Molecule 38: 30S ribosomal protein S5

Chain e: 94% 6%




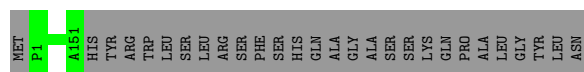
- Molecule 39: 30S ribosomal protein S6

Chain f:  74% 26%



- Molecule 40: 30S ribosomal protein S7

Chain g:  84% 16%



- Molecule 41: 30S ribosomal protein S8

Chain h:  99%




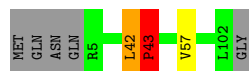
- Molecule 42: 30S ribosomal protein S9

Chain i:  96%




- Molecule 43: 30S ribosomal protein S10

Chain j:  92% ... 5%



- Molecule 44: 30S ribosomal protein S11

Chain k:  90% 10%



- Molecule 45: 30S ribosomal protein S12

Chain l:  99%



- Molecule 46: 30S ribosomal protein S13

Chain m:  94% ...



- Molecule 47: 30S ribosomal protein S14

Chain n:  99% .



- Molecule 48: 30S ribosomal protein S15

Chain o:  99% .




- Molecule 49: 30S ribosomal protein S16

Chain p:  100%


There are no outlier residues recorded for this chain.

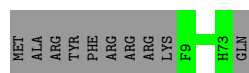
- Molecule 50: 30S ribosomal protein S17

Chain q:  90% ... 5%




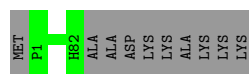
- Molecule 51: 30S ribosomal protein S18

Chain r:  87% 13%



- Molecule 52: 30S ribosomal protein S19

Chain s:  89% 11%



- Molecule 53: 30S ribosomal protein S20

Chain t:  94% ...



- Molecule 54: 30S ribosomal protein S21

Chain u: 89% .. 8%



- Molecule 55: P-site fMet-Phe-tRNA(Phe)

Chain v: 50% 50%



- Molecule 56: P-site fMet-Phe-tRNA(Phe)

Chain w: 75% 18% 5% •



- Molecule 57: mRNA

Chain x: 47% 53%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, NA, CL, 2MA, 3TD, PSU, ZN, OMU, MA6, OMC, 2MG, 4OC, 5MC, G7M, MIA, 1MG, 4SU, UR3, OMG, 6MZ, MG

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	0/450	0.47	0/599
2	1	0.34	0/416	0.49	0/554
3	2	0.36	0/380	0.45	0/498
4	3	0.39	0/513	0.49	0/676
5	4	0.35	0/303	0.46	0/397
6	5	0.27	0/646	0.54	0/898
7	6	0.29	0/531	0.48	0/709
8	A	0.67	9/69263 (0.0%)	0.82	27/108050 (0.0%)
9	B	0.60	2/2873 (0.1%)	0.80	0/4478
10	C	0.40	0/2121	0.50	0/2852
11	D	0.38	0/1586	0.51	0/2134
12	E	0.36	0/1571	0.47	0/2113
13	F	0.34	0/1434	0.51	1/1926 (0.1%)
14	G	0.33	0/1343	0.49	0/1816
15	H	0.32	0/1122	0.57	0/1515
16	I	0.25	0/692	0.49	0/960
17	J	0.38	0/1152	0.47	0/1551
18	K	0.37	0/947	0.51	0/1268
19	L	0.36	0/1054	0.52	0/1403
20	M	0.36	0/1093	0.48	0/1460
21	N	0.36	0/973	0.48	0/1301
22	O	0.33	0/902	0.44	0/1209
23	P	0.36	0/929	0.48	0/1242
24	Q	0.42	0/960	0.42	0/1278
25	R	0.38	0/829	0.50	0/1107
26	S	0.34	0/864	0.48	0/1156
27	T	0.33	0/744	0.47	0/994
28	U	0.33	0/787	0.47	0/1051
29	V	0.36	0/766	0.47	0/1025
30	W	0.37	0/582	0.45	0/769
31	X	0.37	0/635	0.50	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.29	0/510	0.62	1/677 (0.1%)
33	Z	0.32	0/453	0.49	0/605
34	a	0.59	1/36700 (0.0%)	0.81	13/57246 (0.0%)
35	b	0.31	0/1735	0.51	1/2338 (0.0%)
36	c	0.33	0/1651	0.46	0/2225
37	d	0.82	7/1665 (0.4%)	0.79	12/2227 (0.5%)
38	e	0.35	0/1154	0.50	0/1554
39	f	0.35	0/835	0.48	0/1128
40	g	0.29	0/1195	0.46	0/1602
41	h	0.34	0/989	0.49	0/1326
42	i	0.31	0/1034	0.51	0/1375
43	j	0.90	2/796 (0.3%)	0.74	5/1077 (0.5%)
44	k	0.32	0/885	0.46	0/1195
45	l	0.36	0/969	0.53	0/1300
46	m	1.00	6/892 (0.7%)	0.67	3/1193 (0.3%)
47	n	0.31	0/811	0.46	0/1081
48	o	0.31	0/722	0.43	0/964
49	p	0.36	0/659	0.49	0/884
50	q	0.78	3/657 (0.5%)	0.88	5/881 (0.6%)
51	r	0.35	0/544	0.48	0/731
52	s	0.31	0/675	0.47	0/908
53	t	0.78	1/671 (0.1%)	0.65	2/888 (0.2%)
54	u	0.36	0/512	0.84	4/683 (0.6%)
55	v	5.69	3/19 (15.8%)	1.72	0/23
56	w	1.46	28/1650 (1.7%)	1.09	16/2569 (0.6%)
57	x	0.43	0/349	0.85	0/540
All	All	0.61	62/157193 (0.0%)	0.76	90/235057 (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
43	j	0	1
46	m	0	1
50	q	0	2
53	t	0	2
56	w	0	1
All	All	0	7

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	20	U	C2-N3	16.74	1.49	1.37
46	m	65	GLU	CD-OE2	-16.73	1.07	1.25
56	w	16	U	C5-C6	16.73	1.49	1.34
56	w	16	U	C2-N3	16.68	1.49	1.37
56	w	20	U	C5-C6	16.68	1.49	1.34
55	v	102	PHE	C-O	16.33	1.54	1.23
53	t	7	LYS	C-O	-16.32	0.92	1.23
43	j	43	PRO	N-CD	-15.97	1.25	1.47
8	A	2449	U	C5-C6	15.97	1.48	1.34
56	w	75	C	O3'-P	-15.73	1.42	1.61
55	v	101	MET	CG-SD	-15.70	1.40	1.81
8	A	2449	U	C2-N3	15.61	1.48	1.37
56	w	76	A	P-OP2	-15.22	1.23	1.49
37	d	35	GLN	C-O	-14.82	0.95	1.23
43	j	42	LEU	C-O	-14.19	0.96	1.23
46	m	64	VAL	C-O	-12.98	0.98	1.23
56	w	20	U	N1-C2	11.95	1.49	1.38
37	d	37	PRO	N-CA	-11.71	1.27	1.47
46	m	65	GLU	CD-OE1	-11.64	1.12	1.25
37	d	36	ALA	C-O	-11.49	1.01	1.23
50	q	70	LYS	C-O	-11.25	1.01	1.23
56	w	16	U	N1-C2	10.95	1.48	1.38
9	B	1	U	OP3-P	-10.71	1.48	1.61
8	A	1	G	OP3-P	-10.70	1.48	1.61
37	d	37	PRO	N-CD	-10.55	1.33	1.47
56	w	76	A	C5-C6	-10.48	1.31	1.41
8	A	2449	U	N1-C2	10.40	1.48	1.38
56	w	76	A	P-OP1	-10.33	1.31	1.49
37	d	37	PRO	C-O	-9.84	1.03	1.23
46	m	65	GLU	C-O	-9.81	1.04	1.23
56	w	76	A	O4'-C1'	-9.51	1.29	1.41
56	w	20	U	N3-C4	8.65	1.46	1.38
56	w	16	U	N3-C4	8.65	1.46	1.38
50	q	68	LYS	C-O	-8.32	1.07	1.23
56	w	20	U	N1-C6	8.14	1.45	1.38
56	w	16	U	N1-C6	8.03	1.45	1.38
8	A	2449	U	N3-C4	7.45	1.45	1.38
56	w	76	A	C2-N3	-7.15	1.27	1.33
8	A	2449	U	N1-C6	7.11	1.44	1.38
56	w	16	U	C4-C5	7.10	1.50	1.43
56	w	76	A	C4'-O4'	-6.99	1.36	1.45
8	A	2449	U	C4-O4	-6.98	1.18	1.23
56	w	20	U	C4-C5	6.93	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	76	A	P-O5'	-6.82	1.52	1.59
55	v	101	MET	N-CA	-6.66	1.33	1.46
56	w	16	U	C4-O4	-6.32	1.18	1.23
56	w	76	A	C6-N1	-6.27	1.31	1.35
56	w	20	U	C4-O4	-6.25	1.18	1.23
34	a	90	C	N1-C2	6.18	1.46	1.40
37	d	34	GLU	C-O	-6.14	1.11	1.23
8	A	2449	U	C4-C5	5.91	1.48	1.43
37	d	37	PRO	CA-CB	-5.84	1.41	1.53
50	q	69	THR	C-O	-5.84	1.12	1.23
56	w	76	A	C5-C4	-5.83	1.34	1.38
56	w	76	A	N7-C5	-5.76	1.35	1.39
56	w	76	A	N1-C2	-5.73	1.29	1.34
46	m	64	VAL	CB-CG2	-5.70	1.40	1.52
56	w	76	A	C6-N6	-5.59	1.29	1.33
56	w	76	A	C3'-O3'	5.40	1.49	1.42
46	m	65	GLU	CG-CD	-5.37	1.43	1.51
9	B	120	U	C1'-N1	5.27	1.56	1.48
8	A	887	U	C1'-N1	5.11	1.56	1.48

