



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:38 pm GMT

PDB ID : 7PJY
EMDB ID : EMD-13464
Title : Structure of the 70S-EF-G-GDP ribosome complex with tRNAs in chimeric state 1 (CHI1-EF-G-GDP)
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on : 2021-08-24
Resolution : 3.10 Å (reported)
Based on initial models : 4AQY, 6YSS, 5J9Z, 5LZD

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

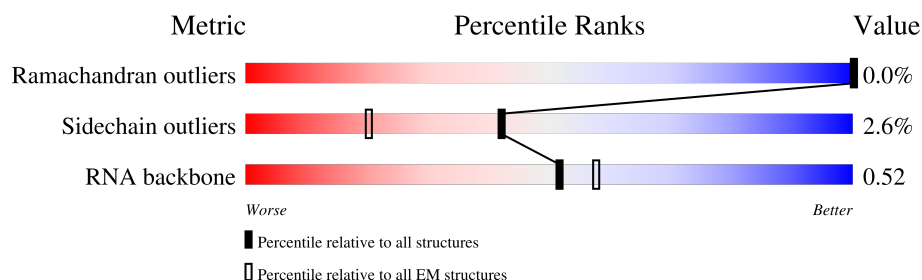
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	57	98% .
2	1	55	91% 9%
3	2	46	98% .
4	3	65	97% ..
5	4	38	100%
6	5	165	79% 21%
7	6	70	89% 6% 6%
8	A	2903	79% 21%
9	B	120	81% 19%



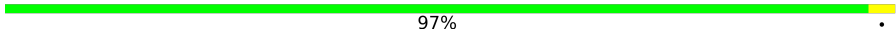
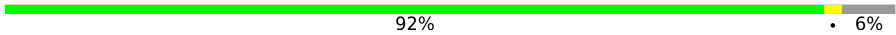


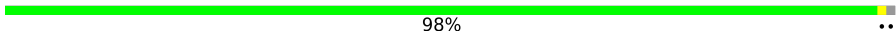
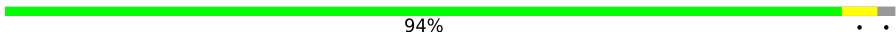
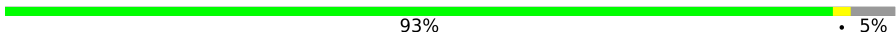

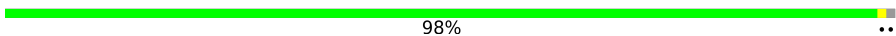
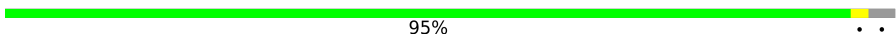
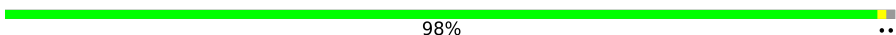
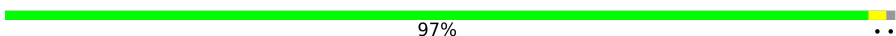
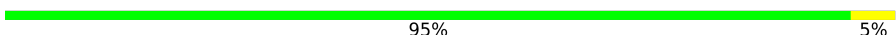



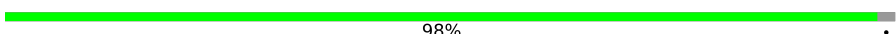






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Mol	Chain	Length	Quality of chain
10	C	273	98% ..
11	D	209	100% ..
12	E	201	99% .
13	F	179	98% ..
14	G	177	99% ..
15	H	149	99% .
16	I	142	99% ..
17	J	142	100% ..
18	K	123	99% .
19	L	144	97% ..
20	M	136	99% .
21	N	127	94% 6% ..
22	O	117	97% ...
23	P	115	99% .
24	Q	118	99% .
25	R	103	97% ..
26	S	110	100% ..
27	T	100	90% . 7%
28	U	104	97% ..
29	V	94	99% .
30	W	85	87% . 12%
31	X	78	97% ..
32	Y	63	98% .
33	Z	59	98% .
34	a	1542	70% 29% .

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Mol	Chain	Length	Quality of chain
35	b	240	 87% . 9%
36	c	233	 88% 12%
37	d	206	 97% .
38	e	167	 92% . 6%
39	f	135	 73% . 26%
40	g	179	 84% . 16%
41	h	130	 98% ..
42	i	130	 94% . .
43	j	103	 93% . 5%
44	k	129	 89% . 10%
45	l	124	 98% ..
46	m	118	 95% . .
47	n	102	 98% ..
48	o	89	 97% ..
49	p	82	 95% 5%
50	q	84	 92% . 5%
51	r	75	 79% 5% . 13%
52	s	92	 87% . 11%
53	t	87	 98% .
54	u	71	 89% . 8%
55	v	77	 62% 34% .
56	w	76	 64% 33% .
57	x	704	 90% 8% .
58	y	2	 50% 50%
59	z	33	 24% 6% 70%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153095 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
			62338	27816	11471	20148	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	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	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	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	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	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	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, fully modified isoform.

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 P0AG59

- 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	697	Total	C	N	O	S		1	0
			5416	3413	938	1040	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	10	Total	C	N	O	P	0	0
			208	93	29	76	10		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total	Mg	0
			1	1	
60	1	1	Total	Mg	0
			1	1	
60	6	1	Total	Mg	0
			1	1	
60	A	267	Total	Mg	0
			267	267	
60	B	6	Total	Mg	0
			6	6	
60	C	3	Total	Mg	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
60	D	1	Total 1	Mg 1	0
60	M	1	Total 1	Mg 1	0
60	O	1	Total 1	Mg 1	0
60	P	1	Total 1	Mg 1	0
60	a	34	Total 34	Mg 34	0
60	w	1	Total 1	Mg 1	0

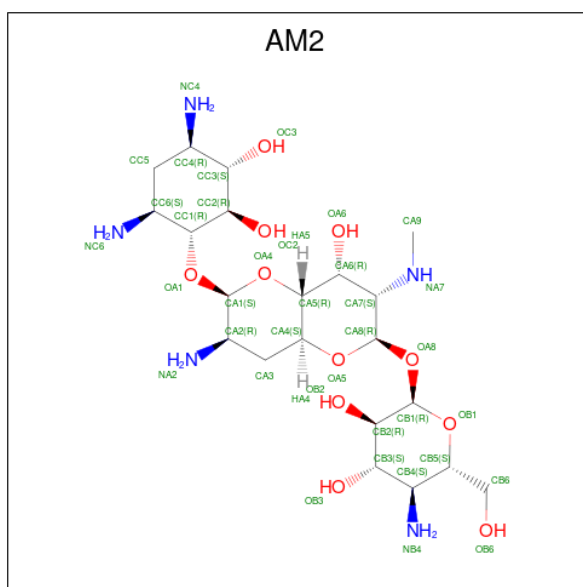
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	4	1	Total 1	Zn 1	0
61	6	1	Total 1	Zn 1	0

- Molecule 62 is SODIUM ION (three-letter code: NA) (formula: Na).

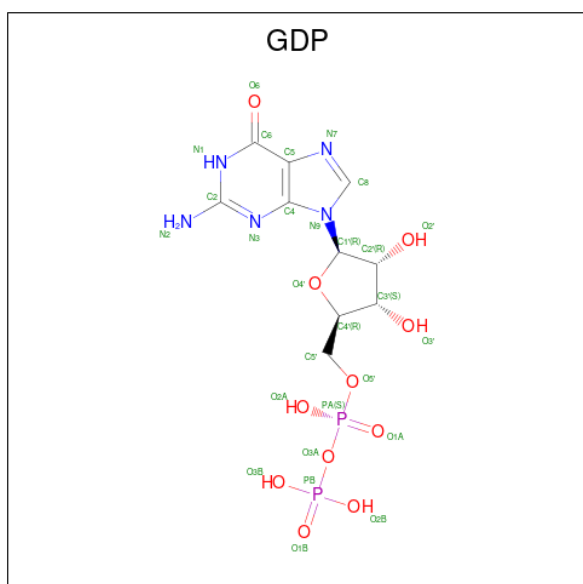
Mol	Chain	Residues	Atoms		AltConf
62	B	1	Total 1	Na 1	0

- Molecule 63 is APRAMYCIN (three-letter code: AM2) (formula: C₂₁H₄₁N₅O₁₁).



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

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

3 Residue-property plots [i](#)

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

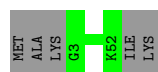
- Molecule 1: 50S ribosomal protein L32

Chain 0:  98% .



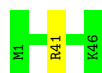
- Molecule 2: 50S ribosomal protein L33

Chain 1:  91% 9%



- Molecule 3: 50S ribosomal protein L34

Chain 2:  98% .



- Molecule 4: 50S ribosomal protein L35

Chain 3:  97% ..




