



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:26 pm GMT

PDB ID : 8PEG
EMDB ID : EMD-17631
Title : Escherichia coli paused disome complex (queueing 70S non-rotated closed PRE state)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-06-13
Resolution : 3.30 Å(reported)
Based on initial model : 7N1P

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

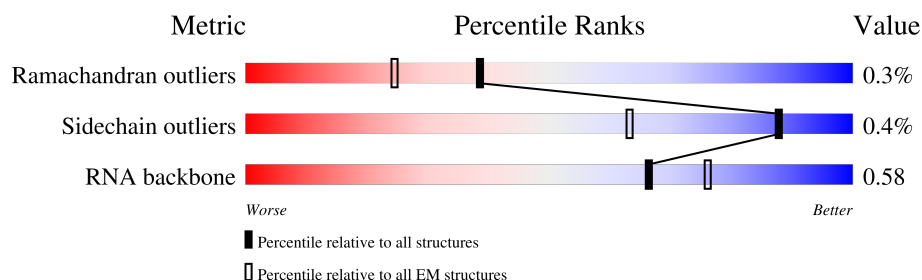
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.




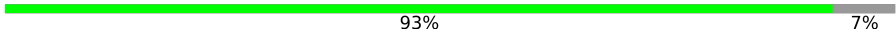

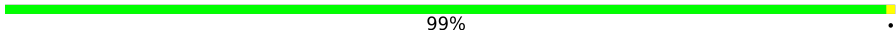
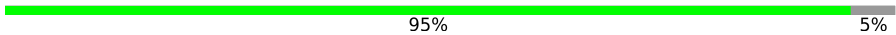


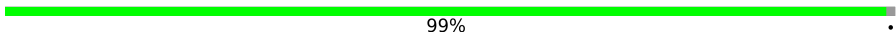
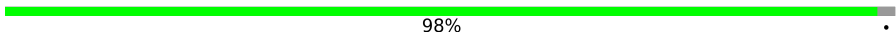
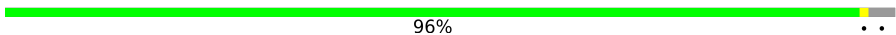


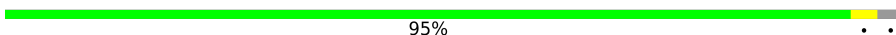

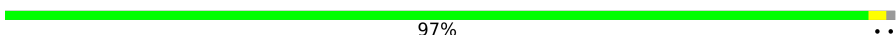
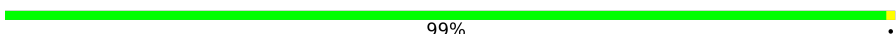
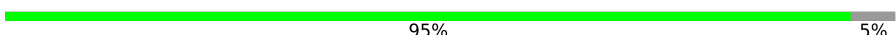
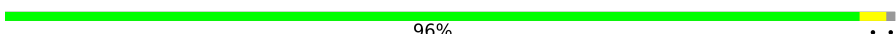

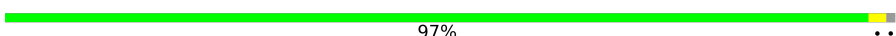
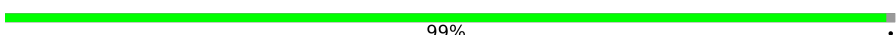




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	38	100%
2	1	78	96% ..
3	2	63	98% .
4	3	59	93% 5% .
5	4	70	94% ..
6	5	57	98% .
7	6	65	98% .
8	7	2903	81% 19% .
9	8	120	85% 13% .



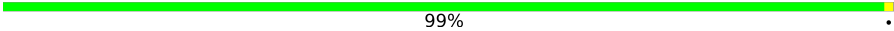
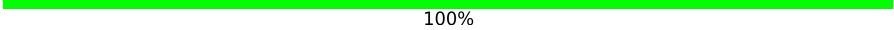
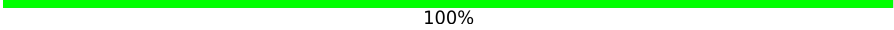
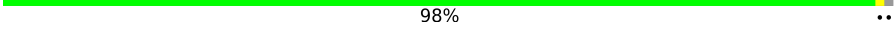
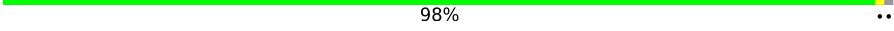
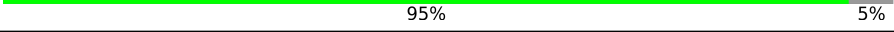
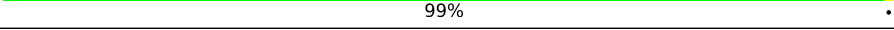
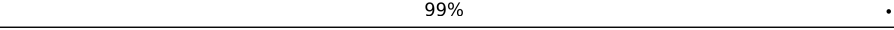

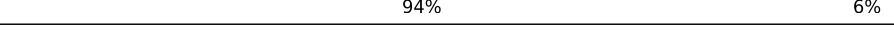
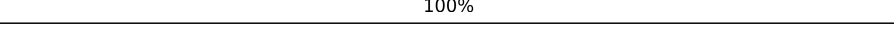
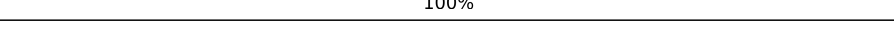
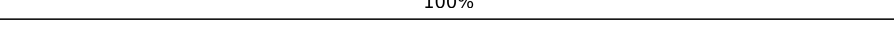
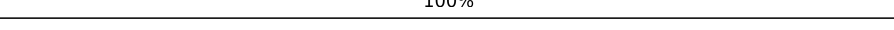
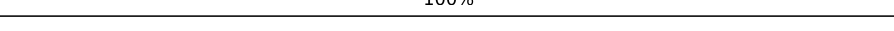
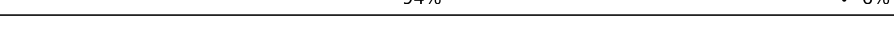
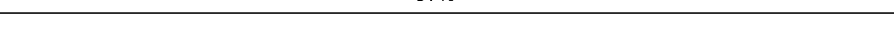
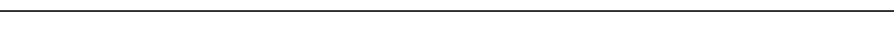

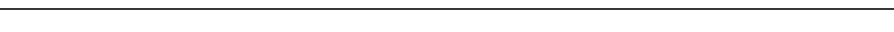
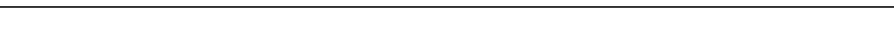


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Mol	Chain	Length	Quality of chain
10	A	1542	
11	B	241	
12	C	233	
13	D	206	
14	E	167	
15	F	135	
16	G	179	
17	H	130	
18	I	130	
19	J	103	
20	K	129	
21	L	124	
22	M	118	
23	N	101	
24	O	89	
25	P	82	
26	Q	84	
27	R	75	
28	S	92	
29	T	87	
30	U	71	
31	V	30	
32	W	76	
33	X	78	
34	Y	76	


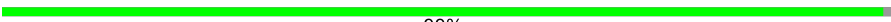
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Mol	Chain	Length	Quality of chain
35	Z	557	 31% 69%
36	a	234	 57% 43%
37	b	273	 99% ..
38	c	209	 100%
39	d	201	 100%
40	e	179	 98% ..
41	f	177	 98% ..
42	g	55	 95% 5%
43	h	136	 99% .
44	i	149	 99% .
45	j	165	 81% . 18%
46	k	142	 94% 6%
47	l	46	 100%
48	m	142	 100%
49	n	123	 100%
50	o	144	 100%
51	p	18	 100%
52	q	127	 94% . 6%
53	r	117	 97% ..
54	s	115	 99% .
55	t	118	 99% .
56	u	103	 99% .
57	v	110	 99% .
58	w	100	 93% 7%
59	x	104	 97% ..

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Mol	Chain	Length	Quality of chain
60	y	94	 100%
61	z	85	 99%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153284 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 L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 2 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 4 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 6 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	2903	Total	C	N	O	P	0	0
			62335	27815	11467	20150	2903		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		

- Molecule 11 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	224	Total	C	N	O	S	0	0
			1751	1108	314	321	8		

- Molecule 12 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 15 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 16 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 20 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 21 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 24 is a protein called 30S ribosomal protein S15.

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

- Molecule 25 is a protein called 30S ribosomal protein S16.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 27 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	74	Total	C	N	O	S	0	0
			624	395	122	105	2		

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 29 is a protein called Small ribosomal subunit protein bS20.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	30	Total	C	N	O	P	0	0
			648	290	124	204	30		

- Molecule 32 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	W	76	Total	C	N	O	P	S	0	0
			1632	731	289	534	76	2		

- Molecule 33 is a RNA chain called tRNA-Ser (E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	X	78	Total	C	N	O	P	S	0	0
			1683	750	304	548	78	3		

- Molecule 34 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
34	Y	76	Total	C	N	O	P	S	0	0
			1631	728	292	534	76	1		

- Molecule 35 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Z	170	Total	C	N	O		
			1319	830	228	261	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	a	134	Total	C	N	O	S	
			1026	645	186	193	2	0

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	e	178	Total	C	N	O	S	
			1420	905	251	258	6	0

- Molecule 41 is a protein called 50S ribosomal protein L6.

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

- Molecule 42 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	g	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 43 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 44 is a protein called 50S ribosomal protein L9.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 46 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	k	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 47 is a protein called 50S ribosomal protein L34.

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

- Molecule 48 is a protein called 50S ribosomal protein L13.

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

- Molecule 49 is a protein called 50S ribosomal protein L14.

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

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

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

- Molecule 51 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	p	18	Total	C	N	O	0	0
			101	63	18	20		

- Molecule 52 is a protein called 50S ribosomal protein L17.

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

- Molecule 53 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	r	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 54 is a protein called 50S ribosomal protein L19.

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

- Molecule 55 is a protein called 50S ribosomal protein L20.

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

- Molecule 56 is a protein called 50S ribosomal protein L21.

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

- Molecule 57 is a protein called 50S ribosomal protein L22.

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

- Molecule 58 is a protein called 50S ribosomal protein L23.

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

- Molecule 59 is a protein called 50S ribosomal protein L24.

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

- Molecule 60 is a protein called 50S ribosomal protein L25.

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

- Molecule 61 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	z	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

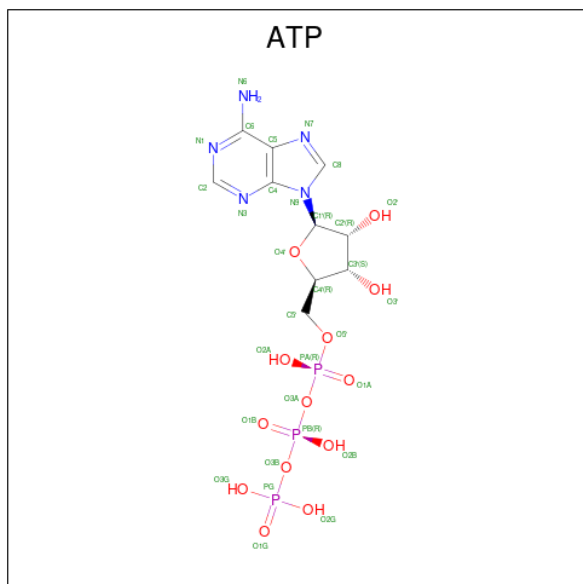
- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	0	1	Total	Zn	0
			1	1	
62	4	1	Total	Zn	0
			1	1	

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
63	7	193	Total	Mg	0
			193	193	
63	A	63	Total	Mg	0
			63	63	
63	X	1	Total	Mg	0
			1	1	
63	Y	1	Total	Mg	0
			1	1	
63	b	1	Total	Mg	0
			1	1	
63	o	1	Total	Mg	0
			1	1	

- Molecule 64 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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 L36

