



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:26 pm GMT

PDB ID : 8RCT  
EMDB ID : EMD-19059  
Title : Escherichia coli paused disome complex (Rotated disome interface class 2)  
Authors : Fluegel, T.; Schacherl, M.  
Deposited on : 2023-12-07  
Resolution : 5.32 Å(reported)  
Based on initial model : 7N1P

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

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

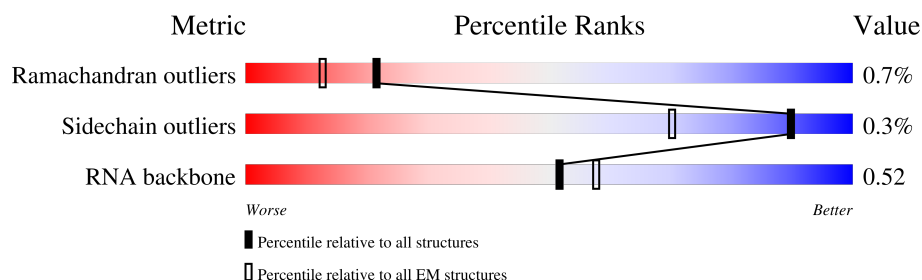
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.32 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.





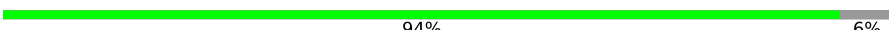







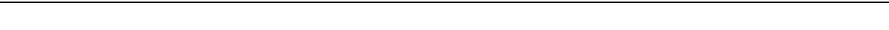

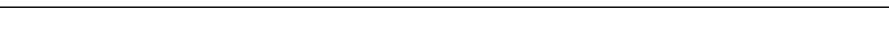
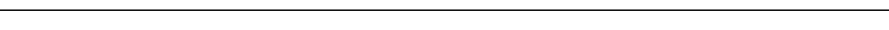
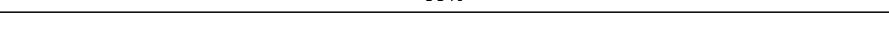
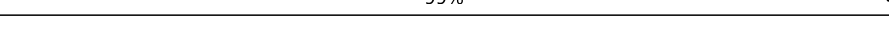
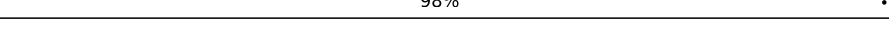
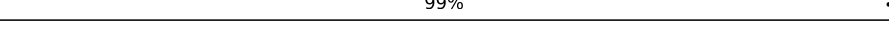
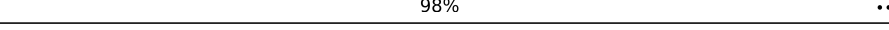
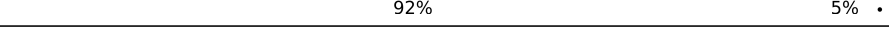


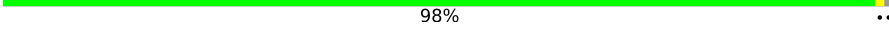
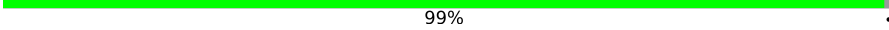
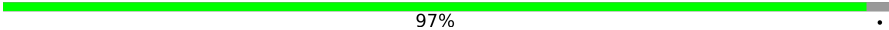
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	12	78	96% ..
2	32	59	97% ..
3	4	70	94% ..
3	41	70	20% 80%
4	62	65	98% .
5	71	2904	. 99%
5	72	2904	83% 17%
6	82	120	80% 19% .
7	A1	1542	70% 30%

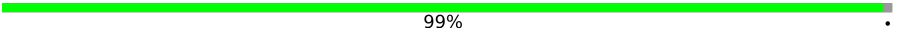
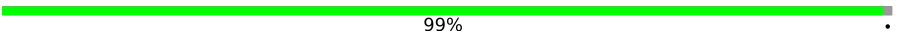
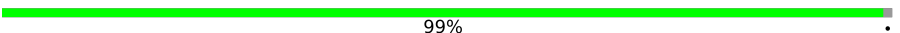
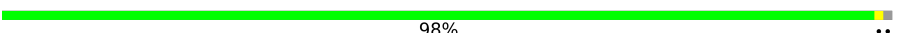
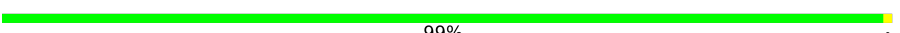
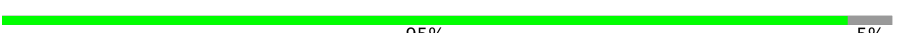