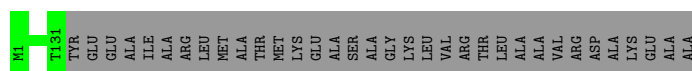
- Molecule 5: 50S ribosomal protein L36

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: 50S ribosomal protein L10

Chain 5:  79% 21%



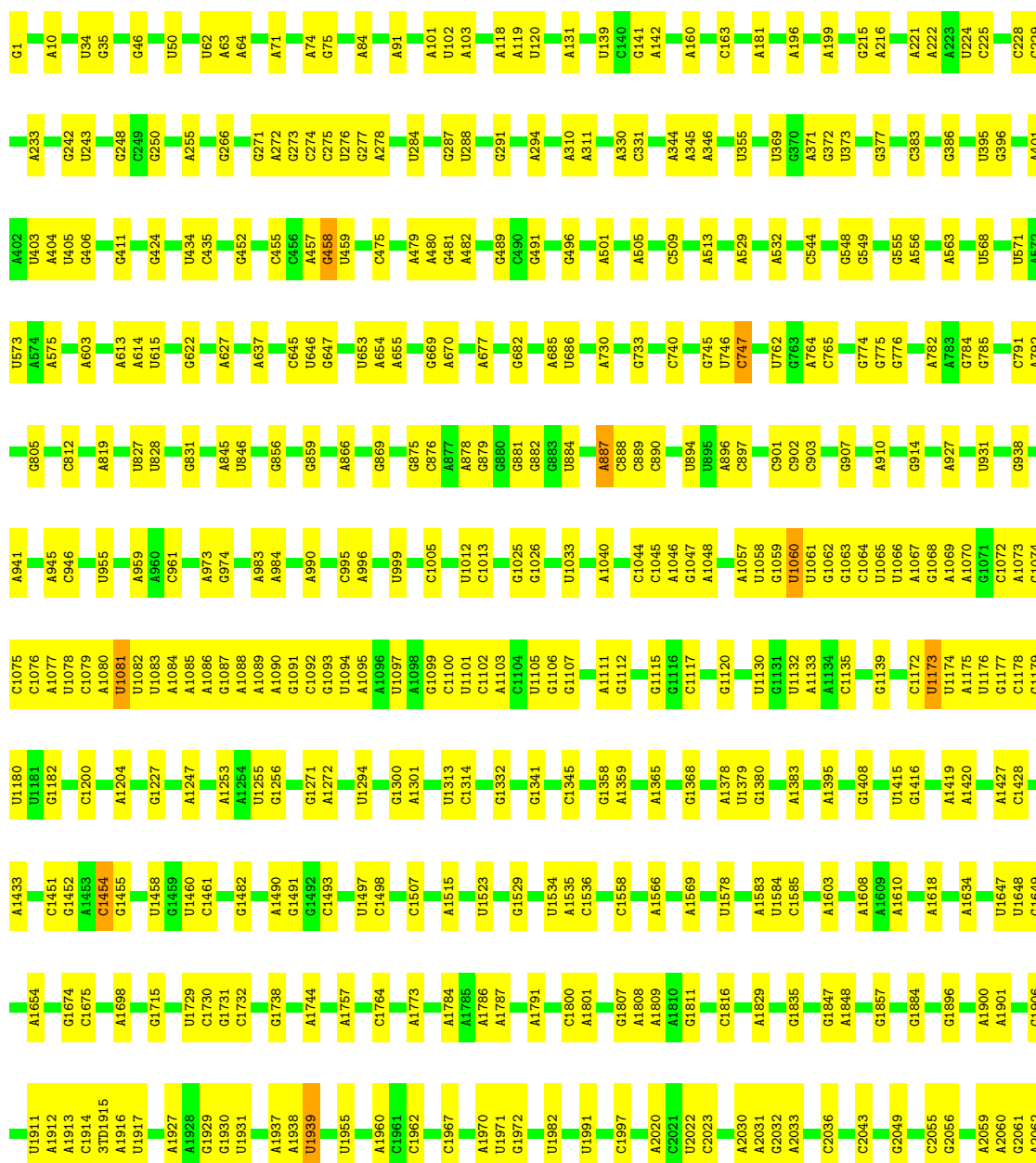
- Molecule 7: 50S ribosomal protein L31

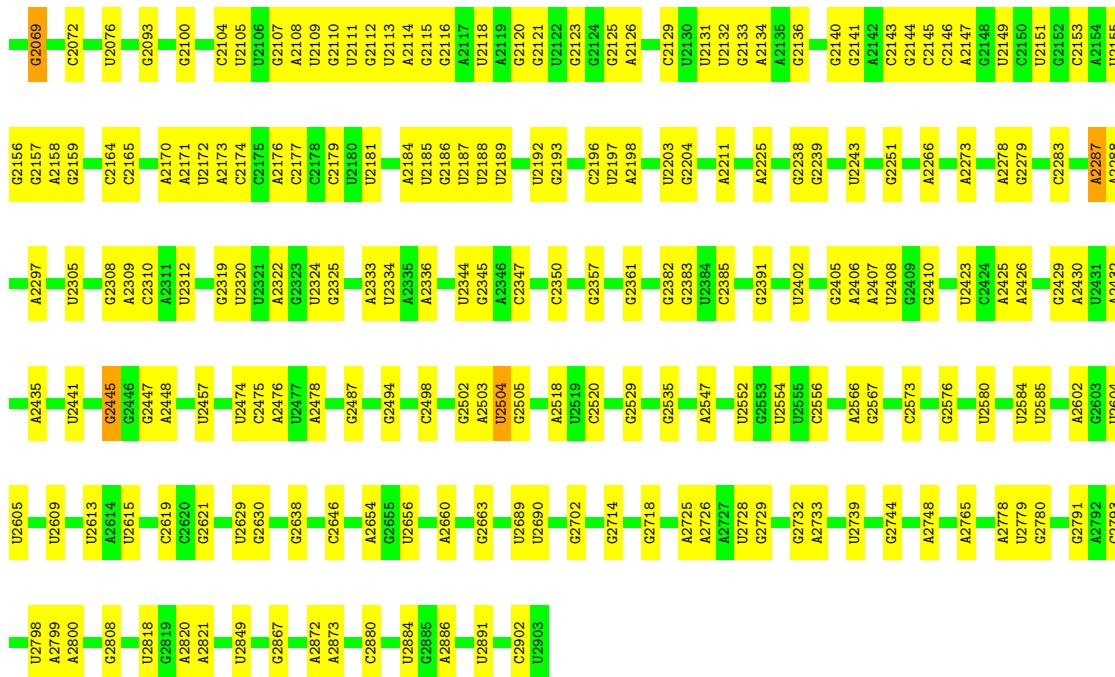
Chain 6: 89% 6% 6%



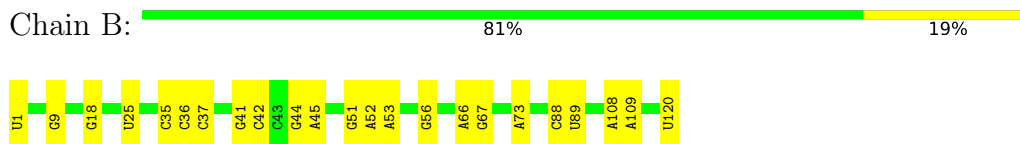
- Molecule 8: 23S ribosomal RNA

Chain A: 79% 21%

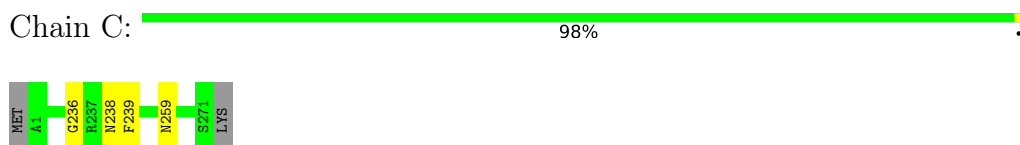




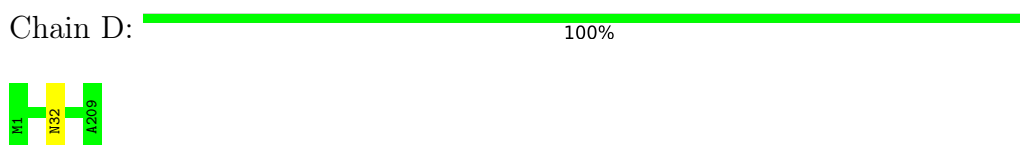
- Molecule 9: 5S ribosomal RNA



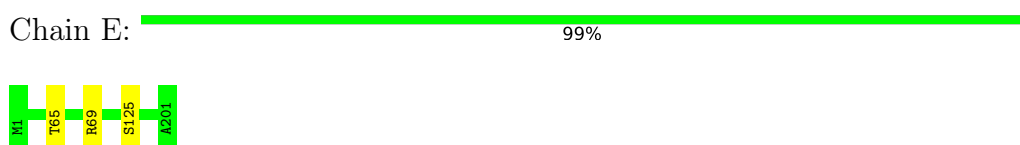
- Molecule 10: 50S ribosomal protein L2



- Molecule 11: 50S ribosomal protein L3



- Molecule 12: 50S ribosomal protein L4



- Molecule 13: 50S ribosomal protein L5

Chain F:  98% ..



- Molecule 14: 50S ribosomal protein L6

Chain G:  99% ..



- Molecule 15: 50S ribosomal protein L9

Chain H:  99% .



- Molecule 16: 50S ribosomal protein L11

Chain I:  99% ..



- Molecule 17: 50S ribosomal protein L13

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L14

Chain K:  99% .



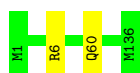
- Molecule 19: 50S ribosomal protein L15

Chain L:  97% ..



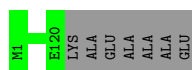
- Molecule 20: 50S ribosomal protein L16

Chain M:  99% .



- Molecule 21: 50S ribosomal protein L17

Chain N: 94% 6%



- Molecule 22: 50S ribosomal protein L18

Chain O: 97% ...



- Molecule 23: 50S ribosomal protein L19

Chain P: 99% .



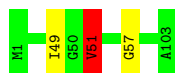
- Molecule 24: 50S ribosomal protein L20

Chain Q: 99% .



- Molecule 25: 50S ribosomal protein L21

Chain R: 97% ..



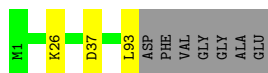
- Molecule 26: 50S ribosomal protein L22

Chain S: 100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L23

Chain T: 90% . 7%



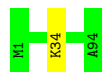
- Molecule 28: 50S ribosomal protein L24

Chain U:  97% ..




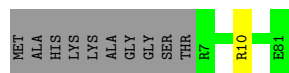
- Molecule 29: 50S ribosomal protein L25

Chain V:  99% .



- Molecule 30: 50S ribosomal protein L27

Chain W:  87% . 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

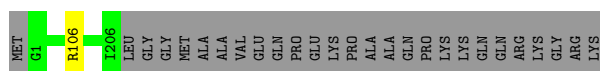
Chain Z:  98% .



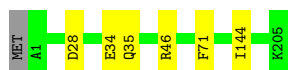
- Molecule 34: 16S ribosomal RNA

Chain a:  70% 29% .

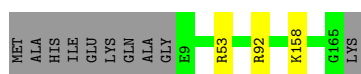




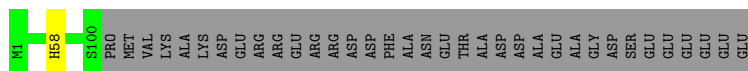
- Molecule 37: 30S ribosomal protein S4



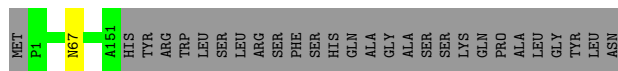
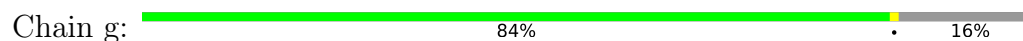
- Molecule 38: 30S ribosomal protein S5



- Molecule 39: 30S ribosomal protein S6, fully modified isoform



- Molecule 40: 30S ribosomal protein S7



- Molecule 41: 30S ribosomal protein S8



- Molecule 42: 30S ribosomal protein S9



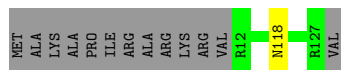
- Molecule 43: 30S ribosomal protein S10





- 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: 95% ..



- Molecule 47: 30S ribosomal protein S14

Chain n: 98% ..



- Molecule 48: 30S ribosomal protein S15

Chain o: 97% ..



- Molecule 49: 30S ribosomal protein S16

Chain p: 95% 5%

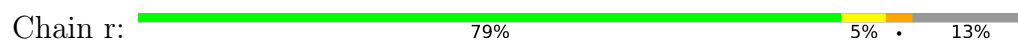


- Molecule 50: 30S ribosomal protein S17

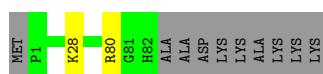
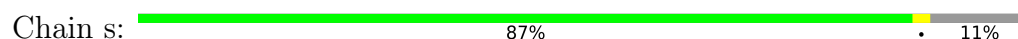
Chain q: 92% 5%



- Molecule 51: 30S ribosomal protein S18



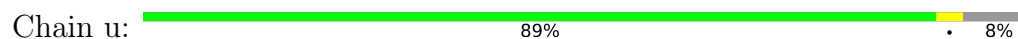
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



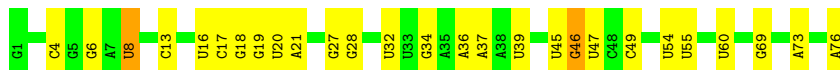
- Molecule 54: 30S ribosomal protein S21



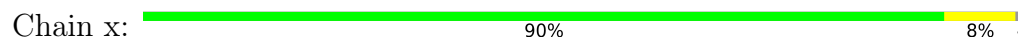
- Molecule 55: P-site tRNA(fMet)

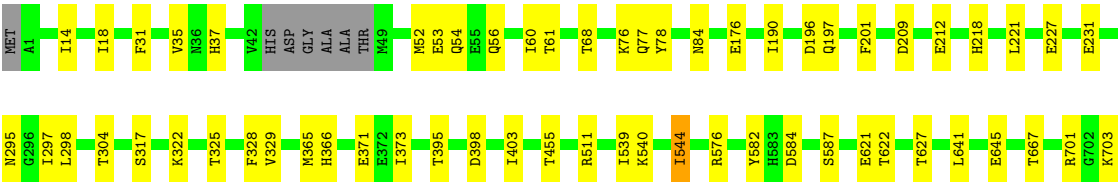


- Molecule 56: P-site fMet-Phe-tRNA(Phe)



- Molecule 57: Elongation factor G





• 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	23737	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: PSU, 5MC, OMU, UR3, GDP, 4OC, 4SU, MIA, 2MA, G7M, OMG, 5MU, NA, MA6, ZN, 3TD, OMC, MG, 6MZ, 1MG, 2MG, FME, AM2

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	0.35	0/450	0.47	0/599
2	1	0.34	0/416	0.47	0/554
3	2	0.34	0/380	0.46	0/498
4	3	0.38	0/513	0.54	0/676
5	4	0.34	0/303	0.53	0/397
6	5	0.28	0/646	0.58	0/898
7	6	0.37	0/531	0.71	1/709 (0.1%)
8	A	0.65	3/69266 (0.0%)	0.84	27/108055 (0.0%)
9	B	0.56	1/2873 (0.0%)	0.83	0/4478
10	C	0.43	0/2121	0.55	2/2852 (0.1%)
11	D	0.39	0/1586	0.50	0/2134
12	E	0.39	0/1571	0.49	0/2113
13	F	0.33	0/1434	0.47	0/1926
14	G	0.32	0/1343	0.48	0/1816
15	H	0.32	0/1122	0.59	0/1515
16	I	0.69	0/692	0.74	0/960
17	J	0.37	0/1152	0.46	0/1551
18	K	0.40	0/947	0.53	0/1268
19	L	0.42	0/1054	0.58	1/1403 (0.1%)
20	M	0.37	0/1093	0.52	0/1460
21	N	0.35	0/973	0.51	0/1301
22	O	0.36	0/902	0.56	2/1209 (0.2%)
23	P	0.38	0/929	0.49	0/1242
24	Q	0.42	0/960	0.41	0/1278
25	R	0.52	1/829 (0.1%)	0.66	2/1107 (0.2%)
26	S	0.35	0/864	0.57	0/1156
27	T	0.39	0/744	0.51	0/994
28	U	0.35	0/787	0.49	0/1051
29	V	0.35	0/766	0.45	0/1025
30	W	0.37	0/582	0.47	0/769
31	X	0.43	1/635 (0.2%)	0.49	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.33	0/510	0.48	0/677
33	Z	0.31	0/453	0.49	0/605
34	a	0.54	9/36725 (0.0%)	0.92	92/57285 (0.2%)
35	b	0.36	0/1735	0.60	0/2338
36	c	0.29	0/1651	0.46	0/2225
37	d	0.36	0/1665	0.55	0/2227
38	e	0.34	0/1154	0.53	0/1554
39	f	0.30	0/835	0.50	0/1128
40	g	0.28	0/1195	0.46	0/1602
41	h	0.34	0/989	0.54	0/1326
42	i	0.39	0/1034	0.58	0/1375
43	j	0.33	0/796	0.55	0/1077
44	k	0.29	0/885	0.46	0/1195
45	l	0.39	0/969	0.58	0/1300
46	m	0.35	0/892	0.56	0/1193
47	n	0.37	0/811	0.54	1/1081 (0.1%)
48	o	0.29	0/722	0.43	0/964
49	p	0.36	0/659	0.56	0/884
50	q	0.39	0/657	0.58	0/881
51	r	0.42	0/544	0.66	3/731 (0.4%)
52	s	0.39	0/675	0.60	1/908 (0.1%)
53	t	0.28	0/671	0.41	0/888
54	u	0.32	0/512	0.58	1/683 (0.1%)
55	v	0.89	8/1767 (0.5%)	0.95	8/2750 (0.3%)
56	w	0.46	1/1650 (0.1%)	0.90	0/2569
57	x	0.54	0/5516	0.76	5/7460 (0.1%)
58	y	0.44	0/11	0.63	0/13
59	z	0.54	0/230	0.79	0/355
All	All	0.56	24/164377 (0.0%)	0.79	146/245116 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	20	U	C5-C6	16.80	1.49	1.34
55	v	20	U	C2-N3	16.49	1.49	1.37
55	v	20	U	N1-C2	11.55	1.49	1.38
55	v	1	C	OP3-P	-10.62	1.48	1.61
9	B	1	U	OP3-P	-10.60	1.48	1.61
8	A	1	G	OP3-P	-10.46	1.48	1.61
34	a	1081	A	O3'-P	10.26	1.73	1.61
55	v	20	U	N3-C4	8.38	1.46	1.38
55	v	20	U	N1-C6	8.31	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	921	U	C5'-C4'	8.27	1.61	1.51
34	a	921	U	P-O5'	8.17	1.68	1.59
55	v	20	U	C4-C5	7.03	1.49	1.43
34	a	1011	C	C5'-C4'	6.83	1.59	1.51
34	a	920	U	O3'-P	6.65	1.69	1.61
34	a	1081	A	C3'-O3'	6.51	1.51	1.42
55	v	20	U	C4-O4	-6.46	1.18	1.23
34	a	1011	C	P-O5'	6.24	1.66	1.59
31	X	28	PHE	C-N	-5.78	1.20	1.34
34	a	1081	A	N9-C4	5.56	1.41	1.37
56	w	34	G	O3'-P	-5.50	1.54	1.61
8	A	902	C	O3'-P	-5.40	1.54	1.61
25	R	57	GLY	CA-C	-5.34	1.43	1.51
8	A	887	A	C1'-N9	-5.32	1.39	1.46
34	a	1011	C	N1-C6	-5.08	1.34	1.37