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 50S ribosomal protein L28

Chain 1:  96%



- Molecule 3: 50S ribosomal protein L29

Chain 2:  98%



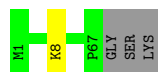
- Molecule 4: 50S ribosomal protein L30

Chain 3:  93% 5%



- Molecule 5: Large ribosomal subunit protein bL31A

Chain 4:  94%



- Molecule 6: 50S ribosomal protein L32

Chain 5:  98%



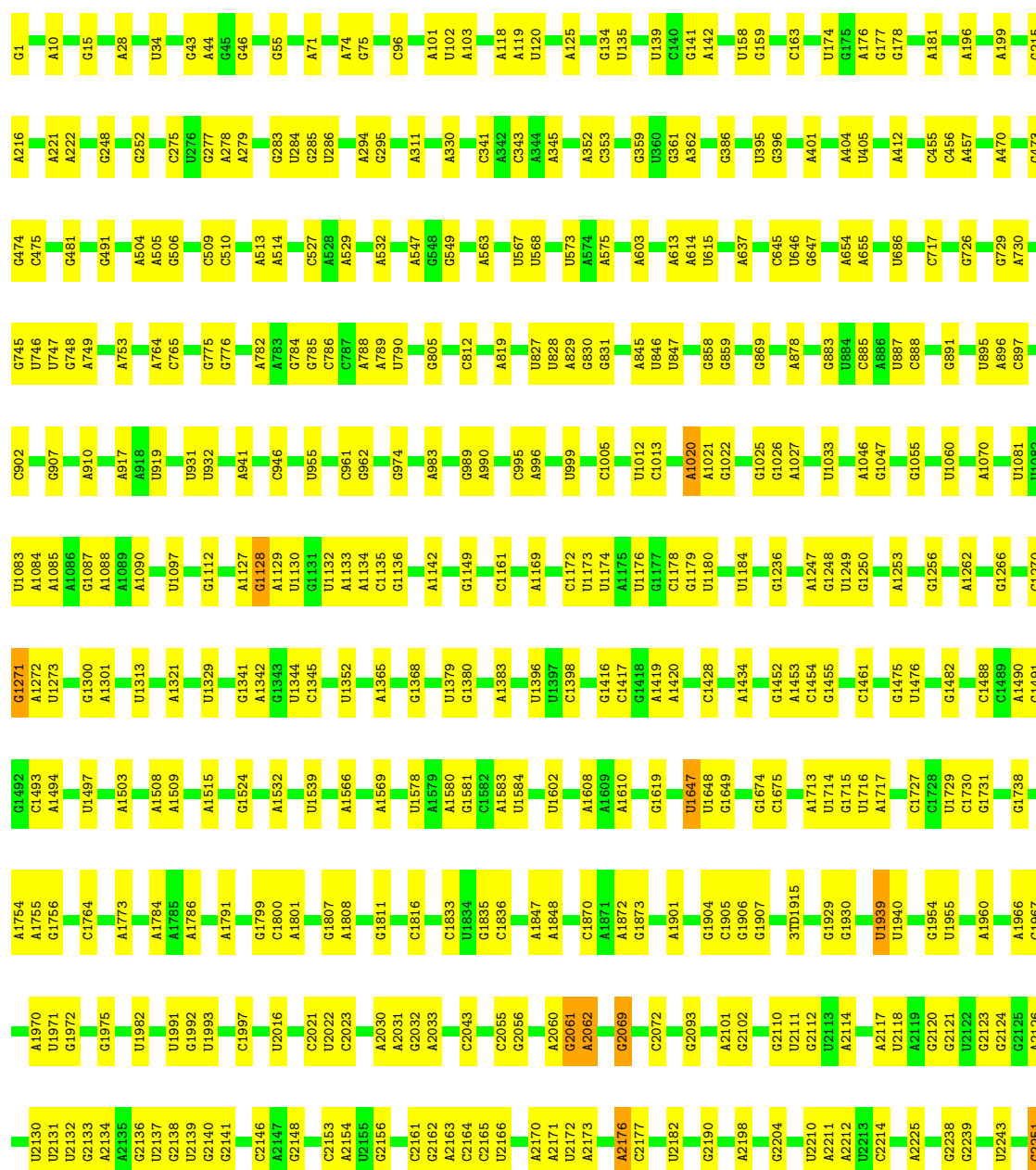
- Molecule 7: 50S ribosomal protein L35

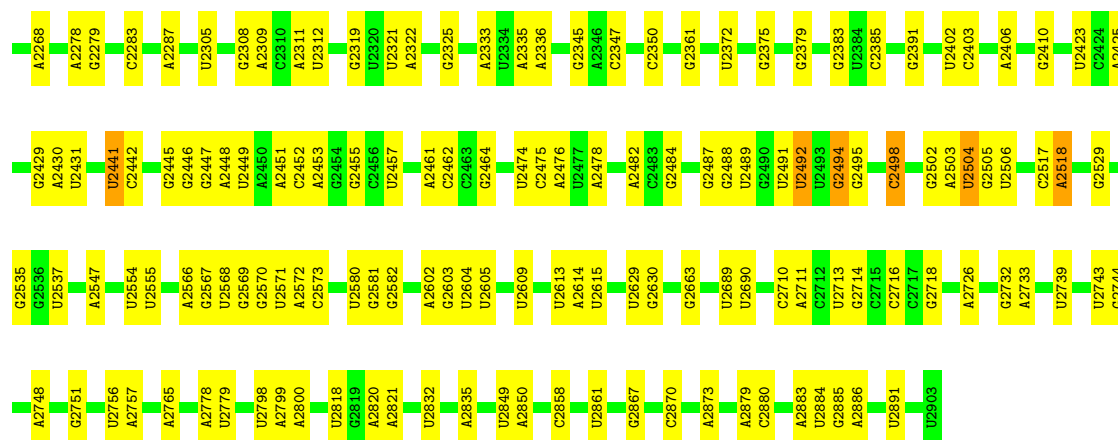
Chain 6: 98%



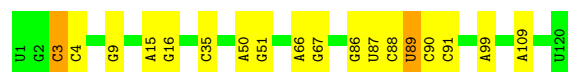
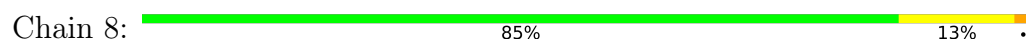
- Molecule 8: 23S ribosomal RNA

Chain 7: 81% 19%

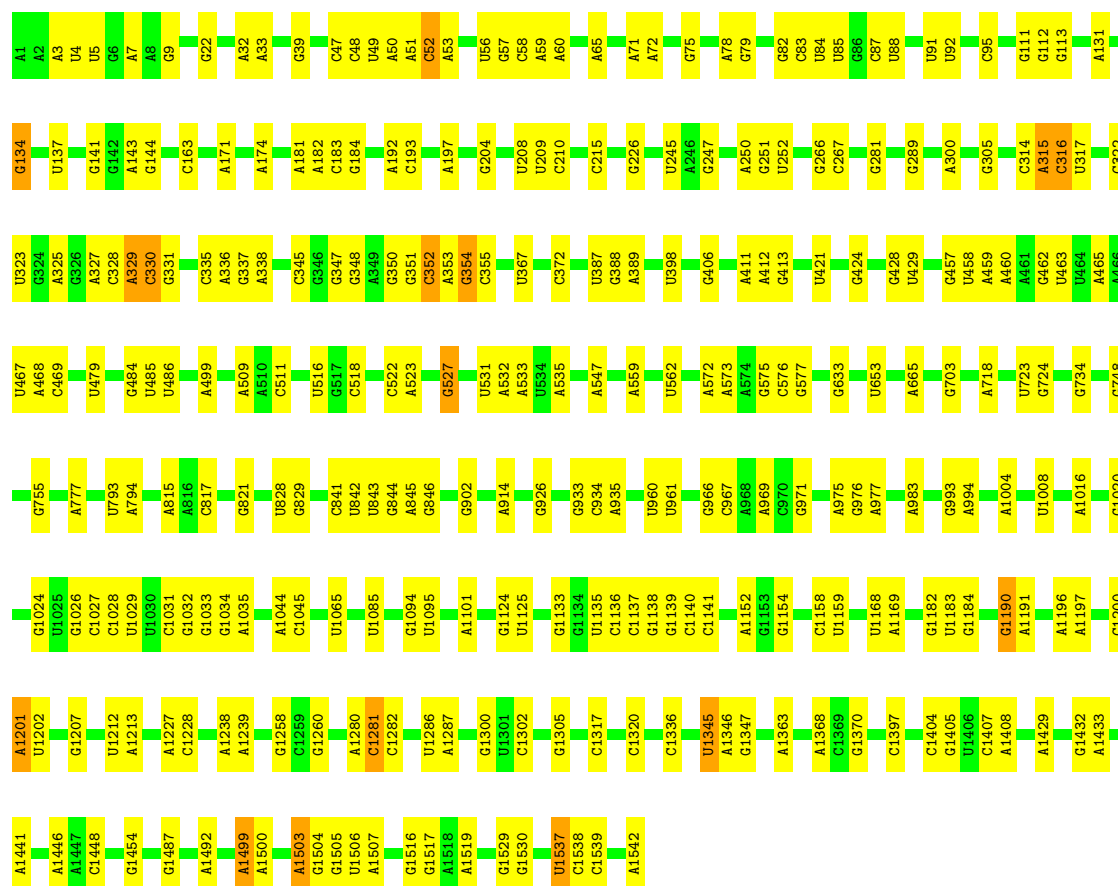
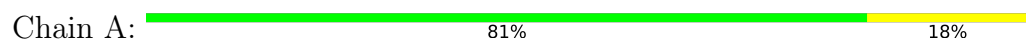




• Molecule 9: 5S ribosomal RNA

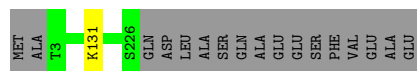


• Molecule 10: 16S ribosomal RNA



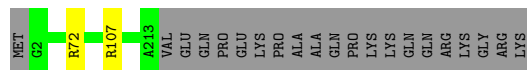
- Molecule 11: Small ribosomal subunit protein uS2

Chain B:  93% 7%



- Molecule 12: Small ribosomal subunit protein uS3

Chain C:  90% 9%



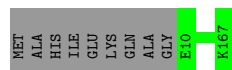
- Molecule 13: Small ribosomal subunit protein uS4

Chain D:  99% 1%




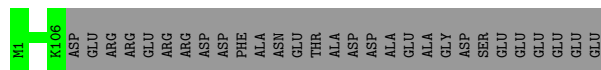
- Molecule 14: Small ribosomal subunit protein uS5

Chain E:  95% 5%




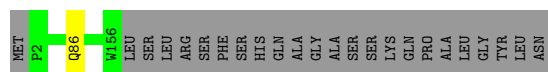
- Molecule 15: 30S ribosomal protein S6

Chain F:  79% 21%



- Molecule 16: 30S ribosomal protein S7

Chain G:  86% 13%



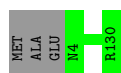
- Molecule 17: Small ribosomal subunit protein uS8

Chain H:  99% 1%



- Molecule 18: Small ribosomal subunit protein uS9

Chain I:  98% .




- Molecule 19: 30S ribosomal protein S10

Chain J:  96% ..



- Molecule 20: Small ribosomal subunit protein uS11

Chain K:  88% . 9%



- Molecule 21: Small ribosomal subunit protein uS12

Chain L:  99% .



- Molecule 22: Small ribosomal subunit protein uS13

Chain M:  95% ..



- Molecule 23: Small ribosomal subunit protein uS14

Chain N:  99% .



- Molecule 24: 30S ribosomal protein S15

Chain O:  97% ..



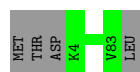
- Molecule 25: 30S ribosomal protein S16

Chain P:  99% .



- Molecule 26: Small ribosomal subunit protein uS17

Chain Q:  95% 5%




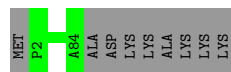
- Molecule 27: Small ribosomal subunit protein bS18

Chain R:  96% ..



- Molecule 28: Small ribosomal subunit protein uS19

Chain S:  90% 10%



- Molecule 29: Small ribosomal subunit protein bS20

Chain T:  97% ..



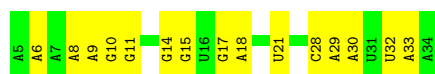
- Molecule 30: 30S ribosomal protein S21

Chain U:  99% .



- Molecule 31: mRNA

Chain V:  50% 50%



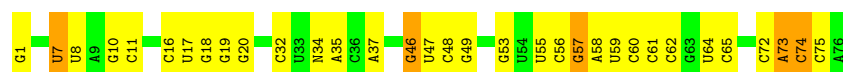
- Molecule 32: tRNA-Phe (P-site)



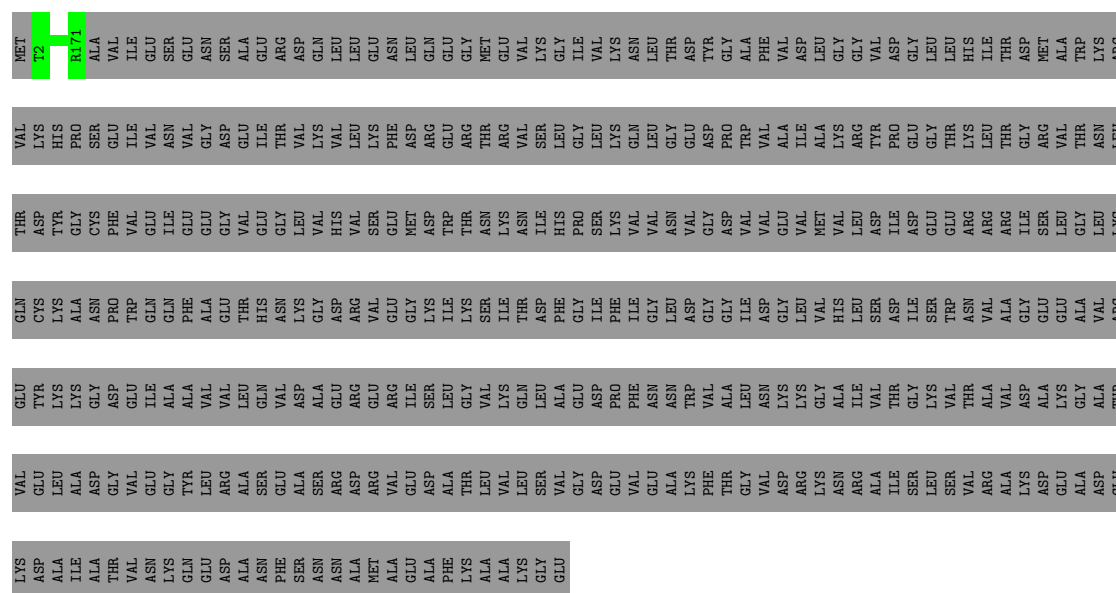
Chain X: 63% 33% .



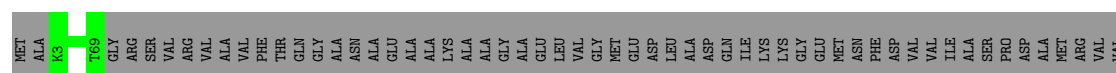
Chain Y: 57% 37% 7%

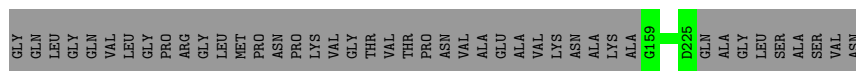


Chain Z: 31% 69%



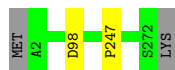
Chain a: 57% 43%





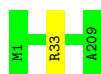
- Molecule 37: 50S ribosomal protein L2

Chain b: 99% ..



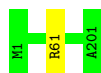
- Molecule 38: 50S ribosomal protein L3

Chain c: 100%



- Molecule 39: 50S ribosomal protein L4

Chain d: 100%



- Molecule 40: 50S ribosomal protein L5

Chain e: 98% ..



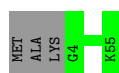
- Molecule 41: 50S ribosomal protein L6

Chain f: 98% ..



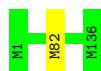
- Molecule 42: 50S ribosomal protein L33

Chain g: 95% 5%



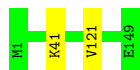
- Molecule 43: 50S ribosomal protein L16

Chain h: 99% .



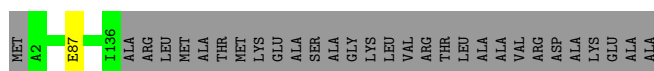
- Molecule 44: 50S ribosomal protein L9

Chain i: 99%



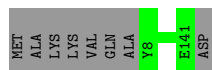
- Molecule 45: Large ribosomal subunit protein uL10

Chain j: 81% 18%



- Molecule 46: 50S ribosomal protein L11

Chain k: 94% 6%



- Molecule 47: 50S ribosomal protein L34

Chain l: 100%

There are no outlier residues recorded for this chain.