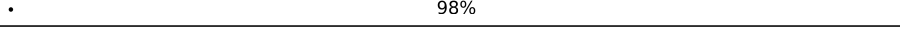
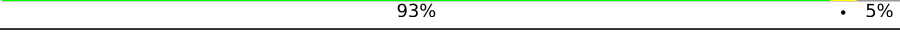
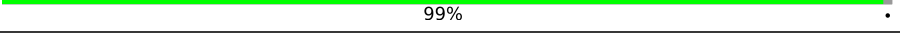
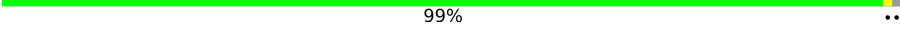
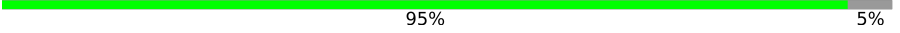
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Mol	Chain	Length	Quality of chain
7	A2	1542	 73%26%
8	B	241	 95%••
8	B2	241	 94%6%
9	C1	233	 88%•9%
9	C2	233	 91%9%
10	D1	206	 98%•
10	D2	206	 98%•
11	E1	167	 95%5%
11	E2	167	 95%5%
12	F1	135	 79%21%
12	F2	135	 78%•21%
13	G1	179	 87%13%
13	G2	179	 80%6%14%
14	H1	130	 99%•
14	H2	130	 99%•
15	I1	130	 98%•
15	I2	130	 99%•
16	J1	103	 98%••
16	J2	103	 92%5%•
17	K1	129	 88%•11%
17	K2	129	 91%•9%
18	L1	124	 98%••
18	L2	124	 99%•
19	M1	118	 97%•
19	M2	118	 99%•

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Mol	Chain	Length	Quality of chain
20	N1	101	 99% .
20	N2	101	 99% .
21	O1	89	 99% .
21	O2	89	 98% ..
22	P1	82	 99% .
23	Q1	84	 95% 5%
23	Q2	84	 94% . 5%
24	R1	75	 97% ..
24	R2	75	 95% . .
25	S1	92	 90% 10%
25	S2	92	 90% 10%
26	T1	87	 94% 5% .
27	U1	71	 97% ..
27	U2	71	 99% .
28	V2	59	 31% 66% .
29	W	76	 54% 37% 9%
30	W1	76	 26% 20% . 53%
31	Y	76	 67% 30% .
32	Y1	76	 38% 8% . 53%
33	Z1	557	 98% .
34	a2	234	 93% . 5%
35	b2	273	 99% .
36	e2	179	 99% ..
37	g2	55	 95% 5%
38	h2	136	 100%

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Mol	Chain	Length	Quality of chain
39	i2	149	<div><div></div><div>95%</div><div>5% •</div></div>
40	l2	46	<div><div></div><div>98%</div><div>•</div></div>
41	o2	144	<div><div></div><div>35%</div><div>65%</div></div>
42	p	10	<div><div></div><div>60%</div><div>40%</div></div>
43	r2	117	<div><div></div><div>99%</div><div>•</div></div>
44	z2	85	<div><div></div><div>89%</div><div>11%</div></div>

## 2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 187381 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 L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	12	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	32	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	68	Total	C	N	O	S	0	0
			533	330	101	96	6		
3	41	14	Total	C	N	O		0	0
			118	74	26	18			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	62	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	71	19	Total	C	N	O	P	0	0
			406	182	73	132	19		
5	72	2904	Total	C	N	O	P	0	0
			62355	27824	11468	20159	2904		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	82	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A1	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		
7	A2	1537	Total	C	N	O	P	0	0
			32990	14721	6049	10683	1537		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	233	Total	C	N	O	S	0	0
			1815	1145	325	337	8		
8	B2	227	Total	C	N	O	S	0	0
			1776	1123	318	327	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C1	213	Total	C	N	O	S	0	0
			1665	1054	312	295	4		
9	C2	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D1	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		
10	D2	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E1	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		
11	E2	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		
12	F2	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G1	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		
13	G2	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
14	H2	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
15	I2	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J1	102	Total	C	N	O	S	0	0
			817	509	157	150	1		
16	J2	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.



Mol	Chain	Residues	Atoms					AltConf	Trace
17	K1	115	Total	C	N	O	S	0	0
			857	528	168	158	3		
17	K2	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L1	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
18	L2	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M1	115	Total	C	N	O	S	0	0
			891	552	179	157	3		
19	M2	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		
20	N2	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
21	O2	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q1	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
23	Q2	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R1	74	Total	C	N	O	S	0	0
			624	395	122	105	2		
24	R2	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S1	83	Total	C	N	O	S	0	0
			663	424	126	111	2		
25	S2	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U1	70	Total	C	N	O	S	0	0
			590	366	125	98	1		
27	U2	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	59	Total	C	N	O	P	0	0
			1272	569	242	402	59		

- Molecule 29 is a RNA chain called tRNA-Trp (P/E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	W	76	Total	C	N	O	P	S	0	0
			1630	730	286	536	76	2		

- Molecule 30 is a RNA chain called tRNA-Phe (P/E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	W1	36	Total	C	N	O	P	S	0	0
			781	352	143	248	36	2		

