



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 05:56 pm GMT

PDB ID : 7PJW  
EMDB ID : EMD-13462  
Title : Structure of the 70S-EF-G-GDP-Pi ribosome complex with tRNAs in hybrid state 2 (H2-EF-G-GDP-Pi)  
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.  
Deposited on : 2021-08-24  
Resolution : 4.00 Å (reported)  
Based on initial models : 6YSS, 4AQY, 5LZD, 5J9Z

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

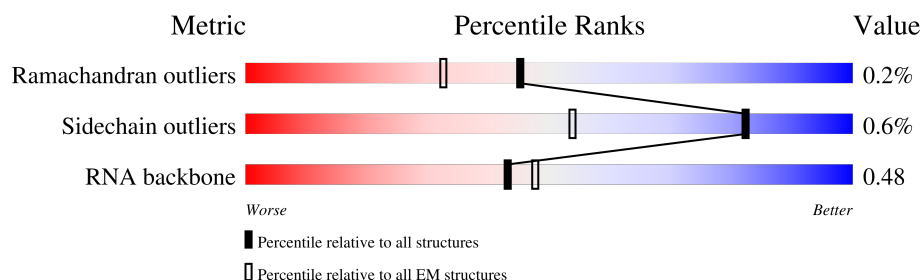
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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.



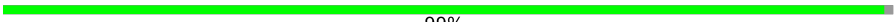













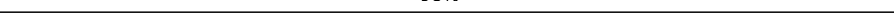
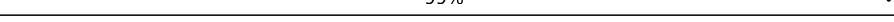
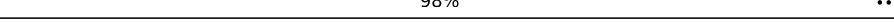
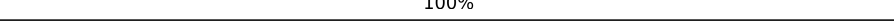

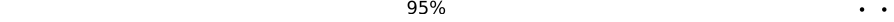
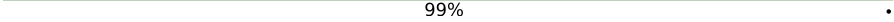

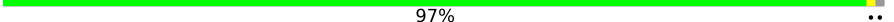
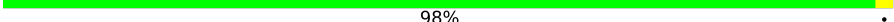
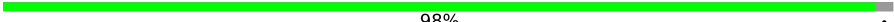
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	



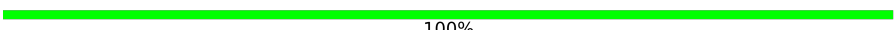
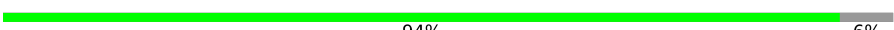






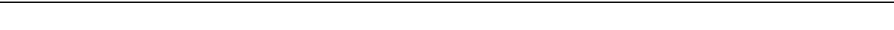

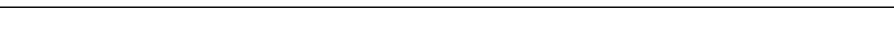
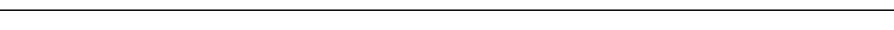
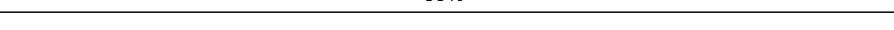
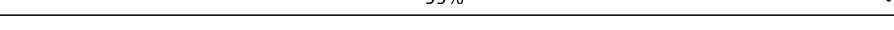
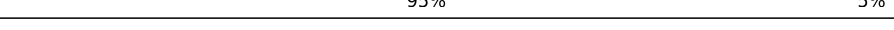


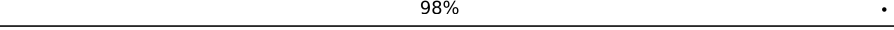



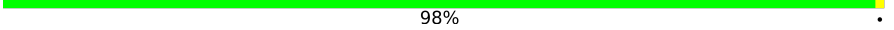

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Mol	Chain	Length	Quality of chain
10	C	273	 99% .
11	D	209	 100%
12	E	201	 100%
13	F	179	 99% .
14	G	177	 99% .
15	H	149	 100%
16	I	142	 99% .
17	J	142	 99% .
18	K	123	 99% .
19	L	144	 99% .
20	M	136	 99% .
21	N	127	 94% . 6%
22	O	117	 99% .
23	P	115	 98% ..
24	Q	118	 99% .
25	R	103	 98% ..
26	S	110	 100%
27	T	100	 93% 7%
28	U	104	 95% . .
29	V	94	 99% .
30	W	85	 88% 12%
31	X	78	 97% ..
32	Y	63	 98% .
33	Z	59	 98% .
34	a	1542	 76% 23% .

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Mol	Chain	Length	Quality of chain
35	b	240	 90% 9%
36	c	233	 88% 12%
37	d	206	 100%
38	e	167	 94% 6%
39	f	135	 74% 26%
40	g	179	 84% 16%
41	h	130	 99% .
42	i	130	 97% ..
43	j	103	 94% . 5%
44	k	129	 89% . 10%
45	l	124	 98% ..
46	m	118	 96% ..
47	n	102	 99% .
48	o	89	 99% .
49	p	82	 99% .
50	q	84	 95% 5%
51	r	75	 87% 13%
52	s	92	 89% 11%
53	t	87	 98% .
54	u	71	 90% . 8%
55	v	77	 68% 30% .
56	w	76	 50% 38% 12%
57	x	704	 98% .
58	y	2	 50% 50%
59	z	33	 . 15% 15% 67%

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152719 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
			62339	27816	11471	20149	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		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		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		
			779	492	146	141	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
34	a	1540	Total	C	N	O	P	
			33050	14748	6057	10705	1540	0

- 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 RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	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 protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	703	Total	C	N	O	S	0	0
			5444	3429	942	1048	25		

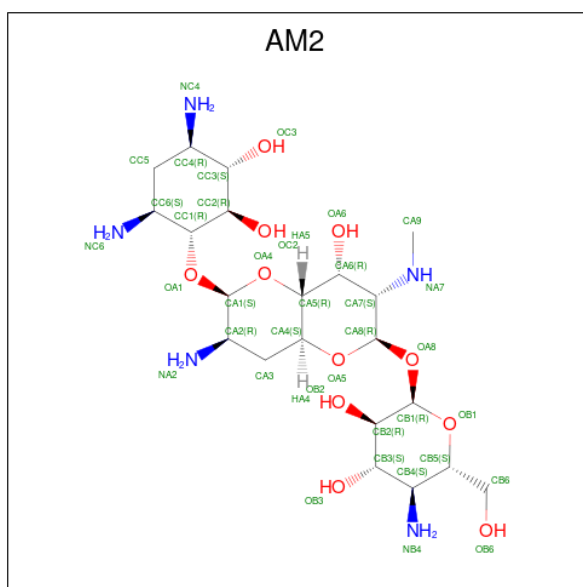
- Molecule 58 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	11	Total	C	N	O	P	0	0
			230	103	35	81	11		

- Molecule 60 is APRAMYCIN (three-letter code: AM2) (formula: C<sub>21</sub>H<sub>41</sub>N<sub>5</sub>O<sub>11</sub>).



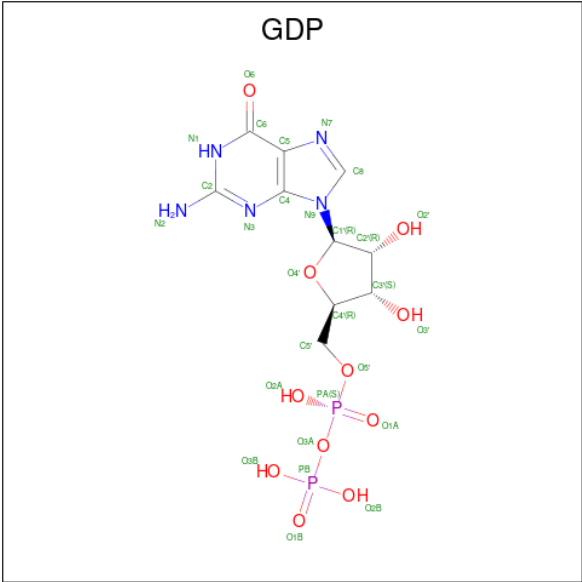
Mol	Chain	Residues	Atoms				AltConf
60	a	1	Total	C	N	O	0
			37	21	5	11	

- Molecule 61 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			AltConf
61	x	1	Total	O	P	0
			5	4	1	

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
62	x	1	Total	C	N	O	P	0
			28	10	5	11	2	

### 3 Residue-property plots


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

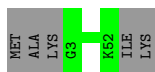
- Molecule 1: 50S ribosomal protein L32

Chain 0:  98% .



- Molecule 2: 50S ribosomal protein L33

Chain 1:  91% 9%



- Molecule 3: 50S ribosomal protein L34

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: 50S ribosomal protein L35

Chain 3:  98% .




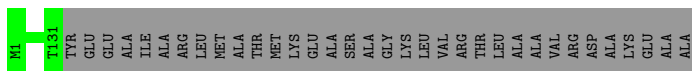
- Molecule 5: 50S ribosomal protein L36

Chain 4:  100%

There are no outlier residues recorded for this chain.