- Molecule 48: 50S ribosomal protein L13

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 49: 50S ribosomal protein L14

Chain n: 100%

There are no outlier residues recorded for this chain.

- Molecule 50: 50S ribosomal protein L15

Chain o: 100%

There are no outlier residues recorded for this chain.

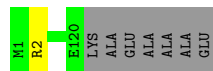
- Molecule 51: Nascent chain

Chain p: 100%

There are no outlier residues recorded for this chain.

- Molecule 52: 50S ribosomal protein L17

Chain q:  94% 6%



- Molecule 53: 50S ribosomal protein L18

Chain r:  97% ..



- Molecule 54: 50S ribosomal protein L19

Chain s:  99% .



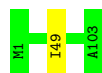
- Molecule 55: 50S ribosomal protein L20

Chain t:  99% .



- Molecule 56: 50S ribosomal protein L21

Chain u:  99% .



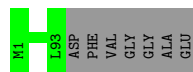
- Molecule 57: 50S ribosomal protein L22

Chain v:  99% .



- Molecule 58: 50S ribosomal protein L23

Chain w:  93% 7%



- Molecule 59: 50S ribosomal protein L24

Chain x:  97% ..



- Molecule 60: 50S ribosomal protein L25

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 61: 50S ribosomal protein L27

Chain z:  99% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32334	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k 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: ZN, PSU, 3TD, 2MG, MA6, OMU, ATP, MIA, UR3, RSP, 12A, 6MZ, 5MU, 5MC, 2MA, 4OC, OMG, CM0, 1MG, G7M, 4SU, OMC, 7MG, MG, H2U

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	0.23	0/303	0.60	0/397
2	1	0.25	0/635	0.63	0/848
3	2	0.25	0/510	0.54	0/677
4	3	0.24	0/453	0.61	0/605
5	4	0.27	0/539	0.58	0/721
6	5	0.25	0/450	0.58	0/599
7	6	0.24	0/513	0.56	0/676
8	7	0.23	1/69284 (0.0%)	0.75	60/108082 (0.1%)
9	8	0.23	0/2872	0.76	6/4478 (0.1%)
10	A	0.23	0/36772	0.75	47/57358 (0.1%)
11	B	0.26	0/1782	0.53	0/2401
12	C	0.26	0/1685	0.57	0/2270
13	D	0.25	0/1665	0.56	0/2227
14	E	0.27	0/1179	0.55	0/1584
15	F	0.25	0/881	0.54	0/1189
16	G	0.27	0/1246	0.55	0/1672
17	H	0.26	0/989	0.57	0/1326
18	I	0.26	0/1034	0.60	0/1375
19	J	0.28	0/813	0.67	0/1100
20	K	0.26	0/900	0.59	0/1215
21	L	0.27	0/969	0.64	0/1300
22	M	0.31	0/900	0.64	0/1204
23	N	0.26	0/817	0.62	0/1088
24	O	0.24	0/722	0.63	0/964
25	P	0.26	0/659	0.62	0/884
26	Q	0.27	0/657	0.61	0/881
27	R	0.30	0/635	0.65	0/849
28	S	0.26	0/680	0.54	0/915
29	T	0.25	0/676	0.55	0/895
30	U	0.30	0/592	0.64	0/785
31	V	0.26	0/727	0.80	0/1132

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	W	0.34	1/1585 (0.1%)	0.86	4/2467 (0.2%)
33	X	0.35	1/1728 (0.1%)	0.91	1/2686 (0.0%)
34	Y	0.43	1/1672 (0.1%)	0.97	7/2599 (0.3%)
35	Z	0.25	0/1334	0.52	0/1799
36	a	0.24	0/1033	0.50	0/1387
37	b	0.26	0/2121	0.63	1/2852 (0.0%)
38	c	0.26	0/1586	0.56	0/2134
39	d	0.25	0/1571	0.53	0/2113
40	e	0.25	0/1444	0.55	0/1937
41	f	0.25	0/1343	0.55	0/1816
42	g	0.25	0/434	0.54	0/576
43	h	0.27	0/1104	0.60	0/1474
44	i	0.25	0/1121	0.54	0/1515
45	j	0.27	0/1037	0.55	0/1400
46	k	0.27	0/993	0.56	0/1341
47	l	0.29	0/380	0.65	0/498
48	m	0.25	0/1152	0.55	0/1551
49	n	0.27	0/955	0.63	0/1279
50	o	0.27	0/1062	0.62	0/1413
51	p	0.82	0/36	1.05	0/48
52	q	0.26	0/973	0.61	0/1301
53	r	0.25	0/901	0.61	0/1209
54	s	0.26	0/929	0.56	0/1242
55	t	0.25	0/960	0.53	0/1278
56	u	0.26	0/829	0.59	0/1107
57	v	0.24	0/864	0.57	0/1156
58	w	0.25	0/744	0.54	0/994
59	x	0.26	0/787	0.54	0/1051
60	y	0.26	0/766	0.54	0/1025
61	z	0.25	0/642	0.56	0/848
All	All	0.25	4/164625 (0.0%)	0.71	126/245793 (0.1%)

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
13	D	0	1
19	J	0	1
20	K	0	1
24	O	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	P	0	1
29	T	0	2
39	d	0	1
41	f	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Y	1	G	OP3-P	-7.60	1.52	1.61
8	7	1	G	OP3-P	-7.55	1.52	1.61
32	W	1	G	OP3-P	-7.52	1.52	1.61
33	X	1	G	OP3-P	-7.50	1.52	1.61

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	1129	A	P-O3'-C3'	-12.54	104.65	119.70
8	7	2605	PSU	P-O3'-C3'	-11.15	106.32	119.70
10	A	1407	5MC	P-O3'-C3'	-10.99	106.51	119.70
8	7	2453	A	P-O3'-C3'	-10.77	106.78	119.70
10	A	1408	A	P-O3'-C3'	-10.70	106.86	119.70
10	A	389	A	P-O3'-C3'	-10.05	107.64	119.70
9	8	89	U	P-O3'-C3'	-9.79	107.95	119.70
10	A	1404	C	P-O3'-C3'	-9.67	108.10	119.70
8	7	2570	G	P-O3'-C3'	-9.59	108.19	119.70
8	7	955	PSU	P-O3'-C3'	-9.49	108.31	119.70
9	8	88	C	P-O3'-C3'	-9.48	108.32	119.70
10	A	335	C	P-O3'-C3'	-9.35	108.48	119.70
10	A	56	U	P-O3'-C3'	-9.33	108.50	119.70
8	7	2462	C	P-O3'-C3'	-9.25	108.60	119.70
8	7	2442	C	P-O3'-C3'	-9.21	108.64	119.70
10	A	1516	2MG	P-O3'-C3'	-9.18	108.69	119.70
10	A	338	A	P-O3'-C3'	-9.16	108.71	119.70
10	A	387	U	P-O3'-C3'	-9.07	108.81	119.70
10	A	112	G	P-O3'-C3'	-9.04	108.85	119.70
8	7	2504	PSU	P-O3'-C3'	-8.98	108.92	119.70
8	7	1905	C	P-O3'-C3'	-8.96	108.95	119.70
10	A	315	A	P-O3'-C3'	-8.95	108.96	119.70
8	7	1836	C	P-O3'-C3'	-8.92	109.00	119.70
8	7	2451	A	P-O3'-C3'	-8.90	109.02	119.70
10	A	516	PSU	P-O3'-C3'	-8.88	109.04	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	2495	G	P-O3'-C3'	-8.85	109.08	119.70
8	7	1647	U	P-O3'-C3'	-8.77	109.17	119.70
10	A	111	G	P-O3'-C3'	-8.74	109.21	119.70
32	W	74	C	P-O3'-C3'	-8.71	109.24	119.70
8	7	1939	5MU	P-O3'-C3'	-8.71	109.25	119.70
10	A	1207	2MG	P-O3'-C3'	-8.70	109.27	119.70
10	A	353	A	P-O3'-C3'	-8.66	109.31	119.70
8	7	2568	U	P-O3'-C3'	-8.58	109.40	119.70
8	7	2487	G	P-O3'-C3'	-8.56	109.43	119.70
8	7	1127	A	P-O3'-C3'	-8.54	109.45	119.70
8	7	2446	G	P-O3'-C3'	-8.54	109.46	119.70
8	7	2498	OMC	P-O3'-C3'	-8.53	109.46	119.70
8	7	2488	G	P-O3'-C3'	-8.52	109.48	119.70
10	A	1500	A	P-O3'-C3'	-8.50	109.50	119.70
10	A	316	C	P-O3'-C3'	-8.48	109.53	119.70
8	7	786	C	P-O3'-C3'	-8.36	109.67	119.70
34	Y	32	C	P-O3'-C3'	-8.31	109.73	119.70
8	7	2441	U	P-O3'-C3'	-8.29	109.75	119.70
8	7	2494	G	P-O3'-C3'	-8.28	109.76	119.70
10	A	336	A	P-O3'-C3'	-8.27	109.78	119.70
10	A	330	C	P-O3'-C3'	-8.24	109.81	119.70
10	A	1504	G	P-O3'-C3'	-8.21	109.84	119.70
8	7	1904	G	P-O3'-C3'	-8.19	109.88	119.70
8	7	2489	U	P-O3'-C3'	-8.15	109.92	119.70
8	7	753	A	P-O3'-C3'	-8.14	109.93	119.70
8	7	567	U	P-O3'-C3'	-8.13	109.94	119.70
10	A	350	G	P-O3'-C3'	-8.10	109.98	119.70
8	7	2517	C	P-O3'-C3'	-8.06	110.03	119.70
34	Y	1	G	P-O3'-C3'	-8.03	110.06	119.70
10	A	355	C	P-O3'-C3'	-7.96	110.15	119.70
8	7	1835	2MG	P-O3'-C3'	-7.92	110.19	119.70
8	7	2062	A	P-O3'-C3'	-7.91	110.21	119.70
34	Y	35	A	P-O3'-C3'	-7.85	110.28	119.70
8	7	2461	A	P-O3'-C3'	-7.84	110.29	119.70
8	7	790	U	P-O3'-C3'	-7.79	110.36	119.70
8	7	2455	G	P-O3'-C3'	-7.76	110.39	119.70
9	8	87	U	P-O3'-C3'	-7.74	110.41	119.70
10	A	57	G	P-O3'-C3'	-7.72	110.43	119.70
8	7	2569	G	P-O3'-C3'	-7.61	110.56	119.70
10	A	1201	A	P-O3'-C3'	7.60	128.82	119.70
10	A	52	C	P-O3'-C3'	-7.56	110.62	119.70
10	A	337	G	P-O3'-C3'	-7.53	110.66	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	317	U	P-O3'-C3'	-7.46	110.74	119.70
10	A	314	C	P-O3'-C3'	-7.46	110.74	119.70
32	W	72	C	P-O3'-C3'	-7.46	110.75	119.70
9	8	86	G	P-O3'-C3'	-7.42	110.80	119.70
8	7	2580	PSU	P-O3'-C3'	-7.38	110.85	119.70
10	A	134	G	P-O3'-C3'	-7.34	110.89	119.70
10	A	1405	G	P-O3'-C3'	-7.24	111.01	119.70
8	7	2452	C	P-O3'-C3'	-7.24	111.01	119.70
10	A	53	A	P-O3'-C3'	-7.22	111.03	119.70
10	A	354	G	P-O3'-C3'	-7.19	111.08	119.70
8	7	2518	A	P-O3'-C3'	-7.16	111.11	119.70
32	W	75	C	P-O3'-C3'	-7.15	111.12	119.70
8	7	1128	G	P-O3'-C3'	-7.08	111.20	119.70
8	7	2457	PSU	P-O3'-C3'	-7.04	111.26	119.70
10	A	58	C	P-O3'-C3'	-7.04	111.26	119.70
10	A	388	G	P-O3'-C3'	-6.96	111.34	119.70
8	7	2492	U	P-O3'-C3'	-6.94	111.37	119.70
34	Y	73	A	P-O3'-C3'	-6.84	111.49	119.70
10	A	1499	A	P-O3'-C3'	-6.83	111.50	119.70
8	7	1271	G	P-O3'-C3'	-6.66	111.70	119.70
8	7	1833	C	P-O3'-C3'	-6.66	111.70	119.70
10	A	113	G	P-O3'-C3'	-6.65	111.72	119.70
10	A	1201	A	OP2-P-O3'	6.63	119.78	105.20
8	7	568	U	P-O3'-C3'	-6.59	111.80	119.70
10	A	329	A	P-O3'-C3'	-6.50	111.90	119.70
8	7	2445	2MG	P-O3'-C3'	-6.50	111.90	119.70
8	7	1020	A	P-O3'-C3'	6.43	127.42	119.70
8	7	2571	U	P-O3'-C3'	-6.34	112.09	119.70
10	A	59	A	P-O3'-C3'	-6.28	112.16	119.70
8	7	2176	A	C2'-C3'-O3'	6.25	123.71	113.70
10	A	1503	A	P-O3'-C3'	-6.15	112.31	119.70
8	7	1270	C	P-O3'-C3'	-6.12	112.35	119.70
8	7	1313	U	C2-N1-C1'	5.95	124.84	117.70
10	A	352	C	P-O3'-C3'	-5.92	112.59	119.70
33	X	89	C	N1-C2-O2	5.85	122.41	118.90
9	8	3	C	OP1-P-O3'	5.84	118.04	105.20
9	8	3	C	P-O3'-C3'	5.76	126.62	119.70
8	7	789	A	P-O3'-C3'	-5.75	112.79	119.70
8	7	2449	H2U	P-O3'-C3'	-5.75	112.80	119.70
8	7	1313	U	N1-C2-O2	5.62	126.74	122.80
10	A	1190	G	P-O3'-C3'	5.62	126.44	119.70
8	7	2176	A	P-O3'-C3'	-5.54	113.06	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	b	98	ASP	CB-CG-OD1	5.54	123.28	118.30
8	7	1020	A	OP2-P-O3'	5.49	117.28	105.20
10	A	1537	U	P-O3'-C3'	5.46	126.25	119.70
10	A	1190	G	OP2-P-O3'	5.41	117.09	105.20
10	A	1505	G	P-O3'-C3'	-5.39	113.24	119.70
8	7	2799	A	C5'-C4'-O4'	5.35	115.52	109.10
10	A	1281	C	OP1-P-O3'	5.35	116.97	105.20
8	7	1313	U	N3-C2-O2	-5.35	118.46	122.20
8	7	2061	G	P-O3'-C3'	-5.31	113.33	119.70
10	A	1345	U	OP2-P-O3'	5.26	116.78	105.20
8	7	2176	A	C5'-C4'-O4'	5.23	115.37	109.10
32	W	73	A	OP1-P-O3'	5.22	116.70	105.20
34	Y	57	G	C3'-C2'-C1'	-5.22	97.33	101.50
8	7	788	A	P-O3'-C3'	-5.16	113.51	119.70
34	Y	72	C	P-O3'-C3'	-5.15	113.53	119.70
34	Y	74	C	C3'-C2'-C1'	-5.13	97.39	101.50
8	7	1675	C	N1-C2-O2	5.03	121.92	118.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	D	104	ARG	Sidechain
19	J	48	ARG	Sidechain
20	K	98	ARG	Sidechain
24	O	84	ARG	Sidechain
25	P	51	ARG	Sidechain
29	T	29	ARG	Sidechain
29	T	60	ARG	Sidechain
39	d	61	ARG	Sidechain
41	f	153	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles ⓘ