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	37	PRO	N-CA-CB	-13.35	87.28	103.30
56	w	76	A	O5'-P-OP1	12.75	126.00	110.70
8	A	1487	U	N3-C4-O4	-12.50	110.65	119.40
56	w	16	U	C2-N3-C4	-12.21	119.67	127.00
8	A	2449	U	C2-N3-C4	-11.81	119.91	127.00
8	A	1487	U	C5-C4-O4	11.24	132.64	125.90
56	w	20	U	C2-N3-C4	-11.13	120.32	127.00
56	w	16	U	C5-C4-O4	-10.18	119.79	125.90
8	A	2449	U	C5-C4-O4	-10.05	119.87	125.90
56	w	20	U	C5-C4-O4	-9.81	120.02	125.90
54	u	12	ASP	O-C-N	9.65	138.14	122.70
56	w	76	A	C5'-C4'-O4'	-9.44	97.77	109.10
8	A	1079	C	N1-C2-O2	9.42	124.55	118.90
50	q	68	LYS	N-CA-CB	-9.15	94.13	110.60
56	w	16	U	N3-C4-C5	9.09	120.05	114.60
8	A	1079	C	C2-N1-C1'	8.94	128.64	118.80
56	w	76	A	O5'-P-OP2	-8.82	97.77	105.70
54	u	12	ASP	CA-C-N	-8.79	97.85	117.20
8	A	2449	U	N3-C4-C5	8.71	119.83	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2449	U	N1-C2-N3	8.68	120.11	114.90
56	w	75	C	P-O3'-C3'	8.58	130.00	119.70
50	q	70	LYS	N-CA-C	-8.55	87.91	111.00
56	w	20	U	N3-C4-C5	8.42	119.65	114.60
46	m	64	VAL	CA-CB-CG1	8.36	123.44	110.90
56	w	16	U	N1-C2-N3	8.36	119.92	114.90
56	w	20	U	N1-C2-N3	8.14	119.78	114.90
8	A	1079	C	N3-C2-O2	-7.71	116.50	121.90
34	a	214	C	C2'-C3'-O3'	7.67	126.37	109.50
8	A	2902	C	N3-C2-O2	-7.62	116.57	121.90
43	j	43	PRO	N-CA-C	7.61	131.88	112.10
50	q	70	LYS	C-N-CA	-7.59	102.71	121.70
46	m	64	VAL	CG1-CB-CG2	-7.47	98.95	110.90
8	A	1502	A	N1-C6-N6	-7.42	114.15	118.60
53	t	7	LYS	N-CA-C	-7.40	91.03	111.00
34	a	89	U	P-O3'-C3'	7.25	128.40	119.70
37	d	79	ALA	N-CA-CB	7.17	120.14	110.10
8	A	2506	U	C2-N1-C1'	7.08	126.20	117.70
8	A	2902	C	N1-C2-O2	7.03	123.12	118.90
56	w	76	A	C1'-C2'-O2'	7.02	131.67	110.60
37	d	34	GLU	CB-CG-CD	-6.96	95.42	114.20
46	m	64	VAL	C-N-CA	6.84	138.79	121.70
8	A	1313	U	C2-N1-C1'	6.79	125.85	117.70
34	a	90	C	O4'-C1'-C2'	-6.63	99.17	105.80
37	d	34	GLU	CB-CA-C	-6.50	97.41	110.40
56	w	76	A	O4'-C1'-N9	-6.46	103.03	108.20
37	d	37	PRO	CA-CB-CG	-6.41	91.81	104.00
8	A	1102	C	N1-C2-O2	6.36	122.72	118.90
8	A	2506	U	N1-C2-O2	6.34	127.24	122.80
8	A	1079	C	C6-N1-C1'	-6.14	113.44	120.80
8	A	2506	U	N3-C2-O2	-6.03	117.98	122.20
53	t	6	ALA	CA-C-O	6.00	132.69	120.10
8	A	889	C	C2-N1-C1'	5.94	125.34	118.80
8	A	1079	C	C6-N1-C2	-5.93	117.93	120.30
43	j	43	PRO	N-CD-CG	-5.93	94.30	103.20
43	j	43	PRO	N-CA-CB	-5.85	96.16	102.60
32	Y	13	GLU	N-CA-CB	5.84	121.11	110.60
13	F	173	ASP	CB-CA-C	5.80	122.00	110.40
56	w	16	U	C5-C6-N1	-5.80	119.80	122.70
8	A	1102	C	C2-N1-C1'	5.66	125.02	118.80
37	d	37	PRO	N-CA-C	5.57	126.59	112.10
8	A	2656	U	C2-N1-C1'	5.55	124.36	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	476	U	N3-C2-O2	-5.52	118.34	122.20
37	d	37	PRO	N-CD-CG	-5.52	94.92	103.20
8	A	1313	U	N1-C2-O2	5.50	126.65	122.80
50	q	70	LYS	CD-CE-NZ	5.46	124.25	111.70
37	d	78	ALA	C-N-CA	5.44	135.29	121.70
8	A	889	C	N1-C2-O2	5.42	122.15	118.90
34	a	481	G	C4-N9-C1'	5.42	133.54	126.50
37	d	149	LYS	C-N-CA	5.40	135.20	121.70
34	a	891	U	C2-N1-C1'	5.39	124.16	117.70
37	d	79	ALA	C-N-CA	-5.36	108.31	121.70
54	u	13	VAL	N-CA-C	-5.28	96.74	111.00
37	d	79	ALA	N-CA-C	-5.26	96.81	111.00
34	a	87	C	C2-N1-C1'	5.25	124.58	118.80
43	j	43	PRO	CA-CB-CG	-5.21	94.10	104.00
50	q	69	THR	CB-CA-C	-5.20	97.55	111.60
43	j	42	LEU	O-C-N	-5.17	111.29	121.10
34	a	471	U	C2-N1-C1'	5.14	123.87	117.70
34	a	998	C	N3-C2-O2	-5.13	118.31	121.90
34	a	891	U	C5-C6-N1	5.12	125.26	122.70
37	d	150	LYS	N-CA-C	-5.12	97.18	111.00
8	A	512	G	O4'-C1'-N9	5.11	112.29	108.20
54	u	13	VAL	CA-CB-CG2	-5.09	103.26	110.90
8	A	1314	C	C2-N1-C1'	5.06	124.36	118.80
34	a	1141	C	N3-C2-O2	-5.04	118.37	121.90
8	A	1313	U	N3-C2-O2	-5.03	118.68	122.20
56	w	16	U	N1-C2-O2	-5.03	119.28	122.80
35	b	87	ASP	CB-CA-C	-5.01	100.37	110.40
34	a	90	C	C4'-C3'-O3'	5.01	123.03	113.00
34	a	999	C	C2-N1-C1'	5.00	124.31	118.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	j	42	LEU	Mainchain
46	m	64	VAL	Mainchain
50	q	69	THR	Mainchain
50	q	70	LYS	Mainchain
53	t	5	SER	Mainchain
53	t	7	LYS	Mainchain
56	w	76	A	Sidechain

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	
1	0	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	44 (100%)	0	0	100	100
4	3	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
5	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
6	5	129/165 (78%)	108 (84%)	21 (16%)	0	100	100
7	6	64/70 (91%)	50 (78%)	14 (22%)	0	100	100
10	C	269/273 (98%)	248 (92%)	20 (7%)	1 (0%)	30	63
11	D	207/209 (99%)	191 (92%)	16 (8%)	0	100	100
12	E	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
13	F	175/179 (98%)	153 (87%)	22 (13%)	0	100	100
14	G	174/177 (98%)	154 (88%)	19 (11%)	1 (1%)	22	53
15	H	147/149 (99%)	111 (76%)	33 (22%)	3 (2%)	6	26
16	I	139/142 (98%)	109 (78%)	30 (22%)	0	100	100
17	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
18	K	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
19	L	141/144 (98%)	124 (88%)	17 (12%)	0	100	100
20	M	134/136 (98%)	125 (93%)	9 (7%)	0	100	100
21	N	118/127 (93%)	112 (95%)	6 (5%)	0	100	100
22	O	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
23	P	112/115 (97%)	102 (91%)	10 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
25	R	101/103 (98%)	89 (88%)	12 (12%)	0	100	100
26	S	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
27	T	91/100 (91%)	81 (89%)	10 (11%)	0	100	100
28	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
29	V	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
30	W	73/85 (86%)	66 (90%)	7 (10%)	0	100	100
31	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
32	Y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	8	31
33	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
35	b	216/240 (90%)	188 (87%)	25 (12%)	3 (1%)	9	34
36	c	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
37	d	203/206 (98%)	167 (82%)	29 (14%)	7 (3%)	3	17
38	e	155/167 (93%)	138 (89%)	17 (11%)	0	100	100
39	f	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
40	g	149/179 (83%)	142 (95%)	7 (5%)	0	100	100
41	h	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/130 (96%)	105 (84%)	20 (16%)	0	100	100
43	j	96/103 (93%)	78 (81%)	16 (17%)	2 (2%)	5	25
44	k	114/129 (88%)	107 (94%)	7 (6%)	0	100	100
45	l	121/124 (98%)	105 (87%)	16 (13%)	0	100	100
46	m	112/118 (95%)	101 (90%)	10 (9%)	1 (1%)	14	45
47	n	99/102 (97%)	86 (87%)	13 (13%)	0	100	100
48	o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
49	p	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
50	q	78/84 (93%)	63 (81%)	13 (17%)	2 (3%)	4	21
51	r	63/75 (84%)	53 (84%)	10 (16%)	0	100	100
52	s	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
53	t	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
54	u	63/71 (89%)	51 (81%)	11 (18%)	1 (2%)	8	31
All	All	5850/6220 (94%)	5250 (90%)	578 (10%)	22 (0%)	32	63