- Molecule 31 is a RNA chain called tRNA-Ala (A/P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Y	76	Total	C	N	O	P		0	0
			1628	726	293	533	76			

- Molecule 32 is a RNA chain called tRNA-Val (A/P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Y1	36	Total	C	N	O	P		0	0
			778	348	142	252	36			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y1	34	CM0	U	variant	GB 1847302804

- Molecule 33 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z1	9	Total	C	N	O	0	0
			75	49	10	16		

- Molecule 34 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	a2	223	Total	C	N	O	S		0	0
			1661	1039	302	314	6			

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e2	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 37 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	g2	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h2	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 39 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i2	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 40 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 41 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o2	51	Total	C	N	O	S	0	0
			377	231	83	62	1		

- Molecule 42 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	p	10	Total	C	N	O	0	0
			76	47	18	11		

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	r2	116	Total	C	N	O	0	0
			891	552	178	161		

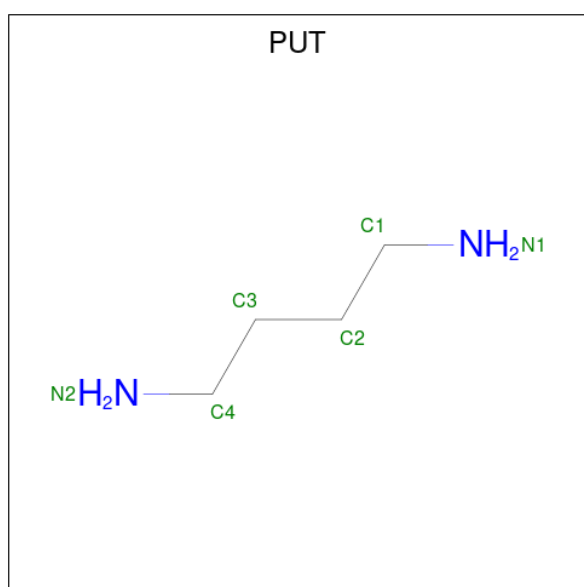
- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z2	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

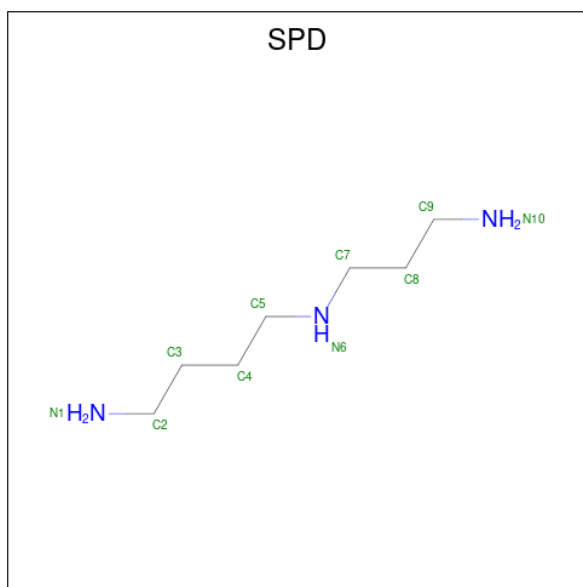
Mol	Chain	Residues	Atoms		AltConf
45	4	1	Total	Zn	0
			1	1	
45	B	1	Total	Zn	0
			1	1	

- Molecule 46 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
46	72	1	Total	C	N	0
			6	4	2	
46	72	1	Total	C	N	0
			6	4	2	

- Molecule 47 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



Mol	Chain	Residues	Atoms			AltConf
47	72	1	Total	C	N	0
			10	7	3	

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	72	163	Total	Mg	0
			163	163	
48	A1	60	Total	Mg	0
			60	60	
48	A2	42	Total	Mg	0
			42	42	
48	Y	2	Total	Mg	0
			2	2	
48	h2	1	Total	Mg	0
			1	1	

### 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 L28

Chain 12:  96% ..



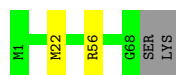
- Molecule 2: 50S ribosomal protein L30

Chain 32:  97% ..



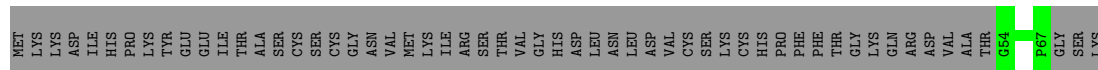
- Molecule 3: Large ribosomal subunit protein bL31A

Chain 4:  94% ..



- Molecule 3: Large ribosomal subunit protein bL31A

Chain 41:  20% 80%



- Molecule 4: 50S ribosomal protein L35

Chain 62:  98% .