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	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
2	1	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
3	2	61/63 (97%)	60 (98%)	0	1 (2%)	8	32
4	3	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3	18
5	4	65/70 (93%)	49 (75%)	16 (25%)	0	100	100
6	5	54/57 (95%)	54 (100%)	0	0	100	100
7	6	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
11	B	222/241 (92%)	209 (94%)	12 (5%)	1 (0%)	25	56
12	C	210/233 (90%)	208 (99%)	2 (1%)	0	100	100
13	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
14	E	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
15	F	104/135 (77%)	103 (99%)	1 (1%)	0	100	100
16	G	153/179 (86%)	149 (97%)	4 (3%)	0	100	100
17	H	127/130 (98%)	127 (100%)	0	0	100	100
18	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
19	J	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
20	K	116/129 (90%)	102 (88%)	11 (10%)	3 (3%)	4	23
21	L	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
22	M	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
23	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
24	O	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	11	38
25	P	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
26	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
27	R	72/75 (96%)	63 (88%)	7 (10%)	2 (3%)	4	22
28	S	81/92 (88%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	T	84/87 (97%)	84 (100%)	0	0	100	100
30	U	68/71 (96%)	61 (90%)	7 (10%)	0	100	100
35	Z	168/557 (30%)	161 (96%)	7 (4%)	0	100	100
36	a	130/234 (56%)	126 (97%)	4 (3%)	0	100	100
37	b	269/273 (98%)	262 (97%)	6 (2%)	1 (0%)	30	61
38	c	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
39	d	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
40	e	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
41	f	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
42	g	50/55 (91%)	50 (100%)	0	0	100	100
43	h	135/136 (99%)	134 (99%)	1 (1%)	0	100	100
44	i	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	19	50
45	j	133/165 (81%)	122 (92%)	11 (8%)	0	100	100
46	k	132/142 (93%)	124 (94%)	8 (6%)	0	100	100
47	l	44/46 (96%)	44 (100%)	0	0	100	100
48	m	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
49	n	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
50	o	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
51	p	4/18 (22%)	3 (75%)	1 (25%)	0	100	100
52	q	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
53	r	114/117 (97%)	105 (92%)	7 (6%)	2 (2%)	7	30
54	s	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
55	t	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
56	u	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	13	42
57	v	108/110 (98%)	96 (89%)	11 (10%)	1 (1%)	14	44
58	w	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
59	x	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
60	y	92/94 (98%)	92 (100%)	0	0	100	100
61	z	82/85 (96%)	77 (94%)	5 (6%)	0	100	100
All	All	6208/7029 (88%)	5944 (96%)	248 (4%)	16 (0%)	38	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	v	64	ALA
4	3	21	LYS
20	K	70	CYS
20	K	80	LYS
53	r	5	SER
3	2	9	LYS
11	B	131	LYS
27	R	16	GLU
53	r	3	LYS
4	3	20	HIS
20	K	74	VAL
24	O	75	VAL
37	b	247	PRO
56	u	49	ILE
27	R	37	GLY
44	i	121	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	34/34 (100%)	34 (100%)	0	100	100
2	1	67/68 (98%)	65 (97%)	2 (3%)	36	62
3	2	55/55 (100%)	55 (100%)	0	100	100
4	3	48/49 (98%)	47 (98%)	1 (2%)	48	70
5	4	60/62 (97%)	59 (98%)	1 (2%)	56	74
6	5	47/48 (98%)	47 (100%)	0	100	100
7	6	51/52 (98%)	51 (100%)	0	100	100
11	B	186/199 (94%)	186 (100%)	0	100	100
12	C	172/190 (90%)	170 (99%)	2 (1%)	67	80
13	D	172/173 (99%)	171 (99%)	1 (1%)	84	90
14	E	120/126 (95%)	120 (100%)	0	100	100
15	F	92/116 (79%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	G	128/147 (87%)	127 (99%)	1 (1%)	79	87
17	H	104/105 (99%)	104 (100%)	0	100	100
18	I	105/107 (98%)	105 (100%)	0	100	100
19	J	88/90 (98%)	88 (100%)	0	100	100
20	K	91/99 (92%)	91 (100%)	0	100	100
21	L	103/104 (99%)	103 (100%)	0	100	100
22	M	93/96 (97%)	90 (97%)	3 (3%)	34	61
23	N	83/84 (99%)	83 (100%)	0	100	100
24	O	76/77 (99%)	76 (100%)	0	100	100
25	P	65/65 (100%)	65 (100%)	0	100	100
26	Q	74/78 (95%)	74 (100%)	0	100	100
27	R	64/65 (98%)	64 (100%)	0	100	100
28	S	72/79 (91%)	72 (100%)	0	100	100
29	T	65/66 (98%)	65 (100%)	0	100	100
30	U	59/61 (97%)	59 (100%)	0	100	100
35	Z	143/461 (31%)	143 (100%)	0	100	100
36	a	110/181 (61%)	110 (100%)	0	100	100
37	b	216/218 (99%)	216 (100%)	0	100	100
38	c	164/164 (100%)	163 (99%)	1 (1%)	84	90
39	d	165/165 (100%)	165 (100%)	0	100	100
40	e	149/150 (99%)	147 (99%)	2 (1%)	65	79
41	f	137/138 (99%)	136 (99%)	1 (1%)	81	88
42	g	47/49 (96%)	47 (100%)	0	100	100
43	h	110/109 (101%)	109 (99%)	1 (1%)	75	85
44	i	114/114 (100%)	113 (99%)	1 (1%)	75	85
45	j	103/123 (84%)	102 (99%)	1 (1%)	73	84
46	k	104/110 (94%)	104 (100%)	0	100	100
47	l	38/38 (100%)	38 (100%)	0	100	100
48	m	116/116 (100%)	116 (100%)	0	100	100
49	n	104/104 (100%)	104 (100%)	0	100	100
50	o	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	p	4/4 (100%)	4 (100%)	0	100	100
52	q	100/103 (97%)	99 (99%)	1 (1%)	73	84
53	r	86/87 (99%)	86 (100%)	0	100	100
54	s	99/100 (99%)	99 (100%)	0	100	100
55	t	89/90 (99%)	89 (100%)	0	100	100
56	u	84/84 (100%)	84 (100%)	0	100	100
57	v	93/93 (100%)	93 (100%)	0	100	100
58	w	80/84 (95%)	80 (100%)	0	100	100
59	x	83/85 (98%)	82 (99%)	1 (1%)	67	80
60	y	78/78 (100%)	78 (100%)	0	100	100
61	z	62/63 (98%)	62 (100%)	0	100	100
All	All	5155/5709 (90%)	5135 (100%)	20 (0%)	88	93

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	72	ARG
2	1	77	LYS
4	3	31	ARG
5	4	8	LYS
12	C	72	ARG
12	C	107	ARG
13	D	44	ARG
16	G	86	GLN
22	M	104	THR
22	M	105	ASN
22	M	113	ARG
38	c	33	ARG
40	e	3	LYS
40	e	178	ARG
41	f	69	ARG
43	h	82	MET
44	i	41	LYS
45	j	87	GLU
52	q	2	ARG
59	x	6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
11	B	120	GLN
15	F	14	GLN
15	F	17	GLN
20	K	119	ASN
21	L	29	GLN
22	M	105	ASN
39	d	115	GLN
41	f	101	ASN
46	k	105	GLN
54	s	10	GLN
54	s	77	HIS
57	v	61	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1538/1542 (99%)	248 (16%)	20 (1%)
31	V	29/30 (96%)	14 (48%)	3 (10%)
32	W	74/76 (97%)	23 (31%)	2 (2%)
33	X	74/78 (94%)	25 (33%)	4 (5%)
34	Y	73/76 (96%)	25 (34%)	7 (9%)
8	7	2898/2903 (99%)	485 (16%)	55 (1%)
9	8	119/120 (99%)	14 (11%)	1 (0%)
All	All	4805/4825 (99%)	834 (17%)	92 (1%)

All (834) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	10	A
8	7	15	G
8	7	28	A
8	7	34	U
8	7	44	A
8	7	46	G
8	7	55	G
8	7	71	A
8	7	74	A
8	7	75	G
8	7	96	C
8	7	101	A
8	7	102	U

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Mol	Chain	Res	Type
8	7	103	A
8	7	118	A
8	7	119	A
8	7	120	U
8	7	125	A
8	7	135	U
8	7	139	U
8	7	141	G
8	7	142	A
8	7	159	G
8	7	163	C
8	7	174	U
8	7	176	A
8	7	177	G
8	7	178	G
8	7	181	A
8	7	196	A
8	7	199	A
8	7	215	G
8	7	216	A
8	7	221	A
8	7	222	A
8	7	248	G
8	7	252	G
8	7	275	C
8	7	277	G
8	7	278	A
8	7	279	A
8	7	283	G
8	7	284	U
8	7	285	G
8	7	286	U
8	7	294	A
8	7	295	G
8	7	311	A
8	7	330	A
8	7	341	C
8	7	343	C
8	7	345	A
8	7	353	C
8	7	359	G
8	7	361	G

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Mol	Chain	Res	Type
8	7	362	A
8	7	386	G
8	7	395	U
8	7	396	G
8	7	401	A
8	7	405	U
8	7	412	A
8	7	455	C
8	7	456	C
8	7	457	A
8	7	470	A
8	7	473	G
8	7	475	C
8	7	481	G
8	7	491	G
8	7	504	A
8	7	505	A
8	7	506	G
8	7	509	C
8	7	510	C
8	7	513	A
8	7	514	A
8	7	527	C
8	7	529	A
8	7	532	A
8	7	547	A
8	7	549	G
8	7	563	A
8	7	573	U
8	7	575	A
8	7	603	A
8	7	613	A
8	7	614	A
8	7	615	U
8	7	637	A
8	7	645	C
8	7	646	U
8	7	647	G
8	7	654	A
8	7	655	A
8	7	686	U
8	7	717	C

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Mol	Chain	Res	Type
8	7	726	G
8	7	729	G
8	7	730	A
8	7	747	5MU
8	7	748	G
8	7	749	A
8	7	764	A
8	7	765	C
8	7	775	G
8	7	776	G
8	7	782	A
8	7	784	G
8	7	785	G
8	7	805	G
8	7	812	C
8	7	819	A
8	7	827	U
8	7	828	U
8	7	830	G
8	7	831	G
8	7	845	A
8	7	846	U
8	7	847	U
8	7	858	G
8	7	859	G
8	7	869	G
8	7	878	A
8	7	883	G
8	7	885	C
8	7	887	U
8	7	888	C
8	7	891	G
8	7	895	U
8	7	896	A
8	7	897	C
8	7	902	C
8	7	907	G
8	7	910	A
8	7	917	A
8	7	919	U
8	7	931	U
8	7	932	U

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Mol	Chain	Res	Type
8	7	941	A
8	7	946	C
8	7	961	C
8	7	962	G
8	7	974	G
8	7	983	A
8	7	990	A
8	7	995	C
8	7	996	A
8	7	999	U
8	7	1005	C
8	7	1012	U
8	7	1013	C
8	7	1021	A
8	7	1022	G
8	7	1025	G
8	7	1026	G
8	7	1027	A
8	7	1033	U
8	7	1046	A
8	7	1047	G
8	7	1055	G
8	7	1060	U
8	7	1070	A
8	7	1081	U
8	7	1083	U
8	7	1084	A
8	7	1085	A
8	7	1087	G
8	7	1088	A
8	7	1090	A
8	7	1097	U
8	7	1112	G
8	7	1130	U
8	7	1132	U
8	7	1133	A
8	7	1134	A
8	7	1135	C
8	7	1136	G
8	7	1142	A
8	7	1149	G
8	7	1161	C

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Mol	Chain	Res	Type
8	7	1169	A
8	7	1172	C
8	7	1173	U
8	7	1174	U
8	7	1176	U
8	7	1178	C
8	7	1179	G
8	7	1180	U
8	7	1184	U
8	7	1236	G
8	7	1247	A
8	7	1248	G
8	7	1249	U
8	7	1250	G
8	7	1253	A
8	7	1256	G
8	7	1262	A
8	7	1271	G
8	7	1272	A
8	7	1273	U
8	7	1300	G
8	7	1301	A
8	7	1321	A
8	7	1329	U
8	7	1341	G
8	7	1342	A
8	7	1345	C
8	7	1352	U
8	7	1365	A
8	7	1368	G
8	7	1379	U
8	7	1380	G
8	7	1383	A
8	7	1396	U
8	7	1398	C
8	7	1416	G
8	7	1417	C
8	7	1419	A
8	7	1420	A
8	7	1428	C
8	7	1434	A
8	7	1452	G