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	b	87	ASP
37	d	34	GLU
37	d	37	PRO
37	d	150	LYS
43	j	43	PRO
32	Y	13	GLU
37	d	79	ALA
50	q	70	LYS
14	G	108	PHE
15	H	104	THR
35	b	20	ARG
43	j	57	VAL
46	m	65	GLU
54	u	12	ASP
35	b	18	GLN
37	d	71	PHE
10	C	240	GLY
15	H	70	GLU
15	H	74	ALA
37	d	144	ILE
37	d	38	GLY
50	q	55	GLY

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	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	44 (98%)	1 (2%)	47	71
3	2	38/38 (100%)	37 (97%)	1 (3%)	41	68
4	3	51/52 (98%)	50 (98%)	1 (2%)	50	74
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	C	216/218 (99%)	216 (100%)	0	100	100
11	D	164/164 (100%)	164 (100%)	0	100	100
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	148 (100%)	0	100	100
14	G	137/138 (99%)	137 (100%)	0	100	100
15	H	114/114 (100%)	111 (97%)	3 (3%)	41	68
17	J	116/116 (100%)	115 (99%)	1 (1%)	75	88
18	K	103/104 (99%)	102 (99%)	1 (1%)	73	86
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	109 (100%)	0	100	100
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	99 (100%)	0	100	100
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	84 (100%)	0	100	100
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	79 (99%)	1 (1%)	65	82
28	U	83/85 (98%)	83 (100%)	0	100	100
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	56 (98%)	1 (2%)	54	76
31	X	67/68 (98%)	67 (100%)	0	100	100
32	Y	55/55 (100%)	53 (96%)	2 (4%)	30	60
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	180 (100%)	0	100	100
36	c	170/190 (90%)	169 (99%)	1 (1%)	84	91
37	d	172/173 (99%)	168 (98%)	4 (2%)	45	70
38	e	114/126 (90%)	114 (100%)	0	100	100
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	124 (100%)	0	100	100
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	105/107 (98%)	103 (98%)	2 (2%)	52	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	j	86/90 (96%)	85 (99%)	1 (1%)	67	83
44	k	89/99 (90%)	89 (100%)	0	100	100
45	l	103/104 (99%)	103 (100%)	0	100	100
46	m	92/96 (96%)	91 (99%)	1 (1%)	70	84
47	n	79/84 (94%)	79 (100%)	0	100	100
48	o	76/77 (99%)	76 (100%)	0	100	100
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	73 (99%)	1 (1%)	62	81
51	r	56/65 (86%)	56 (100%)	0	100	100
52	s	72/79 (91%)	72 (100%)	0	100	100
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	46 (100%)	0	100	100
55	v	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	4628/4831 (96%)	4605 (100%)	23 (0%)	85	92

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	27	ARG
3	2	41	ARG
4	3	32	LEU
15	H	51	ARG
15	H	66	ASN
15	H	104	THR
17	J	95	ARG
18	K	49	ARG
27	T	26	LYS
30	W	10	ARG
32	Y	2	LYS
32	Y	9	LYS
36	c	78	LYS
37	d	37	PRO
37	d	73	ASN
37	d	80	ARG
37	d	150	LYS
42	i	11	ARG
42	i	122	ARG

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Mol	Chain	Res	Type
43	j	43	PRO
46	m	2	ARG
50	q	68	LYS
55	v	101	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	5	ASN
1	0	41	HIS
2	1	25	ASN
3	2	6	GLN
4	3	42	HIS
10	C	52	HIS
10	C	152	GLN
10	C	259	ASN
12	E	41	GLN
12	E	165	HIS
13	F	51	ASN
14	G	44	HIS
18	K	5	GLN
18	K	93	GLN
19	L	54	GLN
21	N	62	ASN
23	P	11	GLN
24	Q	43	GLN
27	T	70	HIS
28	U	52	ASN
28	U	73	ASN
35	b	18	GLN
35	b	169	HIS
36	c	18	ASN
36	c	99	GLN
37	d	125	ASN
38	e	88	HIS
40	g	67	ASN
43	j	56	HIS
47	n	49	GLN
48	o	34	GLN
48	o	79	GLN
49	p	26	ASN
52	s	82	HIS

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Mol	Chain	Res	Type
53	t	83	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1535/1542 (99%)	284 (18%)	0
56	w	74/76 (97%)	13 (17%)	0
57	x	14/15 (93%)	8 (57%)	0
8	A	2898/2903 (99%)	577 (19%)	56 (1%)
9	B	119/120 (99%)	18 (15%)	3 (2%)
All	All	4640/4656 (99%)	900 (19%)	59 (1%)

All (900) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	15	G
8	A	33	C
8	A	35	G
8	A	46	G
8	A	51	G
8	A	63	A
8	A	71	A
8	A	74	A
8	A	75	G
8	A	84	A
8	A	93	G
8	A	102	U
8	A	103	A
8	A	118	A
8	A	119	A
8	A	120	U
8	A	125	A
8	A	131	A
8	A	139	U
8	A	140	C
8	A	141	G
8	A	142	A
8	A	160	A
8	A	163	C
8	A	165	A

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Mol	Chain	Res	Type
8	A	181	A
8	A	196	A
8	A	199	A
8	A	216	A
8	A	221	A
8	A	222	A
8	A	223	A
8	A	228	C
8	A	229	C
8	A	230	G
8	A	242	G
8	A	243	U
8	A	248	G
8	A	250	G
8	A	255	A
8	A	266	G
8	A	275	C
8	A	277	G
8	A	278	A
8	A	281	C
8	A	283	G
8	A	285	G
8	A	294	A
8	A	311	A
8	A	323	C
8	A	324	A
8	A	327	G
8	A	328	U
8	A	330	A
8	A	331	C
8	A	345	A
8	A	346	A
8	A	358	U
8	A	360	U
8	A	361	G
8	A	362	A
8	A	371	A
8	A	372	G
8	A	386	G
8	A	388	G
8	A	395	U
8	A	396	G

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Mol	Chain	Res	Type
8	A	401	A
8	A	404	A
8	A	405	U
8	A	406	G
8	A	411	G
8	A	424	G
8	A	435	C
8	A	455	C
8	A	457	A
8	A	458	G
8	A	473	G
8	A	475	C
8	A	481	G
8	A	491	G
8	A	501	A
8	A	505	A
8	A	509	C
8	A	513	A
8	A	527	C
8	A	529	A
8	A	532	A
8	A	546	U
8	A	548	G
8	A	549	G
8	A	556	A
8	A	563	A
8	A	569	U
8	A	573	U
8	A	575	A
8	A	578	G
8	A	588	U
8	A	603	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	616	A
8	A	627	A
8	A	637	A
8	A	645	C
8	A	646	U
8	A	653	U
8	A	654	A

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Mol	Chain	Res	Type
8	A	655	A
8	A	668	A
8	A	669	G
8	A	677	A
8	A	682	G
8	A	686	U
8	A	695	G
8	A	704	G
8	A	715	A
8	A	717	C
8	A	726	G
8	A	730	A
8	A	738	G
8	A	747	5MC
8	A	764	A
8	A	774	G
8	A	775	G
8	A	776	G
8	A	782	A
8	A	783	A
8	A	784	G
8	A	785	G
8	A	789	A
8	A	791	C
8	A	805	G
8	A	807	U
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	845	A
8	A	846	U
8	A	847	U
8	A	858	G
8	A	859	G
8	A	866	A
8	A	869	G
8	A	877	A
8	A	878	A
8	A	883	G
8	A	884	U
8	A	885	C

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Mol	Chain	Res	Type
8	A	886	A
8	A	887	U
8	A	888	C
8	A	889	C
8	A	890	C
8	A	891	G
8	A	892	A
8	A	893	C
8	A	895	U
8	A	896	A
8	A	897	C
8	A	906	U
8	A	907	G
8	A	910	A
8	A	927	A
8	A	931	U
8	A	934	U
8	A	941	A
8	A	945	A
8	A	946	C
8	A	953	G
8	A	961	C
8	A	973	A
8	A	974	G
8	A	975	A
8	A	983	A
8	A	990	A
8	A	995	C
8	A	996	A
8	A	999	U
8	A	1005	C
8	A	1012	U
8	A	1013	C
8	A	1021	A
8	A	1023	U
8	A	1025	G
8	A	1026	G
8	A	1028	A
8	A	1033	U
8	A	1044	C
8	A	1047	G
8	A	1053	C

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Mol	Chain	Res	Type
8	A	1054	A
8	A	1056	G
8	A	1057	A
8	A	1058	U
8	A	1060	U
8	A	1061	U
8	A	1062	G
8	A	1063	G
8	A	1064	C
8	A	1065	U
8	A	1066	U
8	A	1067	A
8	A	1069	A
8	A	1070	A
8	A	1071	G
8	A	1073	A
8	A	1074	G
8	A	1075	C
8	A	1079	C
8	A	1081	U
8	A	1082	U
8	A	1083	U
8	A	1084	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1089	A
8	A	1090	A
8	A	1091	G
8	A	1093	G
8	A	1094	U
8	A	1098	A
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1109	C
8	A	1111	A
8	A	1112	G
8	A	1115	G
8	A	1119	U
8	A	1130	U
8	A	1131	G