- Molecule 6: 50S ribosomal protein L10

Chain 5:  79% 21%





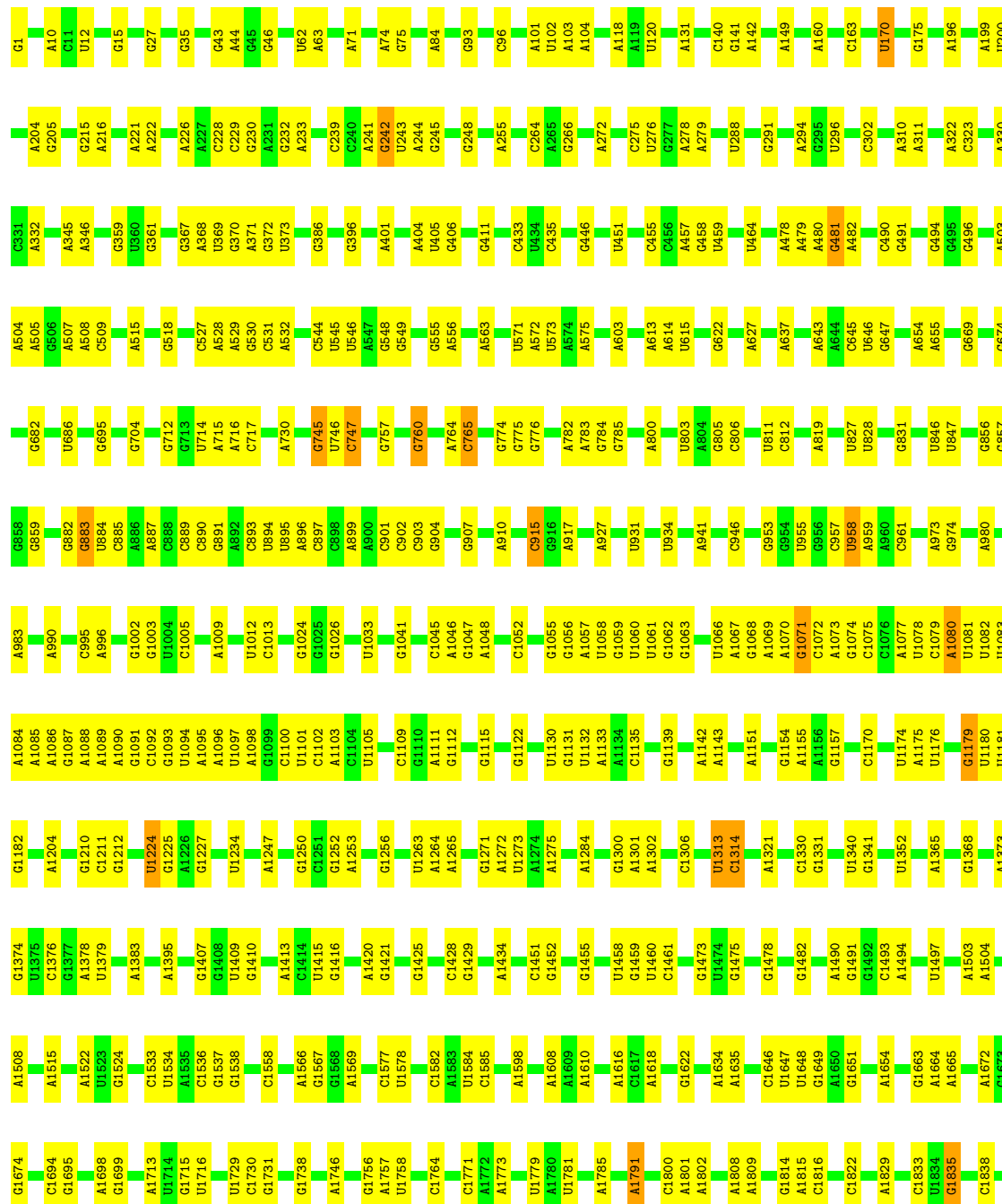
- Molecule 7: 50S ribosomal protein L31

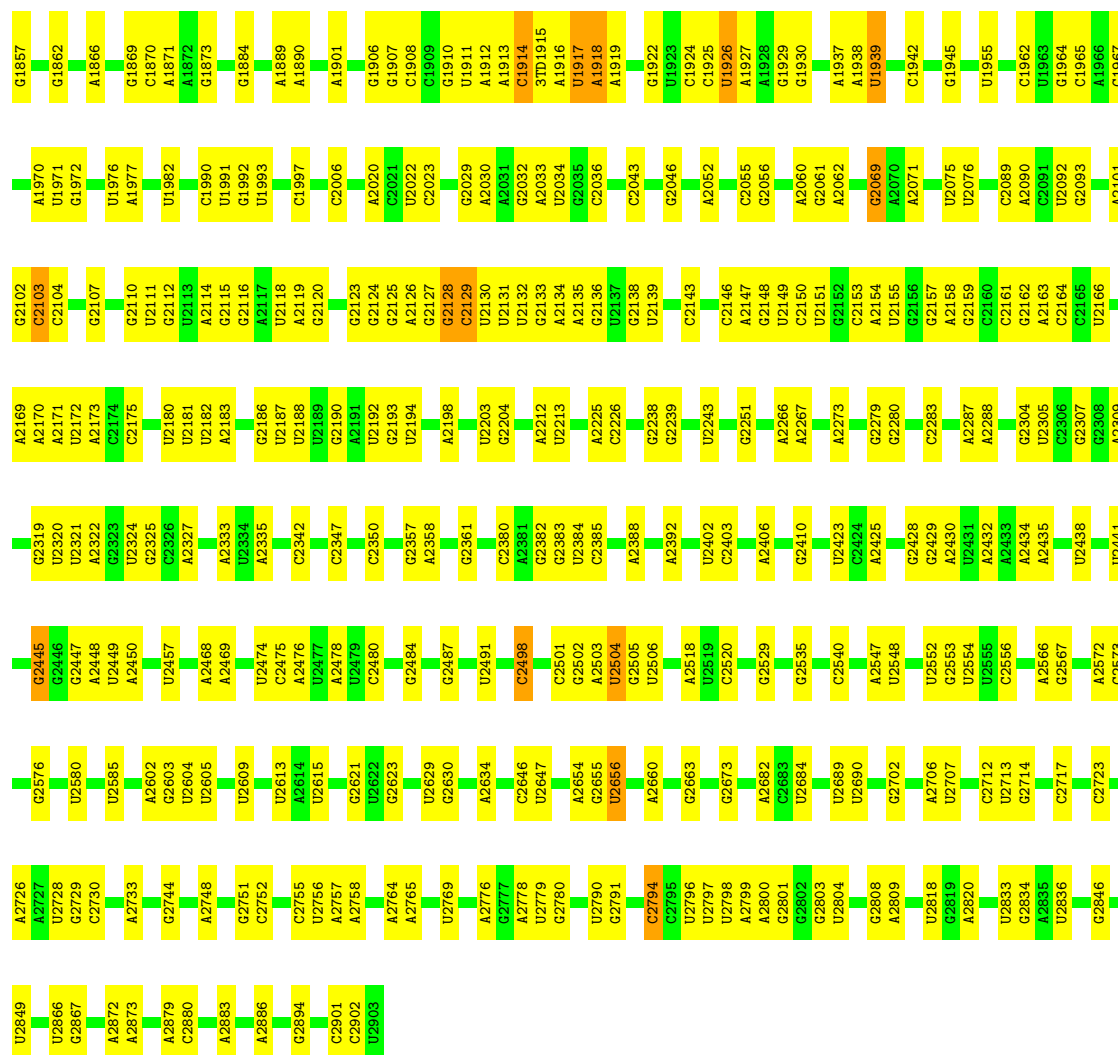
Chain 6:  79% 16% 6%



- Molecule 8: 23S ribosomal RNA

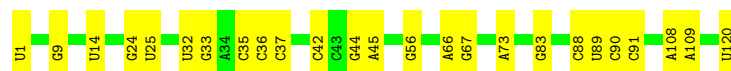
Chain A:  73% 26%





• Molecule 9: 5S ribosomal RNA

Chain B: 79% 21%



- 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:  99%



- Molecule 14: 50S ribosomal protein L6

Chain G:  99%



- Molecule 15: 50S ribosomal protein L9

Chain H:  100%

There are no outlier residues recorded for this chain.

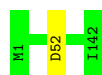
- Molecule 16: 50S ribosomal protein L11

Chain I:  99%



- Molecule 17: 50S ribosomal protein L13

Chain J:  99%



- Molecule 18: 50S ribosomal protein L14

Chain K:  99%



- Molecule 19: 50S ribosomal protein L15

Chain L:  99%



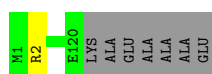
- Molecule 20: 50S ribosomal protein L16

Chain M: 99%



- 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: 98% ..



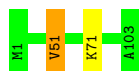
- Molecule 24: 50S ribosomal protein L20

Chain Q: 99%



- Molecule 25: 50S ribosomal protein L21

Chain R: 98% ..



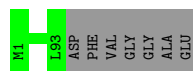
- Molecule 26: 50S ribosomal protein L22

Chain S: 100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L23

Chain T:  93% 7%



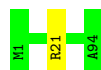
- Molecule 28: 50S ribosomal protein L24

Chain U:  95% . .




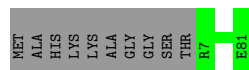
- Molecule 29: 50S ribosomal protein L25

Chain V:  99% .



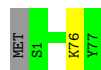
- Molecule 30: 50S ribosomal protein L27

Chain W:  88% 12%



- Molecule 31: 50S ribosomal protein L28

Chain X:  97% ..



- Molecule 32: 50S ribosomal protein L29

Chain Y:  98% .



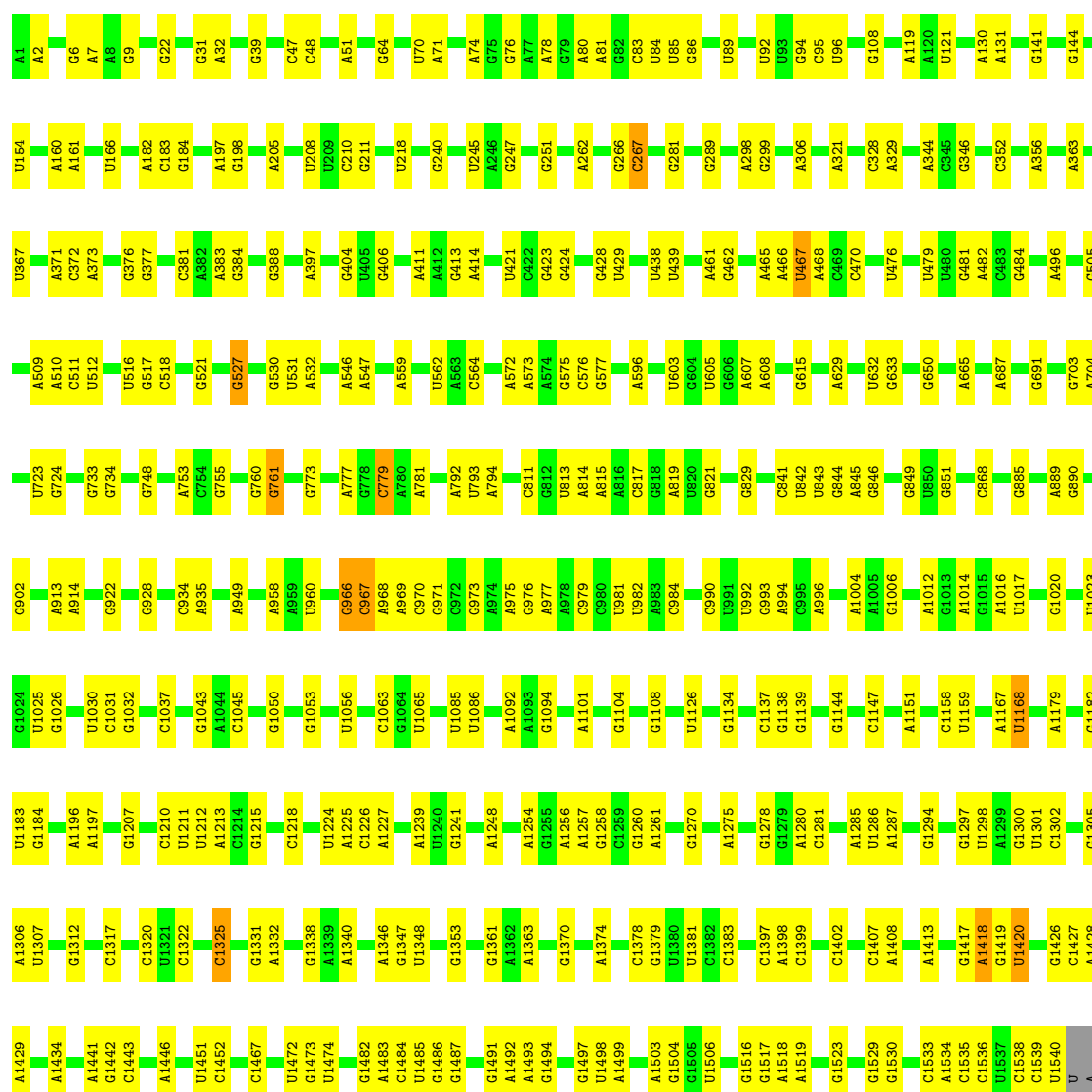
- Molecule 33: 50S ribosomal protein L30

Chain Z:  98% .




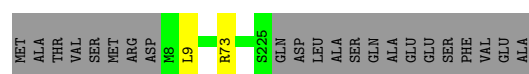
- Molecule 34: 16S ribosomal RNA

Chain a:  76% 23%




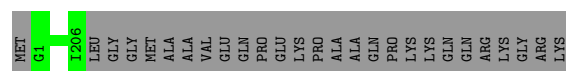
- Molecule 35: 30S ribosomal protein S2

Chain b:  90% 9%



- Molecule 36: 30S ribosomal protein S3

Chain c:  88% 12%



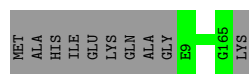
- Molecule 37: 30S ribosomal protein S4

Chain d:  100%



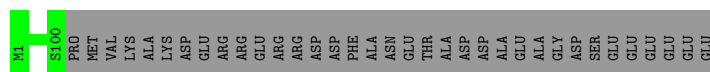
- Molecule 38: 30S ribosomal protein S5

Chain e:  94% 6%




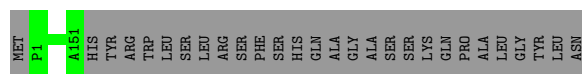
- Molecule 39: 30S ribosomal protein S6

Chain f:  74% 26%



- Molecule 40: 30S ribosomal protein S7

Chain g:  84% 16%



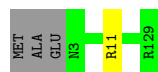
- Molecule 41: 30S ribosomal protein S8

Chain h:  99%



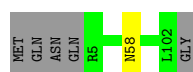
- Molecule 42: 30S ribosomal protein S9

Chain i:  97%




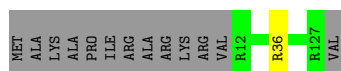
- Molecule 43: 30S ribosomal protein S10

Chain j:  94% 5%



- Molecule 44: 30S ribosomal protein S11

Chain k:  89% • 10%



- Molecule 45: 30S ribosomal protein S12

Chain l:  98% ..



- Molecule 46: 30S ribosomal protein S13

Chain m:  96% ..



- 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:  99% .




- Molecule 50: 30S ribosomal protein S17

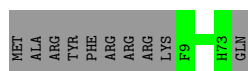
Chain q:  95% 5%




- Molecule 51: 30S ribosomal protein S18

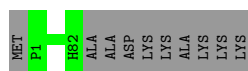


Chain r:  87% 13%



- Molecule 52: 30S ribosomal protein S19

Chain s:  89% 11%



- Molecule 53: 30S ribosomal protein S20

Chain t:  98% .



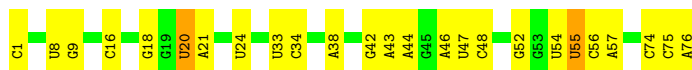
- Molecule 54: 30S ribosomal protein S21

Chain u:  90% . 8%



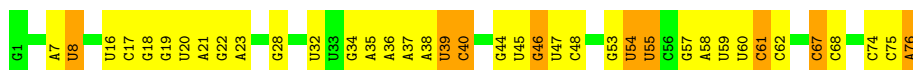
- Molecule 55: P-site tRNA(fMet)

Chain v:  68% 30% .



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

Chain w:  50% 38% 12%

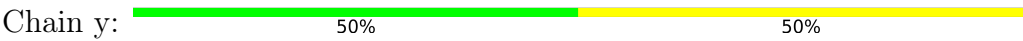


- Molecule 57: Elongation factor G

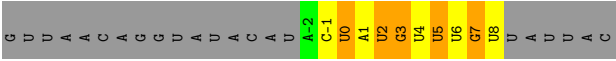
Chain x:  98% .



- Molecule 58: Dipeptide (FME-PHE)



• Molecule 59: mRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9108	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	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: 4SU, 5MC, 5MU, MA6, AM2, PSU, OMU, 2MG, 6MZ, OMC, 2MA, 3TD, UR3, OMG, 4OC, G7M, GDP, PO4, 1MG, FME, MIA, 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	0.39	0/450	0.52	0/599
2	1	0.38	0/416	0.46	0/554
3	2	0.41	0/380	0.53	0/498
4	3	0.47	0/513	0.62	0/676
5	4	0.39	0/303	0.53	0/397
6	5	0.25	0/646	0.50	0/898
7	6	0.45	0/531	0.58	0/709
8	A	0.82	2/69266 (0.0%)	1.00	75/108055 (0.1%)
9	B	0.71	1/2873 (0.0%)	0.90	0/4478
10	C	0.46	0/2121	0.54	0/2852
11	D	0.44	0/1586	0.53	0/2134
12	E	0.43	0/1571	0.53	0/2113
13	F	0.36	0/1434	0.51	0/1926
14	G	0.37	0/1343	0.49	0/1816
15	H	0.30	0/1122	0.57	0/1515
16	I	0.25	0/692	0.49	0/960
17	J	0.44	0/1152	0.49	0/1551
18	K	0.40	0/947	0.53	0/1268
19	L	0.41	0/1054	0.57	0/1403
20	M	0.41	0/1093	0.51	0/1460
21	N	0.43	0/973	0.55	0/1301
22	O	0.40	0/902	0.48	0/1209
23	P	0.44	0/929	0.53	0/1242
24	Q	0.55	0/960	0.52	0/1278
25	R	0.45	0/829	0.58	0/1107
26	S	0.41	0/864	0.56	0/1156
27	T	0.40	0/744	0.54	0/994
28	U	0.43	0/787	0.58	0/1051
29	V	0.42	0/766	0.48	0/1025
30	W	0.44	0/582	0.50	0/769
31	X	0.43	0/635	0.49	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Y	0.34	0/510	0.58	0/677
33	Z	0.38	0/453	0.53	0/605
34	a	0.69	1/36725 (0.0%)	0.97	30/57285 (0.1%)
35	b	0.32	0/1735	0.52	1/2338 (0.0%)
36	c	0.36	0/1651	0.50	0/2225
37	d	0.35	0/1665	0.51	0/2227
38	e	0.37	0/1154	0.52	0/1554
39	f	0.36	0/835	0.49	0/1128
40	g	0.30	0/1195	0.47	0/1602
41	h	0.41	0/989	0.56	0/1326
42	i	0.36	0/1034	0.54	0/1375
43	j	0.34	0/796	0.57	0/1077
44	k	0.37	0/885	0.52	0/1195
45	l	0.40	0/969	0.56	1/1300 (0.1%)
46	m	0.29	0/892	0.49	0/1193
47	n	0.30	0/811	0.44	0/1081
48	o	0.36	0/722	0.49	0/964
49	p	0.38	0/659	0.52	0/884
50	q	0.37	0/657	0.53	0/881
51	r	0.34	0/544	0.50	0/731
52	s	0.33	0/675	0.53	0/908
53	t	0.32	0/671	0.45	0/888
54	u	0.34	0/512	0.54	0/683
55	v	0.65	1/1745 (0.1%)	0.99	5/2716 (0.2%)
56	w	0.61	2/1650 (0.1%)	1.02	6/2569 (0.2%)
57	x	0.37	0/5546	0.55	1/7504 (0.0%)
58	y	0.46	0/11	2.19	0/13
59	z	1.26	2/255 (0.8%)	1.72	7/394 (1.8%)
All	All	0.67	9/164410 (0.0%)	0.88	126/245165 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	1	C	OP3-P	-10.88	1.48	1.61
9	B	1	U	OP3-P	-10.79	1.48	1.61
59	z	1	A	O3'-P	-10.73	1.48	1.61
8	A	1	G	OP3-P	-10.72	1.48	1.61
56	w	34	G	O3'-P	-9.32	1.50	1.61
8	A	2029	G	C3'-O3'	5.63	1.50	1.42
34	a	1494	G	O3'-P	-5.59	1.54	1.61
56	w	76	A	C3'-O3'	5.45	1.49	1.42
59	z	2	U	O3'-P	-5.09	1.55	1.61