- Molecule 5: 23S ribosomal RNA

Chain 71:  99%


G G U U A A C C G G A A C U A A G C C G U A C A C G G A U G C C U G C C A G U C A A G C G G A A C U G  
C U A A U C U G C C G A A A G C G G U C G G U A A A G G U G A U A U G A A C C G U U A U A C C G G C G A A A U  
G G G A A A C C C A A A G U G U G U U C G A A C A A C A A C U U G A A A C C A A A G G U U A A A G G C C G  
A A C C G G G G A A A C U G A A A A A A U U A A G U A C C C A G C G A A A A A C C A A A C C G G A A U C C C C  
A G U A G C G G G A A A C G G A A A A G G A A C A A G C C C A A G A A C C U G A A U G U G U A A G G A A  
G C G U C U G G A A A G G C G G G A U A C A A G G U G A C C C G U A C A A A A A A U G C A A G C U G U  
G A G C U C G A U G A A G G G G G G A A C A A G G U G A C C U G U G A  
C A A G G C U A A A A A C U C C G A A A A A C C G A A U G A  
G A A C C C G G A A G G G A  
A C C G U U A G G C G G U G A  
C A A G G U A A C C G A A A A A G G G G G A  
A G G G U A A G A A C C G A  
A A C U U G G A A G A A C C G A  
A  
A  
G U G A A A U C A A U C C G G G G U A A A C C G A A C U G U U C C C C A A A G G A A A A A A A A A A A A A A  
C C G A A U G C A A A A C U G C G A  
C G U C C G U C G A  
A G U G A  
U U U A  
U A A A C C A U G C C A  
U G U A A A C C C G G A  
C A U U A  
A A C G U A  
G G A  
G U U G G C C G G A