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Mol	Chain	Res	Type
8	A	1132	U
8	A	1133	A
8	A	1135	C
8	A	1142	A
8	A	1169	A
8	A	1171	G
8	A	1173	U
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1178	C
8	A	1180	U
8	A	1181	U
8	A	1186	G
8	A	1195	G
8	A	1206	G
8	A	1211	C
8	A	1212	G
8	A	1227	G
8	A	1236	G
8	A	1242	U
8	A	1247	A
8	A	1248	G
8	A	1250	G
8	A	1253	A
8	A	1255	U
8	A	1256	G
8	A	1271	G
8	A	1272	A
8	A	1273	U
8	A	1290	C
8	A	1300	G
8	A	1301	A
8	A	1302	A
8	A	1306	C
8	A	1321	A
8	A	1352	U
8	A	1365	A
8	A	1368	G
8	A	1378	A
8	A	1379	U
8	A	1383	A

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Mol	Chain	Res	Type
8	A	1392	A
8	A	1395	A
8	A	1416	G
8	A	1420	A
8	A	1421	G
8	A	1427	A
8	A	1428	C
8	A	1452	G
8	A	1454	C
8	A	1459	G
8	A	1461	C
8	A	1482	G
8	A	1485	U
8	A	1486	U
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1497	U
8	A	1498	C
8	A	1502	A
8	A	1503	A
8	A	1504	A
8	A	1507	C
8	A	1508	A
8	A	1509	A
8	A	1515	A
8	A	1522	A
8	A	1523	U
8	A	1524	G
8	A	1533	C
8	A	1534	U
8	A	1535	A
8	A	1536	C
8	A	1537	G
8	A	1538	G
8	A	1554	U
8	A	1558	C
8	A	1566	A
8	A	1569	A
8	A	1578	U
8	A	1583	A
8	A	1584	U

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Mol	Chain	Res	Type
8	A	1608	A
8	A	1610	A
8	A	1626	A
8	A	1627	G
8	A	1634	A
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1672	A
8	A	1674	G
8	A	1675	C
8	A	1715	G
8	A	1716	U
8	A	1726	C
8	A	1729	U
8	A	1730	C
8	A	1731	G
8	A	1736	U
8	A	1738	G
8	A	1744	A
8	A	1764	C
8	A	1773	A
8	A	1776	G
8	A	1781	U
8	A	1782	U
8	A	1784	A
8	A	1786	A
8	A	1787	A
8	A	1800	C
8	A	1801	A
8	A	1808	A
8	A	1816	C
8	A	1848	A
8	A	1866	A
8	A	1867	G
8	A	1869	G
8	A	1884	G
8	A	1900	A
8	A	1906	G
8	A	1913	A
8	A	1914	C
8	A	1919	A

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Mol	Chain	Res	Type
8	A	1927	A
8	A	1929	G
8	A	1930	G
8	A	1937	A
8	A	1938	A
8	A	1955	U
8	A	1965	C
8	A	1967	C
8	A	1970	A
8	A	1971	U
8	A	1972	G
8	A	1982	U
8	A	1991	U
8	A	1996	C
8	A	1997	C
8	A	2020	A
8	A	2022	U
8	A	2023	C
8	A	2031	A
8	A	2032	G
8	A	2033	A
8	A	2043	C
8	A	2046	G
8	A	2052	A
8	A	2055	C
8	A	2056	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2069	G7M
8	A	2072	C
8	A	2093	G
8	A	2100	G
8	A	2101	A
8	A	2105	U
8	A	2106	U
8	A	2108	A
8	A	2111	U
8	A	2112	G
8	A	2113	U
8	A	2114	A
8	A	2115	G

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Mol	Chain	Res	Type
8	A	2116	G
8	A	2118	U
8	A	2119	A
8	A	2120	G
8	A	2121	G
8	A	2124	G
8	A	2125	G
8	A	2126	A
8	A	2127	G
8	A	2128	G
8	A	2129	C
8	A	2131	U
8	A	2134	A
8	A	2135	A
8	A	2136	G
8	A	2137	U
8	A	2138	G
8	A	2139	U
8	A	2140	G
8	A	2141	G
8	A	2142	A
8	A	2143	C
8	A	2144	G
8	A	2145	C
8	A	2146	C
8	A	2147	A
8	A	2149	U
8	A	2151	U
8	A	2152	G
8	A	2154	A
8	A	2155	U
8	A	2156	G
8	A	2157	G
8	A	2158	A
8	A	2159	G
8	A	2162	G
8	A	2163	A
8	A	2164	C
8	A	2165	C
8	A	2166	U
8	A	2167	U
8	A	2170	A

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Mol	Chain	Res	Type
8	A	2171	A
8	A	2172	U
8	A	2173	A
8	A	2174	C
8	A	2175	C
8	A	2176	A
8	A	2177	C
8	A	2178	C
8	A	2180	U
8	A	2181	U
8	A	2183	A
8	A	2186	G
8	A	2189	U
8	A	2193	G
8	A	2198	A
8	A	2203	U
8	A	2204	G
8	A	2211	A
8	A	2212	A
8	A	2225	A
8	A	2238	G
8	A	2239	G
8	A	2251	OMG
8	A	2267	A
8	A	2268	A
8	A	2278	A
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2297	A
8	A	2305	U
8	A	2309	A
8	A	2310	C
8	A	2320	U
8	A	2322	A
8	A	2325	G
8	A	2333	A
8	A	2335	A
8	A	2344	U
8	A	2345	G
8	A	2347	C
8	A	2350	C

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Mol	Chain	Res	Type
8	A	2361	G
8	A	2383	G
8	A	2385	C
8	A	2396	G
8	A	2402	U
8	A	2403	C
8	A	2406	A
8	A	2407	A
8	A	2423	U
8	A	2425	A
8	A	2429	G
8	A	2435	A
8	A	2441	U
8	A	2445	2MG
8	A	2448	A
8	A	2459	A
8	A	2469	A
8	A	2473	U
8	A	2475	C
8	A	2476	A
8	A	2489	U
8	A	2494	G
8	A	2502	G
8	A	2504	PSU
8	A	2505	G
8	A	2513	A
8	A	2518	A
8	A	2529	G
8	A	2547	A
8	A	2554	U
8	A	2566	A
8	A	2567	G
8	A	2569	G
8	A	2573	C
8	A	2582	G
8	A	2585	U
8	A	2586	U
8	A	2602	A
8	A	2609	U
8	A	2610	C
8	A	2613	U
8	A	2615	U

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Mol	Chain	Res	Type
8	A	2629	U
8	A	2630	G
8	A	2633	G
8	A	2655	G
8	A	2656	U
8	A	2663	G
8	A	2685	G
8	A	2689	U
8	A	2690	U
8	A	2702	G
8	A	2714	G
8	A	2716	C
8	A	2718	G
8	A	2726	A
8	A	2727	A
8	A	2729	G
8	A	2732	G
8	A	2733	A
8	A	2739	U
8	A	2744	G
8	A	2748	A
8	A	2757	A
8	A	2761	A
8	A	2765	A
8	A	2777	G
8	A	2778	A
8	A	2779	U
8	A	2791	G
8	A	2797	U
8	A	2800	A
8	A	2808	G
8	A	2809	A
8	A	2818	U
8	A	2820	A
8	A	2821	A
8	A	2833	U
8	A	2861	U
8	A	2867	G
8	A	2868	A
8	A	2873	A
8	A	2879	A
8	A	2880	C

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Mol	Chain	Res	Type
8	A	2884	U
8	A	2886	A
8	A	2891	U
8	A	2894	G
8	A	2901	C
9	B	9	G
9	B	25	U
9	B	35	C
9	B	36	C
9	B	41	G
9	B	42	C
9	B	45	A
9	B	51	G
9	B	53	A
9	B	56	G
9	B	57	A
9	B	67	G
9	B	68	C
9	B	73	A
9	B	88	C
9	B	89	U
9	B	109	A
9	B	120	U
34	a	3	A
34	a	4	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	22	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A
34	a	52	C
34	a	70	U
34	a	71	A
34	a	72	A
34	a	76	G
34	a	78	A
34	a	79	G

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Mol	Chain	Res	Type
34	a	80	A
34	a	81	A
34	a	82	G
34	a	83	C
34	a	84	U
34	a	85	U
34	a	87	C
34	a	88	U
34	a	89	U
34	a	92	U
34	a	93	U
34	a	94	G
34	a	95	C
34	a	96	U
34	a	116	A
34	a	121	U
34	a	129	A
34	a	130	A
34	a	141	G
34	a	144	G
34	a	148	G
34	a	163	C
34	a	164	G
34	a	171	A
34	a	173	U
34	a	177	G
34	a	179	A
34	a	182	A
34	a	184	G
34	a	189	A
34	a	197	A
34	a	198	G
34	a	206	C
34	a	207	C
34	a	208	U
34	a	209	U
34	a	210	C
34	a	211	G
34	a	215	C
34	a	226	G
34	a	240	G
34	a	245	U

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Mol	Chain	Res	Type
34	a	247	G
34	a	251	G
34	a	262	A
34	a	266	G
34	a	267	C
34	a	279	A
34	a	280	C
34	a	289	G
34	a	293	G
34	a	299	G
34	a	301	G
34	a	316	C
34	a	321	A
34	a	328	C
34	a	344	A
34	a	347	G
34	a	348	G
34	a	351	G
34	a	352	C
34	a	354	G
34	a	356	A
34	a	367	U
34	a	372	C
34	a	373	A
34	a	375	U
34	a	382	A
34	a	389	A
34	a	390	U
34	a	392	C
34	a	406	G
34	a	412	A
34	a	413	G
34	a	414	A
34	a	421	U
34	a	424	G
34	a	429	U
34	a	445	G
34	a	461	A
34	a	462	G
34	a	463	U
34	a	465	A
34	a	466	A