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2103	C	N1-C2-O2	10.08	124.95	118.90
59	z	0	U	O5'-P-OP1	9.74	122.39	110.70
56	w	40	C	C2'-C3'-O3'	8.95	129.18	109.50
8	A	2103	C	N3-C2-O2	-8.93	115.65	121.90
8	A	2103	C	C2-N1-C1'	8.18	127.79	118.80
57	x	402	PRO	N-CA-C	-7.95	91.44	112.10
8	A	2129	C	N1-C2-O2	7.88	123.63	118.90
8	A	2129	C	C2-N1-C1'	7.88	127.46	118.80
34	a	979	C	C2-N1-C1'	7.85	127.43	118.80
8	A	1914	C	C2'-C3'-O3'	7.68	126.41	109.50
8	A	1313	U	C2-N1-C1'	7.68	126.91	117.70
55	v	74	C	C2-N1-C1'	7.43	126.97	118.80
8	A	2474	U	N3-C2-O2	-7.37	117.04	122.20
55	v	74	C	N1-C2-O2	7.36	123.32	118.90
56	w	67	C	C2-N1-C1'	7.35	126.89	118.80
8	A	2342	C	N3-C2-O2	-7.15	116.90	121.90
59	z	7	G	C3'-C2'-C1'	-7.13	95.80	101.50
8	A	2103	C	C6-N1-C2	-7.08	117.47	120.30
8	A	1582	C	N3-C2-O2	-7.06	116.96	121.90
56	w	67	C	C6-N1-C1'	-6.90	112.52	120.80
8	A	2474	U	N1-C2-O2	6.86	127.61	122.80
59	z	3	G	C2'-C3'-O3'	-6.68	94.80	109.50
8	A	170	U	C2-N1-C1'	6.67	125.70	117.70
8	A	915	C	C2-N1-C1'	6.54	126.00	118.80
59	z	6	U	C4'-C3'-O3'	6.54	126.08	113.00
8	A	1771	C	C6-N1-C2	-6.46	117.71	120.30
8	A	2474	U	C2-N1-C1'	6.44	125.42	117.70
59	z	5	U	C1'-C2'-O2'	-6.44	91.29	110.60
8	A	1313	U	N3-C2-O2	-6.37	117.74	122.20
56	w	40	C	C5'-C4'-C3'	-6.35	105.84	116.00
56	w	67	C	N1-C2-O2	6.27	122.66	118.90
8	A	1926	U	O4'-C1'-N1	6.23	113.19	108.20
8	A	958	U	N1-C2-O2	6.20	127.14	122.80
8	A	2656	U	C2-N1-C1'	6.13	125.06	117.70
8	A	1157	G	N9-C4-C5	-6.13	102.95	105.40
34	a	811	C	C2-N1-C1'	6.13	125.54	118.80
8	A	1990	C	N3-C2-O2	-6.12	117.62	121.90
34	a	467	U	C2-N1-C1'	6.03	124.94	117.70
34	a	979	C	C6-N1-C1'	-6.02	113.57	120.80
8	A	2129	C	C6-N1-C1'	-5.97	113.64	120.80
8	A	1179	G	C4-N9-C1'	5.93	134.21	126.50
34	a	1168	U	C2-N1-C1'	5.92	124.80	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2129	C	N3-C2-O2	-5.88	117.78	121.90
8	A	883	G	P-O3'-C3'	5.88	126.75	119.70
34	a	1325	C	C2-N1-C1'	5.87	125.25	118.80
34	a	1493	A	C1'-C2'-O2'	-5.87	93.00	110.60
8	A	2723	C	C6-N1-C2	-5.86	117.95	120.30
34	a	1158	C	N1-C2-O2	5.85	122.41	118.90
8	A	1791	A	N1-C2-N3	5.83	132.22	129.30
8	A	2730	C	N3-C2-O2	-5.83	117.82	121.90
8	A	1918	A	C1'-C2'-O2'	-5.82	93.13	110.60
34	a	1420	U	C2-N1-C1'	5.82	124.68	117.70
34	a	979	C	N1-C2-O2	5.79	122.37	118.90
8	A	1170	C	C2-N1-C1'	5.78	125.16	118.80
8	A	2071	A	C6-C5-N7	-5.76	128.27	132.30
55	v	74	C	N3-C2-O2	-5.76	117.87	121.90
34	a	481	G	C4-N9-C1'	5.74	133.97	126.50
8	A	1314	C	C2-N1-C1'	5.73	125.10	118.80
8	A	1080	A	N1-C6-N6	5.71	122.03	118.60
8	A	2006	C	C2-N1-C1'	5.68	125.04	118.80
8	A	1577	C	N3-C2-O2	-5.66	117.94	121.90
34	a	481	G	C6-C5-N7	-5.64	127.02	130.40
8	A	1533	C	N3-C2-O2	-5.63	117.96	121.90
8	A	2071	A	N7-C8-N9	5.63	116.61	113.80
59	z	7	G	C4'-C3'-C2'	-5.62	96.98	102.60
8	A	1945	G	C8-N9-C1'	-5.61	119.70	127.00
8	A	1157	G	C8-N9-C1'	-5.57	119.75	127.00
35	b	9	LEU	CA-CB-CG	5.57	128.10	115.30
34	a	1158	C	N3-C2-O2	-5.56	118.01	121.90
34	a	1418	A	C8-N9-C4	-5.55	103.58	105.80
8	A	2071	A	C4-N9-C1'	5.55	136.28	126.30
34	a	467	U	N1-C2-O2	5.54	126.68	122.80
8	A	765	C	C2-N1-C1'	5.54	124.89	118.80
8	A	1945	G	C4-N9-C1'	5.52	133.68	126.50
34	a	481	G	C4-C5-N7	5.51	113.00	110.80
8	A	958	U	N3-C2-O2	-5.48	118.36	122.20
59	z	5	U	C2'-C3'-O3'	5.42	122.38	113.70
8	A	1582	C	C6-N1-C2	-5.41	118.14	120.30
8	A	1945	G	N3-C4-N9	5.41	129.24	126.00
8	A	528	A	C2-N3-C4	-5.39	107.90	110.60
8	A	1224	U	O4'-C1'-N1	-5.39	103.89	108.20
8	A	2128	G	C4-N9-C1'	5.38	133.49	126.50
8	A	1080	A	N9-C4-C5	-5.37	103.65	105.80
8	A	2540	C	N3-C2-O2	-5.37	118.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2090	A	C5-C6-N1	5.35	120.38	117.70
34	a	438	U	O4'-C1'-N1	5.33	112.47	108.20
8	A	2380	C	N3-C2-O2	-5.33	118.17	121.90
8	A	2075	U	C5-C4-O4	-5.32	122.71	125.90
56	w	61	C	C2-N1-C1'	5.31	124.64	118.80
34	a	95	C	C2-N1-C1'	5.30	124.63	118.80
34	a	949	A	C6-N1-C2	-5.28	115.43	118.60
34	a	603	U	N3-C2-O2	-5.27	118.51	122.20
8	A	2071	A	C4-C5-C6	5.26	119.63	117.00
8	A	1080	A	C5-C6-N6	-5.25	119.50	123.70
8	A	481	G	O4'-C1'-N9	5.25	112.40	108.20
8	A	1170	C	N1-C2-O2	5.25	122.05	118.90
34	a	1418	A	OP1-P-OP2	-5.20	111.80	119.60
8	A	1822	C	N3-C2-O2	-5.18	118.27	121.90
8	A	1313	U	N1-C2-O2	5.16	126.41	122.80
8	A	915	C	C6-N1-C1'	-5.15	114.62	120.80
8	A	2090	A	C6-N1-C2	-5.15	115.51	118.60
8	A	2794	C	C2-N1-C1'	5.15	124.47	118.80
34	a	811	C	C6-N1-C1'	-5.14	114.63	120.80
34	a	1158	C	C2-N1-C1'	5.14	124.45	118.80
34	a	575	G	N3-C4-C5	5.13	131.17	128.60
34	a	481	G	C8-N9-C1'	-5.11	120.36	127.00
8	A	1313	U	C6-N1-C1'	-5.11	114.05	121.20
45	l	102	ASP	CB-CG-OD1	5.11	122.90	118.30
8	A	1870	C	C2-N1-C1'	5.10	124.41	118.80
55	v	74	C	C6-N1-C1'	-5.10	114.69	120.80
8	A	433	C	N3-C2-O2	-5.09	118.33	121.90
8	A	2029	G	C2'-C3'-O3'	5.09	121.85	113.70
8	A	2103	C	C6-N1-C1'	-5.09	114.70	120.80
34	a	779	C	C2-N1-C1'	5.08	124.39	118.80
8	A	242	G	P-O3'-C3'	5.07	125.79	119.70
8	A	1870	C	N3-C2-O2	-5.07	118.35	121.90
34	a	404	G	N3-C4-N9	-5.07	122.96	126.00
34	a	761	G	N3-C4-N9	5.06	129.04	126.00
34	a	267	C	C2-N1-C1'	5.06	124.37	118.80
8	A	1071	G	C4-N9-C1'	5.06	133.08	126.50
8	A	515	A	N1-C2-N3	5.05	131.82	129.30
8	A	1577	C	N1-C2-O2	5.04	121.92	118.90
34	a	476	U	C2-N1-C1'	5.02	123.72	117.70
8	A	760	G	C6-C5-N7	-5.01	127.39	130.40
55	v	74	C	C6-N1-C2	-5.01	118.30	120.30
8	A	2901	C	N3-C2-O2	-5.00	118.40	121.90



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
4	3	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
5	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
6	5	129/165 (78%)	98 (76%)	31 (24%)	0	100	100
7	6	64/70 (91%)	53 (83%)	11 (17%)	0	100	100
10	C	269/273 (98%)	229 (85%)	39 (14%)	1 (0%)	30	66
11	D	207/209 (99%)	172 (83%)	35 (17%)	0	100	100
12	E	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
13	F	175/179 (98%)	143 (82%)	32 (18%)	0	100	100
14	G	174/177 (98%)	154 (88%)	20 (12%)	0	100	100
15	H	147/149 (99%)	117 (80%)	30 (20%)	0	100	100
16	I	139/142 (98%)	103 (74%)	36 (26%)	0	100	100
17	J	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
18	K	120/123 (98%)	98 (82%)	22 (18%)	0	100	100
19	L	141/144 (98%)	113 (80%)	28 (20%)	0	100	100
20	M	134/136 (98%)	114 (85%)	20 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	N	118/127 (93%)	106 (90%)	12 (10%)	0	100	100
22	O	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
23	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
24	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
25	R	101/103 (98%)	86 (85%)	13 (13%)	2 (2%)	6	34
26	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
27	T	91/100 (91%)	79 (87%)	12 (13%)	0	100	100
28	U	100/104 (96%)	85 (85%)	13 (13%)	2 (2%)	6	34
29	V	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
30	W	73/85 (86%)	60 (82%)	13 (18%)	0	100	100
31	X	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
32	Y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	8	38
33	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
35	b	216/240 (90%)	186 (86%)	30 (14%)	0	100	100
36	c	204/233 (88%)	185 (91%)	19 (9%)	0	100	100
37	d	203/206 (98%)	167 (82%)	36 (18%)	0	100	100
38	e	155/167 (93%)	134 (86%)	21 (14%)	0	100	100
39	f	98/135 (73%)	84 (86%)	14 (14%)	0	100	100
40	g	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
41	h	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
42	i	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
43	j	96/103 (93%)	75 (78%)	20 (21%)	1 (1%)	13	47
44	k	114/129 (88%)	97 (85%)	17 (15%)	0	100	100
45	l	121/124 (98%)	95 (78%)	26 (22%)	0	100	100
46	m	112/118 (95%)	96 (86%)	16 (14%)	0	100	100
47	n	99/102 (97%)	83 (84%)	16 (16%)	0	100	100
48	o	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
49	p	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	10	42
50	q	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
51	r	63/75 (84%)	52 (82%)	11 (18%)	0	100	100
52	s	80/92 (87%)	64 (80%)	16 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	51 (81%)	11 (18%)	1 (2%)	8	38
57	x	701/704 (100%)	625 (89%)	74 (11%)	2 (0%)	37	71
All	All	6551/6924 (95%)	5653 (86%)	887 (14%)	11 (0%)	45	76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	U	98	ASN
28	U	16	LYS
57	x	402	PRO
25	R	71	LYS
32	Y	19	LEU
49	p	47	GLU
43	j	58	ASN
54	u	12	ASP
57	x	367	ALA
10	C	240	GLY
25	R	51	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	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	48 (81%)	11 (19%)	1	9
10	C	216/218 (99%)	216 (100%)	0	100	100
11	D	164/164 (100%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	114 (100%)	0	100	100
17	J	116/116 (100%)	115 (99%)	1 (1%)	75	83
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	108 (99%)	1 (1%)	75	83
21	N	100/103 (97%)	99 (99%)	1 (1%)	73	81
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	98 (99%)	1 (1%)	73	81
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	83 (99%)	1 (1%)	67	78
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	80 (100%)	0	100	100
28	U	83/85 (98%)	82 (99%)	1 (1%)	67	78
29	V	78/78 (100%)	77 (99%)	1 (1%)	65	77
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	66 (98%)	1 (2%)	60	75
32	Y	55/55 (100%)	55 (100%)	0	100	100
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	179 (99%)	1 (1%)	84	88
36	c	170/190 (90%)	170 (100%)	0	100	100
37	d	172/173 (99%)	172 (100%)	0	100	100
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%)	104 (99%)	1 (1%)	73	81
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	88 (99%)	1 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	l	103/104 (99%)	103 (100%)	0	100	100
46	m	92/96 (96%)	91 (99%)	1 (1%)	70	80
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%)	74 (100%)	0	100	100
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
57	x	577/578 (100%)	569 (99%)	8 (1%)	62	75
58	y	1/1 (100%)	1 (100%)	0	100	100
All	All	5204/5408 (96%)	5173 (99%)	31 (1%)	82	88

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	6	48	GLN
7	6	49	ARG
7	6	51	VAL
7	6	53	THR
7	6	56	ARG
7	6	57	VAL
7	6	59	ARG
7	6	60	PHE
7	6	62	LYS
7	6	63	ARG
7	6	65	ASN
17	J	52	ASP
20	M	6	ARG
21	N	2	ARG
23	P	88	ARG
25	R	51	VAL
28	U	6	ARG
29	V	21	ARG
31	X	76	LYS
35	b	73	ARG
42	i	11	ARG