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	903	C	P-O3'-C3'	33.07	159.38	119.70
34	a	1082	A	O5'-P-OP2	-17.77	89.37	110.70
34	a	921	U	C5-C6-N1	16.48	130.94	122.70
34	a	921	U	OP1-P-OP2	-16.44	94.94	119.60
34	a	1011	C	C6-N1-C2	-16.11	113.86	120.30
8	A	903	C	OP1-P-O3'	15.85	140.07	105.20
34	a	1011	C	C5-C6-N1	14.80	128.40	121.00
34	a	920	U	OP2-P-O3'	-14.76	72.73	105.20
34	a	1081	A	P-O3'-C3'	13.79	136.24	119.70
34	a	921	U	O5'-P-OP2	13.31	126.67	110.70
34	a	920	U	OP1-P-O3'	13.23	134.31	105.20
34	a	921	U	C6-N1-C2	-13.04	113.18	121.00
55	v	20	U	C2-N3-C4	-11.74	119.95	127.00
34	a	921	U	O4'-C1'-N1	10.50	116.60	108.20
55	v	20	U	C5-C4-O4	-9.81	120.01	125.90
34	a	920	U	P-O3'-C3'	9.55	131.16	119.70
34	a	1011	C	O5'-P-OP1	9.53	122.14	110.70
34	a	920	U	C6-N1-C2	-9.53	115.28	121.00
55	v	20	U	N3-C4-C5	8.87	119.92	114.60
34	a	1081	A	OP2-P-O3'	8.78	124.51	105.20
8	A	903	C	OP2-P-O3'	-8.62	86.23	105.20
34	a	1081	A	O3'-P-O5'	8.56	120.27	104.00
34	a	1011	C	O4'-C1'-N1	8.46	114.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	920	U	N3-C2-O2	-8.46	116.28	122.20
55	v	20	U	N1-C2-N3	8.38	119.93	114.90
34	a	624	C	C6-N1-C2	-8.28	116.99	120.30
34	a	840	C	N3-C2-O2	-8.20	116.16	121.90
34	a	921	U	N3-C4-O4	8.09	125.06	119.40
34	a	1081	A	C4-N9-C1'	8.01	140.72	126.30
34	a	1011	C	OP1-P-OP2	-7.98	107.63	119.60
34	a	920	U	C2-N1-C1'	7.83	127.10	117.70
34	a	920	U	C5-C6-N1	7.77	126.58	122.70
34	a	1098	C	N3-C2-O2	-7.67	116.53	121.90
34	a	1011	C	N1-C1'-C2'	-7.49	103.76	112.00
25	R	51	VAL	CB-CA-C	7.39	125.44	111.40
34	a	1088	G	C5-C6-O6	7.38	133.03	128.60
8	A	1313	U	C2-N1-C1'	7.21	126.36	117.70
57	x	576	ARG	NE-CZ-NH1	-7.18	116.71	120.30
34	a	624	C	N3-C2-O2	-7.05	116.97	121.90
34	a	1081	A	C8-N9-C4	-6.99	103.01	105.80
52	s	28	LYS	N-CA-C	-6.92	92.31	111.00
8	A	1081	U	O4'-C1'-N1	6.92	113.74	108.20
57	x	304	THR	N-CA-C	-6.91	92.33	111.00
34	a	840	C	N1-C2-O2	6.77	122.96	118.90
34	a	1081	A	C8-N9-C1'	-6.77	115.52	127.70
8	A	903	C	O3'-P-O5'	-6.67	91.32	104.00
34	a	921	U	C5-C4-O4	-6.52	121.98	125.90
34	a	1098	C	C6-N1-C2	-6.42	117.73	120.30
57	x	582	TYR	CB-CG-CD2	-6.41	117.16	121.00
34	a	1081	A	N7-C8-N9	6.39	117.00	113.80
57	x	544	ILE	N-CA-C	-6.38	93.78	111.00
34	a	960	U	C2-N1-C1'	6.36	125.33	117.70
34	a	1082	A	C8-N9-C4	-6.36	103.26	105.80
34	a	1010	U	C2'-C3'-O3'	6.34	123.84	113.70
34	a	921	U	C5'-C4'-O4'	6.33	116.70	109.10
47	n	35	ALA	N-CA-C	-6.26	94.11	111.00
34	a	1081	A	N9-C1'-C2'	6.25	122.12	114.00
34	a	1314	C	N3-C2-O2	-6.22	117.55	121.90
55	v	17	C	N1-C1'-C2'	6.21	122.08	114.00
8	A	2474	U	C2-N1-C1'	6.18	125.11	117.70
34	a	1082	A	O4'-C1'-N9	6.17	113.13	108.20
34	a	1011	C	C5'-C4'-O4'	6.16	116.50	109.10
34	a	1210	C	N1-C2-O2	6.12	122.57	118.90
51	r	44	THR	N-CA-C	-6.12	94.48	111.00
34	a	1081	A	N3-C4-C5	-6.11	122.52	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2391	G	O4'-C1'-N9	6.11	113.09	108.20
8	A	1313	U	N1-C2-O2	6.07	127.05	122.80
34	a	177	G	C4-N9-C1'	6.06	134.38	126.50
25	R	51	VAL	C-N-CD	6.06	141.12	128.40
34	a	624	C	C5-C4-N4	6.06	124.44	120.20
34	a	1098	C	N1-C2-N3	6.05	123.43	119.20
8	A	2474	U	N3-C2-O2	-6.04	117.97	122.20
34	a	1098	C	C6-N1-C1'	6.04	128.04	120.80
34	a	1011	C	N1-C2-O2	6.02	122.51	118.90
34	a	462	G	C6-C5-N7	-6.01	126.80	130.40
8	A	544	C	N1-C2-O2	6.00	122.50	118.90
34	a	960	U	N1-C2-O2	5.96	126.97	122.80
34	a	921	U	C5'-C4'-C3'	5.93	125.49	116.00
22	O	34	HIS	N-CA-C	5.93	127.01	111.00
10	C	238	ASN	N-CA-C	5.92	127.00	111.00
34	a	1134	G	N3-C4-N9	-5.88	122.47	126.00
8	A	2474	U	N1-C2-O2	5.87	126.91	122.80
34	a	920	U	O3'-P-O5'	5.87	115.15	104.00
34	a	1262	C	C2-N1-C1'	5.85	125.24	118.80
34	a	921	U	P-O5'-C5'	5.84	130.24	120.90
34	a	1197	A	O5'-P-OP2	-5.81	100.47	105.70
34	a	623	C	N1-C2-O2	5.80	122.38	118.90
34	a	1081	A	N3-C4-N9	5.80	132.04	127.40
34	a	1262	C	N1-C2-O2	5.73	122.34	118.90
8	A	1173	U	C2-N1-C1'	5.73	124.57	117.70
34	a	1314	C	N1-C2-O2	5.68	122.31	118.90
34	a	921	U	O5'-C5'-C4'	5.65	122.44	111.70
19	L	28	GLY	N-CA-C	5.64	127.20	113.10
34	a	1081	A	O4'-C1'-N9	5.60	112.68	108.20
22	O	31	THR	N-CA-C	-5.58	95.92	111.00
8	A	1081	U	C2-N1-C1'	5.57	124.39	117.70
34	a	1011	C	N3-C2-O2	-5.56	118.01	121.90
34	a	623	C	C2-N1-C1'	5.56	124.91	118.80
34	a	1081	A	C5'-C4'-C3'	5.54	124.87	116.00
7	6	56	ARG	CB-CA-C	5.50	121.39	110.40
8	A	2196	C	OP2-P-O3'	5.49	117.28	105.20
10	C	236	GLY	N-CA-C	-5.49	99.38	113.10
55	v	20	U	C5-C6-N1	-5.48	119.96	122.70
57	x	76	LYS	N-CA-C	-5.48	96.20	111.00
34	a	1132	C	N1-C2-O2	5.46	122.18	118.90
34	a	1088	G	N1-C6-O6	-5.43	116.64	119.90
34	a	1088	G	N3-C4-N9	-5.43	122.74	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	617	G	N3-C4-N9	-5.40	122.76	126.00
8	A	1313	U	N3-C2-O2	-5.40	118.42	122.20
34	a	1210	C	C2-N1-C1'	5.39	124.73	118.80
34	a	1082	A	OP1-P-OP2	-5.37	111.55	119.60
34	a	1011	C	C5'-C4'-C3'	5.36	124.58	116.00
34	a	1195	C	O5'-P-OP1	-5.31	100.92	105.70
34	a	1075	U	C2-N1-C1'	5.26	124.02	117.70
54	u	13	VAL	N-CA-C	-5.24	96.84	111.00
34	a	1158	C	N1-C2-O2	5.23	122.04	118.90
51	r	45	GLY	N-CA-C	-5.21	100.06	113.10
34	a	603	U	C2-N1-C1'	5.21	123.95	117.70
34	a	1134	G	N3-C2-N2	-5.20	116.26	119.90
8	A	1060	U	C2-N1-C1'	5.19	123.92	117.70
34	a	624	C	N1-C2-N3	5.17	122.82	119.20
51	r	20	ILE	N-CA-C	-5.17	97.04	111.00
8	A	1507	C	N3-C2-O2	-5.17	118.28	121.90
8	A	2287	A	P-O3'-C3'	5.16	125.90	119.70
55	v	25	C	N1-C2-O2	5.16	122.00	118.90
8	A	2076	U	C2-N1-C1'	5.16	123.89	117.70
34	a	617	G	C5-C6-O6	5.15	131.69	128.60
34	a	1011	C	N3-C4-C5	-5.15	119.84	121.90
8	A	458	G	P-O3'-C3'	5.14	125.87	119.70
34	a	1098	C	C5-C4-N4	5.13	123.79	120.20
34	a	158	G	C4'-C3'-C2'	-5.13	97.47	102.60
34	a	1081	A	C5'-C4'-O4'	-5.12	102.95	109.10
8	A	1451	C	C2-N1-C1'	-5.12	113.17	118.80
55	v	32	C	P-O3'-C3'	5.12	125.84	119.70
34	a	1088	G	N1-C2-N3	5.11	126.97	123.90
8	A	2391	G	C4-N9-C1'	-5.10	119.87	126.50
34	a	214	C	C2-N1-C1'	5.10	124.41	118.80
34	a	1011	C	C2-N3-C4	5.08	122.44	119.90
34	a	1081	A	C2-N3-C4	5.07	113.13	110.60
34	a	624	C	C6-N1-C1'	5.07	126.88	120.80
8	A	2243	U	N3-C2-O2	-5.06	118.66	122.20
8	A	1454	C	P-O3'-C3'	5.06	125.77	119.70
8	A	1314	C	C2-N1-C1'	5.04	124.35	118.80
8	A	2391	G	C8-N9-C1'	5.04	133.55	127.00
34	a	920	U	N1-C2-O2	5.01	126.31	122.80
34	a	481	G	C4-N9-C1'	5.01	133.01	126.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
4	3	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
5	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
6	5	129/165 (78%)	112 (87%)	17 (13%)	0	100	100
7	6	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
10	C	269/273 (98%)	249 (93%)	20 (7%)	0	100	100
11	D	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
12	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
13	F	175/179 (98%)	157 (90%)	18 (10%)	0	100	100
14	G	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
15	H	147/149 (99%)	125 (85%)	22 (15%)	0	100	100
16	I	139/142 (98%)	126 (91%)	12 (9%)	1 (1%)	19	51
17	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	K	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
19	L	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
20	M	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
21	N	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
22	O	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
23	P	112/115 (97%)	106 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
25	R	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	13	42
26	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
27	T	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
28	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
29	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	W	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
31	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
32	Y	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
33	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
35	b	216/240 (90%)	193 (89%)	23 (11%)	0	100	100
36	c	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
37	d	203/206 (98%)	188 (93%)	15 (7%)	0	100	100
38	e	155/167 (93%)	143 (92%)	12 (8%)	0	100	100
39	f	98/135 (73%)	91 (93%)	7 (7%)	0	100	100
40	g	149/179 (83%)	133 (89%)	16 (11%)	0	100	100
41	h	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
42	i	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
43	j	96/103 (93%)	80 (83%)	16 (17%)	0	100	100
44	k	114/129 (88%)	103 (90%)	11 (10%)	0	100	100
45	l	121/124 (98%)	105 (87%)	16 (13%)	0	100	100
46	m	112/118 (95%)	104 (93%)	8 (7%)	0	100	100
47	n	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
48	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
49	p	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
50	q	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
51	r	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
52	s	80/92 (87%)	75 (94%)	5 (6%)	0	100	100
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	55 (87%)	8 (13%)	0	100	100
57	x	694/704 (99%)	632 (91%)	61 (9%)	1 (0%)	48	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6544/6924 (94%)	6062 (93%)	479 (7%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	R	51	VAL
57	x	403	ILE
16	I	22	PRO

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%)	37 (97%)	1 (3%)	41	68
4	3	51/52 (98%)	50 (98%)	1 (2%)	50	74
5	4	34/34 (100%)	34 (100%)	0	100	100
7	6	59/62 (95%)	56 (95%)	3 (5%)	20	49
10	C	216/218 (99%)	214 (99%)	2 (1%)	75	88
11	D	164/164 (100%)	163 (99%)	1 (1%)	84	91
12	E	165/165 (100%)	162 (98%)	3 (2%)	54	76
13	F	148/150 (99%)	147 (99%)	1 (1%)	81	90
14	G	137/138 (99%)	136 (99%)	1 (1%)	81	90
15	H	114/114 (100%)	113 (99%)	1 (1%)	75	88
17	J	116/116 (100%)	116 (100%)	0	100	100
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	100 (98%)	2 (2%)	50	74
20	M	109/109 (100%)	107 (98%)	2 (2%)	54	76
21	N	100/103 (97%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	O	86/87 (99%)	85 (99%)	1 (1%)	67	83
23	P	99/100 (99%)	99 (100%)	0	100	100
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	82 (98%)	2 (2%)	44	70
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	77 (96%)	3 (4%)	28	59
28	U	83/85 (98%)	82 (99%)	1 (1%)	67	83
29	V	78/78 (100%)	77 (99%)	1 (1%)	65	82
30	W	57/63 (90%)	56 (98%)	1 (2%)	54	76
31	X	67/68 (98%)	67 (100%)	0	100	100
32	Y	55/55 (100%)	54 (98%)	1 (2%)	54	76
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	170 (94%)	10 (6%)	17	46
36	c	170/190 (90%)	169 (99%)	1 (1%)	84	91
37	d	172/173 (99%)	166 (96%)	6 (4%)	31	61
38	e	114/126 (90%)	111 (97%)	3 (3%)	41	68
39	f	87/116 (75%)	86 (99%)	1 (1%)	70	84
40	g	124/147 (84%)	123 (99%)	1 (1%)	79	89
41	h	104/105 (99%)	103 (99%)	1 (1%)	73	86
42	i	105/107 (98%)	100 (95%)	5 (5%)	21	51
43	j	86/90 (96%)	84 (98%)	2 (2%)	45	70
44	k	89/99 (90%)	88 (99%)	1 (1%)	70	84
45	l	103/104 (99%)	102 (99%)	1 (1%)	73	86
46	m	92/96 (96%)	90 (98%)	2 (2%)	47	71
47	n	79/84 (94%)	79 (100%)	0	100	100
48	o	76/77 (99%)	74 (97%)	2 (3%)	41	68
49	p	65/65 (100%)	61 (94%)	4 (6%)	15	43
50	q	74/78 (95%)	71 (96%)	3 (4%)	26	57
51	r	56/65 (86%)	51 (91%)	5 (9%)	8	29
52	s	72/79 (91%)	71 (99%)	1 (1%)	62	81
53	t	65/66 (98%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	u	46/61 (75%)	45 (98%)	1 (2%)	47 71
57	x	575/578 (100%)	519 (90%)	56 (10%)	6 25
58	y	1/1 (100%)	1 (100%)	0	100 100
All	All	5202/5408 (96%)	5068 (97%)	134 (3%)	42 68