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Mol	Chain	Res	Type
34	a	467	U
34	a	468	A
34	a	469	C
34	a	470	C
34	a	471	U
34	a	479	U
34	a	481	G
34	a	482	A
34	a	484	G
34	a	495	A
34	a	496	A
34	a	499	A
34	a	509	A
34	a	510	A
34	a	511	C
34	a	512	U
34	a	516	PSU
34	a	518	C
34	a	521	G
34	a	524	G
34	a	527	G7M
34	a	530	G
34	a	532	A
34	a	547	A
34	a	559	A
34	a	562	U
34	a	564	C
34	a	572	A
34	a	573	A
34	a	576	C
34	a	577	G
34	a	579	A
34	a	596	A
34	a	615	G
34	a	632	U
34	a	633	G
34	a	636	U
34	a	641	U
34	a	650	G
34	a	654	G
34	a	665	A
34	a	703	G

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Mol	Chain	Res	Type
34	a	704	A
34	a	721	G
34	a	724	G
34	a	731	G
34	a	748	G
34	a	749	A
34	a	755	G
34	a	777	A
34	a	781	A
34	a	790	A
34	a	794	A
34	a	799	G
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	829	G
34	a	832	G
34	a	836	G
34	a	841	C
34	a	842	U
34	a	843	U
34	a	846	G
34	a	872	A
34	a	884	U
34	a	889	A
34	a	890	G
34	a	891	U
34	a	902	G
34	a	914	A
34	a	926	G
34	a	934	C
34	a	935	A
34	a	960	U
34	a	961	U
34	a	966	2MG
34	a	967	5MC
34	a	969	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	992	U

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Mol	Chain	Res	Type
34	a	993	G
34	a	996	A
34	a	999	C
34	a	1004	A
34	a	1009	U
34	a	1017	U
34	a	1020	G
34	a	1024	G
34	a	1028	C
34	a	1029	U
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1035	A
34	a	1044	A
34	a	1045	C
34	a	1050	G
34	a	1065	U
34	a	1085	U
34	a	1094	G
34	a	1101	A
34	a	1108	G
34	a	1124	G
34	a	1126	U
34	a	1130	A
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1139	G
34	a	1144	G
34	a	1146	A
34	a	1154	G
34	a	1159	U
34	a	1160	G
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1183	U
34	a	1184	G
34	a	1196	A
34	a	1197	A
34	a	1212	U

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Mol	Chain	Res	Type
34	a	1213	A
34	a	1225	A
34	a	1227	A
34	a	1238	A
34	a	1250	A
34	a	1257	A
34	a	1275	A
34	a	1280	A
34	a	1287	A
34	a	1294	G
34	a	1297	G
34	a	1299	A
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1306	A
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1322	C
34	a	1331	G
34	a	1332	A
34	a	1346	A
34	a	1348	U
34	a	1353	G
34	a	1363	A
34	a	1364	U
34	a	1368	A
34	a	1370	G
34	a	1378	C
34	a	1379	G
34	a	1398	A
34	a	1400	C
34	a	1419	G
34	a	1422	G
34	a	1429	A
34	a	1441	A
34	a	1442	G
34	a	1446	A
34	a	1451	U
34	a	1492	A
34	a	1493	A

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Mol	Chain	Res	Type
34	a	1494	G
34	a	1497	G
34	a	1499	A
34	a	1506	U
34	a	1517	G
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1537	U
34	a	1538	C
34	a	1540	U
56	w	9	A
56	w	13	C
56	w	16	U
56	w	17	C
56	w	18	G
56	w	20	U
56	w	21	A
56	w	22	G
56	w	46	G7M
56	w	47	U
56	w	58	A
56	w	75	C
56	w	76	A
57	x	16	U
57	x	19	A
57	x	20	A
57	x	23	U
57	x	24	G
57	x	25	U
57	x	26	U
57	x	27	U

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	102	U
8	A	141	G
8	A	228	C
8	A	242	G

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Mol	Chain	Res	Type
8	A	310	A
8	A	323	C
8	A	456	C
8	A	464	U
8	A	490	C
8	A	547	A
8	A	555	G
8	A	614	A
8	A	784	G
8	A	883	G
8	A	886	A
8	A	887	U
8	A	890	C
8	A	894	U
8	A	1020	A
8	A	1074	G
8	A	1110	G
8	A	1173	U
8	A	1182	G
8	A	1211	C
8	A	1300	G
8	A	1320	C
8	A	1331	G
8	A	1399	C
8	A	1458	U
8	A	1490	A
8	A	1491	G
8	A	1537	G
8	A	1565	C
8	A	1715	G
8	A	1730	C
8	A	1847	G
8	A	2107	G
8	A	2120	G
8	A	2138	G
8	A	2158	A
8	A	2192	U
8	A	2287	A
8	A	2319	G
8	A	2324	U
8	A	2334	U
8	A	2405	G

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Mol	Chain	Res	Type
8	A	2406	A
8	A	2468	A
8	A	2629	U
8	A	2655	G
8	A	2725	A
8	A	2728	U
8	A	2756	U
8	A	2808	G
8	A	2820	A
8	A	2832	U
9	B	44	G
9	B	52	A
9	B	66	A

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

41 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$
8	5MC	A	1962	8	18,22,23	3.63	7 (38%)	26,32,35	1.03	2 (7%)
8	2MA	A	2503	58,8	19,25,26	3.24	7 (36%)	21,37,40	1.78	4 (19%)
8	OMG	A	2251	56,8	18,26,27	2.46	8 (44%)	19,38,41	1.46	4 (21%)
34	4OC	a	1402	34	20,23,24	2.97	8 (40%)	26,32,35	0.92	2 (7%)
56	PSU	w	55	56	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
56	4SU	w	8	56	18,21,22	3.61	7 (38%)	26,30,33	2.22	4 (15%)
8	PSU	A	2604	8	18,21,22	1.33	2 (11%)	22,30,33	1.98	5 (22%)
34	MA6	a	1519	34	18,26,27	1.02	1 (5%)	19,38,41	2.78	2 (10%)
8	3TD	A	1915	58,8	18,22,23	4.33	5 (27%)	22,32,35	1.65	3 (13%)
8	5MC	A	747	8	18,22,23	3.62	7 (38%)	26,32,35	1.13	2 (7%)
56	G7M	w	46	56	20,26,27	2.46	7 (35%)	17,39,42	1.07	1 (5%)
8	1MG	A	745	8	18,26,27	2.63	4 (22%)	19,39,42	1.39	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	5MU	w	54	56	19,22,23	4.80	7 (36%)	28,32,35	3.65	9 (32%)
8	OMC	A	2498	58,8	19,22,23	2.86	7 (36%)	26,31,34	0.82	0
8	PSU	A	2457	8	18,21,22	1.01	2 (11%)	22,30,33	1.95	6 (27%)
8	6MZ	A	2030	8	18,25,26	2.12	3 (16%)	16,36,39	2.32	3 (18%)
8	PSU	A	1911	8	18,21,22	1.08	2 (11%)	22,30,33	1.77	4 (18%)
34	2MG	a	966	34	18,26,27	2.60	7 (38%)	16,38,41	1.59	4 (25%)
8	PSU	A	2605	8	18,21,22	1.33	2 (11%)	22,30,33	1.89	4 (18%)
34	5MC	a	967	34	18,22,23	3.69	7 (38%)	26,32,35	1.00	2 (7%)
56	MIA	w	37	56	24,31,32	2.46	4 (16%)	26,44,47	2.93	9 (34%)
8	G7M	A	2069	8	20,26,27	3.93	9 (45%)	17,39,42	1.14	2 (11%)
8	PSU	A	1917	8	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
34	5MC	a	1407	34	18,22,23	3.65	7 (38%)	26,32,35	0.99	1 (3%)
8	PSU	A	2504	8	18,21,22	1.02	1 (5%)	22,30,33	1.90	5 (22%)
34	G7M	a	527	34	20,26,27	4.02	10 (50%)	17,39,42	1.04	1 (5%)
34	2MG	a	1207	34	18,26,27	2.59	7 (38%)	16,38,41	1.39	4 (25%)
34	UR3	a	1498	34	19,22,23	2.63	6 (31%)	26,32,35	1.49	3 (11%)
56	PSU	w	32	56	18,21,22	1.00	1 (5%)	22,30,33	1.64	5 (22%)
56	PSU	w	39	56	18,21,22	1.01	1 (5%)	22,30,33	1.75	3 (13%)
34	MA6	a	1518	34	18,26,27	1.01	1 (5%)	19,38,41	2.65	2 (10%)
8	PSU	A	2580	8	18,21,22	1.08	2 (11%)	22,30,33	1.92	5 (22%)
8	2MG	A	2445	8	18,26,27	2.58	7 (38%)	16,38,41	1.56	4 (25%)
8	5MU	A	1939	8	19,22,23	4.67	7 (36%)	28,32,35	3.75	10 (35%)
8	6MZ	A	1618	8	18,25,26	2.13	3 (16%)	16,36,39	2.06	3 (18%)
8	PSU	A	955	58,8	18,21,22	1.09	1 (5%)	22,30,33	1.85	5 (22%)
8	PSU	A	746	58,8	18,21,22	1.09	2 (11%)	22,30,33	1.78	4 (18%)
34	PSU	a	516	58,34	18,21,22	0.93	2 (11%)	22,30,33	1.76	5 (22%)
34	2MG	a	1516	34	18,26,27	2.63	7 (38%)	16,38,41	1.47	4 (25%)
8	2MG	A	1835	8	18,26,27	2.57	7 (38%)	16,38,41	1.50	4 (25%)
8	OMU	A	2552	8	19,22,23	2.92	8 (42%)	26,31,34	1.79	5 (19%)