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Mol	Chain	Res	Type
8	7	1453	A
8	7	1454	C
8	7	1455	G
8	7	1461	C
8	7	1476	U
8	7	1482	G
8	7	1488	C
8	7	1490	A
8	7	1491	G
8	7	1493	C
8	7	1494	A
8	7	1497	U
8	7	1503	A
8	7	1508	A
8	7	1509	A
8	7	1515	A
8	7	1524	G
8	7	1532	A
8	7	1539	U
8	7	1566	A
8	7	1569	A
8	7	1578	U
8	7	1581	G
8	7	1583	A
8	7	1584	U
8	7	1602	U
8	7	1608	A
8	7	1610	A
8	7	1619	G
8	7	1647	U
8	7	1648	U
8	7	1649	G
8	7	1674	G
8	7	1714	U
8	7	1715	G
8	7	1716	U
8	7	1717	A
8	7	1727	C
8	7	1729	U
8	7	1730	C
8	7	1731	G
8	7	1738	G

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Mol	Chain	Res	Type
8	7	1754	A
8	7	1755	A
8	7	1756	G
8	7	1764	C
8	7	1773	A
8	7	1784	A
8	7	1786	A
8	7	1791	A
8	7	1799	G
8	7	1800	C
8	7	1801	A
8	7	1807	G
8	7	1808	A
8	7	1811	G
8	7	1816	C
8	7	1848	A
8	7	1870	C
8	7	1872	A
8	7	1873	G
8	7	1901	A
8	7	1906	G
8	7	1907	G
8	7	1929	G
8	7	1930	G
8	7	1940	U
8	7	1954	G
8	7	1955	U
8	7	1960	A
8	7	1966	A
8	7	1967	C
8	7	1970	A
8	7	1971	U
8	7	1972	G
8	7	1975	G
8	7	1982	U
8	7	1991	U
8	7	1992	G
8	7	1993	U
8	7	1997	C
8	7	2016	U
8	7	2021	C
8	7	2022	U

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Mol	Chain	Res	Type
8	7	2023	C
8	7	2031	A
8	7	2032	G
8	7	2033	A
8	7	2043	C
8	7	2055	C
8	7	2056	G
8	7	2060	A
8	7	2061	G
8	7	2062	A
8	7	2069	G7M
8	7	2072	C
8	7	2093	G
8	7	2101	A
8	7	2102	G
8	7	2110	G
8	7	2111	U
8	7	2112	G
8	7	2114	A
8	7	2117	A
8	7	2118	U
8	7	2120	G
8	7	2121	G
8	7	2123	G
8	7	2124	G
8	7	2126	A
8	7	2130	U
8	7	2131	U
8	7	2132	U
8	7	2133	G
8	7	2134	A
8	7	2136	G
8	7	2137	U
8	7	2139	U
8	7	2140	G
8	7	2141	G
8	7	2146	C
8	7	2153	C
8	7	2154	A
8	7	2156	G
8	7	2161	C
8	7	2162	G

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Mol	Chain	Res	Type
8	7	2163	A
8	7	2164	C
8	7	2165	C
8	7	2166	U
8	7	2170	A
8	7	2171	A
8	7	2172	U
8	7	2173	A
8	7	2176	A
8	7	2177	C
8	7	2182	U
8	7	2190	G
8	7	2198	A
8	7	2204	G
8	7	2211	A
8	7	2212	A
8	7	2214	C
8	7	2225	A
8	7	2238	G
8	7	2239	G
8	7	2243	U
8	7	2251	OMG
8	7	2268	A
8	7	2278	A
8	7	2279	G
8	7	2283	C
8	7	2287	A
8	7	2305	U
8	7	2308	G
8	7	2309	A
8	7	2311	A
8	7	2312	U
8	7	2319	G
8	7	2321	U
8	7	2322	A
8	7	2325	G
8	7	2333	A
8	7	2335	A
8	7	2336	A
8	7	2345	G
8	7	2347	C
8	7	2350	C

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Mol	Chain	Res	Type
8	7	2361	G
8	7	2372	U
8	7	2375	G
8	7	2379	G
8	7	2383	G
8	7	2385	C
8	7	2391	G
8	7	2402	U
8	7	2403	C
8	7	2406	A
8	7	2410	G
8	7	2423	U
8	7	2425	A
8	7	2429	G
8	7	2430	A
8	7	2431	U
8	7	2441	U
8	7	2447	G
8	7	2448	A
8	7	2464	G
8	7	2475	C
8	7	2476	A
8	7	2478	A
8	7	2482	A
8	7	2484	G
8	7	2492	U
8	7	2494	G
8	7	2498	OMC
8	7	2502	G
8	7	2504	PSU
8	7	2505	G
8	7	2506	U
8	7	2518	A
8	7	2529	G
8	7	2535	G
8	7	2537	U
8	7	2547	A
8	7	2554	U
8	7	2555	U
8	7	2566	A
8	7	2567	G
8	7	2572	A

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Mol	Chain	Res	Type
8	7	2573	C
8	7	2581	G
8	7	2582	G
8	7	2602	A
8	7	2603	G
8	7	2609	U
8	7	2613	U
8	7	2614	A
8	7	2615	U
8	7	2629	U
8	7	2630	G
8	7	2663	G
8	7	2689	U
8	7	2690	U
8	7	2711	A
8	7	2713	U
8	7	2714	G
8	7	2716	C
8	7	2718	G
8	7	2726	A
8	7	2732	G
8	7	2733	A
8	7	2739	U
8	7	2743	U
8	7	2744	G
8	7	2748	A
8	7	2751	G
8	7	2757	A
8	7	2765	A
8	7	2778	A
8	7	2779	U
8	7	2798	U
8	7	2800	A
8	7	2818	U
8	7	2820	A
8	7	2821	A
8	7	2832	U
8	7	2835	A
8	7	2849	U
8	7	2850	A
8	7	2858	C
8	7	2861	U

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Mol	Chain	Res	Type
8	7	2867	G
8	7	2870	C
8	7	2873	A
8	7	2879	A
8	7	2880	C
8	7	2883	A
8	7	2884	U
8	7	2885	G
8	7	2886	A
8	7	2891	U
9	8	4	C
9	8	9	G
9	8	15	A
9	8	16	G
9	8	35	C
9	8	50	A
9	8	51	G
9	8	66	A
9	8	67	G
9	8	89	U
9	8	90	C
9	8	91	C
9	8	99	A
9	8	109	A
10	A	3	A
10	A	4	U
10	A	5	U
10	A	7	A
10	A	9	G
10	A	22	G
10	A	32	A
10	A	33	A
10	A	39	G
10	A	47	C
10	A	48	C
10	A	49	U
10	A	50	A
10	A	51	A
10	A	52	C
10	A	60	A
10	A	65	A
10	A	71	A

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Mol	Chain	Res	Type
10	A	72	A
10	A	75	G
10	A	78	A
10	A	79	G
10	A	82	G
10	A	83	C
10	A	84	U
10	A	85	U
10	A	87	C
10	A	88	U
10	A	91	U
10	A	92	U
10	A	95	C
10	A	131	A
10	A	134	G
10	A	137	U
10	A	141	G
10	A	143	A
10	A	144	G
10	A	163	C
10	A	171	A
10	A	174	A
10	A	182	A
10	A	183	C
10	A	184	G
10	A	192	A
10	A	193	C
10	A	197	A
10	A	204	G
10	A	208	U
10	A	209	U
10	A	210	C
10	A	215	C
10	A	226	G
10	A	245	U
10	A	247	G
10	A	250	A
10	A	251	G
10	A	252	U
10	A	266	G
10	A	267	C
10	A	281	G

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Mol	Chain	Res	Type
10	A	289	G
10	A	300	A
10	A	305	G
10	A	315	A
10	A	316	C
10	A	322	C
10	A	323	U
10	A	325	A
10	A	327	A
10	A	328	C
10	A	329	A
10	A	330	C
10	A	331	G
10	A	345	C
10	A	347	G
10	A	348	G
10	A	351	G
10	A	352	C
10	A	354	G
10	A	367	U
10	A	372	C
10	A	398	U
10	A	406	G
10	A	411	A
10	A	412	A
10	A	413	G
10	A	421	U
10	A	424	G
10	A	429	U
10	A	458	U
10	A	459	A
10	A	460	A
10	A	462	G
10	A	463	U
10	A	465	A
10	A	467	U
10	A	468	A
10	A	469	C
10	A	479	U
10	A	484	G
10	A	485	U
10	A	486	U

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Mol	Chain	Res	Type
10	A	499	A
10	A	509	A
10	A	511	C
10	A	518	C
10	A	523	A
10	A	527	G7M
10	A	531	U
10	A	532	A
10	A	533	A
10	A	535	A
10	A	547	A
10	A	559	A
10	A	562	U
10	A	572	A
10	A	573	A
10	A	575	G
10	A	576	C
10	A	577	G
10	A	633	G
10	A	653	U
10	A	665	A
10	A	703	G
10	A	718	A
10	A	723	U
10	A	724	G
10	A	734	G
10	A	748	G
10	A	755	G
10	A	777	A
10	A	793	U
10	A	794	A
10	A	815	A
10	A	817	C
10	A	821	G
10	A	828	U
10	A	829	G
10	A	841	C
10	A	842	U
10	A	843	U
10	A	844	G
10	A	845	A
10	A	846	G

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Mol	Chain	Res	Type
10	A	902	G
10	A	914	A
10	A	926	G
10	A	933	G
10	A	934	C
10	A	935	A
10	A	960	U
10	A	961	U
10	A	969	A
10	A	971	G
10	A	975	A
10	A	976	G
10	A	977	A
10	A	983	A
10	A	993	G
10	A	994	A
10	A	1004	A
10	A	1008	U
10	A	1016	A
10	A	1020	G
10	A	1024	G
10	A	1026	G
10	A	1028	C
10	A	1029	U
10	A	1031	C
10	A	1032	G
10	A	1033	G
10	A	1034	G
10	A	1035	A
10	A	1044	A
10	A	1045	C
10	A	1065	U
10	A	1085	U
10	A	1094	G
10	A	1095	U
10	A	1101	A
10	A	1124	G
10	A	1125	U
10	A	1133	G
10	A	1135	U
10	A	1136	C
10	A	1137	C

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Mol	Chain	Res	Type
10	A	1138	G
10	A	1139	G
10	A	1140	C
10	A	1141	C
10	A	1152	A
10	A	1154	G
10	A	1158	C
10	A	1159	U
10	A	1168	U
10	A	1169	A
10	A	1182	G
10	A	1183	U
10	A	1184	G
10	A	1191	A
10	A	1196	A
10	A	1197	A
10	A	1200	C
10	A	1201	A
10	A	1202	U
10	A	1212	U
10	A	1213	A
10	A	1227	A
10	A	1228	C
10	A	1238	A
10	A	1239	A
10	A	1258	G
10	A	1260	G
10	A	1280	A
10	A	1282	C
10	A	1286	U
10	A	1287	A
10	A	1300	G
10	A	1302	C
10	A	1305	G
10	A	1317	C
10	A	1320	C
10	A	1336	C
10	A	1346	A
10	A	1347	G
10	A	1363	A
10	A	1368	A
10	A	1370	G

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Mol	Chain	Res	Type
10	A	1429	A
10	A	1432	G
10	A	1433	A
10	A	1441	A
10	A	1446	A
10	A	1448	C
10	A	1454	G
10	A	1487	G
10	A	1492	A
10	A	1499	A
10	A	1503	A
10	A	1506	U
10	A	1507	A
10	A	1517	G
10	A	1529	G
10	A	1530	G
10	A	1537	U
10	A	1538	C
10	A	1539	C
10	A	1542	A
31	V	6	A
31	V	8	A
31	V	9	A
31	V	10	G
31	V	11	G
31	V	14	G
31	V	15	G
31	V	17	G
31	V	18	A
31	V	21	U
31	V	28	C
31	V	29	A
31	V	30	A
31	V	33	A
32	W	2	C
32	W	4	C
32	W	8	4SU
32	W	11	C
32	W	15	G
32	W	16	H2U
32	W	17	H2U
32	W	18	G

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Mol	Chain	Res	Type
32	W	19	G
32	W	20	H2U
32	W	22	G
32	W	35	A
32	W	44	G
32	W	46	G7M
32	W	47	U
32	W	48	C
32	W	49	C
32	W	52	G
32	W	54	5MU
32	W	58	A
32	W	72	C
32	W	74	C
32	W	76	A
33	X	2	G
33	X	3	U
33	X	7	G
33	X	8	4SU
33	X	9	G
33	X	13	G
33	X	16	A
33	X	17	G
33	X	18	G
33	X	19	C
33	X	20	H2U
33	X	21	G
33	X	22	A
33	X	34	U
33	X	46	A
33	X	47	U
33	X	64	U
33	X	65	C
33	X	66	C
33	X	75	A
33	X	77	U
33	X	82	G
33	X	89	C
33	X	90	G
33	X	93	A
34	Y	7	4SU
34	Y	8	U

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Mol	Chain	Res	Type
34	Y	10	G
34	Y	11	C
34	Y	16	C
34	Y	17	U
34	Y	18	G
34	Y	19	G
34	Y	20	G
34	Y	46	7MG
34	Y	48	C
34	Y	49	G
34	Y	53	G
34	Y	56	C
34	Y	57	G
34	Y	58	A
34	Y	59	U
34	Y	60	C
34	Y	61	C
34	Y	62	C
34	Y	64	U
34	Y	65	C
34	Y	73	A
34	Y	74	C
34	Y	75	C

All (92) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	43	G
8	7	120	U
8	7	134	G
8	7	158	U
8	7	177	G
8	7	277	G
8	7	285	G
8	7	352	A
8	7	404	A
8	7	474	G
8	7	613	A
8	7	748	G
8	7	784	G
8	7	827	U
8	7	829	A

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Mol	Chain	Res	Type
8	7	830	G
8	7	989	G
8	7	1020	A
8	7	1046	A
8	7	1060	U
8	7	1128	G
8	7	1133	A
8	7	1266	G
8	7	1344	U
8	7	1416	G
8	7	1419	A
8	7	1475	G
8	7	1490	A
8	7	1580	A
8	7	1602	U
8	7	1647	U
8	7	1713	A
8	7	1714	U
8	7	1755	A
8	7	1847	A
8	7	1939	5MU
8	7	2031	A
8	7	2110	G
8	7	2136	G
8	7	2138	G
8	7	2139	U
8	7	2148	G
8	7	2162	G
8	7	2163	A
8	7	2176	A
8	7	2177	C
8	7	2210	U
8	7	2211	A
8	7	2430	A
8	7	2474	U
8	7	2491	U
8	7	2506	U
8	7	2581	G
8	7	2710	C
8	7	2756	U
9	8	3	C
10	A	48	C