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	41	ARG
4	3	32	LEU
7	6	20	ASN
7	6	50	ASP
7	6	64	PHE
10	C	239	PHE
10	C	259	ASN
11	D	32	ASN
12	E	65	THR
12	E	69	ARG
12	E	125	SER
13	F	59	ILE
14	G	68	ARG
15	H	138	VAL
19	L	115	GLU
19	L	117	THR
20	M	6	ARG
20	M	60	GLN
22	O	31	THR
25	R	49	ILE
25	R	51	VAL
27	T	26	LYS
27	T	37	ASP
27	T	93	LEU
28	U	73	ASN
29	V	34	LYS
30	W	10	ARG
32	Y	19	LEU
35	b	13	VAL
35	b	14	HIS
35	b	34	ARG
35	b	86	CYS
35	b	87	ASP

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Mol	Chain	Res	Type
35	b	91	VAL
35	b	108	GLN
35	b	183	PHE
35	b	191	ASP
35	b	193	ASP
36	c	106	ARG
37	d	28	ASP
37	d	34	GLU
37	d	35	GLN
37	d	46	ARG
37	d	71	PHE
37	d	144	ILE
38	e	53	ARG
38	e	92	ARG
38	e	158	LYS
39	f	58	HIS
40	g	67	ASN
41	h	17	GLN
42	i	11	ARG
42	i	104	THR
42	i	105	ARG
42	i	110	VAL
42	i	129	ARG
43	j	44	THR
43	j	92	LEU
44	k	118	ASN
45	l	3	VAL
46	m	24	VAL
46	m	106	ARG
48	o	16	ARG
48	o	19	ASN
49	p	8	ARG
49	p	9	HIS
49	p	12	LYS
49	p	45	GLU
50	q	16	MET
50	q	48	GLU
50	q	51	GLU
51	r	13	THR
51	r	17	VAL
51	r	20	ILE
51	r	44	THR

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Mol	Chain	Res	Type
51	r	46	THR
52	s	80	ARG
54	u	12	ASP
57	x	14	ILE
57	x	18	ILE
57	x	31	PHE
57	x	35	VAL
57	x	37	HIS
57	x	52	MET
57	x	53	GLU
57	x	54	GLN
57	x	56	GLN
57	x	60	ILE
57	x	61	THR
57	x	68	THR
57	x	77	GLN
57	x	78	TYR
57	x	84	ASN
57	x	176	GLU
57	x	190	ILE
57	x	196	ASP
57	x	197	GLN
57	x	201	PHE
57	x	209	ASP
57	x	212	GLU
57	x	218	HIS
57	x	221	LEU
57	x	227	GLU
57	x	231	GLU
57	x	295	ASN
57	x	297	ILE
57	x	298	LEU
57	x	317	SER
57	x	322	LYS
57	x	325	THR
57	x	328	PHE
57	x	329	VAL
57	x	365	MET
57	x	366	HIS
57	x	371	GLU
57	x	373	ILE
57	x	395	THR

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Mol	Chain	Res	Type
57	x	398	ASP
57	x	455	THR
57	x	511[A]	ARG
57	x	511[B]	ARG
57	x	539	ILE
57	x	540	LYS
57	x	544	ILE
57	x	584	ASP
57	x	587	SER
57	x	621	GLU
57	x	622	THR
57	x	627	THR
57	x	641	LEU
57	x	645	GLU
57	x	667	THR
57	x	701	ARG
57	x	703	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	441 (28%)	0
55	v	76/77 (98%)	24 (31%)	0
56	w	74/76 (97%)	21 (28%)	0
59	z	9/33 (27%)	2 (22%)	0
8	A	2898/2903 (99%)	572 (19%)	34 (1%)
9	B	119/120 (99%)	21 (17%)	3 (2%)
All	All	4712/4751 (99%)	1081 (22%)	37 (0%)

All (1081) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	34	U
8	A	35	G
8	A	46	G
8	A	50	U
8	A	62	U

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Mol	Chain	Res	Type
8	A	63	A
8	A	64	A
8	A	71	A
8	A	74	A
8	A	75	G
8	A	84	A
8	A	91	A
8	A	101	A
8	A	102	U
8	A	103	A
8	A	118	A
8	A	119	A
8	A	120	U
8	A	131	A
8	A	139	U
8	A	141	G
8	A	142	A
8	A	160	A
8	A	163	C
8	A	181	A
8	A	196	A
8	A	199	A
8	A	215	G
8	A	216	A
8	A	221	A
8	A	222	A
8	A	224	U
8	A	225	C
8	A	228	C
8	A	229	C
8	A	233	A
8	A	242	G
8	A	243	U
8	A	248	G
8	A	250	G
8	A	255	A
8	A	266	G
8	A	271	G
8	A	272	A
8	A	273	G
8	A	274	C
8	A	275	C

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Mol	Chain	Res	Type
8	A	276	U
8	A	277	G
8	A	278	A
8	A	284	U
8	A	287	G
8	A	288	U
8	A	291	G
8	A	294	A
8	A	311	A
8	A	330	A
8	A	331	C
8	A	345	A
8	A	346	A
8	A	355	U
8	A	369	U
8	A	371	A
8	A	372	G
8	A	373	U
8	A	377	G
8	A	383	C
8	A	386	G
8	A	395	U
8	A	396	G
8	A	401	A
8	A	403	U
8	A	404	A
8	A	405	U
8	A	406	G
8	A	411	G
8	A	424	G
8	A	434	U
8	A	435	C
8	A	452	G
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	475	C
8	A	480	A
8	A	481	G
8	A	482	A
8	A	489	G

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Mol	Chain	Res	Type
8	A	491	G
8	A	496	G
8	A	501	A
8	A	505	A
8	A	509	C
8	A	513	A
8	A	529	A
8	A	532	A
8	A	548	G
8	A	549	G
8	A	556	A
8	A	563	A
8	A	568	U
8	A	571	U
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	645	C
8	A	646	U
8	A	647	G
8	A	653	U
8	A	654	A
8	A	655	A
8	A	669	G
8	A	670	A
8	A	677	A
8	A	682	G
8	A	685	A
8	A	686	U
8	A	730	A
8	A	740	C
8	A	747	5MC
8	A	762	U
8	A	764	A
8	A	765	C
8	A	774	G

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Mol	Chain	Res	Type
8	A	775	G
8	A	776	G
8	A	782	A
8	A	784	G
8	A	785	G
8	A	791	C
8	A	792	A
8	A	805	G
8	A	812	C
8	A	819	A
8	A	827	U
8	A	828	U
8	A	831	G
8	A	845	A
8	A	846	U
8	A	856	G
8	A	859	G
8	A	866	A
8	A	869	G
8	A	875	G
8	A	876	C
8	A	878	A
8	A	879	G
8	A	881	G
8	A	882	G
8	A	884	U
8	A	887	A
8	A	888	C
8	A	889	C
8	A	890	C
8	A	894	U
8	A	896	A
8	A	897	C
8	A	901	C
8	A	907	G
8	A	910	A
8	A	914	G
8	A	927	A
8	A	931	U
8	A	938	G
8	A	941	A
8	A	945	A

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Mol	Chain	Res	Type
8	A	946	C
8	A	959	A
8	A	961	C
8	A	973	A
8	A	974	G
8	A	983	A
8	A	984	A
8	A	990	A
8	A	995	C
8	A	996	A
8	A	999	U
8	A	1005	C
8	A	1012	U
8	A	1013	C
8	A	1025	G
8	A	1026	G
8	A	1033	U
8	A	1040	A
8	A	1044	C
8	A	1045	C
8	A	1046	A
8	A	1047	G
8	A	1048	A
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	1064	C
8	A	1065	U
8	A	1066	U
8	A	1067	A
8	A	1068	G
8	A	1069	A
8	A	1070	A
8	A	1072	C
8	A	1073	A
8	A	1074	G
8	A	1075	C
8	A	1077	A

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Mol	Chain	Res	Type
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	1097	U
8	A	1099	G
8	A	1100	C
8	A	1101	U
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1106	G
8	A	1107	G
8	A	1111	A
8	A	1112	G
8	A	1115	G
8	A	1117	C
8	A	1120	G
8	A	1130	U
8	A	1132	U
8	A	1133	A
8	A	1135	C
8	A	1139	G
8	A	1172	C
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1177	G
8	A	1178	C
8	A	1179	G

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Mol	Chain	Res	Type
8	A	1180	U
8	A	1204	A
8	A	1227	G
8	A	1247	A
8	A	1253	A
8	A	1255	U
8	A	1256	G
8	A	1271	G
8	A	1272	A
8	A	1294	U
8	A	1300	G
8	A	1301	A
8	A	1332	G
8	A	1341	G
8	A	1345	C
8	A	1359	A
8	A	1365	A
8	A	1368	G
8	A	1378	A
8	A	1379	U
8	A	1380	G
8	A	1383	A
8	A	1395	A
8	A	1408	G
8	A	1415	U
8	A	1416	G
8	A	1419	A
8	A	1420	A
8	A	1427	A
8	A	1428	C
8	A	1433	A
8	A	1452	G
8	A	1454	C
8	A	1455	G
8	A	1458	U
8	A	1460	U
8	A	1461	C
8	A	1482	G
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1497	U

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Mol	Chain	Res	Type
8	A	1498	C
8	A	1515	A
8	A	1523	U
8	A	1529	G
8	A	1534	U
8	A	1535	A
8	A	1536	C
8	A	1558	C
8	A	1566	A
8	A	1569	A
8	A	1578	U
8	A	1583	A
8	A	1584	U
8	A	1585	C
8	A	1603	A
8	A	1608	A
8	A	1610	A
8	A	1634	A
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1654	A
8	A	1674	G
8	A	1675	C
8	A	1698	A
8	A	1715	G
8	A	1729	U
8	A	1730	C
8	A	1731	G
8	A	1732	C
8	A	1738	G
8	A	1744	A
8	A	1757	A
8	A	1764	C
8	A	1773	A
8	A	1784	A
8	A	1786	A
8	A	1787	A
8	A	1791	A
8	A	1800	C
8	A	1801	A
8	A	1807	G

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Mol	Chain	Res	Type
8	A	1808	A
8	A	1809	A
8	A	1811	G
8	A	1816	C
8	A	1829	A
8	A	1848	A
8	A	1857	G
8	A	1884	G
8	A	1896	G
8	A	1900	A
8	A	1901	A
8	A	1906	G
8	A	1912	A
8	A	1913	A
8	A	1914	C
8	A	1916	A
8	A	1927	A
8	A	1929	G
8	A	1930	G
8	A	1931	U
8	A	1937	A
8	A	1938	A
8	A	1939	5MU
8	A	1955	U
8	A	1960	A
8	A	1967	C
8	A	1970	A
8	A	1971	U
8	A	1972	G
8	A	1982	U
8	A	1991	U
8	A	1997	C
8	A	2020	A
8	A	2022	U
8	A	2023	C
8	A	2031	A
8	A	2032	G
8	A	2033	A
8	A	2036	C
8	A	2043	C
8	A	2049	G
8	A	2055	C

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Mol	Chain	Res	Type
8	A	2056	G
8	A	2059	A
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2069	G7M
8	A	2072	C
8	A	2093	G
8	A	2100	G
8	A	2104	C
8	A	2105	U
8	A	2107	G
8	A	2108	A
8	A	2109	U
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2113	U
8	A	2114	A
8	A	2115	G
8	A	2116	G
8	A	2118	U
8	A	2120	G
8	A	2121	G
8	A	2123	G
8	A	2125	G
8	A	2126	A
8	A	2129	C
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2136	G
8	A	2140	G
8	A	2141	G
8	A	2143	C
8	A	2144	G
8	A	2145	C
8	A	2146	C
8	A	2147	A
8	A	2149	U
8	A	2151	U

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Mol	Chain	Res	Type
8	A	2153	C
8	A	2155	U
8	A	2156	G
8	A	2157	G
8	A	2158	A
8	A	2159	G
8	A	2164	C
8	A	2165	C
8	A	2170	A
8	A	2171	A
8	A	2172	U
8	A	2173	A
8	A	2174	C
8	A	2176	A
8	A	2177	C
8	A	2179	C
8	A	2181	U
8	A	2184	A
8	A	2185	U
8	A	2186	G
8	A	2187	U
8	A	2188	U
8	A	2189	U
8	A	2193	G
8	A	2197	U
8	A	2198	A
8	A	2203	U
8	A	2204	G
8	A	2211	A
8	A	2225	A
8	A	2238	G
8	A	2239	G
8	A	2266	A
8	A	2273	A
8	A	2278	A
8	A	2279	G
8	A	2283	C
8	A	2287	A
8	A	2288	A
8	A	2297	A
8	A	2305	U
8	A	2309	A

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Mol	Chain	Res	Type
8	A	2310	C
8	A	2312	U
8	A	2319	G
8	A	2320	U
8	A	2322	A
8	A	2325	G
8	A	2333	A
8	A	2334	U
8	A	2336	A
8	A	2344	U
8	A	2345	G
8	A	2347	C
8	A	2350	C
8	A	2357	G
8	A	2361	G
8	A	2382	G
8	A	2383	G
8	A	2385	C
8	A	2402	U
8	A	2406	A
8	A	2407	A
8	A	2408	U
8	A	2410	G
8	A	2423	U
8	A	2425	A
8	A	2426	A
8	A	2429	G
8	A	2430	A
8	A	2432	A
8	A	2435	A
8	A	2441	U
8	A	2445	2MG
8	A	2447	G
8	A	2448	A
8	A	2475	C
8	A	2476	A
8	A	2478	A
8	A	2487	G
8	A	2494	G
8	A	2502	G
8	A	2504	PSU
8	A	2505	G

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Mol	Chain	Res	Type
8	A	2518	A
8	A	2520	C
8	A	2529	G
8	A	2535	G
8	A	2547	A
8	A	2554	U
8	A	2556	C
8	A	2566	A
8	A	2567	G
8	A	2573	C
8	A	2576	G
8	A	2584	U
8	A	2585	U
8	A	2602	A
8	A	2609	U
8	A	2613	U
8	A	2615	U
8	A	2619	C
8	A	2621	G
8	A	2629	U
8	A	2630	G
8	A	2638	G
8	A	2646	C
8	A	2654	A
8	A	2656	U
8	A	2660	A
8	A	2663	G
8	A	2689	U
8	A	2690	U
8	A	2702	G
8	A	2714	G
8	A	2718	G
8	A	2725	A
8	A	2726	A
8	A	2729	G
8	A	2732	G
8	A	2733	A
8	A	2739	U
8	A	2744	G
8	A	2748	A
8	A	2765	A
8	A	2778	A

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Mol	Chain	Res	Type
8	A	2779	U
8	A	2780	G
8	A	2791	G
8	A	2793	C
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2808	G
8	A	2818	U
8	A	2820	A
8	A	2821	A
8	A	2849	U
8	A	2867	G
8	A	2872	A
8	A	2873	A
8	A	2880	C
8	A	2884	U
8	A	2886	A
8	A	2891	U
8	A	2902	C
9	B	9	G
9	B	18	G
9	B	25	U
9	B	35	C
9	B	36	C
9	B	37	C
9	B	41	G
9	B	42	C
9	B	44	G
9	B	45	A
9	B	51	G
9	B	52	A
9	B	53	A
9	B	56	G
9	B	67	G
9	B	73	A
9	B	88	C
9	B	89	U
9	B	108	A
9	B	109	A
9	B	120	U
34	a	2	A