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Mol	Chain	Res	Type
44	k	36	ARG
46	m	69	ARG
57	x	103	ARG
57	x	294	ILE
57	x	295	ASN
57	x	336	ARG
57	x	471	ARG
57	x	593	LYS
57	x	601	LYS
57	x	697	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	5	ASN
1	0	37	HIS
1	0	41	HIS
2	1	45	HIS
4	3	30	HIS
10	C	89	ASN
10	C	127	ASN
10	C	225	ASN
10	C	238	ASN
11	D	173	GLN
11	D	185	ASN
12	E	163	ASN
14	G	115	GLN
15	H	66	ASN
15	H	135	HIS
17	J	80	HIS
17	J	136	GLN
18	K	3	GLN
18	K	90	ASN
18	K	93	GLN
19	L	4	ASN
21	N	3	HIS
21	N	11	ASN
21	N	23	ASN
22	O	38	GLN
23	P	11	GLN
24	Q	36	GLN
25	R	43	ASN

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Mol	Chain	Res	Type
26	S	7	HIS
27	T	48	GLN
27	T	59	ASN
27	T	70	HIS
28	U	68	ASN
33	Z	33	HIS
35	b	17	HIS
35	b	167	HIS
36	c	2	GLN
37	d	35	GLN
37	d	39	GLN
37	d	73	ASN
37	d	88	ASN
37	d	135	GLN
38	e	42	ASN
38	e	121	ASN
39	f	52	ASN
40	g	96	ASN
40	g	147	ASN
41	h	17	GLN
43	j	56	HIS
44	k	21	HIS
45	l	76	HIS
47	n	60	GLN
48	o	34	GLN
48	o	37	HIS
49	p	26	ASN
49	p	79	ASN
50	q	44	HIS
50	q	46	HIS
51	r	51	GLN
52	s	13	HIS
52	s	42	ASN
52	s	55	GLN
52	s	56	HIS
53	t	12	GLN
53	t	19	HIS
53	t	47	GLN
53	t	51	ASN
57	x	36	ASN
57	x	121	GLN
57	x	258	ASN

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Mol	Chain	Res	Type
57	x	271	ASN
57	x	427	GLN
57	x	454	GLN
57	x	464	HIS
57	x	516	HIS
57	x	559	GLN
57	x	583	HIS
57	x	626	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	347 (22%)	0
55	v	76/77 (98%)	21 (27%)	0
56	w	74/76 (97%)	35 (47%)	0
59	z	10/33 (30%)	8 (80%)	0
8	A	2898/2903 (99%)	717 (24%)	56 (1%)
9	B	119/120 (99%)	23 (19%)	3 (2%)
All	All	4713/4751 (99%)	1151 (24%)	59 (1%)

All (1151) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	12	U
8	A	15	G
8	A	27	G
8	A	35	G
8	A	43	G
8	A	44	A
8	A	46	G
8	A	62	U
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	96	C
8	A	101	A
8	A	102	U

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Mol	Chain	Res	Type
8	A	103	A
8	A	104	A
8	A	118	A
8	A	120	U
8	A	131	A
8	A	140	C
8	A	141	G
8	A	142	A
8	A	149	A
8	A	160	A
8	A	163	C
8	A	170	U
8	A	175	G
8	A	196	A
8	A	199	A
8	A	200	U
8	A	204	A
8	A	205	G
8	A	215	G
8	A	216	A
8	A	221	A
8	A	222	A
8	A	226	A
8	A	228	C
8	A	229	C
8	A	230	G
8	A	232	G
8	A	233	A
8	A	239	C
8	A	241	A
8	A	242	G
8	A	243	U
8	A	244	A
8	A	245	G
8	A	248	G
8	A	255	A
8	A	264	C
8	A	266	G
8	A	272	A
8	A	275	C
8	A	276	U
8	A	278	A

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Mol	Chain	Res	Type
8	A	279	A
8	A	288	U
8	A	291	G
8	A	294	A
8	A	296	U
8	A	302	C
8	A	311	A
8	A	322	A
8	A	323	C
8	A	330	A
8	A	332	A
8	A	345	A
8	A	346	A
8	A	359	G
8	A	361	G
8	A	367	G
8	A	368	A
8	A	370	G
8	A	371	A
8	A	372	G
8	A	373	U
8	A	386	G
8	A	396	G
8	A	401	A
8	A	404	A
8	A	405	U
8	A	406	G
8	A	411	G
8	A	435	C
8	A	451	U
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	464	U
8	A	478	A
8	A	479	A
8	A	480	A
8	A	481	G
8	A	482	A
8	A	490	C
8	A	491	G

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Mol	Chain	Res	Type
8	A	494	G
8	A	496	G
8	A	504	A
8	A	505	A
8	A	507	A
8	A	508	A
8	A	509	C
8	A	518	G
8	A	527	C
8	A	529	A
8	A	531	C
8	A	532	A
8	A	544	C
8	A	545	U
8	A	546	U
8	A	548	G
8	A	549	G
8	A	556	A
8	A	563	A
8	A	572	A
8	A	573	U
8	A	575	A
8	A	603	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	622	G
8	A	627	A
8	A	637	A
8	A	643	A
8	A	645	C
8	A	646	U
8	A	647	G
8	A	654	A
8	A	655	A
8	A	669	G
8	A	674	G
8	A	682	G
8	A	686	U
8	A	695	G
8	A	704	G
8	A	712	G

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Mol	Chain	Res	Type
8	A	714	U
8	A	716	A
8	A	717	C
8	A	730	A
8	A	745	1MG
8	A	747	5MC
8	A	757	G
8	A	760	G
8	A	764	A
8	A	765	C
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	800	A
8	A	803	U
8	A	805	G
8	A	806	C
8	A	811	U
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	831	G
8	A	846	U
8	A	847	U
8	A	856	G
8	A	857	G
8	A	859	G
8	A	882	G
8	A	883	G
8	A	884	U
8	A	885	C
8	A	887	A
8	A	889	C
8	A	890	C
8	A	891	G
8	A	893	C
8	A	894	U
8	A	895	U

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Mol	Chain	Res	Type
8	A	896	A
8	A	897	C
8	A	899	A
8	A	901	C
8	A	902	C
8	A	903	C
8	A	904	G
8	A	907	G
8	A	910	A
8	A	915	C
8	A	917	A
8	A	927	A
8	A	931	U
8	A	934	U
8	A	941	A
8	A	946	C
8	A	953	G
8	A	957	C
8	A	958	U
8	A	959	A
8	A	961	C
8	A	973	A
8	A	974	G
8	A	980	A
8	A	983	A
8	A	990	A
8	A	995	C
8	A	996	A
8	A	1002	G
8	A	1003	G
8	A	1005	C
8	A	1009	A
8	A	1012	U
8	A	1013	C
8	A	1026	G
8	A	1033	U
8	A	1041	G
8	A	1045	C
8	A	1046	A
8	A	1047	G
8	A	1048	A
8	A	1052	C

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Mol	Chain	Res	Type
8	A	1055	G
8	A	1056	G
8	A	1057	A
8	A	1058	U
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1062	G
8	A	1063	G
8	A	1066	U
8	A	1067	A
8	A	1068	G
8	A	1069	A
8	A	1070	A
8	A	1071	G
8	A	1072	C
8	A	1073	A
8	A	1074	G
8	A	1075	C
8	A	1077	A
8	A	1078	U
8	A	1079	C
8	A	1080	A
8	A	1081	U
8	A	1082	U
8	A	1083	U
8	A	1084	A
8	A	1085	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1089	A
8	A	1091	G
8	A	1092	C
8	A	1093	G
8	A	1094	U
8	A	1095	A
8	A	1096	A
8	A	1097	U
8	A	1098	A
8	A	1100	C
8	A	1101	U

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Mol	Chain	Res	Type
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	1122	G
8	A	1130	U
8	A	1131	G
8	A	1132	U
8	A	1133	A
8	A	1135	C
8	A	1139	G
8	A	1142	A
8	A	1143	A
8	A	1151	A
8	A	1154	G
8	A	1155	A
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1179	G
8	A	1180	U
8	A	1181	U
8	A	1204	A
8	A	1210	G
8	A	1211	C
8	A	1212	G
8	A	1225	G
8	A	1227	G
8	A	1234	U
8	A	1247	A
8	A	1250	G
8	A	1252	G
8	A	1253	A
8	A	1256	G
8	A	1263	U
8	A	1264	A
8	A	1265	A
8	A	1271	G
8	A	1272	A

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Mol	Chain	Res	Type
8	A	1273	U
8	A	1275	A
8	A	1284	A
8	A	1300	G
8	A	1301	A
8	A	1302	A
8	A	1306	C
8	A	1313	U
8	A	1314	C
8	A	1321	A
8	A	1330	C
8	A	1340	U
8	A	1341	G
8	A	1352	U
8	A	1365	A
8	A	1368	G
8	A	1373	A
8	A	1374	G
8	A	1376	C
8	A	1378	A
8	A	1379	U
8	A	1383	A
8	A	1395	A
8	A	1407	G
8	A	1409	U
8	A	1410	G
8	A	1413	A
8	A	1415	U
8	A	1416	G
8	A	1420	A
8	A	1421	G
8	A	1425	G
8	A	1428	C
8	A	1429	G
8	A	1434	A
8	A	1452	G
8	A	1455	G
8	A	1458	U
8	A	1459	G
8	A	1460	U
8	A	1461	C
8	A	1473	G

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Mol	Chain	Res	Type
8	A	1475	G
8	A	1478	G
8	A	1482	G
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1494	A
8	A	1497	U
8	A	1503	A
8	A	1504	A
8	A	1508	A
8	A	1515	A
8	A	1522	A
8	A	1524	G
8	A	1534	U
8	A	1536	C
8	A	1537	G
8	A	1538	G
8	A	1558	C
8	A	1566	A
8	A	1567	G
8	A	1569	A
8	A	1578	U
8	A	1584	U
8	A	1585	C
8	A	1598	A
8	A	1608	A
8	A	1610	A
8	A	1616	A
8	A	1622	G
8	A	1634	A
8	A	1635	A
8	A	1646	C
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1651	G
8	A	1654	A
8	A	1664	A
8	A	1665	A
8	A	1672	A
8	A	1674	G

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Mol	Chain	Res	Type
8	A	1694	C
8	A	1695	G
8	A	1698	A
8	A	1699	G
8	A	1713	A
8	A	1715	G
8	A	1716	U
8	A	1729	U
8	A	1730	C
8	A	1731	G
8	A	1738	G
8	A	1746	A
8	A	1756	G
8	A	1757	A
8	A	1758	U
8	A	1764	C
8	A	1773	A
8	A	1779	U
8	A	1781	U
8	A	1785	A
8	A	1791	A
8	A	1800	C
8	A	1801	A
8	A	1802	A
8	A	1808	A
8	A	1809	A
8	A	1814	G
8	A	1815	A
8	A	1816	C
8	A	1829	A
8	A	1833	C
8	A	1835	2MG
8	A	1838	C
8	A	1857	G
8	A	1862	G
8	A	1866	A
8	A	1869	G
8	A	1871	A
8	A	1873	G
8	A	1884	G
8	A	1889	A
8	A	1890	A

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Mol	Chain	Res	Type
8	A	1901	A
8	A	1906	G
8	A	1908	C
8	A	1910	G
8	A	1912	A
8	A	1913	A
8	A	1914	C
8	A	1916	A
8	A	1917	PSU
8	A	1918	A
8	A	1919	A
8	A	1922	G
8	A	1924	C
8	A	1925	C
8	A	1926	U
8	A	1927	A
8	A	1929	G
8	A	1930	G
8	A	1937	A
8	A	1938	A
8	A	1939	5MU
8	A	1942	C
8	A	1955	U
8	A	1964	G
8	A	1965	C
8	A	1967	C
8	A	1970	A
8	A	1971	U
8	A	1972	G
8	A	1976	U
8	A	1977	A
8	A	1982	U
8	A	1991	U
8	A	1992	G
8	A	1993	U
8	A	1997	C
8	A	2020	A
8	A	2022	U
8	A	2023	C
8	A	2032	G
8	A	2033	A
8	A	2034	U

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Mol	Chain	Res	Type
8	A	2036	C
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	2076	U
8	A	2089	C
8	A	2092	U
8	A	2093	G
8	A	2101	A
8	A	2102	G
8	A	2103	C
8	A	2104	C
8	A	2107	G
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2114	A
8	A	2115	G
8	A	2116	G
8	A	2118	U
8	A	2119	A
8	A	2120	G
8	A	2123	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	2130	U
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2135	A
8	A	2136	G

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Mol	Chain	Res	Type
8	A	2138	G
8	A	2139	U
8	A	2143	C
8	A	2146	C
8	A	2147	A
8	A	2148	G
8	A	2150	C
8	A	2151	U
8	A	2153	C
8	A	2154	A
8	A	2155	U
8	A	2157	G
8	A	2159	G
8	A	2161	C
8	A	2162	G
8	A	2163	A
8	A	2164	C
8	A	2166	U
8	A	2169	A
8	A	2170	A
8	A	2171	A
8	A	2172	U
8	A	2173	A
8	A	2175	C
8	A	2180	U
8	A	2181	U
8	A	2182	U
8	A	2183	A
8	A	2186	G
8	A	2187	U
8	A	2188	U
8	A	2190	G
8	A	2193	G
8	A	2194	U
8	A	2198	A
8	A	2203	U
8	A	2204	G
8	A	2212	A
8	A	2213	U
8	A	2225	A
8	A	2226	C
8	A	2238	G

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Mol	Chain	Res	Type
8	A	2239	G
8	A	2243	U
8	A	2266	A
8	A	2267	A
8	A	2273	A
8	A	2279	G
8	A	2280	G
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2304	G
8	A	2305	U
8	A	2307	G
8	A	2309	A
8	A	2320	U
8	A	2321	U
8	A	2322	A
8	A	2325	G
8	A	2327	A
8	A	2333	A
8	A	2335	A
8	A	2347	C
8	A	2350	C
8	A	2357	G
8	A	2358	A
8	A	2361	G
8	A	2382	G
8	A	2383	G
8	A	2384	U
8	A	2385	C
8	A	2388	A
8	A	2392	A
8	A	2402	U
8	A	2403	C
8	A	2406	A
8	A	2410	G
8	A	2423	U
8	A	2425	A
8	A	2429	G
8	A	2430	A
8	A	2432	A
8	A	2434	A

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Mol	Chain	Res	Type
8	A	2435	A
8	A	2438	U
8	A	2441	U
8	A	2445	2MG
8	A	2447	G
8	A	2448	A
8	A	2449	U
8	A	2450	A
8	A	2469	A
8	A	2475	C
8	A	2476	A
8	A	2478	A
8	A	2480	C
8	A	2484	G
8	A	2487	G
8	A	2491	U
8	A	2498	OMC
8	A	2501	C
8	A	2502	G
8	A	2504	PSU
8	A	2506	U
8	A	2518	A
8	A	2520	C
8	A	2529	G
8	A	2535	G
8	A	2547	A
8	A	2548	U
8	A	2553	G
8	A	2554	U
8	A	2556	C
8	A	2566	A
8	A	2567	G
8	A	2572	A
8	A	2573	C
8	A	2576	G
8	A	2585	U
8	A	2602	A
8	A	2603	G
8	A	2609	U
8	A	2613	U
8	A	2615	U
8	A	2621	G