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Mol	Chain	Res	Type
10	A	84	U
10	A	85	U
10	A	181	A
10	A	251	G
10	A	315	A
10	A	351	G
10	A	428	G
10	A	457	G
10	A	522	C
10	A	845	A
10	A	1027	C
10	A	1124	G
10	A	1137	C
10	A	1190	G
10	A	1201	A
10	A	1281	C
10	A	1345	U
10	A	1397	C
10	A	1432	G
31	V	8	A
31	V	28	C
31	V	32	U
32	W	10	G
32	W	43	C
33	X	2	G
33	X	19	C
33	X	21	G
33	X	46	A
34	Y	7	4SU
34	Y	10	G
34	Y	18	G
34	Y	47	U
34	Y	57	G
34	Y	59	U
34	Y	64	U

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

55 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
32	H2U	W	16	32	18,21,22	3.08	5 (27%)	21,30,33	2.03	5 (23%)
8	3TD	7	1915	8	19,22,23	0.83	1 (5%)	21,32,35	0.59	0
34	PSU	Y	55	34	18,21,22	0.88	1 (5%)	22,30,33	0.58	0
8	2MG	7	1835	8	18,26,27	1.03	2 (11%)	16,38,41	0.79	0
34	5MU	Y	54	34	19,22,23	0.24	0	28,32,35	0.21	0
33	5MU	X	71	33	19,22,23	0.25	0	28,32,35	0.27	0
8	PSU	7	2605	8	18,21,22	0.86	1 (5%)	22,30,33	0.54	0
32	5MU	W	54	32	19,22,23	0.25	0	28,32,35	0.37	0
8	OMU	7	2552	8	19,22,23	0.21	0	26,31,34	0.50	0
8	2MG	7	2445	8	18,26,27	1.02	2 (11%)	16,38,41	0.76	0
33	RSP	X	33	33	17,21,22	4.18	7 (41%)	22,30,33	0.72	0
34	6MZ	Y	37	34	18,25,26	0.66	0	16,36,39	0.58	1 (6%)
33	4SU	X	8	33	18,21,22	3.81	7 (38%)	26,30,33	2.26	4 (15%)
10	PSU	A	516	10,63	18,21,22	0.89	1 (5%)	22,30,33	1.14	3 (13%)
10	5MC	A	967	10	18,22,23	4.04	7 (38%)	26,32,35	1.01	2 (7%)
10	5MC	A	1407	10	18,22,23	0.33	0	26,32,35	0.58	0
8	PSU	7	2504	8	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
8	PSU	7	746	63,8	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
8	PSU	7	955	8	18,21,22	0.86	1 (5%)	22,30,33	0.59	0
34	4SU	Y	7	34	18,21,22	0.37	0	26,30,33	1.35	3 (11%)
32	PSU	W	32	32	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
33	PSU	X	72	33	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
10	4OC	A	1402	10	20,23,24	0.38	0	26,32,35	0.41	0
32	MIA	W	37	32	24,31,32	2.36	3 (12%)	26,44,47	2.55	7 (26%)
33	H2U	X	20	33	18,21,22	3.07	5 (27%)	21,30,33	2.05	4 (19%)
10	UR3	A	1498	10	19,22,23	0.30	0	26,32,35	0.67	0
32	PSU	W	55	32	18,21,22	0.90	1 (5%)	22,30,33	0.70	0
34	CM0	Y	34	34	23,26,27	1.11	1 (4%)	27,37,40	0.56	0
10	MA6	A	1518	10	18,26,27	0.73	0	19,38,41	0.54	0
8	5MC	7	1962	8	18,22,23	0.33	0	26,32,35	0.52	0
34	7MG	Y	46	34	22,26,27	3.88	10 (45%)	29,39,42	2.08	9 (31%)
10	2MG	A	1516	10	18,26,27	1.04	2 (11%)	16,38,41	0.73	0
8	5MU	7	1939	63,8	19,22,23	0.27	0	28,32,35	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	OMG	7	2251	32,8	18,26,27	1.02	2 (11%)	19,38,41	0.69	0
8	5MU	7	747	8	19,22,23	0.23	0	28,32,35	0.33	0
8	PSU	7	2580	8	18,21,22	0.85	1 (5%)	22,30,33	0.97	1 (4%)
8	2MA	7	2503	8	19,25,26	0.88	0	21,37,40	2.04	5 (23%)
8	G7M	7	2069	8	20,26,27	1.12	3 (15%)	17,39,42	0.53	0
8	6MZ	7	2030	8	18,25,26	0.73	0	16,36,39	1.02	2 (12%)
10	G7M	A	527	10	20,26,27	1.13	3 (15%)	17,39,42	0.39	0
8	6MZ	7	1618	8	18,25,26	0.68	0	16,36,39	0.83	0
8	OMC	7	2498	63,8	19,22,23	0.30	0	26,31,34	0.34	0
32	PSU	W	39	32	18,21,22	4.65	8 (44%)	22,30,33	1.89	5 (22%)
10	MA6	A	1519	10	18,26,27	0.75	1 (5%)	19,38,41	0.42	0
8	PSU	7	2457	8	18,21,22	0.85	1 (5%)	22,30,33	0.78	1 (4%)
8	H2U	7	2449	8	18,21,22	4.41	14 (77%)	21,30,33	2.21	5 (23%)
33	12A	X	38	10,33	29,36,37	4.79	16 (55%)	34,52,55	3.02	9 (26%)
32	H2U	W	20	32	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
32	G7M	W	46	32	20,26,27	2.81	7 (35%)	17,39,42	1.13	1 (5%)
10	2MG	A	966	10	18,26,27	2.83	7 (38%)	16,38,41	1.43	4 (25%)
32	4SU	W	8	32	18,21,22	3.79	7 (38%)	26,30,33	2.23	5 (19%)
10	2MG	A	1207	10	18,26,27	1.01	3 (16%)	16,38,41	0.88	1 (6%)
8	PSU	7	2604	8	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
32	H2U	W	17	32	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
8	1MG	7	745	8	18,26,27	0.97	1 (5%)	19,39,42	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	H2U	W	16	32	-	1/7/38/39	0/2/2/2
8	3TD	7	1915	8	-	0/7/25/26	0/2/2/2
34	PSU	Y	55	34	-	4/7/25/26	0/2/2/2
8	2MG	7	1835	8	-	1/5/27/28	0/3/3/3
34	5MU	Y	54	34	-	0/7/25/26	0/2/2/2
33	5MU	X	71	33	-	0/7/25/26	0/2/2/2
8	PSU	7	2605	8	-	0/7/25/26	0/2/2/2
32	5MU	W	54	32	-	4/7/25/26	0/2/2/2
8	OMU	7	2552	8	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MG	7	2445	8	-	2/5/27/28	0/3/3/3
33	RSP	X	33	33	-	1/7/25/26	0/2/2/2
34	6MZ	Y	37	34	-	0/5/27/28	0/3/3/3
33	4SU	X	8	33	-	2/7/25/26	0/2/2/2
10	PSU	A	516	10,63	-	0/7/25/26	0/2/2/2
10	5MC	A	967	10	-	0/7/25/26	0/2/2/2
10	5MC	A	1407	10	-	0/7/25/26	0/2/2/2
8	PSU	7	2504	8	-	0/7/25/26	0/2/2/2
8	PSU	7	746	63,8	-	6/7/25/26	0/2/2/2
8	PSU	7	955	8	-	0/7/25/26	0/2/2/2
34	4SU	Y	7	34	-	0/7/25/26	0/2/2/2
32	PSU	W	32	32	-	0/7/25/26	0/2/2/2
33	PSU	X	72	33	-	0/7/25/26	0/2/2/2
10	4OC	A	1402	10	-	0/9/29/30	0/2/2/2
32	MIA	W	37	32	-	4/11/33/34	0/3/3/3
33	H2U	X	20	33	-	5/7/38/39	0/2/2/2
10	UR3	A	1498	10	-	2/7/25/26	0/2/2/2
32	PSU	W	55	32	-	0/7/25/26	0/2/2/2
34	CM0	Y	34	34	-	2/12/30/31	0/2/2/2
10	MA6	A	1518	10	-	0/7/29/30	0/3/3/3
8	5MC	7	1962	8	-	4/7/25/26	0/2/2/2
34	7MG	Y	46	34	-	1/7/37/38	0/3/3/3
10	2MG	A	1516	10	-	1/5/27/28	0/3/3/3
8	5MU	7	1939	63,8	-	0/7/25/26	0/2/2/2
8	OMG	7	2251	32,8	-	3/5/27/28	0/3/3/3
8	5MU	7	747	8	-	0/7/25/26	0/2/2/2
8	PSU	7	2580	8	-	0/7/25/26	0/2/2/2
8	2MA	7	2503	8	-	0/3/25/26	0/3/3/3
8	G7M	7	2069	8	-	1/3/25/26	0/3/3/3
8	6MZ	7	2030	8	-	1/5/27/28	0/3/3/3
10	G7M	A	527	10	-	2/3/25/26	0/3/3/3
8	6MZ	7	1618	8	-	2/5/27/28	0/3/3/3
8	OMC	7	2498	63,8	-	2/9/27/28	0/2/2/2
32	PSU	W	39	32	-	0/7/25/26	0/2/2/2
10	MA6	A	1519	10	-	4/7/29/30	0/3/3/3
8	PSU	7	2457	8	-	0/7/25/26	0/2/2/2
8	H2U	7	2449	8	-	0/7/38/39	0/2/2/2
33	12A	X	38	10,33	-	10/21/43/44	0/3/3/3
32	H2U	W	20	32	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	W	46	32	-	3/3/25/26	0/3/3/3
10	2MG	A	966	10	-	0/5/27/28	0/3/3/3
32	4SU	W	8	32	-	2/7/25/26	0/2/2/2
10	2MG	A	1207	10	-	0/5/27/28	0/3/3/3
8	PSU	7	2604	8	-	0/7/25/26	0/2/2/2
32	H2U	W	17	32	-	6/7/38/39	0/2/2/2
8	1MG	7	745	8	-	0/3/25/26	0/3/3/3