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Mol	Chain	Res	Type
34	a	5	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	16	A
34	a	22	G
34	a	31	G
34	a	32	A
34	a	37	U
34	a	39	G
34	a	46	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A
34	a	64	G
34	a	69	G
34	a	71	A
34	a	73	C
34	a	74	A
34	a	77	A
34	a	78	A
34	a	79	G
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	88	U
34	a	89	U
34	a	90	C
34	a	92	U
34	a	94	G
34	a	97	G
34	a	114	U
34	a	121	U
34	a	131	A
34	a	133	U
34	a	140	U
34	a	141	G
34	a	144	G

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Mol	Chain	Res	Type
34	a	145	G
34	a	146	G
34	a	148	G
34	a	152	A
34	a	158	G
34	a	160	A
34	a	163	C
34	a	164	G
34	a	166	U
34	a	169	C
34	a	170	U
34	a	171	A
34	a	173	U
34	a	174	A
34	a	179	A
34	a	180	U
34	a	182	A
34	a	183	C
34	a	186	C
34	a	188	C
34	a	189	A
34	a	197	A
34	a	198	G
34	a	201	G
34	a	202	G
34	a	204	G
34	a	205	A
34	a	206	C
34	a	207	C
34	a	208	U
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	213	G
34	a	214	C
34	a	216	U
34	a	219	U
34	a	221	C
34	a	224	U
34	a	226	G
34	a	240	G

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Mol	Chain	Res	Type
34	a	245	U
34	a	246	A
34	a	247	G
34	a	251	G
34	a	253	A
34	a	262	A
34	a	266	G
34	a	267	C
34	a	271	C
34	a	279	A
34	a	281	G
34	a	289	G
34	a	298	A
34	a	299	G
34	a	301	G
34	a	316	C
34	a	317	U
34	a	321	A
34	a	322	C
34	a	328	C
34	a	330	C
34	a	342	C
34	a	343	U
34	a	344	A
34	a	345	C
34	a	346	G
34	a	347	G
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	363	A
34	a	367	U
34	a	372	C
34	a	373	A
34	a	374	A
34	a	375	U
34	a	376	G
34	a	384	G
34	a	388	G
34	a	392	C
34	a	397	A

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Mol	Chain	Res	Type
34	a	405	U
34	a	406	G
34	a	411	A
34	a	414	A
34	a	415	A
34	a	421	U
34	a	422	C
34	a	423	G
34	a	428	G
34	a	429	U
34	a	430	A
34	a	435	A
34	a	436	C
34	a	439	U
34	a	442	G
34	a	443	C
34	a	447	G
34	a	448	A
34	a	454	G
34	a	457	G
34	a	458	U
34	a	460	A
34	a	462	G
34	a	463	U
34	a	464	U
34	a	467	U
34	a	468	A
34	a	469	C
34	a	470	C
34	a	471	U
34	a	472	U
34	a	473	U
34	a	476	U
34	a	477	C
34	a	479	U
34	a	482	A
34	a	484	G
34	a	492	C
34	a	495	A
34	a	496	A
34	a	497	G
34	a	505	G

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Mol	Chain	Res	Type
34	a	509	A
34	a	510	A
34	a	511	C
34	a	512	U
34	a	515	G
34	a	516	PSU
34	a	518	C
34	a	524	G
34	a	530	G
34	a	532	A
34	a	547	A
34	a	560	A
34	a	562	U
34	a	564	C
34	a	570	G
34	a	572	A
34	a	573	A
34	a	574	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	583	A
34	a	596	A
34	a	607	A
34	a	614	C
34	a	618	C
34	a	620	C
34	a	623	C
34	a	624	C
34	a	633	G
34	a	635	A
34	a	636	U
34	a	639	G
34	a	641	U
34	a	650	G
34	a	661	G
34	a	662	U
34	a	665	A
34	a	676	A
34	a	686	U
34	a	687	A
34	a	690	G

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Mol	Chain	Res	Type
34	a	693	G
34	a	695	A
34	a	700	G
34	a	702	A
34	a	703	G
34	a	710	G
34	a	721	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G
34	a	734	G
34	a	736	C
34	a	739	C
34	a	753	A
34	a	755	G
34	a	777	A
34	a	781	A
34	a	782	A
34	a	793	U
34	a	794	A
34	a	799	G
34	a	812	G
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	820	U
34	a	821	G
34	a	833	G
34	a	836	G
34	a	837	U
34	a	840	C
34	a	842	U
34	a	843	U
34	a	845	A
34	a	849	G
34	a	864	A
34	a	865	A
34	a	872	A
34	a	876	C
34	a	885	G

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Mol	Chain	Res	Type
34	a	890	G
34	a	891	U
34	a	902	G
34	a	914	A
34	a	920	U
34	a	921	U
34	a	926	G
34	a	927	G
34	a	934	C
34	a	935	A
34	a	945	G
34	a	946	A
34	a	958	A
34	a	960	U
34	a	961	U
34	a	964	A
34	a	965	U
34	a	966	2MG
34	a	967	5MC
34	a	969	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	979	C
34	a	980	C
34	a	982	U
34	a	984	C
34	a	989	U
34	a	992	U
34	a	993	G
34	a	994	A
34	a	995	C
34	a	996	A
34	a	997	U
34	a	1000	A
34	a	1002	G
34	a	1004	A
34	a	1008	U
34	a	1011	C
34	a	1012	A
34	a	1022	A
34	a	1023	U

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Mol	Chain	Res	Type
34	a	1026	G
34	a	1027	C
34	a	1028	C
34	a	1029	U
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1033	G
34	a	1034	G
34	a	1037	C
34	a	1041	G
34	a	1045	C
34	a	1049	U
34	a	1050	G
34	a	1064	G
34	a	1065	U
34	a	1075	U
34	a	1080	A
34	a	1081	A
34	a	1082	A
34	a	1083	U
34	a	1084	G
34	a	1085	U
34	a	1086	U
34	a	1094	G
34	a	1100	C
34	a	1101	A
34	a	1102	A
34	a	1105	A
34	a	1108	G
34	a	1120	C
34	a	1124	G
34	a	1126	U
34	a	1127	G
34	a	1130	A
34	a	1131	G
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1140	C

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Mol	Chain	Res	Type
34	a	1142	G
34	a	1143	G
34	a	1145	A
34	a	1146	A
34	a	1154	G
34	a	1159	U
34	a	1160	G
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1173	U
34	a	1176	A
34	a	1183	U
34	a	1184	G
34	a	1193	G
34	a	1196	A
34	a	1197	A
34	a	1200	C
34	a	1201	A
34	a	1202	U
34	a	1210	C
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1227	A
34	a	1228	C
34	a	1236	A
34	a	1239	A
34	a	1242	G
34	a	1249	C
34	a	1250	A
34	a	1257	A
34	a	1260	G
34	a	1261	A
34	a	1262	C
34	a	1263	C
34	a	1264	U
34	a	1267	C
34	a	1269	A
34	a	1270	G
34	a	1274	A
34	a	1275	A

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Mol	Chain	Res	Type
34	a	1280	A
34	a	1285	A
34	a	1287	A
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1303	C
34	a	1312	G
34	a	1317	C
34	a	1318	A
34	a	1319	A
34	a	1320	C
34	a	1322	C
34	a	1330	U
34	a	1331	G
34	a	1332	A
34	a	1333	A
34	a	1335	U
34	a	1336	C
34	a	1338	G
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1349	A
34	a	1353	G
34	a	1360	A
34	a	1366	C
34	a	1370	G
34	a	1378	C
34	a	1381	U
34	a	1394	A
34	a	1395	C
34	a	1397	C
34	a	1398	A
34	a	1400	C
34	a	1419	G
34	a	1422	G
34	a	1441	A
34	a	1444	U
34	a	1446	A
34	a	1447	A
34	a	1450	U

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Mol	Chain	Res	Type
34	a	1452	C
34	a	1453	G
34	a	1454	G
34	a	1456	A
34	a	1472	U
34	a	1492	A
34	a	1494	G
34	a	1497	G
34	a	1499	A
34	a	1503	A
34	a	1506	U
34	a	1517	G
34	a	1520	C
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1536	C
34	a	1538	C
34	a	1539	C
34	a	1540	U
55	v	8	4SU
55	v	9	G
55	v	17(A)	U
55	v	19	G
55	v	20	U
55	v	21	A
55	v	22	G
55	v	23	C
55	v	33	U
55	v	34	C
55	v	36	U
55	v	38	A
55	v	40	C
55	v	41	C
55	v	47	U
55	v	48	C
55	v	54	5MU
55	v	56	C
55	v	60	U
55	v	68	C
55	v	73	A
55	v	74	C

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Mol	Chain	Res	Type
55	v	75	C
55	v	76	A
56	w	4	C
56	w	6	G
56	w	8	4SU
56	w	13	C
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	27	G
56	w	28	G
56	w	36	A
56	w	45	U
56	w	46	G7M
56	w	47	U
56	w	49	C
56	w	60	U
56	w	69	G
56	w	73	A
56	w	76	A
59	z	4	U
59	z	9	U

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	102	U
8	A	141	G
8	A	242	G
8	A	310	A
8	A	344	A
8	A	479	A
8	A	555	G
8	A	733	G
8	A	784	G
8	A	1076	C
8	A	1078	U
8	A	1085	A
8	A	1090	A

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Mol	Chain	Res	Type
8	A	1091	G
8	A	1173	U
8	A	1178	C
8	A	1182	G
8	A	1200	C
8	A	1300	G
8	A	1358	G
8	A	1454	C
8	A	1490	A
8	A	1730	C
8	A	1847	G
8	A	1913	A
8	A	2192	U
8	A	2287	A
8	A	2308	G
8	A	2324	U
8	A	2405	G
8	A	2406	A
8	A	2728	U
8	A	2779	U
8	A	2820	A
9	B	44	G
9	B	52	A
9	B	66	A

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

45 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	PSU	A	2580	8,60	18,21,22	1.11	3 (16%)	22,30,33	1.89	6 (27%)
8	OMU	A	2552	8,60	19,22,23	2.94	8 (42%)	26,31,34	1.78	5 (19%)
34	PSU	a	516	34	18,21,22	0.99	1 (5%)	22,30,33	1.79	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	6MZ	A	2030	8	18,25,26	2.16	3 (16%)	16,36,39	2.26	3 (18%)
34	UR3	a	1498	34,60	19,22,23	2.69	6 (31%)	26,32,35	1.57	4 (15%)
8	2MG	A	2445	8	18,26,27	1.14	1 (5%)	16,38,41	1.48	4 (25%)
34	2MG	a	1516	34	18,26,27	2.64	7 (38%)	16,38,41	1.47	4 (25%)
8	3TD	A	1915	8	18,22,23	7.37	11 (61%)	22,32,35	1.72	3 (13%)
8	5MC	A	747	8	18,22,23	3.62	7 (38%)	26,32,35	1.14	1 (3%)
8	PSU	A	2604	8	18,21,22	1.06	1 (5%)	22,30,33	1.72	2 (9%)
34	G7M	a	527	34	20,26,27	2.44	7 (35%)	17,39,42	1.16	1 (5%)
56	4SU	w	8	56	18,21,22	3.62	7 (38%)	26,30,33	2.22	4 (15%)
34	2MG	a	1207	34	18,26,27	2.62	7 (38%)	16,38,41	1.36	3 (18%)
55	4SU	v	8	55	18,21,22	3.61	7 (38%)	26,30,33	2.32	5 (19%)
56	G7M	w	46	56	20,26,27	2.49	7 (35%)	17,39,42	1.16	1 (5%)
8	PSU	A	2605	8	18,21,22	1.02	1 (5%)	22,30,33	1.78	2 (9%)
8	PSU	A	1917	8	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
55	5MU	v	54	55	19,22,23	4.85	7 (36%)	28,32,35	3.60	9 (32%)
8	PSU	A	2457	8	18,21,22	0.98	2 (11%)	22,30,33	1.88	6 (27%)
8	2MG	A	1835	8	18,26,27	2.57	7 (38%)	16,38,41	1.46	4 (25%)
8	G7M	A	2069	8	20,26,27	2.35	7 (35%)	17,39,42	1.06	1 (5%)
34	4OC	a	1402	34	20,23,24	3.00	8 (40%)	26,32,35	0.82	1 (3%)
8	1MG	A	745	8	18,26,27	2.66	4 (22%)	19,39,42	1.50	4 (21%)
56	MIA	w	37	56	24,31,32	2.58	4 (16%)	26,44,47	3.68	9 (34%)
8	OMC	A	2498	8,60	19,22,23	2.92	7 (36%)	26,31,34	0.83	0
58	FME	y	101	58	8,9,10	0.96	0	7,9,11	1.17	1 (14%)
8	PSU	A	746	8,60	18,21,22	1.09	2 (11%)	22,30,33	1.81	5 (22%)
8	5MU	A	1939	8	19,22,23	4.68	7 (36%)	28,32,35	3.76	9 (32%)
8	OMG	A	2251	8,56,60	18,26,27	2.46	8 (44%)	19,38,41	1.55	4 (21%)
8	PSU	A	1911	8	18,21,22	1.39	3 (16%)	22,30,33	2.01	4 (18%)
8	PSU	A	2504	8	18,21,22	1.14	2 (11%)	22,30,33	1.84	4 (18%)
8	2MA	A	2503	8,60	19,25,26	3.25	6 (31%)	21,37,40	1.77	4 (19%)
56	PSU	w	55	56	18,21,22	1.43	2 (11%)	22,30,33	1.98	3 (13%)
34	2MG	a	966	34	18,26,27	1.19	1 (5%)	16,38,41	1.35	3 (18%)
56	PSU	w	39	56	18,21,22	1.04	1 (5%)	22,30,33	1.72	4 (18%)
8	5MC	A	1962	8	18,22,23	3.65	7 (38%)	26,32,35	0.97	1 (3%)
34	5MC	a	967	34	18,22,23	3.73	7 (38%)	26,32,35	1.03	2 (7%)
56	5MU	w	54	56	19,22,23	1.40	4 (21%)	28,32,35	1.94	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	v	55	55	18,21,22	1.36	3 (16%)	22,30,33	1.96	4 (18%)
34	MA6	a	1518	34	18,26,27	1.02	1 (5%)	19,38,41	2.64	2 (10%)
8	6MZ	A	1618	8	18,25,26	2.13	3 (16%)	16,36,39	2.11	3 (18%)
8	PSU	A	955	8	18,21,22	1.07	2 (11%)	22,30,33	1.75	4 (18%)
34	5MC	a	1407	34	18,22,23	1.03	2 (11%)	26,32,35	1.57	7 (26%)
56	PSU	w	32	56	18,21,22	1.03	1 (5%)	22,30,33	1.71	4 (18%)
34	MA6	a	1519	34	18,26,27	0.98	1 (5%)	19,38,41	2.79	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PSU	A	2580	8,60	-	0/7/25/26	0/2/2/2
8	OMU	A	2552	8,60	-	2/9/27/28	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
34	UR3	a	1498	34,60	-	4/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	3TD	A	1915	8	-	3/7/25/26	0/2/2/2
8	5MC	A	747	8	-	1/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
34	G7M	a	527	34	-	0/3/25/26	0/3/3/3
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
56	G7M	w	46	56	-	2/3/25/26	0/3/3/3
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
34	4OC	a	1402	34	-	0/9/29/30	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
8	OMC	A	2498	8,60	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	FME	y	101	58	-	5/7/9/11	-
8	PSU	A	746	8,60	-	2/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	2/7/25/26	0/2/2/2
8	OMG	A	2251	8,56,60	-	1/5/27/28	0/3/3/3
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
8	2MA	A	2503	8,60	-	2/3/25/26	0/3/3/3
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	2/5/27/28	0/3/3/3
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	2/7/25/26	0/2/2/2
34	5MC	a	967	34	-	2/7/25/26	0/2/2/2
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	1/7/29/30	0/3/3/3
8	6MZ	A	1618	8	-	0/5/27/28	0/3/3/3
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	1/7/29/30	0/3/3/3