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
8	5MC	A	1962	8	-	0/7/25/26	0/2/2/2
8	2MA	A	2503	58,8	-	2/3/25/26	0/3/3/3
8	OMG	A	2251	56,8	-	3/5/27/28	0/3/3/3
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	1/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	1/7/29/30	0/3/3/3
8	3TD	A	1915	58,8	-	3/7/25/26	0/2/2/2
8	5MC	A	747	8	-	4/7/25/26	0/2/2/2
56	G7M	w	46	56	-	3/3/25/26	0/3/3/3
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
56	5MU	w	54	56	-	2/7/25/26	0/2/2/2
8	OMC	A	2498	58,8	-	0/9/27/28	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	0/5/27/28	0/3/3/3
8	PSU	A	2605	8	-	1/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
34	G7M	a	527	34	-	3/3/25/26	0/3/3/3
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
8	5MU	A	1939	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	1/5/27/28	0/3/3/3
8	PSU	A	955	58,8	-	0/7/25/26	0/2/2/2
8	PSU	A	746	58,8	-	1/7/25/26	0/2/2/2
34	PSU	a	516	58,34	-	3/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	OMU	A	2552	8	-	2/9/27/28	0/2/2/2

All (195) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C6-C5	13.20	1.50	1.35
56	w	54	5MU	C2-N1	10.85	1.55	1.38
56	w	54	5MU	C6-N1	10.39	1.55	1.38
8	A	1939	5MU	C2-N1	10.23	1.54	1.38
8	A	1939	5MU	C6-N1	10.22	1.55	1.38
56	w	54	5MU	C4-C5	10.04	1.61	1.44
34	a	527	G7M	C8-N7	9.99	1.51	1.33
8	A	2069	G7M	C8-N7	9.96	1.51	1.33
34	a	527	G7M	C8-N9	9.66	1.50	1.33
8	A	2069	G7M	C8-N9	9.65	1.50	1.33
8	A	1915	3TD	C2-N1	9.53	1.49	1.37
8	A	1939	5MU	C4-C5	9.49	1.60	1.44
34	a	1407	5MC	C6-C5	9.35	1.50	1.34
34	a	967	5MC	C6-C5	9.19	1.49	1.34
8	A	747	5MC	C6-C5	9.00	1.49	1.34
8	A	1962	5MC	C6-C5	8.95	1.49	1.34
8	A	2503	2MA	C4-N3	8.57	1.49	1.35
56	w	8	4SU	C4-N3	8.27	1.46	1.37
8	A	1939	5MU	C4-N3	-8.05	1.23	1.38
56	w	54	5MU	C4-N3	-7.82	1.24	1.38
8	A	1618	6MZ	C6-N6	7.58	1.47	1.35
8	A	2030	6MZ	C6-N6	7.39	1.47	1.35
8	A	745	1MG	C2-N2	7.25	1.47	1.34
56	w	8	4SU	C2-N1	7.19	1.50	1.38
56	w	37	MIA	C13-C14	7.15	1.52	1.32
8	A	1962	5MC	C4-N3	6.88	1.45	1.34
34	a	967	5MC	C4-N3	6.88	1.45	1.34
8	A	2552	OMU	C2-N1	6.81	1.49	1.38
8	A	747	5MC	C4-N3	6.76	1.45	1.34
8	A	2503	2MA	C2-N3	6.74	1.46	1.34
34	a	1498	UR3	C2-N1	6.64	1.48	1.38
34	a	1402	4OC	C4-N3	6.60	1.44	1.32
56	w	37	MIA	C2-S10	6.56	1.81	1.75
34	a	1407	5MC	C4-N3	6.50	1.45	1.34
8	A	2552	OMU	C2-N3	6.39	1.49	1.38
8	A	1962	5MC	C2-N3	6.20	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2498	OMC	C2-N3	6.13	1.48	1.36
34	a	967	5MC	C2-N3	6.13	1.48	1.36
34	a	1207	2MG	C2-N2	6.13	1.47	1.33
8	A	747	5MC	C2-N3	6.12	1.48	1.36
34	a	1516	2MG	C2-N2	6.11	1.47	1.33
8	A	2498	OMC	C6-C5	6.11	1.49	1.35
34	a	966	2MG	C2-N2	6.08	1.46	1.33
34	a	1402	4OC	C6-C5	6.07	1.49	1.35
34	a	1407	5MC	C2-N3	6.03	1.48	1.36
8	A	1835	2MG	C2-N2	6.01	1.46	1.33
34	a	1498	UR3	C6-C5	5.97	1.48	1.35
8	A	1915	3TD	C6-N1	5.91	1.46	1.36
8	A	2445	2MG	C2-N2	5.88	1.46	1.33
56	w	8	4SU	C6-C5	5.85	1.48	1.35
56	w	54	5MU	C6-C5	5.83	1.44	1.34
8	A	1939	5MU	C6-C5	5.75	1.44	1.34
56	w	46	G7M	C2-N3	5.75	1.47	1.33
34	a	527	G7M	C2-N3	5.73	1.47	1.33
56	w	8	4SU	C2-N3	5.67	1.48	1.38
8	A	2498	OMC	C4-N3	5.63	1.45	1.34
8	A	2503	2MA	C2-N1	5.60	1.44	1.34
56	w	37	MIA	C6-N6	5.59	1.44	1.34
34	a	1402	4OC	C2-N3	5.57	1.47	1.36
8	A	745	1MG	C2-N3	5.47	1.44	1.34
8	A	2552	OMU	C6-C5	5.42	1.47	1.35
8	A	2069	G7M	C2-N3	5.34	1.46	1.33
8	A	2503	2MA	C6-N1	5.12	1.43	1.33
56	w	8	4SU	C4-S4	-5.12	1.58	1.68
8	A	2251	OMG	C2-N3	5.00	1.45	1.33
34	a	966	2MG	C4-N3	4.96	1.49	1.37
56	w	46	G7M	C4-N3	4.94	1.49	1.37
34	a	967	5MC	C4-N4	4.93	1.46	1.34
34	a	1516	2MG	C4-N3	4.93	1.49	1.37
34	a	1207	2MG	C4-N3	4.88	1.49	1.37
34	a	1407	5MC	C4-N4	4.85	1.46	1.34
34	a	527	G7M	C6-N1	4.81	1.45	1.37
8	A	745	1MG	C4-N3	4.81	1.49	1.37
8	A	1835	2MG	C4-N3	4.80	1.49	1.37
8	A	2251	OMG	C4-N3	4.78	1.49	1.37
8	A	1962	5MC	C4-N4	4.77	1.46	1.34
8	A	747	5MC	C4-N4	4.77	1.46	1.34
8	A	2445	2MG	C4-N3	4.75	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C2-N3	4.73	1.49	1.38
34	a	527	G7M	C2-N2	4.71	1.45	1.34
34	a	1498	UR3	C2-N3	4.63	1.48	1.39
8	A	2069	G7M	C6-N1	4.55	1.44	1.37
34	a	1407	5MC	C6-N1	4.55	1.45	1.38
34	a	1516	2MG	C2-N1	4.54	1.44	1.36
8	A	2069	G7M	C2-N2	4.50	1.44	1.34
34	a	967	5MC	C6-N1	4.43	1.45	1.38
34	a	1207	2MG	C2-N1	4.42	1.43	1.36
8	A	2251	OMG	C2-N2	4.41	1.44	1.34
8	A	1962	5MC	C6-N1	4.40	1.45	1.38
8	A	1835	2MG	C2-N1	4.37	1.43	1.36
56	w	46	G7M	C2-N2	4.36	1.44	1.34
8	A	2445	2MG	C2-N1	4.34	1.43	1.36
34	a	966	2MG	C2-N1	4.34	1.43	1.36
34	a	967	5MC	C2-N1	4.20	1.49	1.40
8	A	747	5MC	C6-N1	4.19	1.45	1.38
34	a	527	G7M	C4-N3	4.14	1.47	1.37
8	A	747	5MC	C2-N1	4.10	1.48	1.40
8	A	1962	5MC	C2-N1	4.07	1.48	1.40
34	a	1402	4OC	C4-N4	4.06	1.44	1.35
34	a	1407	5MC	C2-N1	4.01	1.48	1.40
8	A	2069	G7M	C4-N3	3.90	1.46	1.37
34	a	1402	4OC	C5-C4	3.88	1.49	1.40
8	A	2498	OMC	C4-N4	3.83	1.42	1.33
8	A	2552	OMU	C4-N3	3.74	1.45	1.38
56	w	46	G7M	C6-N1	3.74	1.43	1.37
34	a	527	G7M	C2-N1	3.72	1.46	1.37
34	a	1402	4OC	C2-N1	3.59	1.47	1.40
34	a	1516	2MG	C6-N1	3.55	1.43	1.37
8	A	2069	G7M	C2-N1	3.51	1.46	1.37
8	A	2251	OMG	C6-N1	3.44	1.43	1.37
34	a	1207	2MG	C6-N1	3.43	1.43	1.37
8	A	2498	OMC	C2-N1	3.38	1.47	1.40
8	A	747	5MC	O2-C2	-3.33	1.17	1.23
34	a	966	2MG	C6-N1	3.33	1.42	1.37
56	w	46	G7M	C5-C6	3.33	1.54	1.45
8	A	2445	2MG	C5-C4	-3.30	1.34	1.43
8	A	1835	2MG	C6-N1	3.30	1.42	1.37
8	A	2498	OMC	C6-N1	3.29	1.45	1.38
34	a	967	5MC	O2-C2	-3.28	1.17	1.23
56	w	55	PSU	C6-C5	3.23	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1962	5MC	O2-C2	-3.20	1.17	1.23
8	A	2605	PSU	C6-C5	3.18	1.39	1.35
8	A	2445	2MG	O6-C6	-3.17	1.16	1.23
8	A	2604	PSU	C6-C5	3.16	1.39	1.35
56	w	8	4SU	C5-C4	3.15	1.46	1.42
34	a	1407	5MC	O2-C2	-3.13	1.17	1.23
8	A	2445	2MG	C6-N1	3.13	1.42	1.37
8	A	2552	OMU	O4-C4	-3.11	1.18	1.24
8	A	1911	PSU	C6-C5	3.11	1.38	1.35
8	A	2030	6MZ	C5-C4	-3.10	1.32	1.40
8	A	1835	2MG	C5-C4	-3.10	1.35	1.43
8	A	1835	2MG	O6-C6	-3.07	1.17	1.23
34	a	1516	2MG	C5-C4	-3.07	1.35	1.43
34	a	1402	4OC	O2-C2	-3.06	1.18	1.23
8	A	955	PSU	C6-C5	3.04	1.38	1.35
8	A	1917	PSU	C6-C5	3.03	1.38	1.35
34	a	966	2MG	C5-C4	-2.99	1.35	1.43
34	a	966	2MG	C5-C6	2.99	1.53	1.47
8	A	2251	OMG	C5-C6	2.98	1.53	1.47
34	a	1516	2MG	O6-C6	-2.98	1.17	1.23
8	A	1618	6MZ	C5-C4	-2.96	1.33	1.40
34	a	1402	4OC	C6-N1	2.96	1.45	1.38
8	A	2504	PSU	C6-C5	2.94	1.38	1.35
34	a	1207	2MG	C5-C4	-2.94	1.35	1.43
34	a	966	2MG	O6-C6	-2.92	1.17	1.23
8	A	2498	OMC	O2-C2	-2.92	1.18	1.23
56	w	37	MIA	C5-C4	-2.91	1.33	1.40
34	a	1207	2MG	O6-C6	-2.89	1.17	1.23
56	w	32	PSU	C6-C5	2.89	1.38	1.35
34	a	1207	2MG	C5-C6	2.88	1.53	1.47
8	A	2580	PSU	C6-C5	2.85	1.38	1.35
8	A	745	1MG	C5-C4	-2.84	1.35	1.43
8	A	2251	OMG	C5-C4	-2.84	1.35	1.43
34	a	1498	UR3	C6-N1	2.82	1.44	1.38
8	A	1915	3TD	C4-N3	2.82	1.46	1.40
34	a	1516	2MG	C5-C6	2.81	1.53	1.47
8	A	746	PSU	C6-C5	2.79	1.38	1.35
8	A	1835	2MG	C5-C6	2.79	1.53	1.47
8	A	1939	5MU	O2-C2	-2.79	1.17	1.23
34	a	1519	MA6	C5-C4	-2.79	1.33	1.40
56	w	46	G7M	C2-N1	2.75	1.44	1.37
8	A	1939	5MU	O4-C4	-2.74	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	54	5MU	O4-C4	-2.72	1.18	1.23
8	A	1618	6MZ	C2-N3	2.71	1.36	1.32
34	a	1518	MA6	C5-C4	-2.69	1.33	1.40
56	w	39	PSU	C6-C5	2.67	1.38	1.35
8	A	2604	PSU	C4-N3	-2.67	1.33	1.38
8	A	2552	OMU	C6-N1	2.66	1.44	1.38
34	a	527	G7M	C5-C6	2.64	1.52	1.45
8	A	2552	OMU	O2-C2	-2.64	1.18	1.23
8	A	2605	PSU	C4-N3	-2.60	1.34	1.38
8	A	2445	2MG	C5-C6	2.59	1.52	1.47
56	w	8	4SU	O2-C2	-2.57	1.18	1.23
8	A	2030	6MZ	C2-N3	2.55	1.36	1.32
56	w	54	5MU	O2-C2	-2.54	1.18	1.23
8	A	2503	2MA	C6-C5	2.51	1.52	1.43
8	A	2503	2MA	C6-N6	-2.46	1.24	1.34
8	A	2069	G7M	C5-C6	2.42	1.51	1.45
34	a	1498	UR3	O2-C2	-2.39	1.18	1.22
8	A	2069	G7M	O6-C6	-2.38	1.18	1.23
8	A	2251	OMG	C2-N1	2.35	1.43	1.37
34	a	516	PSU	C6-C5	2.33	1.38	1.35
34	a	1498	UR3	O4-C4	-2.33	1.18	1.23
34	a	527	G7M	O6-C6	-2.32	1.18	1.23
8	A	2457	PSU	C6-C5	2.32	1.38	1.35
8	A	746	PSU	C4-C5	-2.23	1.37	1.44
8	A	2251	OMG	O6-C6	-2.20	1.18	1.23
8	A	2580	PSU	O4'-C1'	-2.20	1.40	1.43
56	w	46	G7M	O6-C6	-2.19	1.18	1.23
8	A	2552	OMU	C5-C4	2.17	1.48	1.43
34	a	527	G7M	C5-C4	2.12	1.43	1.39
8	A	1911	PSU	C4-C5	-2.07	1.38	1.44
8	A	2457	PSU	O4'-C1'	-2.07	1.41	1.43
8	A	2503	2MA	C5-C4	-2.03	1.35	1.40
34	a	516	PSU	C4-C5	-2.01	1.38	1.44