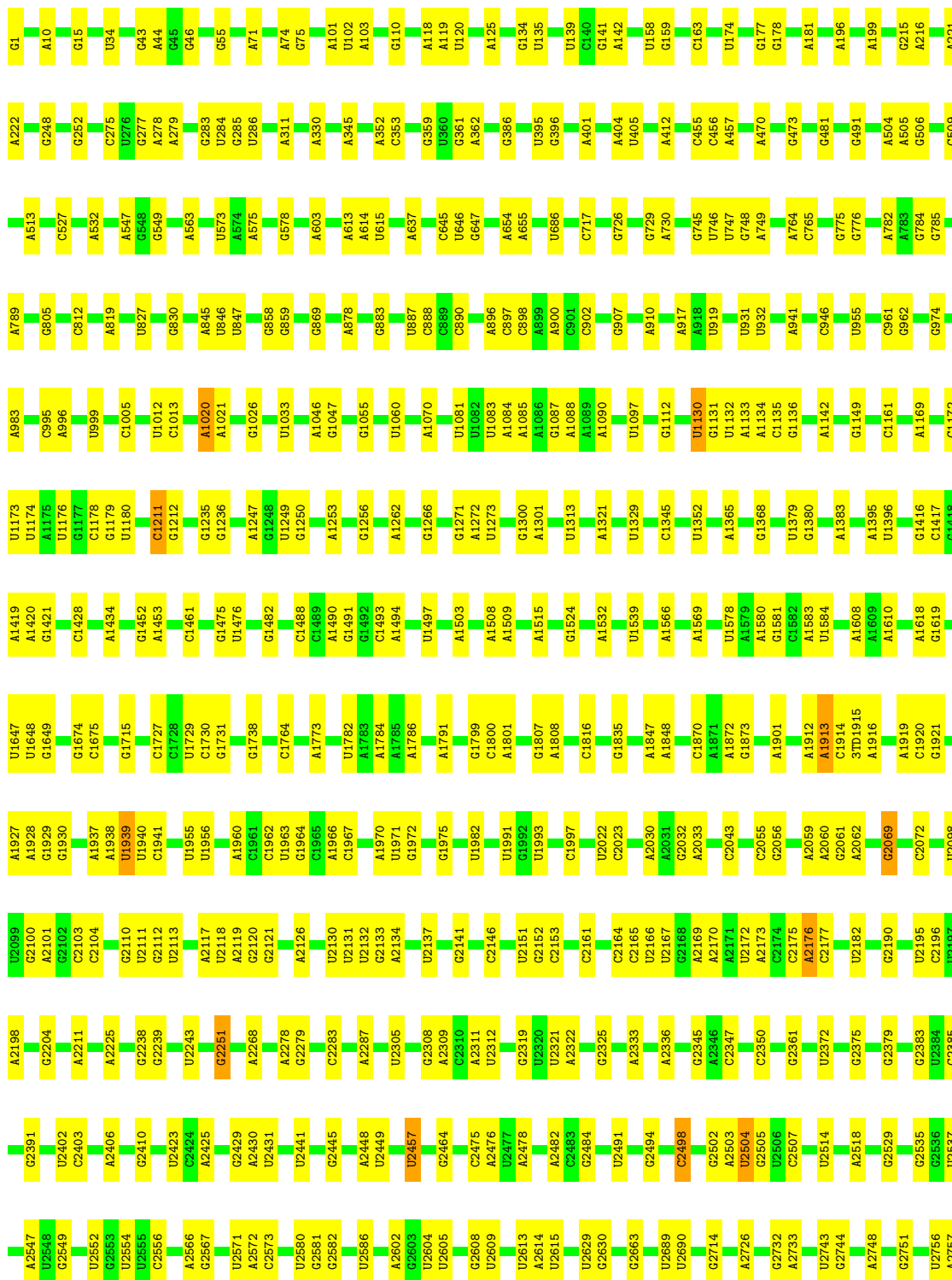


C	G	A	A	A	A	U	C	A	A	G	A	G	C	U	G	A	G	G	C	G	U	G	A	G	A	C	G	A	G	A	C	A	C	U	A	C	G	U	G	G	C	U	U	G	A	A	C	A	A	U	G	C	C	U	G	
C	U	U	C	C	A	G	G	A	A	A	A	G	C	C	U	C	U	A	A	G	C	A	A	G	C	A	G	U	A	A	C	A	A	C	A	A	U	C	C	U	U	A	C	C	G	A	A	C	C	6M2	G					
U	G	U	U	C	A	G	G	U	A	A	G	A	A	A	A	C	C	A	A	A	G	G	A	C	C	U	U	G	A	A	C	A	A	U	C	G	G	G	U	U	A	A	C	C	U	A	G	G	C	A	A	U				
G	G	U	G	C	C	A	A	G	C	U	C	G	A	A	U	A	C	C	U	U	G	A	A	C	U	U	G	A	A	C	U	A	U	A	A	A	C	C	U	C	C	G	A	A	C	C	U	G	A	G						
C	U	G	A	A	A	U	C	A	A	G	U	C	G	A	A	U	A	C	C	A	G	C	C	U	G	C	C	A	A	C	U	U	A	U	A	A	A	A	C	A	C	C	G	A	A	C	U	U	G	C						
A	A	A	C	A	C	G	A	A	A	G	U	G	G	A	A	U	A	A	C	A	G	G	U	G	C	C	A	A	C	U	U	A	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U	G					
G	G	U	U	U	A	G	C	G	G	A	A	G	C	C	U	C	A	U	C	U	U	C	A	U	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C							
C	G	A	A	5MU	U	C	C	U	U	A	G	U	C	G	G	A	A	A	U	U	C	C	G	A	A	U	G	C	C	A	U	U	A	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U							
C	U	C	C	A	A	U	G	A	A	C	C	C	G	U	A	A	G	A	U	U	C	C	G	A	A	U	G	C	A	U	U	A	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U						
A	C	G	G	A	A	U	G	G	A	C	C	C	G	U	A	A	C	C	U	U	A	C	U	A	A	A	U	C	C	U	U	A	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U						
A	G	G	A	A	U	G	G	A	A	G	G	A	U	U	G	U	A	A	A	U	G	U	A	A	A	U	C	C	A	U	U	A	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U						
C	C	A	C	C	C	U	U	A	A	C	U	U	G	A	U	U	G	U	C	U	A	A	C	C	U	U	A	A	C	C	U	U	A	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U					
G	G	U	G	G	A	G	U	U	U	A	A	U	C	A	U	U	G	G	C	U	C	C	U	A	A	A	U	C	C	U	U	A	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U					
G	C	U	A	A	U	C	C	G	G	U	A	A	U	C	A	A	G	A	U	C	A	G	U	U	C	C	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U						
C	G	U	G	A	C	A	C	A	A	PSU	PSU	C	G	U	U	C	C	A	U	C	C	A	U	C	C	A	U	C	C	A	U	C	C	A	U	C	C	A	U	C	C	A	U	C	C	A	U	C	C	A	U					
A	G	U	A	C	G	A	A	C	C	G	G	A	A	C	C	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U					
G	C	C	G	G	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	C							

G A U A A G G C C G G G U U G U G U U A A A G C C G A U U G C G U U G A A G C U A A C C G G U A C U A A U G A A C C C G U G A  
 G G C C U U U A A U C C U