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Mol	Chain	Res	Type
8	A	2623	G
8	A	2629	U
8	A	2630	G
8	A	2634	A
8	A	2646	C
8	A	2647	U
8	A	2654	A
8	A	2655	G
8	A	2656	U
8	A	2660	A
8	A	2663	G
8	A	2673	G
8	A	2682	A
8	A	2684	U
8	A	2689	U
8	A	2690	U
8	A	2702	G
8	A	2707	U
8	A	2712	C
8	A	2713	U
8	A	2714	G
8	A	2717	C
8	A	2726	A
8	A	2729	G
8	A	2733	A
8	A	2744	G
8	A	2748	A
8	A	2751	G
8	A	2752	C
8	A	2755	C
8	A	2757	A
8	A	2758	A
8	A	2764	A
8	A	2765	A
8	A	2769	U
8	A	2776	A
8	A	2778	A
8	A	2779	U
8	A	2780	G
8	A	2790	U
8	A	2791	G
8	A	2794	C

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Mol	Chain	Res	Type
8	A	2796	U
8	A	2797	U
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2801	G
8	A	2803	G
8	A	2804	U
8	A	2808	G
8	A	2809	A
8	A	2818	U
8	A	2820	A
8	A	2833	U
8	A	2834	G
8	A	2836	U
8	A	2846	G
8	A	2849	U
8	A	2866	U
8	A	2867	G
8	A	2872	A
8	A	2873	A
8	A	2879	A
8	A	2880	C
8	A	2883	A
8	A	2886	A
8	A	2894	G
8	A	2902	C
9	B	9	G
9	B	14	U
9	B	24	G
9	B	25	U
9	B	32	U
9	B	33	G
9	B	35	C
9	B	37	C
9	B	42	C
9	B	44	G
9	B	45	A
9	B	56	G
9	B	66	A
9	B	67	G
9	B	73	A

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Mol	Chain	Res	Type
9	B	83	G
9	B	88	C
9	B	89	U
9	B	90	C
9	B	91	C
9	B	108	A
9	B	109	A
9	B	120	U
34	a	2	A
34	a	6	G
34	a	7	A
34	a	9	G
34	a	22	G
34	a	31	G
34	a	32	A
34	a	39	G
34	a	47	C
34	a	48	C
34	a	51	A
34	a	64	G
34	a	70	U
34	a	71	A
34	a	74	A
34	a	76	G
34	a	78	A
34	a	80	A
34	a	81	A
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	89	U
34	a	92	U
34	a	94	G
34	a	96	U
34	a	108	G
34	a	119	A
34	a	121	U
34	a	130	A
34	a	131	A
34	a	141	G
34	a	144	G

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Mol	Chain	Res	Type
34	a	154	U
34	a	160	A
34	a	161	A
34	a	166	U
34	a	182	A
34	a	183	C
34	a	184	G
34	a	197	A
34	a	198	G
34	a	205	A
34	a	208	U
34	a	210	C
34	a	211	G
34	a	218	U
34	a	240	G
34	a	245	U
34	a	247	G
34	a	251	G
34	a	262	A
34	a	266	G
34	a	267	C
34	a	281	G
34	a	289	G
34	a	298	A
34	a	299	G
34	a	306	A
34	a	321	A
34	a	328	C
34	a	329	A
34	a	344	A
34	a	346	G
34	a	352	C
34	a	356	A
34	a	363	A
34	a	367	U
34	a	371	A
34	a	372	C
34	a	373	A
34	a	376	G
34	a	377	G
34	a	381	C
34	a	383	A

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Mol	Chain	Res	Type
34	a	384	G
34	a	388	G
34	a	397	A
34	a	406	G
34	a	411	A
34	a	413	G
34	a	414	A
34	a	421	U
34	a	423	G
34	a	424	G
34	a	428	G
34	a	429	U
34	a	439	U
34	a	461	A
34	a	462	G
34	a	465	A
34	a	466	A
34	a	467	U
34	a	468	A
34	a	470	C
34	a	479	U
34	a	482	A
34	a	484	G
34	a	496	A
34	a	505	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	512	U
34	a	517	G
34	a	518	C
34	a	521	G
34	a	527	G7M
34	a	530	G
34	a	531	U
34	a	532	A
34	a	546	A
34	a	547	A
34	a	559	A
34	a	562	U
34	a	564	C
34	a	572	A

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Mol	Chain	Res	Type
34	a	573	A
34	a	576	C
34	a	577	G
34	a	596	A
34	a	605	U
34	a	607	A
34	a	608	A
34	a	615	G
34	a	629	A
34	a	632	U
34	a	633	G
34	a	650	G
34	a	665	A
34	a	687	A
34	a	691	G
34	a	703	G
34	a	704	A
34	a	723	U
34	a	724	G
34	a	733	G
34	a	734	G
34	a	748	G
34	a	753	A
34	a	755	G
34	a	760	G
34	a	761	G
34	a	773	G
34	a	777	A
34	a	779	C
34	a	781	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	813	U
34	a	814	A
34	a	815	A
34	a	817	C
34	a	819	A
34	a	821	G
34	a	829	G
34	a	841	C
34	a	842	U

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Mol	Chain	Res	Type
34	a	843	U
34	a	844	G
34	a	845	A
34	a	846	G
34	a	849	G
34	a	851	G
34	a	868	C
34	a	885	G
34	a	889	A
34	a	890	G
34	a	902	G
34	a	913	A
34	a	914	A
34	a	922	G
34	a	928	G
34	a	934	C
34	a	935	A
34	a	958	A
34	a	960	U
34	a	966	2MG
34	a	967	5MC
34	a	968	A
34	a	969	A
34	a	970	C
34	a	971	G
34	a	973	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	981	U
34	a	982	U
34	a	984	C
34	a	990	C
34	a	992	U
34	a	993	G
34	a	994	A
34	a	996	A
34	a	1004	A
34	a	1006	G
34	a	1012	A
34	a	1014	A
34	a	1016	A

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Mol	Chain	Res	Type
34	a	1017	U
34	a	1020	G
34	a	1023	U
34	a	1025	U
34	a	1026	G
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1037	C
34	a	1043	G
34	a	1045	C
34	a	1050	G
34	a	1053	G
34	a	1056	U
34	a	1063	C
34	a	1065	U
34	a	1085	U
34	a	1086	U
34	a	1092	A
34	a	1094	G
34	a	1101	A
34	a	1104	G
34	a	1108	G
34	a	1126	U
34	a	1134	G
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1144	G
34	a	1147	C
34	a	1151	A
34	a	1159	U
34	a	1167	A
34	a	1168	U
34	a	1179	A
34	a	1182	G
34	a	1183	U
34	a	1184	G
34	a	1196	A
34	a	1197	A
34	a	1210	C
34	a	1211	U

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Mol	Chain	Res	Type
34	a	1212	U
34	a	1213	A
34	a	1215	G
34	a	1218	C
34	a	1224	U
34	a	1225	A
34	a	1226	C
34	a	1227	A
34	a	1239	A
34	a	1241	G
34	a	1248	A
34	a	1254	A
34	a	1256	A
34	a	1257	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1270	G
34	a	1275	A
34	a	1278	G
34	a	1280	A
34	a	1281	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1294	G
34	a	1297	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1305	G
34	a	1306	A
34	a	1307	U
34	a	1312	G
34	a	1317	C
34	a	1320	C
34	a	1322	C
34	a	1325	C
34	a	1331	G
34	a	1332	A
34	a	1338	G

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Mol	Chain	Res	Type
34	a	1340	A
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1353	G
34	a	1361	G
34	a	1363	A
34	a	1370	G
34	a	1374	A
34	a	1378	C
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1408	A
34	a	1413	A
34	a	1417	G
34	a	1418	A
34	a	1419	G
34	a	1420	U
34	a	1426	G
34	a	1427	C
34	a	1428	A
34	a	1429	A
34	a	1434	A
34	a	1441	A
34	a	1442	G
34	a	1443	C
34	a	1446	A
34	a	1451	U
34	a	1452	C
34	a	1467	C
34	a	1472	U
34	a	1473	G
34	a	1474	U
34	a	1482	G
34	a	1483	A
34	a	1484	C
34	a	1485	U
34	a	1486	G

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Mol	Chain	Res	Type
34	a	1487	G
34	a	1491	G
34	a	1492	A
34	a	1497	G
34	a	1499	A
34	a	1503	A
34	a	1504	G
34	a	1506	U
34	a	1517	G
34	a	1523	G
34	a	1529	G
34	a	1530	G
34	a	1533	C
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1538	C
34	a	1539	C
34	a	1540	U
55	v	9	G
55	v	16	C
55	v	18	G
55	v	20	H2U
55	v	21	A
55	v	24	U
55	v	33	U
55	v	34	C
55	v	38	A
55	v	42	G
55	v	43	A
55	v	44	A
55	v	46	A
55	v	47	U
55	v	48	C
55	v	52	G
55	v	55	PSU
55	v	56	C
55	v	57	A
55	v	75	C
55	v	76	A
56	w	7	A
56	w	8	4SU

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Mol	Chain	Res	Type
56	w	16	U
56	w	17	C
56	w	18	G
56	w	19	G
56	w	20	U
56	w	21	A
56	w	22	G
56	w	23	A
56	w	28	G
56	w	35	A
56	w	36	A
56	w	38	A
56	w	39	PSU
56	w	40	C
56	w	44	G
56	w	45	U
56	w	46	G7M
56	w	47	U
56	w	48	C
56	w	53	G
56	w	54	5MU
56	w	55	PSU
56	w	57	G
56	w	58	A
56	w	59	U
56	w	60	U
56	w	61	C
56	w	62	C
56	w	67	C
56	w	68	C
56	w	74	C
56	w	75	C
56	w	76	A
59	z	-1	C
59	z	0	U
59	z	2	U
59	z	3	G
59	z	4	U
59	z	5	U
59	z	7	G
59	z	8	U

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	242	G
8	A	310	A
8	A	369	U
8	A	446	G
8	A	458	G
8	A	479	A
8	A	481	G
8	A	503	A
8	A	530	G
8	A	545	U
8	A	555	G
8	A	571	U
8	A	715	A
8	A	774	G
8	A	784	G
8	A	883	G
8	A	894	U
8	A	1024	G
8	A	1062	G
8	A	1082	U
8	A	1090	A
8	A	1093	G
8	A	1182	G
8	A	1224	U
8	A	1300	G
8	A	1331	G
8	A	1451	C
8	A	1473	G
8	A	1490	A
8	A	1647	U
8	A	1663	G
8	A	1715	G
8	A	1730	C
8	A	1907	G
8	A	1912	A
8	A	1917	PSU
8	A	1918	A
8	A	1926	U
8	A	1939	5MU
8	A	2149	U
8	A	2150	C
8	A	2158	A
8	A	2192	U

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Mol	Chain	Res	Type
8	A	2287	A
8	A	2319	G
8	A	2324	U
8	A	2428	G
8	A	2449	U
8	A	2468	A
8	A	2505	G
8	A	2655	G
8	A	2706	A
8	A	2728	U
8	A	2756	U
8	A	2796	U
8	A	2808	G
9	B	36	C
9	B	66	A
9	B	89	U

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

46 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
58	FME	y	101	58	8,9,10	0.48	0	7,9,11	1.04	1 (14%)
8	PSU	A	1911	8	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
8	PSU	A	2604	8	18,21,22	1.09	2 (11%)	22,30,33	1.90	5 (22%)
8	OMG	A	2251	8	18,26,27	1.08	1 (5%)	19,38,41	1.14	2 (10%)
8	2MG	A	2445	8	18,26,27	1.19	1 (5%)	16,38,41	1.32	3 (18%)
56	5MU	w	54	56	19,22,23	1.46	5 (26%)	28,32,35	2.23	8 (28%)
8	PSU	A	2457	8	18,21,22	1.06	2 (11%)	22,30,33	1.98	5 (22%)
34	2MG	a	1516	34	18,26,27	2.59	7 (38%)	16,38,41	1.38	4 (25%)
8	3TD	A	1915	8	22,23,23	6.54	9 (40%)	29,35,35	4.35	14 (48%)
55	PSU	v	55	55	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PSU	A	955	8	18,21,22	1.00	1 (5%)	22,30,33	1.69	4 (18%)
34	4OC	a	1402	34	20,23,24	2.98	8 (40%)	26,32,35	0.79	0
56	PSU	w	32	56	18,21,22	1.79	5 (27%)	22,30,33	2.48	8 (36%)
8	G7M	A	2069	8	20,26,27	2.33	7 (35%)	17,39,42	1.05	1 (5%)
8	2MG	A	1835	8	18,26,27	2.60	7 (38%)	16,38,41	1.40	3 (18%)
8	PSU	A	1917	8	18,21,22	2.72	5 (27%)	22,30,33	2.98	9 (40%)
55	5MU	v	54	55	19,22,23	4.81	7 (36%)	28,32,35	3.52	11 (39%)
8	6MZ	A	2030	8	18,25,26	1.28	2 (11%)	16,36,39	2.30	6 (37%)
8	6MZ	A	1618	8	18,25,26	2.17	4 (22%)	16,36,39	2.03	3 (18%)
55	H2U	v	20	55	18,21,22	3.03	5 (27%)	21,30,33	2.04	5 (23%)
34	5MC	a	967	34	18,22,23	3.73	7 (38%)	26,32,35	0.95	1 (3%)
34	MA6	a	1519	34	18,26,27	1.02	1 (5%)	19,38,41	2.60	2 (10%)
8	OMU	A	2552	8	19,22,23	2.94	8 (42%)	26,31,34	1.76	4 (15%)
8	2MA	A	2503	8	19,25,26	3.18	6 (31%)	21,37,40	1.46	3 (14%)
56	4SU	w	8	56	18,21,22	3.57	7 (38%)	26,30,33	2.32	5 (19%)
34	G7M	a	527	34	20,26,27	2.39	7 (35%)	17,39,42	1.09	1 (5%)
8	PSU	A	2504	8	18,21,22	1.14	2 (11%)	22,30,33	1.83	4 (18%)
56	G7M	w	46	56	20,26,27	2.46	7 (35%)	17,39,42	1.11	1 (5%)
34	PSU	a	516	34	18,21,22	1.42	3 (16%)	22,30,33	2.13	4 (18%)
56	PSU	w	55	56	18,21,22	1.41	3 (16%)	22,30,33	1.93	4 (18%)
8	OMC	A	2498	8	19,22,23	0.89	1 (5%)	26,31,34	1.20	1 (3%)
56	PSU	w	39	56	18,21,22	2.13	8 (44%)	22,30,33	3.11	13 (59%)
55	4SU	v	8	55	18,21,22	3.44	7 (38%)	26,30,33	2.44	5 (19%)
8	1MG	A	745	8	18,26,27	2.62	4 (22%)	19,39,42	1.34	3 (15%)
8	PSU	A	2605	8	18,21,22	1.12	2 (11%)	22,30,33	1.81	4 (18%)
34	2MG	a	1207	34	18,26,27	2.57	7 (38%)	16,38,41	1.36	4 (25%)
34	UR3	a	1498	34	19,22,23	2.58	6 (31%)	26,32,35	1.43	3 (11%)
34	2MG	a	966	34	18,26,27	2.60	7 (38%)	16,38,41	1.51	4 (25%)
8	5MC	A	1962	8	18,22,23	3.55	7 (38%)	26,32,35	1.10	2 (7%)
34	5MC	a	1407	34	18,22,23	3.69	7 (38%)	26,32,35	0.95	1 (3%)
8	5MU	A	1939	8	19,22,23	4.62	7 (36%)	28,32,35	3.76	10 (35%)
8	5MC	A	747	8	18,22,23	3.46	7 (38%)	26,32,35	1.12	2 (7%)
8	PSU	A	746	8	18,21,22	1.07	2 (11%)	22,30,33	1.67	4 (18%)
34	MA6	a	1518	34	18,26,27	1.04	1 (5%)	19,38,41	2.49	2 (10%)
8	PSU	A	2580	8	18,21,22	1.09	3 (16%)	22,30,33	1.90	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	MIA	w	37	56	24,31,32	3.90	9 (37%)	26,44,47	3.57	14 (53%)