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	38	12A	C2-S2	14.59	1.88	1.75
32	W	32	PSU	C6-C5	12.17	1.49	1.35
32	W	39	PSU	C6-C5	12.14	1.49	1.35
33	X	33	RSP	C2-N3	11.88	1.49	1.36
33	X	38	12A	C2'-C3'	-10.51	1.24	1.53
8	7	2449	H2U	C2'-C3'	-10.35	1.25	1.53
10	A	967	5MC	C6-C5	9.89	1.50	1.34
34	Y	46	7MG	C8-N9	9.86	1.51	1.46
33	X	20	H2U	C2-N1	9.61	1.49	1.35
32	W	39	PSU	C2-N1	9.55	1.49	1.36
32	W	32	PSU	C2-N1	9.54	1.49	1.36
32	W	20	H2U	C2-N1	9.47	1.49	1.35
32	W	16	H2U	C2-N1	9.45	1.49	1.35
32	W	17	H2U	C2-N1	9.41	1.49	1.35
8	7	2449	H2U	C2-N1	9.25	1.48	1.35
33	X	8	4SU	C4-N3	8.95	1.47	1.37
32	W	8	4SU	C4-N3	8.84	1.47	1.37
33	X	38	12A	C2'-C1'	8.58	1.66	1.53
32	W	32	PSU	C2-N3	8.26	1.51	1.37
32	W	39	PSU	C2-N3	8.23	1.51	1.37
34	Y	46	7MG	C5-N7	7.85	1.44	1.35
32	W	37	MIA	C2-S10	7.82	1.82	1.75
33	X	38	12A	O3'-C3'	7.75	1.61	1.43
10	A	967	5MC	C4-N3	7.48	1.46	1.34
33	X	38	12A	O4'-C1'	-7.45	1.30	1.41
10	A	967	5MC	C2-N3	6.95	1.50	1.36
32	W	8	4SU	C2-N3	6.95	1.50	1.38
33	X	33	RSP	C6-C5	6.91	1.51	1.35
32	W	37	MIA	C6-N6	6.90	1.47	1.34
33	X	8	4SU	C2-N3	6.89	1.50	1.38
33	X	33	RSP	C4-N4	6.67	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	46	G7M	C2-N2	6.57	1.49	1.34
32	W	17	H2U	C2-N3	6.53	1.49	1.38
32	W	16	H2U	C2-N3	6.51	1.49	1.38
32	W	20	H2U	C2-N3	6.51	1.49	1.38
10	A	966	2MG	C2-N2	6.44	1.47	1.33
33	X	20	H2U	C2-N3	6.40	1.49	1.38
8	7	2449	H2U	C2-N3	6.29	1.49	1.38
33	X	8	4SU	C4-S4	-6.10	1.56	1.68
32	W	8	4SU	C4-S4	-6.01	1.57	1.68
34	Y	46	7MG	C2-N3	5.92	1.47	1.33
34	Y	46	7MG	C4-N9	5.90	1.44	1.37
33	X	8	4SU	C2-N1	5.89	1.47	1.38
32	W	32	PSU	C6-N1	5.86	1.46	1.36
32	W	46	G7M	C2-N3	5.82	1.47	1.33
32	W	8	4SU	C6-C5	5.80	1.48	1.35
32	W	39	PSU	C6-N1	5.78	1.45	1.36
33	X	8	4SU	C6-C5	5.77	1.48	1.35
32	W	8	4SU	C2-N1	5.77	1.47	1.38
33	X	38	12A	CC-N	5.75	1.48	1.35
10	A	967	5MC	C4-N4	5.71	1.49	1.34
34	Y	46	7MG	C4-N3	5.57	1.47	1.34
10	A	967	5MC	C6-N1	5.55	1.47	1.38
10	A	966	2MG	C4-N3	5.53	1.50	1.37
32	W	46	G7M	C4-N3	5.35	1.50	1.37
10	A	966	2MG	C2-N1	5.35	1.45	1.36
33	X	33	RSP	C4-N3	5.31	1.45	1.34
33	X	38	12A	C6-N6	5.27	1.45	1.36
32	W	17	H2U	C4-N3	4.99	1.46	1.37
32	W	20	H2U	C4-N3	4.98	1.46	1.37
32	W	16	H2U	C4-N3	4.94	1.46	1.37
34	Y	46	7MG	C2-N2	4.77	1.45	1.34
33	X	20	H2U	C4-N3	4.72	1.45	1.37
8	7	2449	H2U	C4-N3	4.71	1.45	1.37
34	Y	34	CM0	C6-C5	4.66	1.39	1.34
33	X	38	12A	C3'-C4'	4.60	1.64	1.53
8	7	2449	H2U	O4'-C1'	-4.58	1.31	1.42
10	A	967	5MC	C2-N1	4.57	1.49	1.40
32	W	32	PSU	C4-N3	4.39	1.47	1.38
32	W	46	G7M	C6-N1	4.38	1.44	1.37
32	W	39	PSU	C4-N3	4.37	1.46	1.38
10	A	966	2MG	C6-N1	4.06	1.43	1.37
10	A	966	2MG	C5-C6	3.89	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Y	46	7MG	C2-N1	3.80	1.47	1.37
33	X	33	RSP	C5-C4	3.60	1.51	1.42
34	Y	46	7MG	C5-C6	3.54	1.52	1.43
32	W	8	4SU	C5-C4	3.51	1.47	1.42
32	W	55	PSU	C6-C5	3.51	1.39	1.35
32	W	46	G7M	C5-C6	3.47	1.54	1.45
33	X	8	4SU	C5-C4	3.45	1.47	1.42
8	7	2069	G7M	C8-N9	3.44	1.39	1.33
32	W	8	4SU	C6-N1	3.44	1.46	1.38
34	Y	55	PSU	C6-C5	3.43	1.39	1.35
33	X	8	4SU	C6-N1	3.42	1.46	1.38
10	A	527	G7M	C8-N9	3.40	1.39	1.33
8	7	1915	3TD	C6-C5	3.39	1.39	1.35
34	Y	46	7MG	C6-N1	3.37	1.45	1.38
33	X	72	PSU	C6-C5	3.37	1.39	1.35
8	7	746	PSU	C6-C5	3.35	1.39	1.35
8	7	2449	H2U	C5'-C4'	-3.35	1.41	1.51
8	7	2504	PSU	C6-C5	3.33	1.39	1.35
8	7	955	PSU	C6-C5	3.30	1.39	1.35
8	7	2605	PSU	C6-C5	3.28	1.39	1.35
8	7	2580	PSU	C6-C5	3.28	1.39	1.35
8	7	2457	PSU	C6-C5	3.27	1.39	1.35
8	7	2604	PSU	C6-C5	3.26	1.39	1.35
33	X	38	12A	O4'-C4'	3.26	1.52	1.45
33	X	33	RSP	C6-N1	3.26	1.45	1.38
8	7	2449	H2U	C2'-C1'	3.24	1.63	1.53
33	X	33	RSP	C2-S2	-3.21	1.59	1.67
8	7	2449	H2U	O3'-C3'	3.19	1.50	1.43
32	W	39	PSU	O4-C4	-3.19	1.17	1.23
10	A	516	PSU	C6-C5	3.17	1.39	1.35
32	W	32	PSU	O4-C4	-3.12	1.17	1.23
32	W	46	G7M	C2-N1	2.97	1.45	1.37
33	X	38	12A	CA-N	2.76	1.51	1.45
8	7	2251	OMG	C5-C6	-2.73	1.41	1.47
33	X	38	12A	CC-N6	2.70	1.43	1.37
32	W	32	PSU	C1'-C5	2.69	1.56	1.50
32	W	39	PSU	C1'-C5	2.64	1.56	1.50
10	A	1207	2MG	C5-C6	-2.61	1.42	1.47
8	7	1835	2MG	C5-C6	-2.60	1.42	1.47
33	X	38	12A	C5-C4	-2.59	1.34	1.40
10	A	1516	2MG	C5-C6	-2.59	1.42	1.47
8	7	2449	H2U	O2'-C2'	2.57	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	2445	2MG	C5-C6	-2.56	1.42	1.47
33	X	38	12A	O-C	2.55	1.29	1.22
32	W	39	PSU	O2-C2	-2.55	1.18	1.23
32	W	32	PSU	O2-C2	-2.54	1.18	1.23
34	Y	46	7MG	O6-C6	-2.46	1.18	1.23
33	X	20	H2U	O2-C2	-2.46	1.18	1.23
10	A	527	G7M	C8-N7	2.46	1.37	1.33
8	7	2449	H2U	O4-C4	-2.45	1.18	1.23
10	A	966	2MG	C5-C4	-2.44	1.36	1.43
8	7	2449	H2U	O2-C2	-2.43	1.18	1.23
8	7	2449	H2U	C3'-C4'	2.40	1.59	1.53
8	7	2069	G7M	C8-N7	2.37	1.37	1.33
33	X	38	12A	O2'-C2'	2.35	1.48	1.43
32	W	37	MIA	C5-C4	-2.33	1.34	1.40
8	7	2449	H2U	O4'-C4'	2.27	1.50	1.45
32	W	17	H2U	O2-C2	-2.27	1.18	1.23
33	X	38	12A	C5'-C4'	-2.27	1.44	1.51
32	W	16	H2U	O2-C2	-2.25	1.18	1.23
8	7	745	1MG	C5-C4	-2.24	1.37	1.43
10	A	967	5MC	O2-C2	-2.23	1.19	1.23
8	7	2449	H2U	C1'-N1	-2.23	1.42	1.46
8	7	2251	OMG	C8-N7	-2.22	1.31	1.35
33	X	38	12A	C6-N1	2.21	1.35	1.32
33	X	20	H2U	O4-C4	-2.21	1.18	1.23
32	W	20	H2U	O2-C2	-2.20	1.19	1.23
10	A	527	G7M	C5-C6	-2.18	1.39	1.45
32	W	16	H2U	O4-C4	-2.15	1.18	1.23
32	W	46	G7M	O6-C6	-2.14	1.18	1.23
32	W	17	H2U	O4-C4	-2.13	1.18	1.23
32	W	20	H2U	O4-C4	-2.13	1.18	1.23
8	7	1835	2MG	C8-N7	-2.13	1.31	1.35
8	7	2069	G7M	C5-C6	-2.10	1.40	1.45
10	A	1516	2MG	C8-N7	-2.10	1.31	1.35
10	A	1207	2MG	C5-C4	-2.10	1.37	1.43
8	7	2445	2MG	C8-N7	-2.09	1.31	1.35
10	A	1207	2MG	C8-N7	-2.05	1.31	1.35
10	A	966	2MG	O6-C6	-2.02	1.19	1.23
10	A	1519	MA6	C8-N7	-2.02	1.31	1.34

All (92) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	X	38	12A	N6-C6-N1	-11.23	98.72	118.84
32	W	37	MIA	C11-S10-C2	9.96	109.70	102.27
33	X	38	12A	C2M-S2-C2	9.30	109.21	102.27
33	X	8	4SU	C4-N3-C2	-7.94	119.63	127.34
32	W	8	4SU	C4-N3-C2	-7.83	119.74	127.34
8	7	2449	H2U	C4-N3-C2	-7.64	119.46	125.79
32	W	16	H2U	C4-N3-C2	-7.15	119.86	125.79
32	W	17	H2U	C4-N3-C2	-6.95	120.03	125.79
32	W	20	H2U	C4-N3-C2	-6.95	120.03	125.79
33	X	20	H2U	C4-N3-C2	-6.71	120.22	125.79
8	7	2503	2MA	C5-C6-N1	-6.39	116.82	121.01
33	X	8	4SU	C5-C4-N3	5.86	120.13	114.69
32	W	8	4SU	C5-C4-N3	5.48	119.78	114.69
34	Y	46	7MG	C5-C6-N1	5.00	119.81	110.99
32	W	39	PSU	C4-N3-C2	-4.64	119.65	126.34
33	X	38	12A	N6-CC-N	4.57	120.14	113.76
34	Y	46	7MG	C2-N3-C4	4.54	120.38	112.30
8	7	2503	2MA	C5-C6-N6	4.51	127.20	120.35
32	W	32	PSU	C4-N3-C2	-4.47	119.90	126.34
34	Y	7	4SU	C4-N3-C2	-4.41	123.06	127.34
34	Y	46	7MG	C5-C4-N3	-4.24	120.06	128.13
32	W	39	PSU	N1-C2-N3	4.22	119.91	115.13
32	W	32	PSU	N1-C2-N3	4.08	119.75	115.13
32	W	8	4SU	N3-C2-N1	3.82	119.97	114.89
33	X	8	4SU	N3-C2-N1	3.67	119.77	114.89
33	X	20	H2U	N3-C2-N1	3.64	120.50	116.65
32	W	37	MIA	C12-C13-C14	-3.62	120.09	127.14
33	X	8	4SU	C5-C4-S4	-3.61	119.82	124.47
10	A	966	2MG	C5-C6-N1	3.56	120.23	113.95
33	X	38	12A	OO-CC-N6	-3.55	117.62	123.62
32	W	37	MIA	N3-C2-N1	-3.48	120.57	126.98
32	W	8	4SU	C5-C4-S4	-3.45	120.03	124.47
32	W	39	PSU	C6-C5-C4	3.38	120.56	118.20
32	W	37	MIA	C2-N3-C4	3.36	119.95	115.32
10	A	967	5MC	C5-C6-N1	-3.33	119.92	123.34
8	7	2580	PSU	C3'-C2'-C1'	3.29	105.46	101.64
32	W	16	H2U	N3-C2-N1	3.25	120.09	116.65
8	7	2449	H2U	C5-C4-N3	3.25	120.30	116.65
34	Y	46	7MG	C4-C5-N7	3.23	110.01	105.53
33	X	38	12A	CA-N-CC	3.18	127.23	121.94
8	7	2449	H2U	N3-C2-N1	3.17	120.01	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	17	H2U	N3-C2-N1	3.16	120.00	116.65
32	W	46	G7M	C2-N1-C6	-3.16	119.28	125.10
32	W	20	H2U	N3-C2-N1	3.13	119.97	116.65
32	W	32	PSU	C6-C5-C4	3.08	120.36	118.20
10	A	516	PSU	C4-N3-C2	-3.05	121.94	126.34
33	X	38	12A	O3'-C3'-C4'	3.03	119.80	111.05
33	X	20	H2U	C5-C6-N1	2.93	121.26	111.61
34	Y	46	7MG	N9-C4-N3	2.91	129.82	125.47
32	W	32	PSU	C6-N1-C2	-2.91	119.71	122.68
32	W	37	MIA	S10-C2-N3	2.91	126.19	116.10
34	Y	46	7MG	C5-C4-N9	2.91	110.12	106.35
34	Y	46	7MG	C2-N1-C6	-2.88	119.85	125.10
34	Y	7	4SU	C5-C4-N3	2.87	117.35	114.69
32	W	39	PSU	C6-N1-C2	-2.84	119.78	122.68
32	W	16	H2U	C5-C4-N3	2.83	119.83	116.65
34	Y	46	7MG	O6-C6-C5	-2.82	120.62	127.54
34	Y	7	4SU	C3'-C2'-C1'	2.80	106.74	101.43
33	X	38	12A	C2-N3-C4	2.79	119.17	115.32
33	X	38	12A	C3'-C2'-C1'	2.79	105.17	100.98
32	W	20	H2U	C5-C4-N3	2.78	119.78	116.65
32	W	17	H2U	C5-C4-N3	2.74	119.72	116.65
33	X	38	12A	N3-C2-N1	-2.71	122.00	126.98
8	7	2503	2MA	C2-N1-C6	2.70	122.29	118.08
8	7	2503	2MA	CM2-C2-N1	2.69	121.35	117.15
32	W	20	H2U	C5-C6-N1	2.67	120.42	111.61
32	W	17	H2U	C5-C6-N1	2.66	120.39	111.61
32	W	16	H2U	C5-C6-N1	2.62	120.25	111.61
8	7	2449	H2U	C5-C6-N1	2.61	120.23	111.61
10	A	966	2MG	C8-N7-C5	2.61	107.97	102.99
33	X	20	H2U	C5-C4-N3	2.59	119.56	116.65
32	W	39	PSU	O2-C2-N1	-2.53	120.01	122.79
32	W	32	PSU	O2-C2-N1	-2.51	120.03	122.79
32	W	16	H2U	O2-C2-N1	-2.46	120.02	123.11
34	Y	46	7MG	N9-C8-N7	2.41	106.83	103.38
32	W	37	MIA	C16-C14-C15	2.40	119.91	114.60
8	7	2503	2MA	N3-C2-N1	-2.38	121.38	125.73
8	7	2449	H2U	O2-C2-N1	-2.38	120.12	123.11
8	7	2457	PSU	C3'-C2'-C1'	2.35	104.38	101.64
10	A	966	2MG	O6-C6-C5	-2.34	119.79	124.37
8	7	2030	6MZ	C9-N6-C6	-2.34	120.86	122.87
32	W	37	MIA	C1'-N9-C4	-2.33	122.55	126.64
32	W	17	H2U	O2-C2-N1	-2.29	120.23	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	W	20	H2U	O2-C2-N1	-2.24	120.29	123.11
10	A	1207	2MG	CM2-N2-C2	-2.21	118.99	123.86
10	A	516	PSU	C5-C6-N1	-2.19	118.82	122.11
10	A	967	5MC	CM5-C5-C6	-2.12	120.01	122.85
8	7	2030	6MZ	C2-N1-C6	2.12	118.41	116.59
10	A	966	2MG	CM2-N2-C2	-2.11	119.19	123.86
10	A	516	PSU	N1-C2-N3	2.08	117.49	115.13
34	Y	37	6MZ	C2-N1-C6	2.02	118.32	116.59
32	W	8	4SU	O2-C2-N1	-2.02	120.10	122.79