- Molecule 5: 23S ribosomal RNA

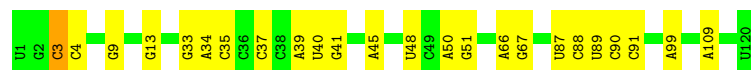
Chain 72:  83% 17%





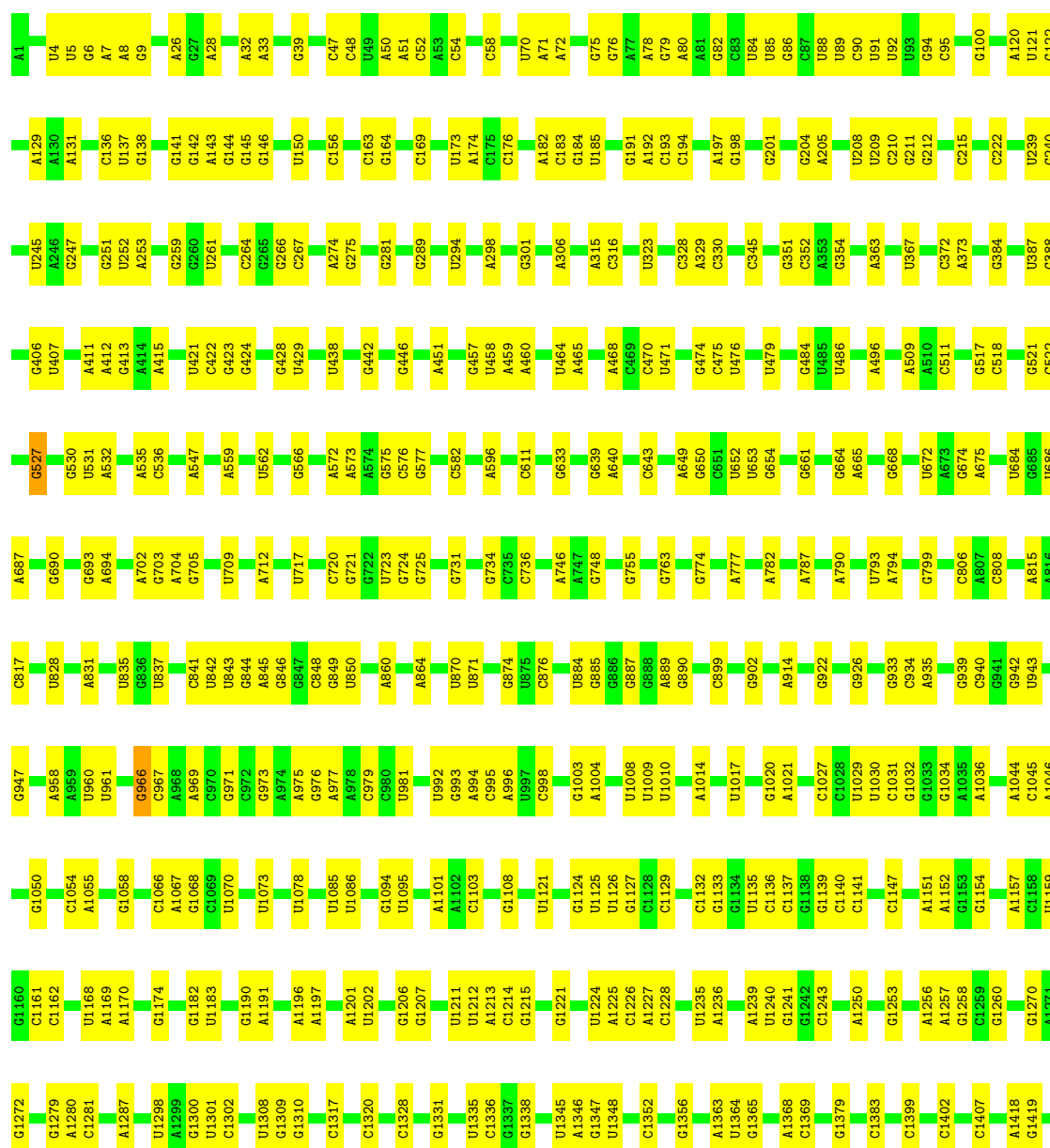
• Molecule 6: 5S ribosomal RNA

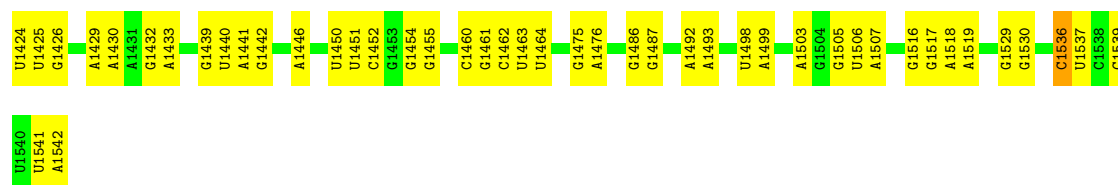
Chain 82: 80% 19%



• Molecule 7: 16S ribosomal RNA

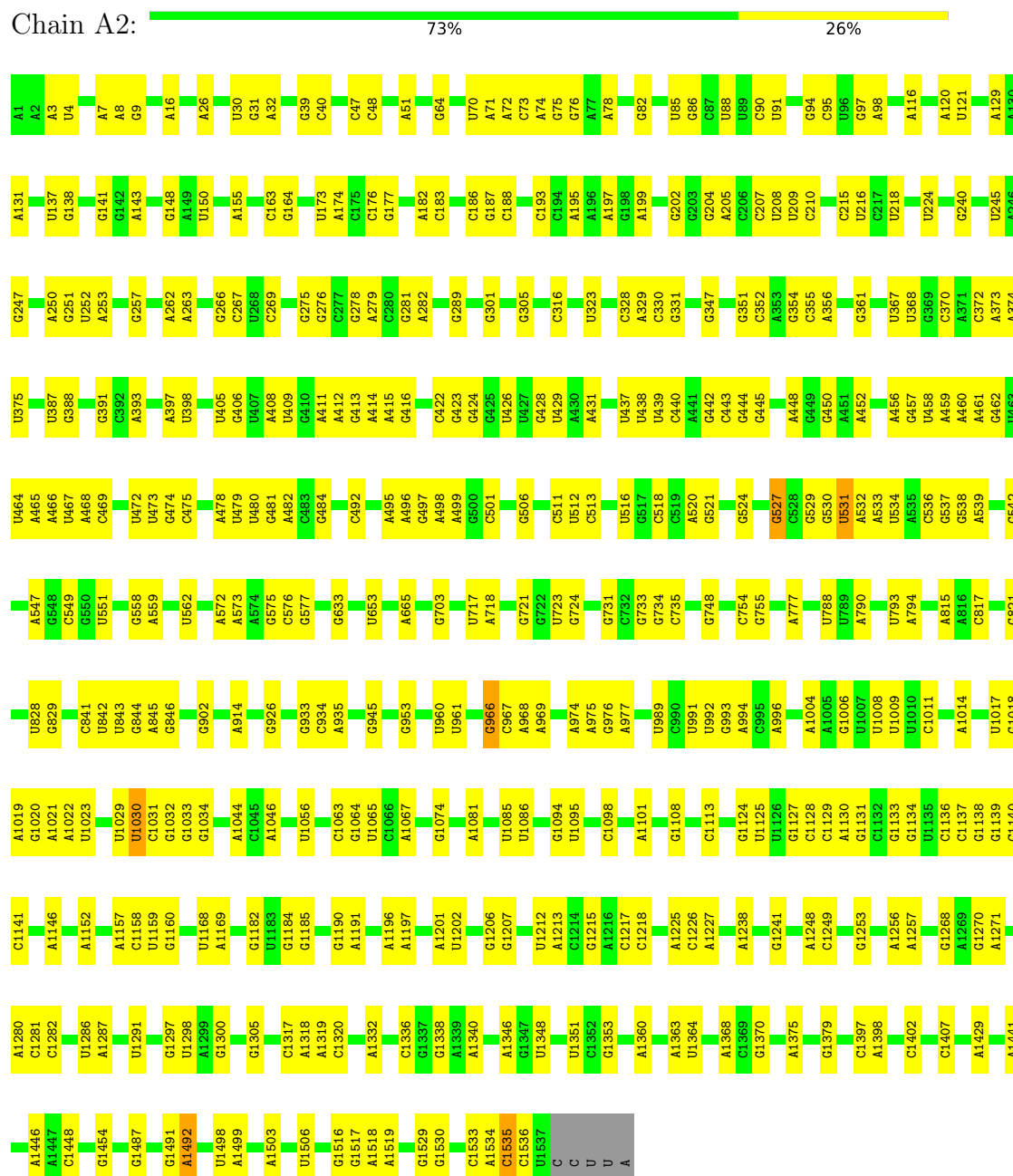
Chain A1: 70% 30%





• Molecule 7: 16S ribosomal RNA

Chain A2:



• Molecule 8: Small ribosomal subunit protein uS2

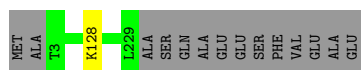
Chain B:

95%



- Molecule 8: Small ribosomal subunit protein uS2

Chain B2: 94% 6%



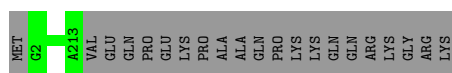
- Molecule 9: Small ribosomal subunit protein uS3

Chain C1: 88% 9%



- Molecule 9: Small ribosomal subunit protein uS3

Chain C2: 91% 9%



- Molecule 10: Small ribosomal subunit protein uS4

Chain D1: 98%



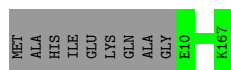
- Molecule 10: Small ribosomal subunit protein uS4

Chain D2: 98%



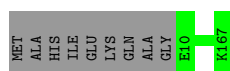
- Molecule 11: Small ribosomal subunit protein uS5

Chain E1: 95% 5%



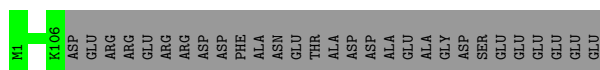
- Molecule 11: Small ribosomal subunit protein uS5