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
58	FME	y	101	58	-	4/7/9/11	-
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	1/7/25/26	0/2/2/2
8	OMG	A	2251	8	-	2/5/27/28	0/3/3/3
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
56	5MU	w	54	56	-	1/7/25/26	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	3TD	A	1915	8	-	4/10/26/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	3/9/29/30	0/2/2/2
56	PSU	w	32	56	-	4/7/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	PSU	A	1917	8	-	5/7/25/26	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	5/5/27/28	0/3/3/3
8	6MZ	A	1618	8	-	2/5/27/28	0/3/3/3
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
34	5MC	a	967	34	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	3/7/29/30	0/3/3/3
8	OMU	A	2552	8	-	3/9/27/28	0/2/2/2
8	2MA	A	2503	8	-	2/3/25/26	0/3/3/3
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
34	G7M	a	527	34	-	2/3/25/26	0/3/3/3
8	PSU	A	2504	8	-	2/7/25/26	0/2/2/2
56	G7M	w	46	56	-	2/3/25/26	0/3/3/3
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
56	PSU	w	55	56	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OMC	A	2498	8	-	1/9/27/28	0/2/2/2
56	PSU	w	39	56	-	5/7/25/26	0/2/2/2
55	4SU	v	8	55	-	1/7/25/26	0/2/2/2
8	1MG	A	745	8	-	2/3/25/26	0/3/3/3
8	PSU	A	2605	8	-	1/7/25/26	0/2/2/2
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
34	2MG	a	966	34	-	2/5/27/28	0/3/3/3
8	5MC	A	1962	8	-	4/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	2/7/25/26	0/2/2/2
8	5MC	A	747	8	-	0/7/25/26	0/2/2/2
8	PSU	A	746	8	-	2/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	3/7/29/30	0/3/3/3
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
56	MIA	w	37	56	-	6/11/33/34	0/3/3/3

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C2'-C1'	-19.15	1.28	1.53
8	A	1915	3TD	O4'-C1'	15.38	1.64	1.43
56	w	37	MIA	C2-S10	-15.05	1.62	1.75
8	A	1915	3TD	C6-C5	11.52	1.48	1.35
55	v	54	5MU	C2-N1	11.13	1.56	1.38
55	v	54	5MU	C6-N1	10.33	1.55	1.38
8	A	1939	5MU	C6-N1	9.91	1.55	1.38
8	A	1939	5MU	C2-N1	9.74	1.54	1.38
55	v	54	5MU	C4-C5	9.51	1.60	1.44
34	a	967	5MC	C6-C5	9.49	1.50	1.34
8	A	1939	5MU	C4-C5	9.37	1.60	1.44
34	a	1407	5MC	C6-C5	9.33	1.49	1.34
55	v	20	H2U	C2-N1	9.24	1.48	1.35
8	A	1962	5MC	C6-C5	8.83	1.49	1.34
8	A	747	5MC	C6-C5	8.81	1.49	1.34
8	A	1939	5MU	C4-N3	-8.32	1.23	1.38
55	v	54	5MU	C4-N3	-8.10	1.23	1.38
8	A	2503	2MA	C4-N3	8.04	1.48	1.35
8	A	1915	3TD	C2-N1	8.01	1.47	1.37
56	w	8	4SU	C4-N3	7.83	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	8	4SU	C4-N3	7.52	1.45	1.37
8	A	1618	6MZ	C6-N6	7.47	1.47	1.35
56	w	8	4SU	C2-N1	7.28	1.50	1.38
8	A	745	1MG	C2-N2	7.27	1.47	1.34
56	w	37	MIA	C13-C14	7.24	1.53	1.32
8	A	1915	3TD	O4'-C4'	-7.06	1.29	1.45
34	a	1402	4OC	C4-N3	6.97	1.44	1.32
8	A	2503	2MA	C2-N3	6.91	1.46	1.34
55	v	8	4SU	C2-N1	6.86	1.49	1.38
8	A	1962	5MC	C4-N3	6.81	1.45	1.34
8	A	2552	OMU	C2-N1	6.75	1.49	1.38
34	a	1407	5MC	C4-N3	6.74	1.45	1.34
8	A	2552	OMU	C2-N3	6.68	1.49	1.38
34	a	967	5MC	C4-N3	6.64	1.45	1.34
8	A	1915	3TD	O3'-C3'	-6.48	1.27	1.43
8	A	747	5MC	C4-N3	6.40	1.45	1.34
55	v	20	H2U	C2-N3	6.34	1.49	1.38
34	a	1516	2MG	C2-N2	6.28	1.47	1.33
34	a	1407	5MC	C2-N3	6.26	1.49	1.36
34	a	1498	UR3	C2-N1	6.20	1.47	1.38
34	a	1207	2MG	C2-N2	6.20	1.47	1.33
8	A	1835	2MG	C2-N2	6.19	1.47	1.33
34	a	967	5MC	C2-N3	6.16	1.48	1.36
34	a	966	2MG	C2-N2	6.13	1.47	1.33
8	A	1962	5MC	C2-N3	6.11	1.48	1.36
55	v	54	5MU	C6-C5	6.09	1.44	1.34
34	a	1498	UR3	C6-C5	6.03	1.49	1.35
8	A	1917	PSU	C2'-C1'	-6.00	1.45	1.53
8	A	1939	5MU	C6-C5	5.98	1.44	1.34
56	w	8	4SU	C6-C5	5.93	1.48	1.35
8	A	747	5MC	C2-N3	5.86	1.48	1.36
34	a	1402	4OC	C2-N3	5.82	1.48	1.36
34	a	1402	4OC	C6-C5	5.76	1.48	1.35
8	A	2503	2MA	C2-N1	5.73	1.44	1.34
56	w	46	G7M	C2-N3	5.71	1.47	1.33
34	a	527	G7M	C2-N3	5.67	1.47	1.33
8	A	745	1MG	C2-N3	5.65	1.44	1.34
55	v	8	4SU	C6-C5	5.63	1.48	1.35
56	w	37	MIA	C2'-C1'	-5.56	1.45	1.53
8	A	2552	OMU	C6-C5	5.54	1.47	1.35
56	w	8	4SU	C2-N3	5.48	1.47	1.38
8	A	2069	G7M	C2-N3	5.36	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	8	4SU	C2-N3	5.31	1.47	1.38
55	v	8	4SU	C4-S4	-5.28	1.58	1.68
56	w	39	PSU	C2'-C1'	-5.19	1.47	1.53
56	w	8	4SU	C4-S4	-5.06	1.58	1.68
34	a	966	2MG	C4-N3	4.98	1.49	1.37
55	v	20	H2U	C4-N3	4.98	1.46	1.37
56	w	46	G7M	C4-N3	4.95	1.49	1.37
8	A	1835	2MG	C4-N3	4.92	1.49	1.37
34	a	1207	2MG	C4-N3	4.91	1.49	1.37
34	a	527	G7M	C4-N3	4.91	1.49	1.37
8	A	1917	PSU	C4-N3	-4.87	1.29	1.38
8	A	2503	2MA	C6-N1	4.85	1.42	1.33
8	A	1917	PSU	C2-N1	-4.78	1.30	1.36
8	A	745	1MG	C4-N3	4.78	1.49	1.37
34	a	967	5MC	C4-N4	4.77	1.46	1.34
34	a	1498	UR3	C2-N3	4.71	1.48	1.39
34	a	967	5MC	C6-N1	4.70	1.46	1.38
8	A	2069	G7M	C4-N3	4.68	1.48	1.37
34	a	1407	5MC	C4-N4	4.68	1.46	1.34
8	A	747	5MC	C4-N4	4.67	1.46	1.34
8	A	1962	5MC	C4-N4	4.67	1.46	1.34
34	a	1407	5MC	C6-N1	4.62	1.45	1.38
34	a	1516	2MG	C2-N1	4.60	1.44	1.36
34	a	1516	2MG	C4-N3	4.56	1.48	1.37
34	a	1207	2MG	C2-N1	4.52	1.43	1.36
34	a	966	2MG	C2-N1	4.51	1.43	1.36
8	A	1915	3TD	C6-N1	4.33	1.43	1.36
34	a	527	G7M	C2-N2	4.33	1.44	1.34
56	w	46	G7M	C2-N2	4.29	1.44	1.34
8	A	1835	2MG	C2-N1	4.29	1.43	1.36
34	a	967	5MC	C2-N1	4.25	1.49	1.40
34	a	1402	4OC	C4-N4	4.19	1.44	1.35
8	A	2069	G7M	C2-N2	4.15	1.44	1.34
8	A	1962	5MC	C6-N1	4.09	1.45	1.38
56	w	46	G7M	C6-N1	3.90	1.43	1.37
34	a	1407	5MC	C2-N1	3.87	1.48	1.40
8	A	1917	PSU	C2-N3	-3.81	1.31	1.37
8	A	1917	PSU	C6-N1	-3.77	1.30	1.36
8	A	747	5MC	C6-N1	3.69	1.44	1.38
8	A	1962	5MC	C2-N1	3.67	1.48	1.40
34	a	1402	4OC	C2-N1	3.66	1.47	1.40
8	A	2552	OMU	C4-N3	3.59	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	747	5MC	O2-C2	-3.58	1.17	1.23
8	A	2030	6MZ	O3'-C3'	3.56	1.51	1.43
56	w	8	4SU	C5-C4	3.52	1.47	1.42
34	a	1402	4OC	C5-C4	3.52	1.48	1.40
55	v	55	PSU	C6-C5	3.46	1.39	1.35
56	w	32	PSU	C4-N3	-3.46	1.32	1.38
34	a	966	2MG	C6-N1	3.45	1.43	1.37
34	a	527	G7M	C6-N1	3.44	1.43	1.37
34	a	967	5MC	O2-C2	-3.43	1.17	1.23
56	w	55	PSU	C6-C5	3.37	1.39	1.35
34	a	1407	5MC	O2-C2	-3.35	1.17	1.23
8	A	2069	G7M	C6-N1	3.32	1.42	1.37
34	a	1207	2MG	C6-N1	3.31	1.42	1.37
34	a	1516	2MG	C6-N1	3.30	1.42	1.37
8	A	2504	PSU	C6-C5	3.29	1.39	1.35
8	A	747	5MC	C2-N1	3.22	1.47	1.40
8	A	1835	2MG	O6-C6	-3.22	1.16	1.23
56	w	39	PSU	C6-C5	3.21	1.39	1.35
8	A	2552	OMU	O4-C4	-3.21	1.18	1.24
8	A	1962	5MC	O2-C2	-3.20	1.17	1.23
34	a	516	PSU	C6-C5	3.19	1.39	1.35
8	A	2605	PSU	C6-C5	3.15	1.39	1.35
56	w	37	MIA	C4-N3	-3.14	1.30	1.35
8	A	1835	2MG	C6-N1	3.11	1.42	1.37
56	w	32	PSU	C2-N1	-3.10	1.32	1.36
55	v	8	4SU	C5-C4	3.09	1.46	1.42
8	A	1835	2MG	C5-C4	-3.06	1.35	1.43
8	A	2445	2MG	C6-N1	-3.05	1.33	1.37
8	A	1911	PSU	C6-C5	3.04	1.38	1.35
34	a	527	G7M	C5-C6	3.03	1.53	1.45
8	A	2069	G7M	C5-C6	3.02	1.53	1.45
34	a	1516	2MG	C5-C4	-2.99	1.35	1.43
8	A	746	PSU	C6-C5	2.99	1.38	1.35
8	A	2604	PSU	C6-C5	2.98	1.38	1.35
56	w	46	G7M	C5-C6	2.98	1.53	1.45
8	A	1618	6MZ	C5-C4	-2.95	1.33	1.40
34	a	1516	2MG	O6-C6	-2.95	1.17	1.23
34	a	1402	4OC	O2-C2	-2.94	1.18	1.23
34	a	516	PSU	C4-N3	-2.94	1.33	1.38
34	a	1207	2MG	O6-C6	-2.93	1.17	1.23
34	a	966	2MG	O6-C6	-2.92	1.17	1.23
8	A	1939	5MU	O4-C4	-2.92	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	966	2MG	C5-C6	2.89	1.53	1.47
56	w	55	PSU	C4-N3	-2.88	1.33	1.38
34	a	1402	4OC	C6-N1	2.86	1.44	1.38
34	a	1207	2MG	C5-C4	-2.83	1.35	1.43
8	A	2251	OMG	C6-N1	-2.80	1.33	1.37
56	w	46	G7M	C2-N1	2.80	1.44	1.37
8	A	1939	5MU	O2-C2	-2.76	1.18	1.23
34	a	966	2MG	C5-C4	-2.74	1.36	1.43
55	v	8	4SU	O2-C2	-2.74	1.18	1.23
34	a	1518	MA6	C5-C4	-2.74	1.33	1.40
8	A	2580	PSU	O4'-C1'	-2.73	1.40	1.43
56	w	37	MIA	C2'-C3'	-2.72	1.45	1.53
56	w	54	5MU	C4-N3	-2.72	1.33	1.38
56	w	39	PSU	C2-N1	-2.70	1.33	1.36
34	a	1516	2MG	C5-C6	2.70	1.52	1.47
56	w	54	5MU	C6-C5	2.70	1.39	1.34
8	A	745	1MG	C5-C4	-2.69	1.36	1.43
34	a	1498	UR3	C6-N1	2.68	1.44	1.38
56	w	39	PSU	C4-N3	-2.68	1.33	1.38
56	w	39	PSU	C1'-C5	-2.67	1.44	1.50
55	v	54	5MU	O4-C4	-2.67	1.18	1.23
34	a	1519	MA6	C5-C4	-2.64	1.34	1.40
8	A	1618	6MZ	C2-N3	2.62	1.36	1.32
55	v	54	5MU	O2-C2	-2.61	1.18	1.23
8	A	2457	PSU	O4'-C1'	-2.60	1.40	1.43
56	w	8	4SU	O2-C2	-2.58	1.18	1.23
8	A	1915	3TD	C2-N3	2.57	1.44	1.38
8	A	955	PSU	C6-C5	2.56	1.38	1.35
8	A	2552	OMU	C6-N1	2.56	1.44	1.38
8	A	1835	2MG	C5-C6	2.54	1.52	1.47
56	w	32	PSU	C6-N1	-2.52	1.32	1.36
56	w	54	5MU	C6-N1	-2.52	1.33	1.38
34	a	1498	UR3	O2-C2	-2.52	1.17	1.22
8	A	2069	G7M	C2-N1	2.51	1.43	1.37
56	w	46	G7M	O6-C6	-2.50	1.18	1.23
8	A	2503	2MA	C6-C5	2.48	1.52	1.43
34	a	527	G7M	O6-C6	-2.48	1.18	1.23
34	a	1207	2MG	C5-C6	2.48	1.52	1.47
34	a	527	G7M	C2-N1	2.46	1.43	1.37
56	w	37	MIA	C3'-C4'	-2.44	1.46	1.53
56	w	39	PSU	C3'-C4'	-2.44	1.46	1.53
8	A	2069	G7M	O6-C6	-2.42	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2552	OMU	O2-C2	-2.41	1.18	1.23
8	A	1915	3TD	C1'-C5	-2.40	1.44	1.50
34	a	1498	UR3	O4-C4	-2.40	1.18	1.23
8	A	1618	6MZ	C6-N1	-2.40	1.30	1.34
8	A	2503	2MA	C6-N6	-2.36	1.25	1.34
8	A	2457	PSU	C4-C5	-2.35	1.37	1.44
55	v	20	H2U	O4-C4	-2.35	1.18	1.23
56	w	32	PSU	C1'-C5	-2.32	1.44	1.50
56	w	54	5MU	C4-C5	2.30	1.48	1.44
56	w	37	MIA	O5'-C5'	-2.29	1.39	1.44
56	w	54	5MU	C2-N1	2.27	1.42	1.38
55	v	20	H2U	O2-C2	-2.26	1.18	1.23
8	A	2580	PSU	C4-C5	-2.22	1.37	1.44
8	A	2605	PSU	C4-C5	-2.18	1.37	1.44
8	A	2580	PSU	C6-C5	2.14	1.37	1.35
8	A	2030	6MZ	C5-C4	2.14	1.46	1.40
8	A	2504	PSU	C4-C5	-2.13	1.38	1.44
56	w	32	PSU	O5'-C5'	-2.12	1.39	1.44
56	w	37	MIA	O4'-C4'	-2.11	1.40	1.45
8	A	746	PSU	C4-C5	-2.08	1.38	1.44
56	w	55	PSU	C2-N3	-2.07	1.34	1.37
56	w	39	PSU	O4'-C1'	-2.07	1.41	1.43
34	a	516	PSU	C2-N3	-2.07	1.34	1.37
8	A	2552	OMU	C5-C4	2.06	1.48	1.43
56	w	37	MIA	C2-N3	-2.06	1.30	1.34
8	A	2604	PSU	C4-C5	-2.02	1.38	1.44
8	A	2498	OMC	C5-C4	-2.02	1.38	1.42
56	w	39	PSU	C6-N1	-2.01	1.32	1.36