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	O4'-C1'	18.04	1.68	1.43
8	A	1915	3TD	C2'-C1'	-15.17	1.34	1.53
8	A	1915	3TD	C6-C5	13.53	1.51	1.35
55	v	54	5MU	C2-N1	11.31	1.56	1.38
55	v	54	5MU	C6-N1	10.57	1.56	1.38
8	A	1939	5MU	C6-N1	10.26	1.55	1.38
8	A	1939	5MU	C2-N1	10.03	1.54	1.38
55	v	54	5MU	C4-C5	9.95	1.61	1.44
8	A	1915	3TD	C2-N1	9.60	1.49	1.37
8	A	1939	5MU	C4-C5	9.58	1.60	1.44
34	a	967	5MC	C6-C5	9.37	1.50	1.34
8	A	747	5MC	C6-C5	9.07	1.49	1.34
8	A	1962	5MC	C6-C5	9.05	1.49	1.34
56	w	37	MIA	C2-S10	-8.93	1.68	1.75
8	A	2503	2MA	C4-N3	8.61	1.49	1.35
56	w	8	4SU	C4-N3	8.21	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1939	5MU	C4-N3	-8.17	1.23	1.38
55	v	8	4SU	C4-N3	8.13	1.46	1.37
55	v	54	5MU	C4-N3	-7.74	1.24	1.38
55	v	8	4SU	C2-N1	7.59	1.50	1.38
8	A	2030	6MZ	C6-N6	7.54	1.47	1.35
8	A	1618	6MZ	C6-N6	7.52	1.47	1.35
56	w	8	4SU	C2-N1	7.32	1.50	1.38
8	A	745	1MG	C2-N2	7.28	1.47	1.34
34	a	967	5MC	C4-N3	6.99	1.45	1.34
34	a	1498	UR3	C2-N1	6.96	1.48	1.38
8	A	2503	2MA	C2-N3	6.92	1.46	1.34
8	A	1962	5MC	C4-N3	6.87	1.45	1.34
8	A	2552	OMU	C2-N1	6.82	1.49	1.38
34	a	1402	4OC	C4-N3	6.81	1.44	1.32
8	A	747	5MC	C4-N3	6.79	1.45	1.34
56	w	37	MIA	C13-C14	6.56	1.51	1.32
8	A	2552	OMU	C2-N3	6.52	1.49	1.38
8	A	1962	5MC	C2-N3	6.32	1.49	1.36
34	a	967	5MC	C2-N3	6.26	1.49	1.36
34	a	1207	2MG	C2-N2	6.23	1.47	1.33
8	A	1915	3TD	O4'-C4'	-6.21	1.31	1.45
8	A	2498	OMC	C6-C5	6.21	1.49	1.35
8	A	747	5MC	C2-N3	6.19	1.48	1.36
8	A	2498	OMC	C2-N3	6.18	1.48	1.36
34	a	1516	2MG	C2-N2	6.16	1.47	1.33
8	A	1835	2MG	C2-N2	6.13	1.47	1.33
34	a	1498	UR3	C6-C5	5.98	1.49	1.35
8	A	1915	3TD	C6-N1	5.95	1.46	1.36
34	a	1402	4OC	C6-C5	5.90	1.48	1.35
56	w	8	4SU	C6-C5	5.87	1.48	1.35
55	v	54	5MU	C6-C5	5.85	1.44	1.34
34	a	1402	4OC	C2-N3	5.83	1.48	1.36
56	w	46	G7M	C2-N3	5.81	1.47	1.33
8	A	1939	5MU	C6-C5	5.80	1.44	1.34
56	w	8	4SU	C2-N3	5.76	1.48	1.38
55	v	8	4SU	C6-C5	5.74	1.48	1.35
8	A	2498	OMC	C4-N3	5.68	1.45	1.34
34	a	527	G7M	C2-N3	5.66	1.46	1.33
55	v	8	4SU	C2-N3	5.58	1.47	1.38
8	A	2503	2MA	C2-N1	5.51	1.43	1.34
8	A	2552	OMU	C6-C5	5.51	1.47	1.35
8	A	745	1MG	C2-N3	5.47	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2069	G7M	C2-N3	5.30	1.46	1.33
34	a	1207	2MG	C4-N3	5.11	1.49	1.37
56	w	8	4SU	C4-S4	-5.09	1.58	1.68
8	A	2251	OMG	C2-N3	5.05	1.45	1.33
55	v	8	4SU	C4-S4	-5.04	1.58	1.68
8	A	2503	2MA	C6-N1	5.02	1.42	1.33
8	A	1915	3TD	C2-N3	5.01	1.49	1.38
34	a	527	G7M	C4-N3	4.96	1.49	1.37
8	A	1835	2MG	C4-N3	4.92	1.49	1.37
56	w	46	G7M	C4-N3	4.90	1.49	1.37
34	a	1498	UR3	C2-N3	4.88	1.48	1.39
34	a	967	5MC	C4-N4	4.86	1.46	1.34
34	a	1516	2MG	C4-N3	4.84	1.49	1.37
8	A	745	1MG	C4-N3	4.82	1.49	1.37
8	A	2069	G7M	C4-N3	4.81	1.49	1.37
8	A	2251	OMG	C4-N3	4.74	1.48	1.37
8	A	1962	5MC	C4-N4	4.72	1.46	1.34
8	A	1915	3TD	O3'-C3'	-4.71	1.31	1.43
8	A	747	5MC	C4-N4	4.67	1.46	1.34
34	a	1516	2MG	C2-N1	4.60	1.44	1.36
8	A	2251	OMG	C2-N2	4.53	1.45	1.34
34	a	967	5MC	C6-N1	4.53	1.45	1.38
8	A	1962	5MC	C6-N1	4.45	1.45	1.38
34	a	527	G7M	C2-N2	4.40	1.44	1.34
34	a	1207	2MG	C2-N1	4.39	1.43	1.36
8	A	1835	2MG	C2-N1	4.37	1.43	1.36
8	A	747	5MC	C6-N1	4.29	1.45	1.38
8	A	2069	G7M	C2-N2	4.27	1.44	1.34
56	w	46	G7M	C2-N2	4.25	1.44	1.34
34	a	1402	4OC	C4-N4	4.18	1.44	1.35
34	a	967	5MC	C2-N1	4.12	1.48	1.40
8	A	1962	5MC	C2-N1	3.99	1.48	1.40
8	A	747	5MC	C2-N1	3.97	1.48	1.40
8	A	2498	OMC	C4-N4	3.93	1.43	1.33
56	w	46	G7M	C6-N1	3.92	1.43	1.37
8	A	2552	OMU	C4-N3	3.80	1.45	1.38
56	w	37	MIA	C2'-C1'	-3.80	1.48	1.53
34	a	1402	4OC	C5-C4	3.75	1.48	1.40
34	a	1402	4OC	C2-N1	3.72	1.48	1.40
8	A	2069	G7M	C6-N1	3.56	1.43	1.37
8	A	2498	OMC	C6-N1	3.55	1.46	1.38
8	A	2498	OMC	C2-N1	3.55	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1516	2MG	C6-N1	3.53	1.43	1.37
56	w	46	G7M	C5-C6	3.51	1.54	1.45
34	a	527	G7M	C6-N1	3.50	1.43	1.37
34	a	527	G7M	C5-C6	3.35	1.54	1.45
8	A	2504	PSU	C6-C5	3.34	1.39	1.35
56	w	39	PSU	C6-C5	3.33	1.39	1.35
8	A	2251	OMG	C6-N1	3.29	1.42	1.37
34	a	1207	2MG	C6-N1	3.28	1.42	1.37
56	w	55	PSU	C6-C5	3.27	1.39	1.35
8	A	747	5MC	O2-C2	-3.26	1.17	1.23
8	A	2030	6MZ	C5-C4	-3.24	1.32	1.40
8	A	1835	2MG	C6-N1	3.22	1.42	1.37
34	a	967	5MC	O2-C2	-3.22	1.17	1.23
55	v	8	4SU	C5-C4	3.21	1.46	1.42
56	w	32	PSU	C6-C5	3.20	1.39	1.35
8	A	1917	PSU	C6-C5	3.17	1.39	1.35
56	w	8	4SU	C5-C4	3.15	1.46	1.42
34	a	1516	2MG	C5-C4	-3.10	1.35	1.43
8	A	1962	5MC	O2-C2	-3.10	1.18	1.23
8	A	2069	G7M	C5-C6	3.08	1.53	1.45
8	A	1835	2MG	C5-C4	-3.05	1.35	1.43
34	a	1207	2MG	C5-C6	3.04	1.53	1.47
8	A	2552	OMU	O4-C4	-3.03	1.18	1.24
8	A	1618	6MZ	C5-C4	-3.03	1.32	1.40
56	w	55	PSU	C4-N3	-3.01	1.33	1.38
34	a	1402	4OC	C6-N1	3.01	1.45	1.38
8	A	1911	PSU	C6-C5	3.00	1.38	1.35
8	A	1915	3TD	C4-N3	2.99	1.46	1.40
34	a	966	2MG	C6-N1	-2.99	1.33	1.37
34	a	1516	2MG	O6-C6	-2.98	1.17	1.23
8	A	2445	2MG	C6-N1	-2.98	1.33	1.37
34	a	1207	2MG	O6-C6	-2.98	1.17	1.23
8	A	1835	2MG	O6-C6	-2.98	1.17	1.23
34	a	1516	2MG	C5-C6	2.98	1.53	1.47
8	A	2498	OMC	O2-C2	-2.98	1.18	1.23
8	A	745	1MG	C5-C4	-2.98	1.35	1.43
55	v	55	PSU	C4-N3	-2.97	1.33	1.38
34	a	516	PSU	C6-C5	2.96	1.38	1.35
56	w	54	5MU	C4-N3	-2.89	1.33	1.38
8	A	1911	PSU	C4-N3	-2.87	1.33	1.38
34	a	1498	UR3	C6-N1	2.86	1.44	1.38
8	A	2251	OMG	C5-C4	-2.85	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1939	5MU	O2-C2	-2.84	1.17	1.23
8	A	746	PSU	C6-C5	2.83	1.38	1.35
8	A	2604	PSU	C6-C5	2.83	1.38	1.35
34	a	1207	2MG	C5-C4	-2.82	1.35	1.43
8	A	1939	5MU	O4-C4	-2.81	1.18	1.23
34	a	1402	4OC	O2-C2	-2.80	1.18	1.23
8	A	2605	PSU	C6-C5	2.77	1.38	1.35
8	A	955	PSU	C6-C5	2.76	1.38	1.35
8	A	2251	OMG	C5-C6	2.76	1.53	1.47
56	w	46	G7M	C2-N1	2.75	1.44	1.37
8	A	2580	PSU	C6-C5	2.74	1.38	1.35
8	A	1835	2MG	C5-C6	2.72	1.52	1.47
56	w	37	MIA	O4'-C4'	-2.66	1.39	1.45
8	A	2503	2MA	C6-C5	2.61	1.53	1.43
34	a	1407	5MC	C6-C5	2.61	1.38	1.34
55	v	54	5MU	O4-C4	-2.60	1.18	1.23
8	A	2552	OMU	O2-C2	-2.60	1.18	1.23
8	A	2552	OMU	C6-N1	2.59	1.44	1.38
8	A	2580	PSU	O4'-C1'	-2.59	1.40	1.43
34	a	1518	MA6	C5-C4	-2.58	1.34	1.40
34	a	1519	MA6	C5-C4	-2.56	1.34	1.40
8	A	2069	G7M	C2-N1	2.56	1.44	1.37
8	A	1618	6MZ	C2-N3	2.50	1.36	1.32
34	a	1498	UR3	O2-C2	-2.49	1.18	1.22
34	a	527	G7M	C2-N1	2.48	1.43	1.37
56	w	54	5MU	C6-C5	2.47	1.38	1.34
56	w	8	4SU	O2-C2	-2.45	1.18	1.23
55	v	8	4SU	O2-C2	-2.42	1.18	1.23
55	v	55	PSU	C6-C5	2.42	1.38	1.35
8	A	1915	3TD	C3'-C4'	2.41	1.59	1.53
8	A	2251	OMG	C2-N1	2.38	1.43	1.37
8	A	2503	2MA	C6-N6	-2.38	1.25	1.34
56	w	54	5MU	C2-N3	-2.33	1.33	1.38
34	a	527	G7M	O6-C6	-2.33	1.18	1.23
56	w	54	5MU	C6-N1	-2.31	1.34	1.38
34	a	1407	5MC	C6-N1	-2.31	1.34	1.38
34	a	1498	UR3	O4-C4	-2.31	1.18	1.23
56	w	46	G7M	O6-C6	-2.28	1.18	1.23
8	A	2030	6MZ	C2-N3	2.27	1.35	1.32
55	v	54	5MU	O2-C2	-2.26	1.18	1.23
8	A	2069	G7M	O6-C6	-2.24	1.18	1.23
8	A	2251	OMG	O6-C6	-2.24	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	746	PSU	C4-C5	-2.23	1.37	1.44
8	A	2457	PSU	C6-C5	2.21	1.37	1.35
55	v	55	PSU	C2-N3	-2.21	1.33	1.37
8	A	955	PSU	C4-C5	-2.20	1.37	1.44
8	A	2552	OMU	C5-C4	2.14	1.48	1.43
8	A	1911	PSU	C2-N3	-2.10	1.33	1.37
8	A	2457	PSU	O4'-C1'	-2.09	1.40	1.43
8	A	2580	PSU	C4-C5	-2.07	1.38	1.44
8	A	2504	PSU	C4-C5	-2.05	1.38	1.44
8	A	1915	3TD	O5'-C5'	-2.05	1.39	1.44