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1939	5MU	C5-C4-N3	12.36	125.86	115.31
56	w	54	5MU	C5-C4-N3	12.15	125.69	115.31
8	A	1939	5MU	C5-C6-N1	-10.72	112.31	123.34
34	a	1519	MA6	N1-C6-N6	-10.32	106.19	117.06
56	w	54	5MU	C5-C6-N1	-10.32	112.72	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	37	MIA	C12-C13-C14	-9.95	107.78	127.14
34	a	1518	MA6	N1-C6-N6	-9.80	106.74	117.06
56	w	8	4SU	C4-N3-C2	-7.69	119.87	127.34
8	A	2604	PSU	N1-C2-N3	6.03	121.96	115.13
8	A	2605	PSU	N1-C2-N3	5.98	121.91	115.13
8	A	2030	6MZ	C9-N6-C6	-5.90	117.79	122.87
34	a	1519	MA6	N3-C2-N1	-5.74	119.71	128.68
8	A	2503	2MA	C2-N3-C4	5.72	120.17	115.52
34	a	1518	MA6	N3-C2-N1	-5.57	119.98	128.68
8	A	1939	5MU	O4-C4-C5	-5.54	118.47	124.90
8	A	2030	6MZ	N3-C2-N1	-5.43	120.18	128.68
56	w	8	4SU	C5-C4-N3	5.43	119.72	114.69
8	A	1618	6MZ	N3-C2-N1	-5.32	120.36	128.68
56	w	37	MIA	C11-S10-C2	5.28	106.21	102.27
8	A	1939	5MU	C4-N3-C2	-5.19	120.64	127.35
8	A	2552	OMU	C4-N3-C2	-5.16	119.77	126.58
8	A	1915	3TD	N1-C2-N3	5.08	120.15	116.14
8	A	1618	6MZ	C9-N6-C6	-5.03	118.54	122.87
8	A	2504	PSU	N1-C2-N3	5.02	120.82	115.13
56	w	54	5MU	O4-C4-C5	-4.98	119.13	124.90
8	A	2457	PSU	N1-C2-N3	4.90	120.68	115.13
8	A	2457	PSU	C4-N3-C2	-4.89	119.29	126.34
8	A	2580	PSU	N1-C2-N3	4.85	120.63	115.13
8	A	746	PSU	C4-N3-C2	-4.84	119.36	126.34
56	w	54	5MU	C4-N3-C2	-4.78	121.17	127.35
8	A	955	PSU	C4-N3-C2	-4.77	119.47	126.34
8	A	955	PSU	N1-C2-N3	4.71	120.46	115.13
56	w	39	PSU	C4-N3-C2	-4.68	119.59	126.34
56	w	55	PSU	N1-C2-N3	4.67	120.42	115.13
8	A	1939	5MU	N3-C2-N1	4.63	121.04	114.89
8	A	1911	PSU	C4-N3-C2	-4.61	119.69	126.34
8	A	1917	PSU	C4-N3-C2	-4.58	119.74	126.34
8	A	2504	PSU	C4-N3-C2	-4.55	119.79	126.34
8	A	2580	PSU	C4-N3-C2	-4.55	119.79	126.34
56	w	37	MIA	C16-C14-C13	-4.52	109.59	122.65
34	a	516	PSU	C4-N3-C2	-4.48	119.88	126.34
56	w	37	MIA	C15-C14-C13	-4.48	109.71	122.65
56	w	39	PSU	N1-C2-N3	4.48	120.20	115.13
34	a	1498	UR3	C4-N3-C2	-4.45	120.38	124.56
8	A	1917	PSU	N1-C2-N3	4.40	120.11	115.13
8	A	746	PSU	N1-C2-N3	4.40	120.11	115.13
8	A	1911	PSU	N1-C2-N3	4.35	120.06	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	32	PSU	C4-N3-C2	-4.35	120.08	126.34
56	w	55	PSU	C4-N3-C2	-4.30	120.14	126.34
56	w	54	5MU	N3-C2-N1	4.20	120.46	114.89
34	a	516	PSU	N1-C2-N3	4.19	119.88	115.13
8	A	2030	6MZ	C1'-N9-C4	-4.10	119.43	126.64
56	w	32	PSU	N1-C2-N3	4.10	119.78	115.13
8	A	1915	3TD	C4-N3-C2	-4.04	120.23	124.61
8	A	745	1MG	C5-C6-N1	3.97	119.88	113.90
56	w	54	5MU	C5M-C5-C6	-3.96	117.56	122.85
8	A	2605	PSU	C4-N3-C2	-3.94	120.67	126.34
8	A	2604	PSU	C4-N3-C2	-3.88	120.75	126.34
56	w	54	5MU	C5M-C5-C4	3.84	122.99	118.77
8	A	2552	OMU	N3-C2-N1	3.81	119.95	114.89
56	w	8	4SU	C5-C4-S4	-3.72	119.67	124.47
8	A	1939	5MU	C5M-C5-C6	-3.65	117.97	122.85
8	A	2445	2MG	C5-C6-N1	3.62	120.35	113.95
56	w	8	4SU	N3-C2-N1	3.61	119.69	114.89
8	A	1835	2MG	C5-C6-N1	3.57	120.25	113.95
34	a	1498	UR3	C1'-N1-C2	3.52	122.93	116.99
8	A	2605	PSU	O2-C2-N1	-3.48	118.96	122.79
8	A	2604	PSU	O2-C2-N1	-3.47	118.97	122.79
34	a	966	2MG	C5-C6-N1	3.45	120.05	113.95
34	a	1516	2MG	C5-C6-N1	3.45	120.03	113.95
8	A	2503	2MA	N3-C2-N1	-3.43	119.47	125.73
8	A	2251	OMG	C5-C6-N1	3.42	119.99	113.95
56	w	37	MIA	N3-C2-N1	-3.42	120.69	126.98
56	w	37	MIA	C2-N3-C4	3.41	120.03	115.32
34	a	1207	2MG	C5-C6-N1	3.41	119.97	113.95
8	A	2552	OMU	C5-C4-N3	3.33	119.83	114.84
8	A	2445	2MG	CM2-N2-C2	-3.26	116.67	123.86
34	a	967	5MC	C5-C6-N1	-3.24	120.01	123.34
8	A	1939	5MU	C5M-C5-C4	3.22	122.31	118.77
8	A	747	5MC	C5-C6-N1	-3.21	120.04	123.34
56	w	37	MIA	C12-N6-C6	-3.18	117.83	122.55
8	A	2580	PSU	O2-C2-N1	-3.18	119.29	122.79
56	w	55	PSU	O2-C2-N1	-3.06	119.42	122.79
34	a	1407	5MC	C5-C6-N1	-3.04	120.21	123.34
8	A	2251	OMG	C2-N1-C6	-3.03	119.52	125.10
56	w	46	G7M	C2-N1-C6	-3.02	119.54	125.10
8	A	1939	5MU	O2-C2-N1	-3.00	118.79	122.79
8	A	1835	2MG	CM2-N2-C2	-2.95	117.34	123.86
8	A	2552	OMU	C1'-N1-C2	2.94	122.90	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2457	PSU	O2-C2-N1	-2.92	119.58	122.79
56	w	37	MIA	S10-C2-N1	2.89	126.03	116.01
8	A	1618	6MZ	C1'-N9-C4	-2.86	121.62	126.64
34	a	516	PSU	O2-C2-N1	-2.82	119.68	122.79
8	A	2580	PSU	C6-N1-C2	-2.81	119.81	122.68
8	A	745	1MG	C8-N7-C5	2.80	108.32	102.99
8	A	1917	PSU	O2-C2-N1	-2.78	119.73	122.79
34	a	966	2MG	CM2-N2-C2	-2.77	117.74	123.86
8	A	2504	PSU	C6-N1-C2	-2.75	119.87	122.68
8	A	2552	OMU	O4-C4-C5	-2.73	120.36	125.16
56	w	55	PSU	C6-C5-C4	2.70	120.09	118.20
34	a	966	2MG	C8-N7-C5	2.70	108.13	102.99
34	a	527	G7M	C2-N1-C6	-2.67	120.18	125.10
8	A	2445	2MG	C8-N7-C5	2.67	108.08	102.99
8	A	2604	PSU	C3'-C2'-C1'	2.67	104.74	101.64
8	A	2503	2MA	C1'-N9-C4	-2.67	121.95	126.64
34	a	1516	2MG	C8-N7-C5	2.65	108.03	102.99
8	A	1962	5MC	C5-C6-N1	-2.63	120.63	123.34
8	A	2069	G7M	C2-N1-C6	-2.61	120.30	125.10
56	w	55	PSU	C6-N1-C2	-2.61	120.02	122.68
56	w	54	5MU	O4-C4-N3	-2.57	115.19	120.12
8	A	2457	PSU	C6-C5-C4	2.57	120.00	118.20
8	A	1835	2MG	C8-N7-C5	2.56	107.87	102.99
8	A	2504	PSU	O2-C2-N1	-2.53	120.01	122.79
8	A	2251	OMG	C8-N7-C5	2.53	107.80	102.99
8	A	2457	PSU	C6-N1-C2	-2.48	120.14	122.68
34	a	1207	2MG	C8-N7-C5	2.47	107.69	102.99
34	a	516	PSU	C6-N1-C2	-2.46	120.17	122.68
34	a	1498	UR3	C6-N1-C2	-2.44	119.61	121.79
8	A	1911	PSU	O2-C2-N1	-2.40	120.15	122.79
8	A	747	5MC	CM5-C5-C6	-2.40	119.64	122.85
34	a	1516	2MG	CM2-N2-C2	-2.38	118.60	123.86
8	A	2580	PSU	O4'-C1'-C2'	2.37	108.48	105.14
8	A	1835	2MG	O6-C6-C5	-2.37	119.75	124.37
8	A	2445	2MG	O6-C6-C5	-2.36	119.76	124.37
8	A	746	PSU	C6-C5-C4	2.36	119.85	118.20
8	A	2504	PSU	C6-C5-C4	2.35	119.84	118.20
8	A	1939	5MU	O4-C4-N3	-2.32	115.67	120.12
8	A	955	PSU	C6-N1-C2	-2.32	120.31	122.68
8	A	955	PSU	O2-C2-N1	-2.32	120.24	122.79
34	a	1516	2MG	O6-C6-C5	-2.31	119.86	124.37
8	A	1911	PSU	C6-N1-C2	-2.30	120.34	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1917	PSU	C6-N1-C2	-2.29	120.34	122.68
56	w	32	PSU	O2-C2-N1	-2.27	120.29	122.79
56	w	39	PSU	C6-N1-C2	-2.24	120.39	122.68
34	a	1207	2MG	O6-C6-C5	-2.21	120.05	124.37
34	a	1207	2MG	CM2-N2-C2	-2.21	118.99	123.86
8	A	2457	PSU	O4'-C1'-C2'	2.20	108.25	105.14
56	w	54	5MU	O2-C2-N1	-2.18	119.89	122.79
8	A	2251	OMG	O6-C6-C5	-2.18	120.12	124.37
56	w	37	MIA	C16-C14-C15	-2.18	109.80	114.60
34	a	1402	4OC	C6-C5-C4	2.16	119.60	116.96
56	w	32	PSU	C6-N1-C2	-2.14	120.49	122.68
34	a	966	2MG	O6-C6-C5	-2.10	120.27	124.37
8	A	746	PSU	O2-C2-N1	-2.10	120.48	122.79
34	a	516	PSU	O4'-C1'-C2'	2.08	108.08	105.14
8	A	955	PSU	C6-C5-C4	2.07	119.64	118.20
8	A	1962	5MC	CM5-C5-C6	-2.06	120.10	122.85
8	A	1915	3TD	O4'-C1'-C2'	2.05	108.04	105.14
34	a	1402	4OC	CM4-N4-C4	-2.05	118.45	122.45
8	A	745	1MG	O6-C6-C5	-2.04	120.58	124.19
8	A	2503	2MA	CM2-C2-N1	2.03	120.32	117.15
8	A	2069	G7M	N2-C2-N1	2.03	121.03	116.71
56	w	32	PSU	O4'-C1'-C2'	2.02	108.00	105.14
34	a	967	5MC	CM5-C5-C6	-2.02	120.15	122.85
8	A	2605	PSU	C5-C6-N1	-2.01	119.09	122.11
8	A	1939	5MU	C6-C5-C4	2.01	119.71	118.03
8	A	2604	PSU	C5-C6-N1	-2.00	119.11	122.11