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1915	3TD	O9-P-O5'	-12.58	73.25	106.73
8	A	1939	5MU	C5-C4-N3	12.18	125.71	115.31
55	v	54	5MU	C5-C4-N3	11.21	124.88	115.31
8	A	1939	5MU	C5-C6-N1	-10.68	112.35	123.34
8	A	1915	3TD	O9-P-OP1	-10.59	67.16	107.64
55	v	54	5MU	C5-C6-N1	-9.80	113.26	123.34
34	a	1519	MA6	N1-C6-N6	-9.71	106.83	117.06
34	a	1518	MA6	N1-C6-N6	-8.97	107.61	117.06
55	v	8	4SU	C4-N3-C2	-8.58	119.01	127.34
56	w	8	4SU	C4-N3-C2	-8.29	119.29	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	37	MIA	C12-C13-C14	-8.14	111.30	127.14
56	w	39	PSU	N1-C2-N3	7.75	123.92	115.13
8	A	1915	3TD	O4-C4-N3	-7.24	107.03	120.30
8	A	1915	3TD	OP1-P-O5'	7.18	125.84	106.73
55	v	20	H2U	C4-N3-C2	-7.05	119.94	125.79
56	w	32	PSU	N1-C2-N3	6.28	122.24	115.13
56	w	39	PSU	O4'-C1'-C2'	-6.26	96.32	105.14
8	A	2030	6MZ	C2-N1-C6	6.16	121.87	116.59
34	a	516	PSU	N1-C2-N3	6.11	122.05	115.13
8	A	1915	3TD	N1-C2-N3	5.99	120.86	116.14
8	A	1915	3TD	C3'-C2'-C1'	5.96	108.58	101.64
8	A	1917	PSU	N1-C2-N3	5.96	121.88	115.13
55	v	8	4SU	C5-C4-N3	5.93	120.19	114.69
56	w	37	MIA	C11-S10-C2	-5.90	97.86	102.27
56	w	55	PSU	N1-C2-N3	5.89	121.80	115.13
56	w	37	MIA	O3'-C3'-C2'	-5.85	92.88	111.82
56	w	37	MIA	C5-C6-N1	-5.64	116.13	120.81
56	w	8	4SU	C5-C4-N3	5.61	119.89	114.69
8	A	1618	6MZ	C9-N6-C6	-5.59	118.06	122.87
8	A	2552	OMU	C4-N3-C2	-5.43	119.42	126.58
8	A	1939	5MU	C4-N3-C2	-5.41	120.34	127.35
56	w	37	MIA	O2'-C2'-C3'	-5.41	94.31	111.82
34	a	1518	MA6	N3-C2-N1	-5.36	120.30	128.68
56	w	32	PSU	O2-C2-N1	-5.27	116.99	122.79
56	w	54	5MU	C4-N3-C2	-5.23	120.59	127.35
55	v	54	5MU	N3-C2-N1	5.18	121.76	114.89
8	A	1939	5MU	N3-C2-N1	5.15	121.73	114.89
34	a	1519	MA6	N3-C2-N1	-5.10	120.70	128.68
8	A	1917	PSU	C3'-C2'-C1'	5.10	107.58	101.64
56	w	54	5MU	N3-C2-N1	5.10	121.66	114.89
8	A	1939	5MU	O4-C4-C5	-5.07	119.03	124.90
8	A	1917	PSU	O2'-C2'-C1'	-4.93	99.47	111.23
8	A	1915	3TD	C4-N3-C2	-4.93	119.26	124.61
55	v	54	5MU	O4-C4-C5	-4.92	119.20	124.90
56	w	37	MIA	O4'-C1'-C2'	-4.86	99.83	106.93
8	A	1917	PSU	O4'-C1'-C2'	-4.85	98.31	105.14
8	A	1618	6MZ	N3-C2-N1	-4.83	121.13	128.68
8	A	2604	PSU	C4-N3-C2	-4.83	119.39	126.34
8	A	2457	PSU	C4-N3-C2	-4.82	119.39	126.34
55	v	54	5MU	C4-N3-C2	-4.77	121.18	127.35
8	A	2604	PSU	N1-C2-N3	4.74	120.50	115.13
8	A	1917	PSU	C6-C5-C4	-4.73	114.89	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1911	PSU	C4-N3-C2	-4.70	119.56	126.34
56	w	32	PSU	C2'-C3'-C4'	-4.67	93.56	102.64
8	A	2605	PSU	C4-N3-C2	-4.64	119.65	126.34
56	w	39	PSU	O2-C2-N1	-4.60	117.72	122.79
8	A	2605	PSU	N1-C2-N3	4.59	120.33	115.13
56	w	37	MIA	C3'-C2'-C1'	4.53	107.79	100.98
34	a	1498	UR3	C4-N3-C2	-4.51	120.32	124.56
8	A	2504	PSU	N1-C2-N3	4.49	120.22	115.13
8	A	746	PSU	C4-N3-C2	-4.48	119.88	126.34
8	A	2580	PSU	C4-N3-C2	-4.47	119.90	126.34
56	w	37	MIA	C15-C14-C13	-4.40	109.94	122.65
8	A	2457	PSU	N1-C2-N3	4.40	120.11	115.13
8	A	2503	2MA	C2-N3-C4	4.39	119.09	115.52
8	A	2504	PSU	C4-N3-C2	-4.37	120.05	126.34
8	A	2580	PSU	N1-C2-N3	4.29	119.99	115.13
55	v	55	PSU	C4-N3-C2	-4.27	120.18	126.34
8	A	1911	PSU	N1-C2-N3	4.24	119.94	115.13
55	v	55	PSU	N1-C2-N3	4.22	119.91	115.13
8	A	1917	PSU	C4-N3-C2	-4.16	120.35	126.34
34	a	516	PSU	C4-N3-C2	-4.07	120.47	126.34
8	A	955	PSU	C4-N3-C2	-4.07	120.47	126.34
56	w	54	5MU	C5-C4-N3	4.07	118.78	115.31
55	v	8	4SU	C5-C4-S4	-4.04	119.27	124.47
8	A	955	PSU	N1-C2-N3	4.02	119.69	115.13
56	w	8	4SU	N3-C2-N1	4.00	120.19	114.89
8	A	746	PSU	N1-C2-N3	3.97	119.63	115.13
55	v	8	4SU	N3-C2-N1	3.97	120.16	114.89
8	A	1939	5MU	O2-C2-N1	-3.92	117.58	122.79
8	A	2552	OMU	N3-C2-N1	3.91	120.08	114.89
8	A	2030	6MZ	C9-N6-C6	-3.90	119.52	122.87
56	w	54	5MU	C5-C6-N1	-3.86	119.36	123.34
8	A	2498	OMC	C2'-C1'-N1	-3.85	106.75	114.22
8	A	745	1MG	C5-C6-N1	3.82	119.64	113.90
8	A	1915	3TD	O9-P-OP2	-3.78	95.88	110.68
8	A	1917	PSU	O2-C2-N1	-3.78	118.63	122.79
56	w	37	MIA	C4-C5-N7	-3.77	105.47	109.40
56	w	54	5MU	O4-C4-C5	-3.76	120.55	124.90
56	w	37	MIA	C2'-C3'-C4'	-3.73	95.39	102.64
56	w	55	PSU	C4-N3-C2	-3.73	120.96	126.34
56	w	39	PSU	C6-C5-C4	3.68	120.77	118.20
55	v	54	5MU	C5M-C5-C6	-3.66	117.97	122.85
8	A	747	5MC	C5-C6-N1	-3.65	119.58	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1835	2MG	C5-C6-N1	3.64	120.38	113.95
8	A	955	PSU	O2-C2-N1	-3.62	118.81	122.79
56	w	39	PSU	C4-N3-C2	-3.60	121.15	126.34
8	A	2504	PSU	O2-C2-N1	-3.60	118.83	122.79
8	A	1962	5MC	C5-C6-N1	-3.60	119.64	123.34
8	A	2457	PSU	O2-C2-N1	-3.55	118.88	122.79
8	A	2552	OMU	C5-C4-N3	3.48	120.05	114.84
8	A	2580	PSU	O2-C2-N1	-3.47	118.97	122.79
8	A	1915	3TD	O2-C2-N3	-3.43	116.76	121.83
34	a	1207	2MG	C5-C6-N1	3.41	119.98	113.95
34	a	966	2MG	C5-C6-N1	3.41	119.98	113.95
56	w	37	MIA	O2'-C2'-C1'	-3.38	98.39	110.85
8	A	1915	3TD	C10-N3-C2	3.37	125.85	118.30
34	a	516	PSU	O2-C2-N1	-3.32	119.13	122.79
8	A	1939	5MU	C5M-C5-C6	-3.28	118.47	122.85
34	a	527	G7M	C2-N1-C6	-3.23	119.14	125.10
56	w	39	PSU	C3'-C2'-C1'	-3.20	97.90	101.64
56	w	8	4SU	C5-C4-S4	-3.20	120.34	124.47
56	w	46	G7M	C2-N1-C6	-3.18	119.25	125.10
34	a	1516	2MG	C5-C6-N1	3.17	119.56	113.95
8	A	2030	6MZ	C4-C5-N7	-3.16	106.10	109.40
56	w	37	MIA	C16-C14-C13	-3.14	113.58	122.65
56	w	39	PSU	O4'-C4'-C3'	-3.12	98.94	105.11
34	a	516	PSU	C3'-C2'-C1'	3.10	105.25	101.64
8	A	1915	3TD	O2'-C2'-C1'	-3.10	103.83	111.23
55	v	20	H2U	N3-C2-N1	3.09	119.92	116.65
8	A	2069	G7M	C2-N1-C6	-3.08	119.42	125.10
8	A	2457	PSU	C6-C5-C4	3.05	120.33	118.20
56	w	32	PSU	C4'-O4'-C1'	-3.05	100.89	108.55
8	A	746	PSU	O2-C2-N1	-3.02	119.46	122.79
34	a	1498	UR3	C1'-N1-C2	2.99	122.04	116.99
56	w	55	PSU	O2-C2-N1	-2.96	119.53	122.79
8	A	2504	PSU	C6-N1-C2	-2.96	119.66	122.68
55	v	20	H2U	C5-C4-N3	2.94	119.95	116.65
56	w	32	PSU	C6-N1-C2	-2.92	119.69	122.68
8	A	2030	6MZ	N3-C2-N1	-2.92	124.11	128.68
8	A	2552	OMU	O4-C4-C5	-2.88	120.09	125.16
56	w	39	PSU	C6-N1-C2	-2.85	119.76	122.68
8	A	2604	PSU	O2-C2-N1	-2.82	119.69	122.79
56	w	32	PSU	C4-N3-C2	-2.80	122.31	126.34
55	v	54	5MU	C5M-C5-C4	2.79	121.84	118.77
55	v	55	PSU	O2-C2-N1	-2.78	119.73	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1911	PSU	O2-C2-N1	-2.73	119.78	122.79
8	A	1939	5MU	C5M-C5-C4	2.70	121.74	118.77
8	A	2580	PSU	O4'-C1'-C2'	2.69	108.94	105.14
55	v	20	H2U	C5-C6-N1	2.68	120.44	111.61
58	y	101	FME	O-C-CA	-2.68	117.77	124.78
34	a	1498	UR3	C6-N1-C2	-2.67	119.39	121.79
8	A	2445	2MG	CM2-N2-C2	-2.66	117.98	123.86
34	a	1407	5MC	C5-C6-N1	-2.66	120.60	123.34
8	A	2503	2MA	N3-C2-N1	-2.65	120.89	125.73
34	a	1516	2MG	CM2-N2-C2	-2.65	118.01	123.86
55	v	20	H2U	O2-C2-N1	-2.64	119.79	123.11
8	A	1915	3TD	C5'-C4'-C3'	-2.61	105.40	115.18
55	v	54	5MU	O2-C2-N1	-2.61	119.32	122.79
8	A	1915	3TD	C5-C6-N1	-2.61	118.20	122.11
55	v	54	5MU	C6-C5-C4	2.58	120.19	118.03
8	A	2580	PSU	C6-N1-C2	-2.58	120.05	122.68
34	a	966	2MG	CM2-N2-C2	-2.57	118.18	123.86
8	A	2251	OMG	C8-N7-C5	2.57	107.88	102.99
55	v	54	5MU	C6-N1-C2	-2.55	118.71	121.30
56	w	54	5MU	C3'-C2'-C1'	2.54	106.25	101.43
8	A	2605	PSU	O2-C2-N1	-2.54	119.99	122.79
8	A	1939	5MU	O4-C4-N3	-2.53	115.27	120.12
34	a	1207	2MG	O6-C6-C5	-2.53	119.44	124.37
8	A	1962	5MC	C5-C4-N4	-2.53	117.70	121.48
56	w	32	PSU	O4'-C1'-C2'	2.52	108.70	105.14
56	w	55	PSU	C3'-C2'-C1'	2.52	104.57	101.64
34	a	966	2MG	C8-N7-C5	2.52	107.78	102.99
34	a	967	5MC	C5-C6-N1	-2.51	120.76	123.34
8	A	955	PSU	C6-N1-C2	-2.50	120.12	122.68
56	w	39	PSU	O4-C4-N3	2.46	124.84	120.12
8	A	745	1MG	C8-N7-C5	2.46	107.67	102.99
8	A	1915	3TD	O4'-C1'-C2'	-2.45	101.70	105.14
8	A	747	5MC	CM5-C5-C6	-2.44	119.58	122.85
8	A	2251	OMG	C5-C6-N1	2.41	118.22	113.95
8	A	2457	PSU	O4'-C1'-C2'	2.41	108.54	105.14
56	w	54	5MU	O4'-C1'-N1	2.40	113.86	108.36
8	A	2605	PSU	C6-N1-C2	-2.39	120.23	122.68
8	A	2030	6MZ	C2'-C3'-C4'	-2.39	98.00	102.64
34	a	1516	2MG	C8-N7-C5	2.36	107.49	102.99
8	A	1835	2MG	C8-N7-C5	2.36	107.49	102.99
56	w	37	MIA	O4'-C4'-C3'	-2.36	100.45	105.11
34	a	966	2MG	O6-C6-C5	-2.36	119.77	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	39	PSU	C4'-O4'-C1'	-2.34	102.67	108.55
34	a	1207	2MG	C8-N7-C5	2.34	107.45	102.99
8	A	1835	2MG	O6-C6-C5	-2.32	119.84	124.37
8	A	2445	2MG	C5-C6-N1	2.31	118.02	113.95
8	A	1917	PSU	O4'-C4'-C3'	-2.31	100.55	105.11
56	w	32	PSU	C5'-C4'-C3'	-2.30	106.54	115.18
8	A	2604	PSU	C6-N1-C2	-2.30	120.33	122.68
56	w	54	5MU	O2-C2-N1	-2.29	119.74	122.79
55	v	55	PSU	C6-N1-C2	-2.27	120.36	122.68
56	w	39	PSU	O5'-C5'-C4'	2.27	116.70	108.99
55	v	54	5MU	O4-C4-N3	-2.20	115.90	120.12
56	w	39	PSU	C2'-C3'-C4'	2.20	106.91	102.64
8	A	2604	PSU	C6-C5-C4	2.19	119.73	118.20
8	A	2503	2MA	C5-C6-N1	-2.19	119.58	121.01
8	A	745	1MG	O6-C6-C5	-2.18	120.34	124.19
34	a	1516	2MG	O6-C6-C5	-2.18	120.12	124.37
8	A	1618	6MZ	C1'-N9-C4	-2.16	122.85	126.64
56	w	39	PSU	C5-C6-N1	-2.14	118.89	122.11
8	A	1939	5MU	C6-C5-C4	2.10	119.79	118.03
55	v	8	4SU	O2-C2-N1	-2.10	119.99	122.79
8	A	1911	PSU	C6-N1-C2	-2.10	120.54	122.68
56	w	8	4SU	O2-C2-N1	-2.09	120.00	122.79
8	A	2445	2MG	C8-N7-C5	2.06	106.92	102.99
34	a	1207	2MG	CM2-N2-C2	-2.06	119.31	123.86
56	w	37	MIA	C2-N1-C6	2.03	120.81	117.19
8	A	1917	PSU	C6-N1-C2	-2.02	120.61	122.68
8	A	2030	6MZ	O4'-C1'-C2'	-2.01	103.99	106.93
8	A	746	PSU	C6-N1-C2	-2.01	120.63	122.68