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	527	G7M	O4'-C4'-C5'-O5'
10	A	527	G7M	C3'-C4'-C5'-O5'
10	A	1516	2MG	N3-C2-N2-CM2
10	A	1519	MA6	C5-C6-N6-C10
8	7	746	PSU	C2'-C1'-C5-C4
8	7	746	PSU	C2'-C1'-C5-C6
8	7	2251	OMG	C1'-C2'-O2'-CM2
32	W	17	H2U	O4'-C1'-N1-C6
32	W	17	H2U	C2'-C1'-N1-C2
32	W	17	H2U	C2'-C1'-N1-C6
32	W	37	MIA	O4'-C4'-C5'-O5'
32	W	37	MIA	C3'-C4'-C5'-O5'
32	W	37	MIA	N1-C2-S10-C11
32	W	37	MIA	N3-C2-S10-C11
33	X	8	4SU	C3'-C4'-C5'-O5'
33	X	8	4SU	O4'-C4'-C5'-O5'
33	X	20	H2U	C4'-C5'-O5'-P
33	X	20	H2U	O4'-C4'-C5'-O5'
33	X	20	H2U	C3'-C4'-C5'-O5'
33	X	20	H2U	O4'-C1'-N1-C6
33	X	38	12A	C3'-C4'-C5'-O5'
33	X	38	12A	C5-C6-N6-CC
33	X	38	12A	N1-C2-S2-C2M
33	X	38	12A	N3-C2-S2-C2M
33	X	38	12A	CB-CA-N-CC
33	X	38	12A	N-CA-CB-OG1
33	X	38	12A	N-CA-CB-CG2
33	X	38	12A	C-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
33	X	38	12A	C-CA-CB-CG2
34	Y	34	CM0	O5-C7-C8-O8
34	Y	55	PSU	C2'-C1'-C5-C4
34	Y	34	CM0	O5-C7-C8-O9
8	7	2498	OMC	C3'-C4'-C5'-O5'
8	7	2498	OMC	O4'-C4'-C5'-O5'
32	W	8	4SU	O4'-C4'-C5'-O5'
33	X	38	12A	O4'-C4'-C5'-O5'
33	X	20	H2U	O4'-C1'-N1-C2
10	A	1498	UR3	O4'-C4'-C5'-O5'
8	7	2251	OMG	O4'-C4'-C5'-O5'
8	7	2445	2MG	C3'-C4'-C5'-O5'
32	W	8	4SU	C3'-C4'-C5'-O5'
10	A	1498	UR3	C3'-C4'-C5'-O5'
8	7	1618	6MZ	O4'-C4'-C5'-O5'
8	7	2251	OMG	C3'-C4'-C5'-O5'
10	A	1519	MA6	C5-C6-N6-C9
10	A	1519	MA6	N1-C6-N6-C10
8	7	2030	6MZ	O4'-C4'-C5'-O5'
8	7	2445	2MG	O4'-C4'-C5'-O5'
32	W	17	H2U	C4'-C5'-O5'-P
32	W	46	G7M	C4'-C5'-O5'-P
34	Y	46	7MG	C4'-C5'-O5'-P
8	7	1618	6MZ	C3'-C4'-C5'-O5'
32	W	46	G7M	O4'-C4'-C5'-O5'
32	W	54	5MU	C4'-C5'-O5'-P
32	W	17	H2U	O4'-C1'-N1-C2
32	W	54	5MU	C3'-C4'-C5'-O5'
32	W	16	H2U	C4'-C5'-O5'-P
8	7	746	PSU	O4'-C1'-C5-C4
34	Y	55	PSU	O4'-C1'-C5-C4
8	7	1962	5MC	O4'-C1'-N1-C6
32	W	54	5MU	C2'-C1'-N1-C2
8	7	1962	5MC	C2'-C1'-N1-C6
32	W	54	5MU	C2'-C1'-N1-C6
8	7	2069	G7M	O4'-C4'-C5'-O5'
34	Y	55	PSU	O4'-C4'-C5'-O5'
8	7	1835	2MG	O4'-C4'-C5'-O5'
32	W	17	H2U	O4'-C4'-C5'-O5'
8	7	746	PSU	O4'-C1'-C5-C6
32	W	20	H2U	O4'-C1'-N1-C6
32	W	20	H2U	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
34	Y	55	PSU	O4'-C1'-C5-C6
8	7	1962	5MC	O4'-C1'-N1-C2
32	W	20	H2U	C4'-C5'-O5'-P
8	7	746	PSU	O4'-C4'-C5'-O5'
8	7	746	PSU	C3'-C4'-C5'-O5'
32	W	46	G7M	C3'-C4'-C5'-O5'
10	A	1519	MA6	O4'-C4'-C5'-O5'
33	X	33	RSP	C3'-C4'-C5'-O5'
8	7	1962	5MC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 264 ligands modelled in this entry, 262 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
64	ATP	7	3194	-	26,33,33	3.46	10 (38%)	31,52,52	2.19	7 (22%)
64	ATP	7	3193	-	26,33,33	3.48	10 (38%)	31,52,52	2.24	7 (22%)

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
64	ATP	7	3194	-	-	4/18/38/38	0/3/3/3
64	ATP	7	3193	-	-	6/18/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	7	3194	ATP	C2'-C3'	-10.66	1.24	1.53
64	7	3193	ATP	C2'-C3'	-10.60	1.24	1.53
64	7	3194	ATP	O4'-C1'	7.46	1.51	1.41
64	7	3193	ATP	O4'-C1'	7.46	1.51	1.41
64	7	3193	ATP	O4'-C4'	-6.45	1.30	1.45
64	7	3194	ATP	O4'-C4'	-6.22	1.31	1.45
64	7	3194	ATP	C3'-C4'	5.45	1.66	1.53
64	7	3193	ATP	C3'-C4'	5.39	1.66	1.53
64	7	3193	ATP	C2'-C1'	4.92	1.61	1.53
64	7	3194	ATP	C2'-C1'	4.62	1.60	1.53
64	7	3194	ATP	O2'-C2'	3.32	1.50	1.43
64	7	3193	ATP	O2'-C2'	3.30	1.50	1.43
64	7	3193	ATP	C6-N6	3.23	1.45	1.34
64	7	3194	ATP	C6-N6	3.22	1.45	1.34
64	7	3194	ATP	C5-C4	-2.65	1.33	1.40
64	7	3193	ATP	C5-C4	-2.64	1.33	1.40
64	7	3193	ATP	C2-N3	2.24	1.35	1.32
64	7	3194	ATP	C2-N3	2.22	1.35	1.32
64	7	3193	ATP	O3'-C3'	2.19	1.48	1.43
64	7	3194	ATP	O3'-C3'	2.19	1.48	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	7	3193	ATP	C5-C6-N6	6.65	130.46	120.35
64	7	3194	ATP	C5-C6-N6	6.60	130.39	120.35
64	7	3194	ATP	N3-C2-N1	-5.50	120.08	128.68
64	7	3193	ATP	N3-C2-N1	-5.46	120.14	128.68
64	7	3193	ATP	C1'-N9-C4	4.93	135.31	126.64
64	7	3194	ATP	C1'-N9-C4	4.75	134.99	126.64
64	7	3193	ATP	N6-C6-N1	-4.43	109.38	118.57
64	7	3194	ATP	N6-C6-N1	-4.42	109.39	118.57
64	7	3193	ATP	C3'-C2'-C1'	2.98	105.47	100.98
64	7	3194	ATP	PB-O3B-PG	-2.66	123.71	132.83
64	7	3193	ATP	PB-O3B-PG	-2.65	123.74	132.83
64	7	3193	ATP	PA-O3A-PB	-2.64	123.77	132.83
64	7	3194	ATP	PA-O3A-PB	-2.12	125.54	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	7	3194	ATP	C3'-C2'-C1'	2.04	104.05	100.98

There are no chirality outliers.

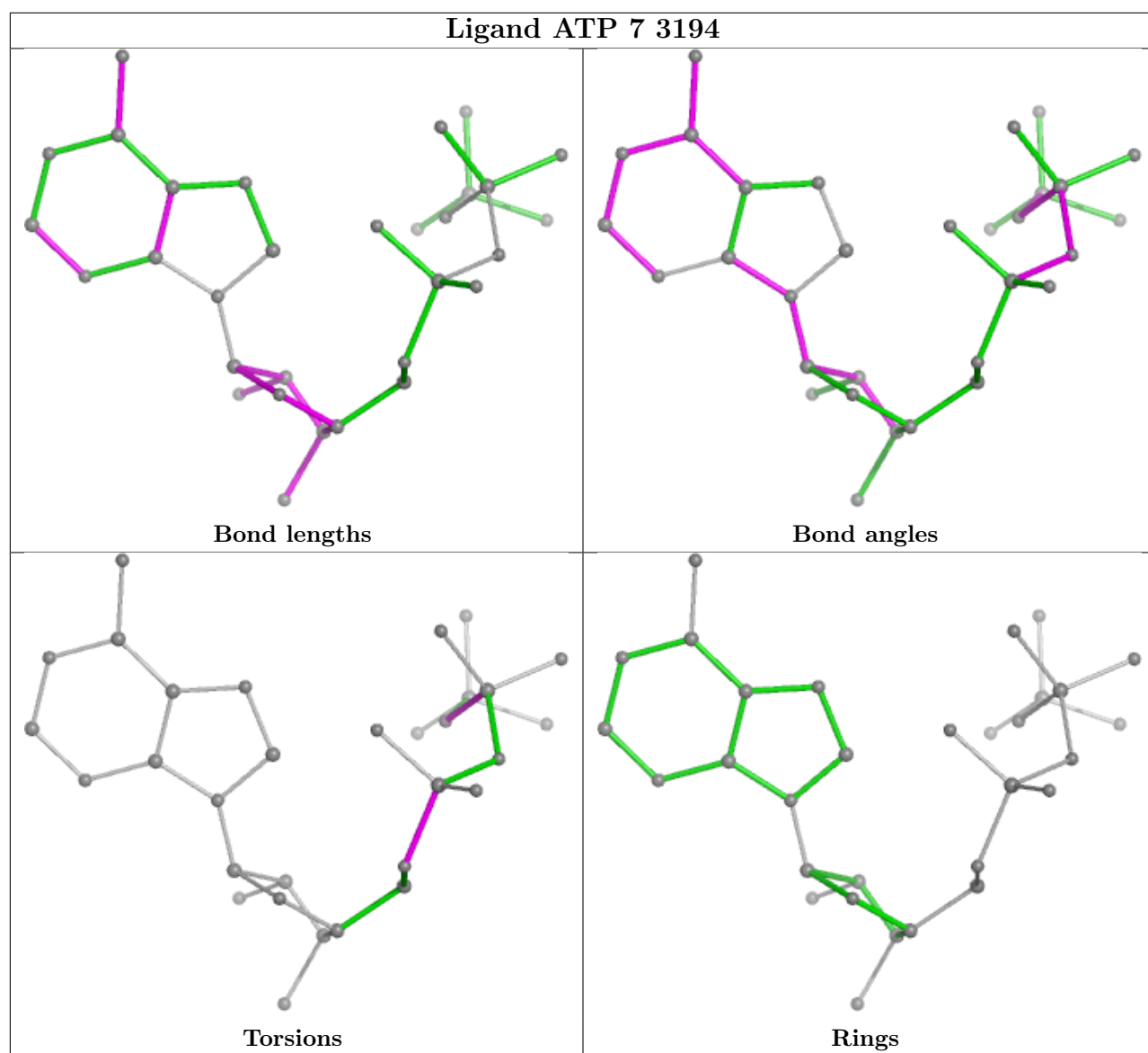
All (10) torsion outliers are listed below:

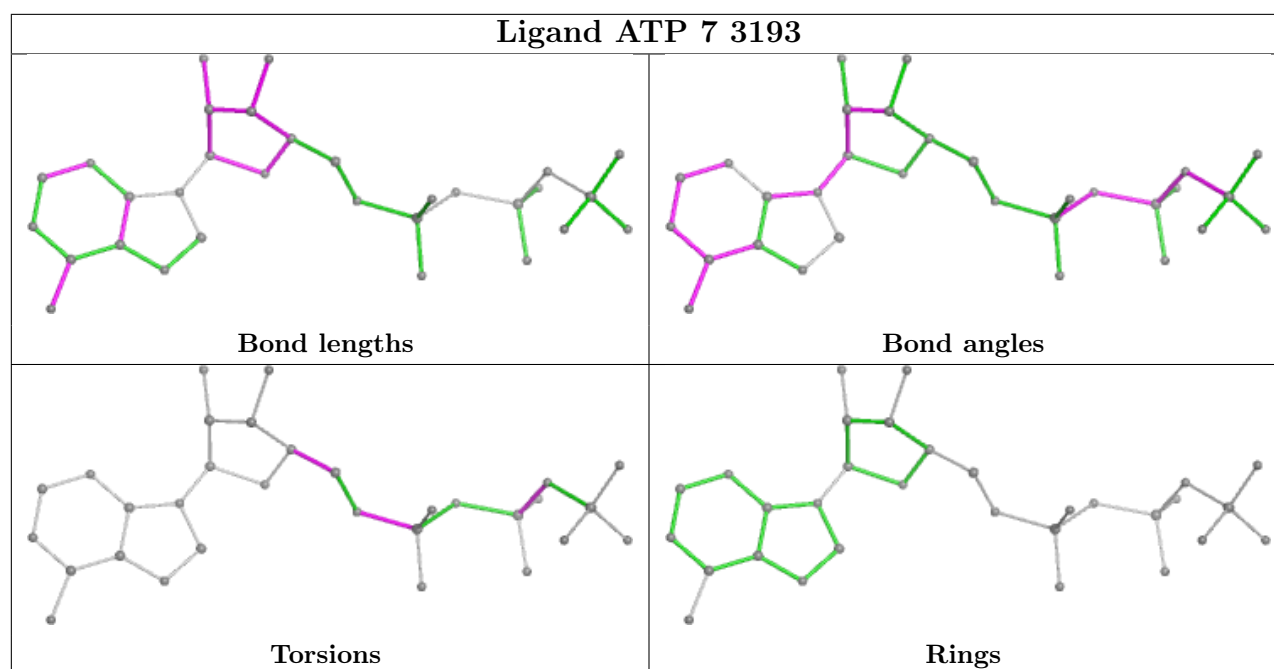
Mol	Chain	Res	Type	Atoms
64	7	3193	ATP	C5'-O5'-PA-O1A
64	7	3194	ATP	C5'-O5'-PA-O3A
64	7	3193	ATP	C3'-C4'-C5'-O5'
64	7	3193	ATP	C5'-O5'-PA-O3A
64	7	3193	ATP	C5'-O5'-PA-O2A
64	7	3194	ATP	C5'-O5'-PA-O1A
64	7	3194	ATP	C5'-O5'-PA-O2A
64	7	3193	ATP	O4'-C4'-C5'-O5'
64	7	3193	ATP	PG-O3B-PB-O2B
64	7	3194	ATP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	47:U	O3'	63:A	P	17.15