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	37	MIA	C11-S10-C2	-12.51	92.92	102.27
8	A	1939	5MU	C5-C4-N3	12.43	125.92	115.31
55	v	54	5MU	C5-C4-N3	12.19	125.72	115.31
8	A	1939	5MU	C5-C6-N1	-10.67	112.36	123.34
34	a	1519	MA6	N1-C6-N6	-10.39	106.12	117.06
55	v	54	5MU	C5-C6-N1	-9.94	113.12	123.34
34	a	1518	MA6	N1-C6-N6	-9.78	106.76	117.06
56	w	37	MIA	C12-C13-C14	-9.61	108.45	127.14
55	v	8	4SU	C4-N3-C2	-8.10	119.47	127.34
56	w	8	4SU	C4-N3-C2	-7.58	119.98	127.34
8	A	1911	PSU	N1-C2-N3	6.08	122.02	115.13
56	w	55	PSU	N1-C2-N3	6.08	122.02	115.13
34	a	1519	MA6	N3-C2-N1	-5.78	119.64	128.68
55	v	8	4SU	C5-C4-N3	5.65	119.93	114.69
8	A	2030	6MZ	N3-C2-N1	-5.59	119.94	128.68
34	a	1518	MA6	N3-C2-N1	-5.56	119.99	128.68
56	w	8	4SU	C5-C4-N3	5.53	119.82	114.69
8	A	2503	2MA	C2-N3-C4	5.52	120.00	115.52
8	A	1618	6MZ	C9-N6-C6	-5.47	118.16	122.87
55	v	55	PSU	N1-C2-N3	5.46	121.32	115.13
8	A	1618	6MZ	N3-C2-N1	-5.27	120.44	128.68
8	A	2552	OMU	C4-N3-C2	-5.27	119.63	126.58
8	A	1939	5MU	C4-N3-C2	-5.24	120.57	127.35
8	A	1939	5MU	O4-C4-C5	-5.23	118.84	124.90
55	v	54	5MU	O4-C4-C5	-5.21	118.87	124.90
8	A	2605	PSU	C4-N3-C2	-4.96	119.19	126.34
8	A	2030	6MZ	C9-N6-C6	-4.95	118.61	122.87
8	A	2504	PSU	N1-C2-N3	4.91	120.70	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	746	PSU	C4-N3-C2	-4.75	119.49	126.34
8	A	2457	PSU	N1-C2-N3	4.74	120.50	115.13
8	A	1939	5MU	N3-C2-N1	4.71	121.15	114.89
8	A	1915	3TD	C4-N3-C2	-4.69	119.52	124.61
8	A	2457	PSU	C4-N3-C2	-4.67	119.61	126.34
55	v	54	5MU	C4-N3-C2	-4.63	121.35	127.35
34	a	516	PSU	N1-C2-N3	4.63	120.38	115.13
8	A	2604	PSU	C4-N3-C2	-4.61	119.70	126.34
56	w	32	PSU	C4-N3-C2	-4.54	119.80	126.34
8	A	2030	6MZ	C1'-N9-C4	-4.52	118.71	126.64
8	A	2580	PSU	N1-C2-N3	4.48	120.21	115.13
8	A	1917	PSU	N1-C2-N3	4.47	120.19	115.13
8	A	2580	PSU	C4-N3-C2	-4.46	119.91	126.34
56	w	39	PSU	N1-C2-N3	4.45	120.17	115.13
56	w	54	5MU	N3-C2-N1	4.45	120.79	114.89
8	A	955	PSU	C4-N3-C2	-4.42	119.97	126.34
56	w	54	5MU	C4-N3-C2	-4.42	121.64	127.35
56	w	37	MIA	C2-N3-C4	4.40	121.39	115.32
8	A	746	PSU	N1-C2-N3	4.40	120.11	115.13
34	a	516	PSU	C4-N3-C2	-4.40	120.00	126.34
56	w	32	PSU	N1-C2-N3	4.39	120.11	115.13
56	w	39	PSU	C4-N3-C2	-4.35	120.07	126.34
56	w	37	MIA	C15-C14-C13	-4.33	110.14	122.65
8	A	2605	PSU	N1-C2-N3	4.32	120.02	115.13
8	A	1911	PSU	C4-N3-C2	-4.29	120.16	126.34
8	A	2504	PSU	C4-N3-C2	-4.28	120.17	126.34
8	A	955	PSU	N1-C2-N3	4.25	119.95	115.13
8	A	1917	PSU	C4-N3-C2	-4.23	120.24	126.34
8	A	745	1MG	C5-C6-N1	4.22	120.24	113.90
8	A	2604	PSU	N1-C2-N3	4.21	119.90	115.13
55	v	55	PSU	C4-N3-C2	-4.19	120.30	126.34
56	w	54	5MU	C5-C4-N3	4.12	118.83	115.31
56	w	37	MIA	C16-C14-C13	-4.12	110.75	122.65
8	A	1915	3TD	N1-C2-N3	4.10	119.37	116.14
55	v	54	5MU	N3-C2-N1	4.09	120.32	114.89
34	a	1498	UR3	C4-N3-C2	-4.08	120.72	124.56
56	w	55	PSU	C4-N3-C2	-4.04	120.52	126.34
34	a	1498	UR3	C6-N1-C2	-4.03	118.18	121.79
8	A	747	5MC	C5-C6-N1	-4.00	119.23	123.34
8	A	2552	OMU	N3-C2-N1	3.90	120.07	114.89
56	w	8	4SU	C5-C4-S4	-3.84	119.52	124.47
56	w	54	5MU	O4-C4-C5	-3.82	120.47	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	8	4SU	C5-C4-S4	-3.78	119.59	124.47
34	a	1498	UR3	C1'-N1-C2	3.77	123.36	116.99
55	v	54	5MU	C5M-C5-C6	-3.74	117.85	122.85
55	v	8	4SU	N3-C2-N1	3.74	119.86	114.89
55	v	54	5MU	C5M-C5-C4	3.65	122.78	118.77
34	a	967	5MC	C5-C6-N1	-3.62	119.62	123.34
8	A	1939	5MU	C5M-C5-C6	-3.58	118.06	122.85
56	w	8	4SU	N3-C2-N1	3.58	119.64	114.89
8	A	2251	OMG	C5-C6-N1	3.56	120.23	113.95
34	a	1207	2MG	C5-C6-N1	3.49	120.11	113.95
8	A	1835	2MG	C5-C6-N1	3.48	120.09	113.95
34	a	1516	2MG	C5-C6-N1	3.47	120.07	113.95
56	w	55	PSU	O2-C2-N1	-3.45	118.99	122.79
8	A	2552	OMU	C5-C4-N3	3.39	119.91	114.84
8	A	1939	5MU	O2-C2-N1	-3.36	118.31	122.79
8	A	2503	2MA	N3-C2-N1	-3.35	119.62	125.73
8	A	1911	PSU	O2-C2-N1	-3.30	119.16	122.79
56	w	46	G7M	C2-N1-C6	-3.29	119.04	125.10
8	A	1939	5MU	C5M-C5-C4	3.25	122.34	118.77
34	a	527	G7M	C2-N1-C6	-3.25	119.12	125.10
8	A	2504	PSU	C6-N1-C2	-3.22	119.39	122.68
8	A	2445	2MG	CM2-N2-C2	-3.18	116.84	123.86
8	A	2457	PSU	O2-C2-N1	-3.17	119.30	122.79
8	A	1962	5MC	C5-C6-N1	-3.13	120.12	123.34
34	a	516	PSU	O2-C2-N1	-3.12	119.36	122.79
56	w	37	MIA	C4-C5-N7	-3.05	106.22	109.40
56	w	54	5MU	C5-C6-N1	-3.02	120.23	123.34
8	A	2552	OMU	O4-C4-C5	-2.98	119.92	125.16
34	a	1407	5MC	C5-C6-N1	-2.96	120.29	123.34
8	A	1618	6MZ	C1'-N9-C4	-2.96	121.45	126.64
55	v	55	PSU	O2-C2-N1	-2.96	119.54	122.79
8	A	2251	OMG	C2-N1-C6	-2.95	119.66	125.10
8	A	746	PSU	C6-C5-C4	2.92	120.24	118.20
8	A	2069	G7M	C2-N1-C6	-2.80	119.94	125.10
34	a	1407	5MC	C5-C4-N3	-2.77	118.68	121.67
34	a	516	PSU	C6-N1-C2	-2.77	119.85	122.68
8	A	745	1MG	C8-N7-C5	2.76	108.26	102.99
8	A	2580	PSU	O4'-C1'-C2'	2.76	109.03	105.14
8	A	1915	3TD	O4'-C4'-C3'	-2.70	99.77	105.11
8	A	1835	2MG	CM2-N2-C2	-2.69	117.92	123.86
8	A	2552	OMU	C1'-N1-C2	2.69	122.44	117.57
8	A	1917	PSU	C6-N1-C2	-2.68	119.94	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	966	2MG	C3'-C2'-C1'	2.68	105.02	100.98
8	A	2251	OMG	C8-N7-C5	2.68	108.10	102.99
8	A	2503	2MA	C1'-N9-C4	-2.65	121.98	126.64
34	a	1516	2MG	CM2-N2-C2	-2.65	118.01	123.86
8	A	2580	PSU	C6-N1-C2	-2.63	119.99	122.68
34	a	1407	5MC	O3'-C3'-C4'	2.62	118.62	111.05
8	A	955	PSU	O2-C2-N1	-2.61	119.92	122.79
34	a	1407	5MC	O4'-C4'-C3'	-2.61	99.96	105.11
34	a	1516	2MG	C8-N7-C5	2.58	107.91	102.99
34	a	1407	5MC	O2-C2-N3	-2.58	118.14	122.33
34	a	1207	2MG	C8-N7-C5	2.57	107.88	102.99
8	A	2445	2MG	C5-C6-N1	2.56	118.47	113.95
8	A	1835	2MG	O6-C6-C5	-2.56	119.38	124.37
8	A	1835	2MG	C8-N7-C5	2.55	107.86	102.99
56	w	37	MIA	C5-C6-N1	-2.55	118.69	120.81
56	w	37	MIA	O4'-C4'-C3'	-2.55	100.07	105.11
8	A	1939	5MU	O4-C4-N3	-2.54	115.25	120.12
8	A	2504	PSU	O2-C2-N1	-2.51	120.02	122.79
8	A	1911	PSU	C3'-C2'-C1'	2.50	104.55	101.64
56	w	39	PSU	C6-N1-C2	-2.49	120.14	122.68
8	A	1917	PSU	O2-C2-N1	-2.48	120.06	122.79
34	a	966	2MG	C5-C6-N1	2.47	118.31	113.95
56	w	32	PSU	O2-C2-N1	-2.46	120.08	122.79
8	A	2580	PSU	O2-C2-N1	-2.46	120.08	122.79
8	A	955	PSU	C6-N1-C2	-2.46	120.17	122.68
55	v	54	5MU	O4-C4-N3	-2.45	115.42	120.12
8	A	746	PSU	O2-C2-N1	-2.38	120.17	122.79
8	A	2251	OMG	O6-C6-C5	-2.36	119.77	124.37
34	a	1498	UR3	O2-C2-N3	-2.35	118.03	121.34
8	A	2503	2MA	CM2-C2-N3	2.34	120.79	117.16
8	A	2457	PSU	C6-N1-C2	-2.32	120.31	122.68
56	w	39	PSU	O2-C2-N1	-2.32	120.24	122.79
8	A	745	1MG	CM1-N1-C6	2.31	120.72	117.55
34	a	1516	2MG	O6-C6-C5	-2.31	119.86	124.37
55	v	55	PSU	C6-C5-C4	-2.29	116.60	118.20
56	w	32	PSU	C6-N1-C2	-2.27	120.37	122.68
8	A	745	1MG	O6-C6-C5	-2.24	120.23	124.19
34	a	1407	5MC	C2'-C1'-N1	-2.24	106.88	113.22
8	A	2457	PSU	C6-C5-C4	2.23	119.75	118.20
8	A	2445	2MG	C8-N7-C5	2.21	107.20	102.99
58	y	101	FME	C-CA-N	2.15	113.61	109.73
8	A	2580	PSU	C6-C5-C4	2.13	119.69	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	O4'-C1'-C2'	2.12	108.14	105.14
8	A	2457	PSU	O4'-C1'-C2'	2.12	108.13	105.14
34	a	966	2MG	C8-N7-C5	2.11	107.00	102.99
56	w	54	5MU	O2-C2-N1	-2.09	120.01	122.79
8	A	2445	2MG	O6-C6-C5	-2.07	120.34	124.37
8	A	746	PSU	C6-N1-C2	-2.06	120.58	122.68
56	w	37	MIA	N3-C2-N1	-2.03	123.25	126.98
34	a	1207	2MG	O6-C6-C5	-2.03	120.41	124.37
34	a	967	5MC	CM5-C5-C6	-2.03	120.14	122.85
34	a	1402	4OC	C6-C5-C4	2.02	119.44	116.96
55	v	54	5MU	C1'-N1-C2	2.02	121.22	117.57
55	v	8	4SU	C1'-N1-C2	2.01	121.21	117.57
34	a	1407	5MC	C2'-C3'-C4'	2.00	106.53	102.64

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	a	967	5MC	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
55	v	54	5MU	C3'-C4'-C5'-O5'
55	v	54	5MU	O4'-C4'-C5'-O5'
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
8	A	746	PSU	C2'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C1'-N1-C2
8	A	2552	OMU	O4'-C1'-N1-C6
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	C12-C13-C14-C16
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	C2'-C1'-C5-C6
56	w	39	PSU	O4'-C1'-C5-C6
58	y	101	FME	O1-CN-N-CA
58	y	101	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
58	y	101	FME	C-CA-CB-CG
58	y	101	FME	O-C-CA-CB
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	966	2MG	C3'-C4'-C5'-O5'
8	A	1939	5MU	O4'-C4'-C5'-O5'
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2503	2MA	O4'-C4'-C5'-O5'
58	y	101	FME	CB-CG-SD-CE
8	A	1939	5MU	C3'-C4'-C5'-O5'
8	A	2503	2MA	C3'-C4'-C5'-O5'
56	w	37	MIA	N1-C6-N6-C12
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	2445	2MG	O4'-C4'-C5'-O5'
34	a	1518	MA6	C5-C6-N6-C10
8	A	1835	2MG	C3'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C4'-C5'-O5'
56	w	46	G7M	C4'-C5'-O5'-P
8	A	1915	3TD	C3'-C4'-C5'-O5'
56	w	46	G7M	C3'-C4'-C5'-O5'
34	a	1519	MA6	C4'-C5'-O5'-P
34	a	1498	UR3	C3'-C4'-C5'-O5'
8	A	747	5MC	C4'-C5'-O5'-P
8	A	1962	5MC	C2'-C1'-N1-C6
8	A	1962	5MC	O4'-C1'-N1-C6
8	A	2251	OMG	O4'-C4'-C5'-O5'
8	A	746	PSU	O4'-C1'-C5-C6
8	A	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 326 ligands modelled in this entry, 321 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	AM2	a	1628	-	40,40,40	0.18	0	53,60,60	0.57	0
64	GDP	x	801	-	24,30,30	1.38	3 (12%)	30,47,47	1.80	8 (26%)
63	AM2	a	1620	-	40,40,40	0.50	0	53,60,60	0.92	2 (3%)
63	AM2	a	1626	-	40,40,40	0.20	0	53,60,60	0.83	1 (1%)
63	AM2	a	1636	-	40,40,40	0.15	0	53,60,60	0.64	1 (1%)

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
63	AM2	a	1628	-	-	4/12/84/84	1/4/4/4
64	GDP	x	801	-	-	2/12/32/32	0/3/3/3
63	AM2	a	1620	-	-	5/12/84/84	0/4/4/4
63	AM2	a	1626	-	-	3/12/84/84	1/4/4/4
63	AM2	a	1636	-	-	7/12/84/84	1/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	x	801	GDP	C6-N1	-4.04	1.31	1.37
64	x	801	GDP	C2'-C1'	-2.50	1.50	1.53
64	x	801	GDP	C2-N1	-2.07	1.32	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	x	801	GDP	PA-O3A-PB	-4.02	119.04	132.83
63	a	1626	AM2	CA5-CA6-CA7	-3.50	102.47	110.62
64	x	801	GDP	O2B-PB-O3A	2.96	114.56	104.64
64	x	801	GDP	O3A-PB-O1B	-2.89	95.17	111.19
63	a	1620	AM2	CC2-CC3-CC4	-2.89	106.49	111.37
64	x	801	GDP	C8-N7-C5	2.72	108.17	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	a	1620	AM2	CA8-CA7-NA7	2.63	115.72	111.00
64	x	801	GDP	C5-C6-N1	2.53	118.41	113.95
64	x	801	GDP	O6-C6-N1	-2.42	117.79	120.65
64	x	801	GDP	C3'-C2'-C1'	2.33	104.49	100.98
63	a	1636	AM2	OA1-CC1-CC2	2.28	113.34	107.28
64	x	801	GDP	O3'-C3'-C2'	-2.12	104.96	111.82

There are no chirality outliers.