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	55	PSU	O4'-C1'-C5-C6
8	A	745	1MG	O4'-C4'-C5'-O5'
8	A	746	PSU	C2'-C1'-C5-C4
8	A	746	PSU	C2'-C1'-C5-C6
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	1917	PSU	C2'-C1'-C5-C4
8	A	1917	PSU	C2'-C1'-C5-C6
8	A	2030	6MZ	N1-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	2251	OMG	C1'-C2'-O2'-CM2
8	A	2504	PSU	C3'-C4'-C5'-O5'
8	A	2504	PSU	O4'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C1'-N1-C2
8	A	2552	OMU	O4'-C1'-N1-C6
8	A	2552	OMU	C1'-C2'-O2'-CM2
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
34	a	967	5MC	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
34	a	1402	4OC	C1'-C2'-O2'-CM2
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	1518	MA6	C5-C6-N6-C9
34	a	1518	MA6	C5-C6-N6-C10
34	a	1519	MA6	C3'-C4'-C5'-O5'
56	w	32	PSU	C2'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C5-C6-N6-C12
56	w	37	MIA	N1-C6-N6-C12
56	w	37	MIA	N1-C2-S10-C11
56	w	37	MIA	N3-C2-S10-C11
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	O4'-C1'-C5-C6
56	w	39	PSU	C3'-C4'-C5'-O5'
56	w	39	PSU	C4'-C5'-O5'-P
56	w	55	PSU	C3'-C4'-C5'-O5'
58	y	101	FME	O1-CN-N-CA
58	y	101	FME	N-CA-CB-CG
58	y	101	FME	C-CA-CB-CG
8	A	745	1MG	C3'-C4'-C5'-O5'
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	1939	5MU	C3'-C4'-C5'-O5'
8	A	1939	5MU	O4'-C4'-C5'-O5'
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2498	OMC	O4'-C4'-C5'-O5'
8	A	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
34	a	1402	4OC	O4'-C4'-C5'-O5'
56	w	39	PSU	O4'-C4'-C5'-O5'
56	w	55	PSU	O4'-C4'-C5'-O5'
8	A	1915	3TD	O4'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
34	a	1519	MA6	O4'-C4'-C5'-O5'
34	a	1518	MA6	N1-C6-N6-C10
8	A	2030	6MZ	C4'-C5'-O5'-P
8	A	1962	5MC	C2'-C1'-N1-C6
8	A	2445	2MG	O4'-C4'-C5'-O5'
8	A	1835	2MG	C3'-C4'-C5'-O5'
34	a	527	G7M	C3'-C4'-C5'-O5'
58	y	101	FME	CB-CG-SD-CE
8	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	527	G7M	C4'-C5'-O5'-P
34	a	1519	MA6	C4'-C5'-O5'-P
56	w	54	5MU	C4'-C5'-O5'-P
8	A	1917	PSU	C3'-C4'-C5'-O5'
8	A	1962	5MC	C2'-C1'-N1-C2
55	v	55	PSU	C4'-C5'-O5'-P
8	A	1618	6MZ	C3'-C4'-C5'-O5'
8	A	1962	5MC	O4'-C1'-N1-C6
8	A	1962	5MC	O4'-C1'-N1-C2
8	A	2251	OMG	C4'-C5'-O5'-P
56	w	46	G7M	C4'-C5'-O5'-P
56	w	46	G7M	C3'-C4'-C5'-O5'
8	A	1917	PSU	O4'-C1'-C5-C4
8	A	2604	PSU	O4'-C1'-C5-C4
8	A	2605	PSU	O4'-C1'-C5-C4
8	A	1618	6MZ	O4'-C4'-C5'-O5'
56	w	32	PSU	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C5-C6-N6-C9
55	v	8	4SU	O4'-C4'-C5'-O5'
8	A	1917	PSU	O4'-C1'-C5-C6
8	A	2069	G7M	O4'-C4'-C5'-O5'
8	A	1915	3TD	C3'-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](#)

3 ligands 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	$\# Z  > 2$
61	PO4	x	802	-	4,4,4	1.11	0	6,6,6	0.44	0
60	AM2	a	2001	-	40,40,40	0.83	1 (2%)	53,60,60	1.73	12 (22%)
62	GDP	x	801	-	24,30,30	1.00	1 (4%)	30,47,47	1.68	5 (16%)

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
62	GDP	x	801	-	-	5/12/32/32	0/3/3/3
60	AM2	a	2001	-	-	4/12/84/84	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	x	801	GDP	C6-N1	-2.87	1.33	1.37
60	a	2001	AM2	CA6-CA7	-2.62	1.48	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	x	801	GDP	PA-O3A-PB	-5.36	114.44	132.83
60	a	2001	AM2	OA6-CA6-CA7	-4.20	101.18	109.66
60	a	2001	AM2	CA8-CA7-CA6	-3.87	98.68	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	a	2001	AM2	CC2-CC3-CC4	-3.81	104.93	111.37
60	a	2001	AM2	OA4-CA1-CA2	3.76	118.62	110.25
60	a	2001	AM2	CA8-CA7-NA7	-3.52	104.71	111.00
60	a	2001	AM2	CA1-OA4-CA5	3.47	118.65	113.06
60	a	2001	AM2	CB5-CB4-NB4	-2.70	105.33	110.92
62	x	801	GDP	C5-C6-N1	2.68	118.68	113.95
62	x	801	GDP	C8-N7-C5	2.63	108.01	102.99
60	a	2001	AM2	CA5-CA6-CA7	-2.51	104.77	110.62
62	x	801	GDP	C2'-C3'-C4'	2.48	107.46	102.64
60	a	2001	AM2	CA6-CA7-NA7	-2.32	104.83	111.28
60	a	2001	AM2	CA1-OA1-CC1	-2.32	112.22	117.96
60	a	2001	AM2	CA6-CA5-CA4	-2.16	105.97	110.93
62	x	801	GDP	O2B-PB-O3A	2.02	111.41	104.64
60	a	2001	AM2	OA8-CB1-CB2	-2.01	102.88	108.10

There are no chirality outliers.

All (9) torsion outliers are listed below:

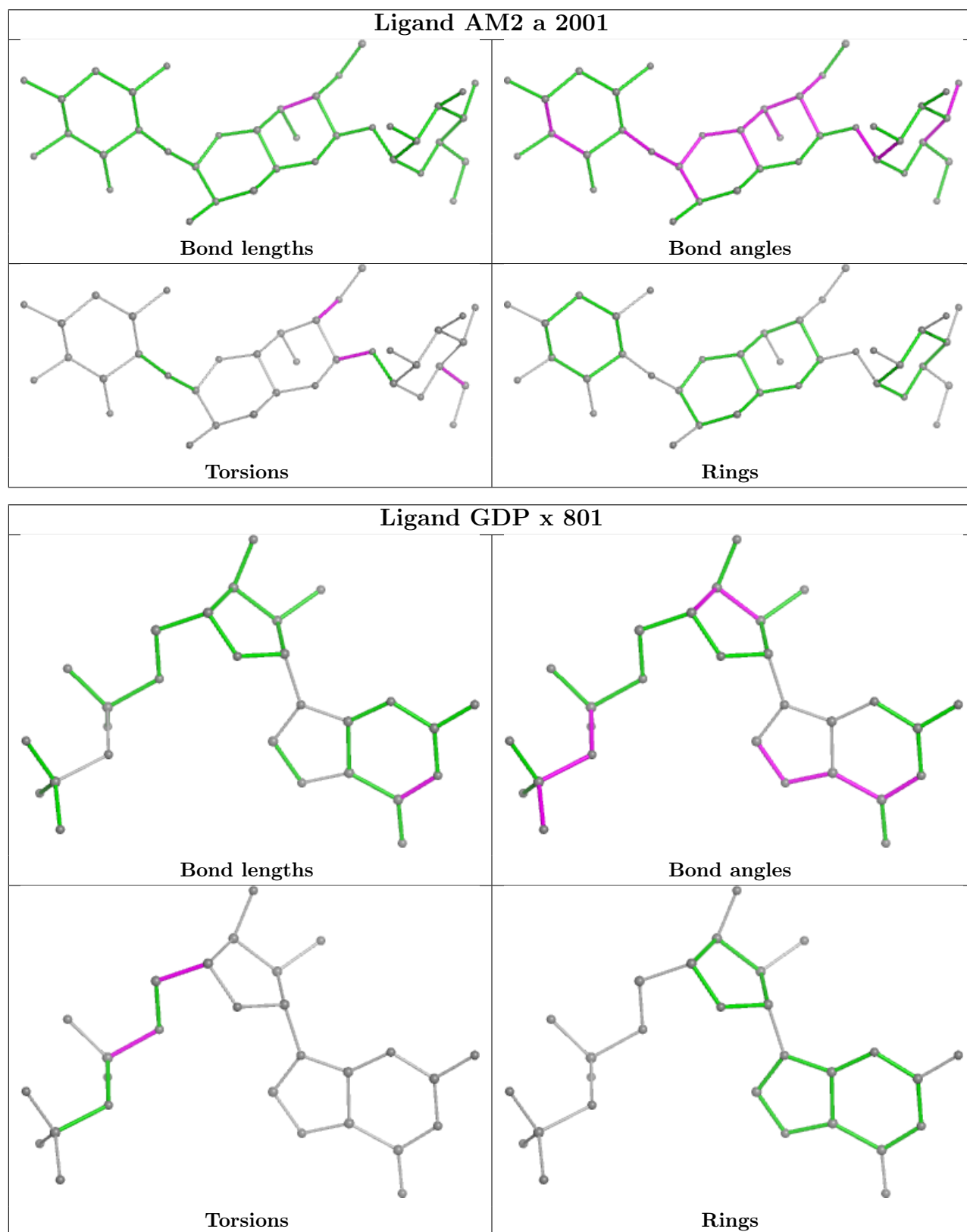
Mol	Chain	Res	Type	Atoms
62	x	801	GDP	C5'-O5'-PA-O1A
62	x	801	GDP	C5'-O5'-PA-O2A
60	a	2001	AM2	OB1-CB5-CB6-OB6
62	x	801	GDP	O4'-C4'-C5'-O5'
60	a	2001	AM2	CB4-CB5-CB6-OB6
62	x	801	GDP	C3'-C4'-C5'-O5'
60	a	2001	AM2	CA8-CA7-NA7-CA9
60	a	2001	AM2	OA5-CA8-OA8-CB1
62	x	801	GDP	C5'-O5'-PA-O3A

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](#)

There are no chain breaks in this entry.