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1618	6MZ	N1-C6-N6-C9
8	A	1915	3TD	C2'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2251	OMG	O4'-C4'-C5'-O5'
8	A	2251	OMG	C3'-C4'-C5'-O5'
8	A	2251	OMG	C1'-C2'-O2'-CM2
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C1'-N1-C2
8	A	2552	OMU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	C2'-C1'-C5-C6
56	w	39	PSU	O4'-C1'-C5-C6
56	w	46	G7M	O4'-C4'-C5'-O5'
8	A	2069	G7M	O4'-C4'-C5'-O5'
8	A	2503	2MA	O4'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
56	w	46	G7M	C3'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	2445	2MG	O4'-C4'-C5'-O5'
34	a	527	G7M	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
8	A	747	5MC	C3'-C4'-C5'-O5'
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	1835	2MG	C3'-C4'-C5'-O5'
8	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	527	G7M	O4'-C4'-C5'-O5'
34	a	516	PSU	O4'-C4'-C5'-O5'
8	A	747	5MC	C4'-C5'-O5'-P
34	a	1519	MA6	C4'-C5'-O5'-P
8	A	747	5MC	O4'-C4'-C5'-O5'
34	a	516	PSU	C3'-C4'-C5'-O5'
56	w	37	MIA	C3'-C4'-C5'-O5'
8	A	2604	PSU	C3'-C4'-C5'-O5'
34	a	527	G7M	C4'-C5'-O5'-P
8	A	2605	PSU	O4'-C1'-C5-C4
34	a	516	PSU	O4'-C1'-C5-C4
56	w	55	PSU	O4'-C1'-C5-C4
56	w	54	5MU	C3'-C4'-C5'-O5'
8	A	747	5MC	C2'-C1'-N1-C2
8	A	746	PSU	O4'-C1'-C5-C6
56	w	46	G7M	C4'-C5'-O5'-P
56	w	54	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 337 ligands modelled in this entry, 337 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 [i](#)

There are no chain breaks in this entry.