All (21) torsion outliers are listed below:

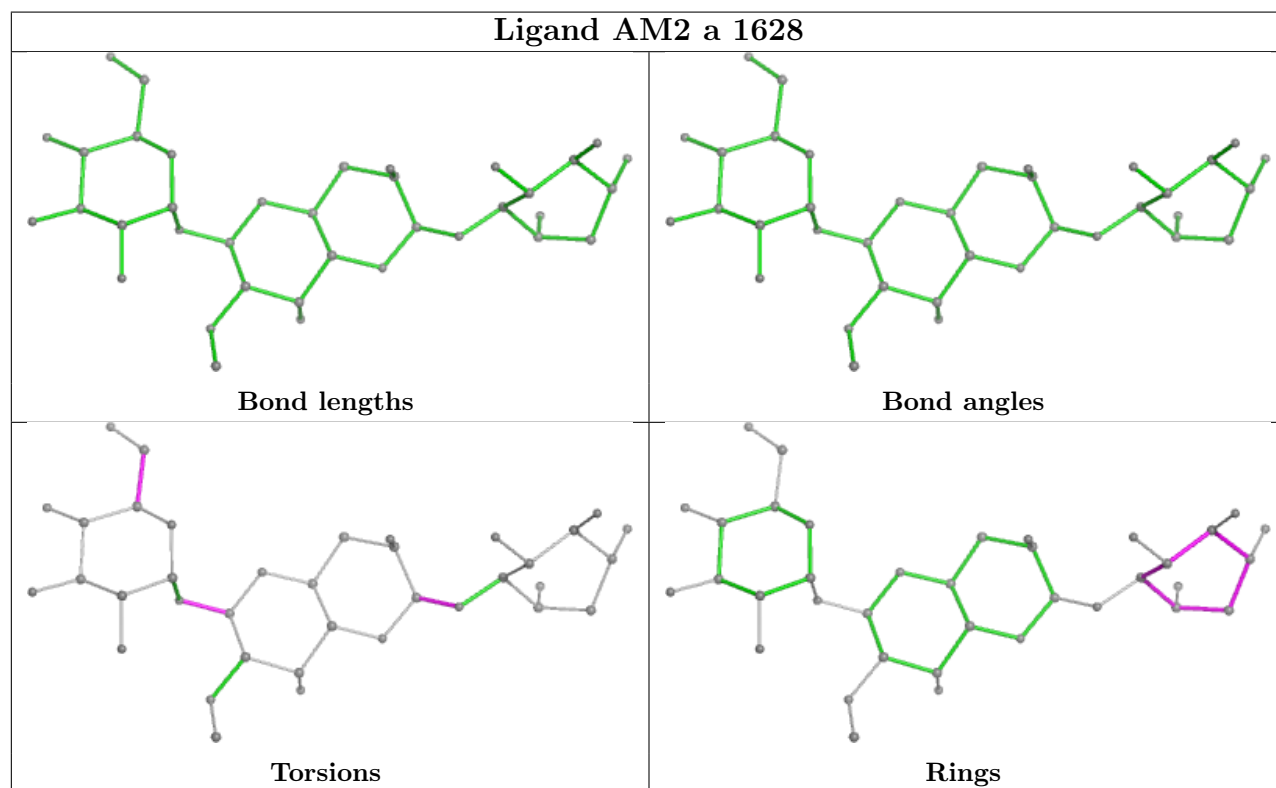
Mol	Chain	Res	Type	Atoms
63	a	1620	AM2	CA8-CA7-NA7-CA9
63	a	1626	AM2	CA2-CA1-OA1-CC1
63	a	1628	AM2	CA2-CA1-OA1-CC1
63	a	1628	AM2	CA7-CA8-OA8-CB1
63	a	1636	AM2	CA7-CA8-OA8-CB1
63	a	1636	AM2	OB1-CB1-OA8-CA8
63	a	1626	AM2	OA4-CA1-OA1-CC1
63	a	1636	AM2	OA4-CA1-OA1-CC1
63	a	1628	AM2	OA4-CA1-OA1-CC1
63	a	1636	AM2	OA5-CA8-OA8-CB1
63	a	1636	AM2	CB2-CB1-OA8-CA8
63	a	1620	AM2	OA5-CA8-OA8-CB1
63	a	1626	AM2	OB1-CB5-CB6-OB6
63	a	1628	AM2	OB1-CB5-CB6-OB6
63	a	1636	AM2	CC2-CC1-OA1-CA1
63	a	1620	AM2	OB1-CB5-CB6-OB6
63	a	1620	AM2	CB4-CB5-CB6-OB6
64	x	801	GDP	O4'-C4'-C5'-O5'
63	a	1620	AM2	OA4-CA1-OA1-CC1
63	a	1636	AM2	CA8-CA7-NA7-CA9
64	x	801	GDP	C5'-O5'-PA-O1A

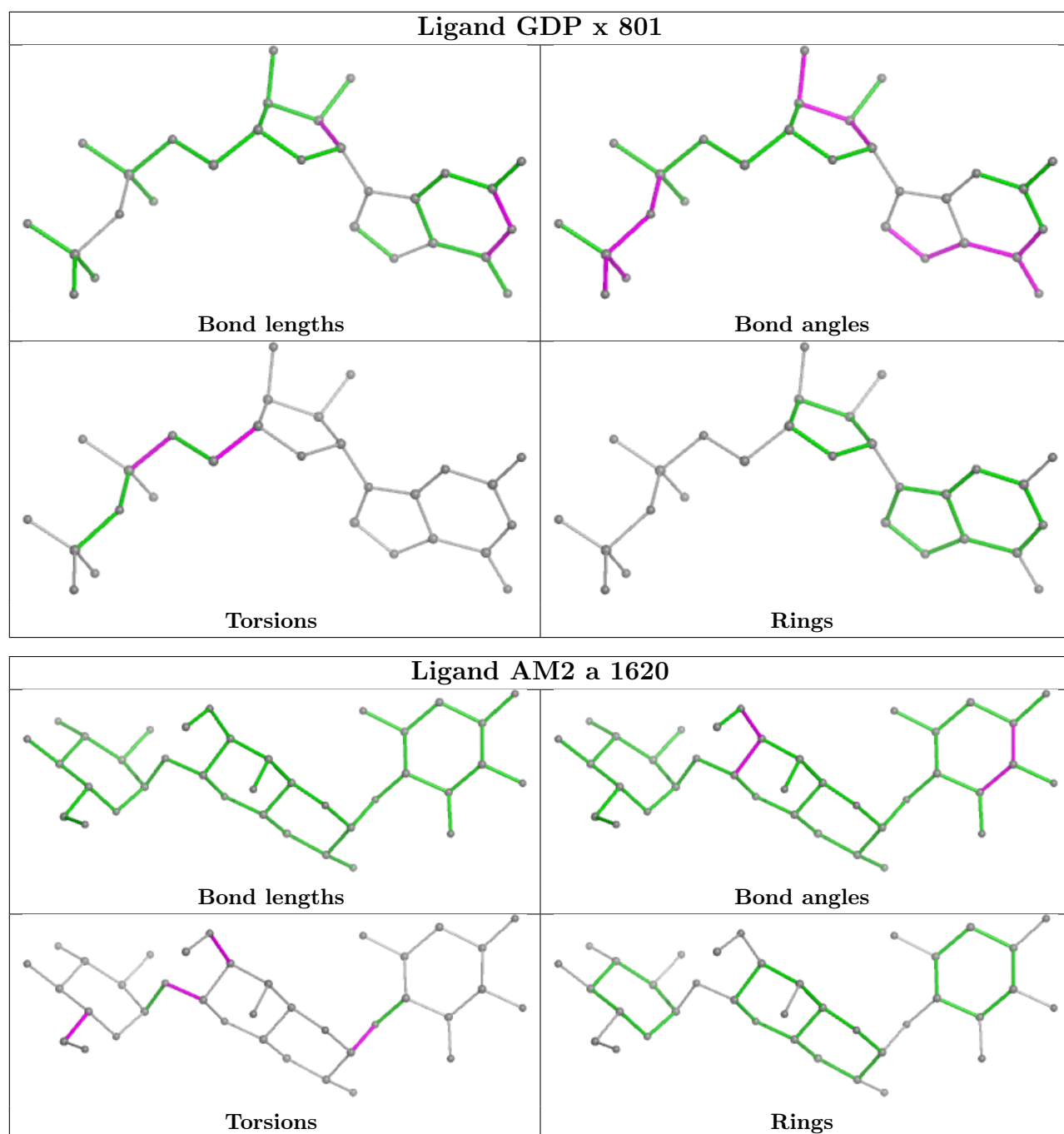
All (3) ring outliers are listed below:

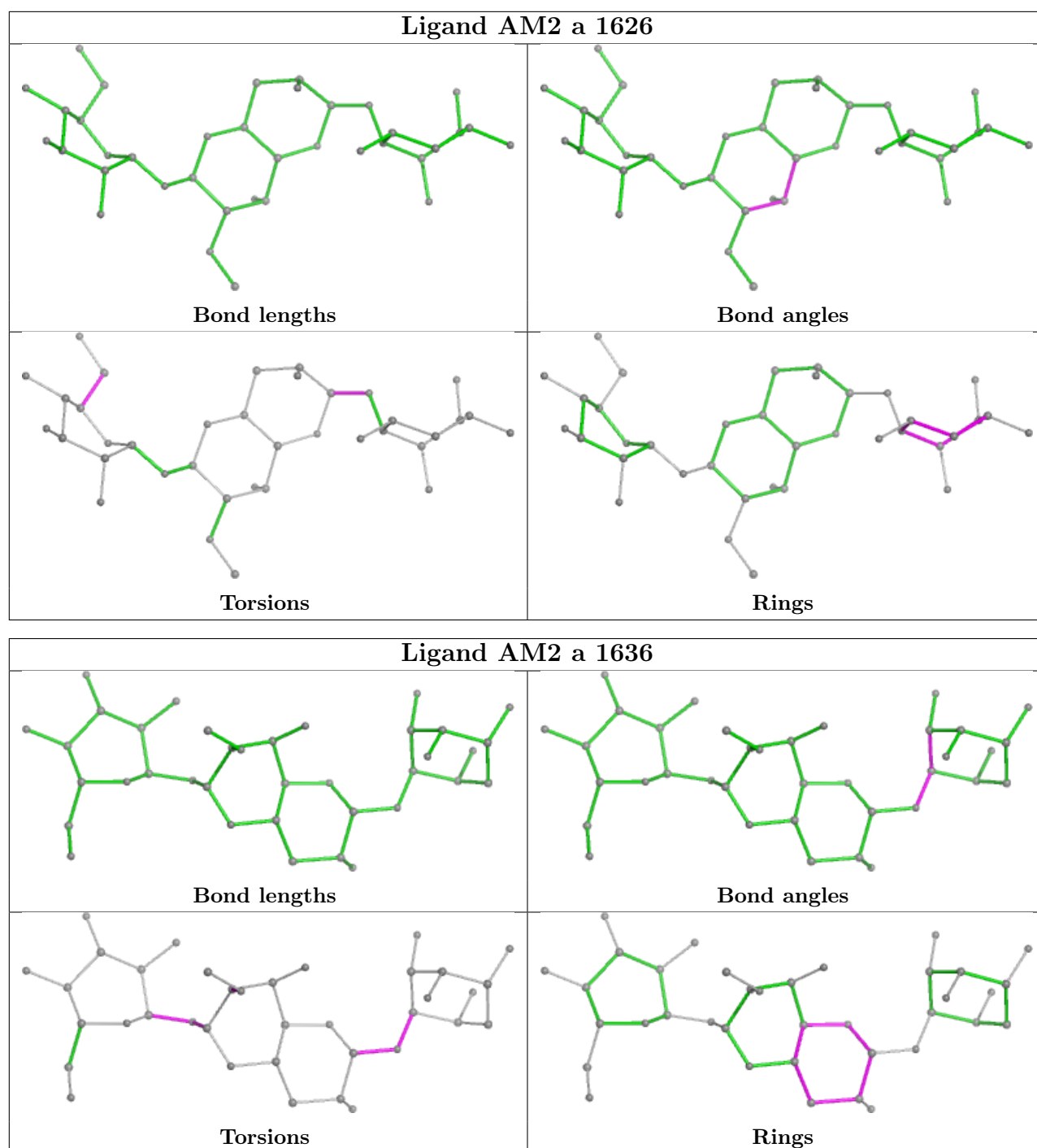
Mol	Chain	Res	Type	Atoms
63	a	1626	AM2	CC1-CC2-CC3-CC4-CC5-CC6
63	a	1628	AM2	CC1-CC2-CC3-CC4-CC5-CC6
63	a	1636	AM2	CA1-CA2-CA3-CA4-CA5-OA4

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.