Chain E2: 95% 5%



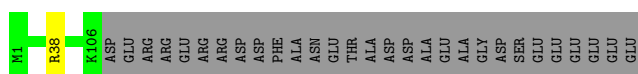
- Molecule 12: 30S ribosomal protein S6

Chain F1: 79% 21%



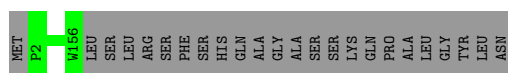
- Molecule 12: 30S ribosomal protein S6

Chain F2: 78% 21%



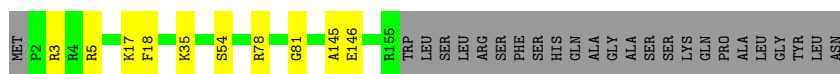
- Molecule 13: 30S ribosomal protein S7

Chain G1: 87% 13%



- Molecule 13: 30S ribosomal protein S7

Chain G2: 80% 6% 14%



- Molecule 14: Small ribosomal subunit protein uS8

Chain H1: 99%



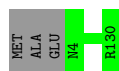
- Molecule 14: Small ribosomal subunit protein uS8

Chain H2: 99%



- Molecule 15: Small ribosomal subunit protein uS9

Chain I1: 98%



- Molecule 15: Small ribosomal subunit protein uS9

Chain I2: 99% .



- Molecule 16: 30S ribosomal protein S10

Chain J1: 98% ..



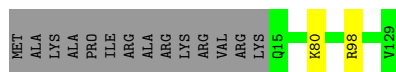
- Molecule 16: 30S ribosomal protein S10

Chain J2: 92% 5% .



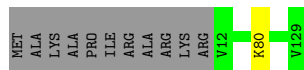
- Molecule 17: Small ribosomal subunit protein uS11

Chain K1: 88% . 11%



- Molecule 17: Small ribosomal subunit protein uS11

Chain K2: 91% . 9%



- Molecule 18: Small ribosomal subunit protein uS12

Chain L1: 98% ..



- Molecule 18: Small ribosomal subunit protein uS12

Chain L2: 99% .



- Molecule 19: Small ribosomal subunit protein uS13

Chain M1:  97%



- Molecule 19: Small ribosomal subunit protein uS13

Chain M2:  99%



- Molecule 20: Small ribosomal subunit protein uS14

Chain N1:  99%



- Molecule 20: Small ribosomal subunit protein uS14

Chain N2:  99%



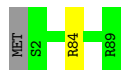
- Molecule 21: 30S ribosomal protein S15

Chain O1:  99%



- Molecule 21: 30S ribosomal protein S15

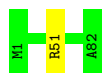
Chain O2:  98%



- Molecule 22: 30S ribosomal protein S16

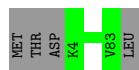
Chain P1:  99%





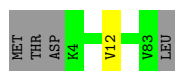
- Molecule 23: Small ribosomal subunit protein uS17

Chain Q1: 95% 5%



- Molecule 23: Small ribosomal subunit protein uS17

Chain Q2: 94% 5%



- Molecule 24: Small ribosomal subunit protein bS18

Chain R1: 97% ..



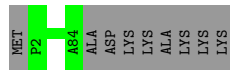
- Molecule 24: Small ribosomal subunit protein bS18

Chain R2: 95% ..



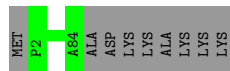
- Molecule 25: Small ribosomal subunit protein uS19

Chain S1: 90% 10%



- Molecule 25: Small ribosomal subunit protein uS19

Chain S2: 90% 10%



- Molecule 26: Small ribosomal subunit protein bS20

Chain T1: 94% 5%



- Molecule 27: 30S ribosomal protein S21

Chain U1: 97%



- Molecule 27: 30S ribosomal protein S21

Chain U2: 99%



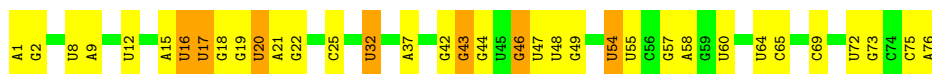
- Molecule 28: messenger RNA

Chain V2: 31% 66%



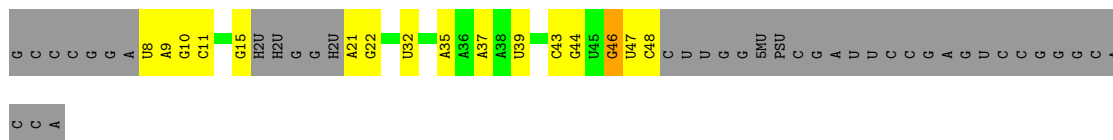
- Molecule 29: tRNA-Trp (P/E-site)

Chain W: 54% 37% 9%



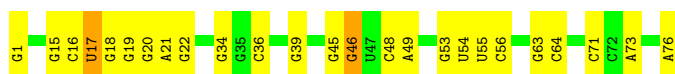
- Molecule 30: tRNA-Phe (P/E-site)

Chain W1: 26% 20% 53%



- Molecule 31: tRNA-Ala (A/P-site)

Chain Y: 67% 30%



- Molecule 32: tRNA-Val (A/P-site)



Chain e2:  99% ..



- Molecule 37: 50S ribosomal protein L33

Chain g2:  95% 5%



- Molecule 38: 50S ribosomal protein L16

Chain h2:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 50S ribosomal protein L9

Chain i2:  95% 5% •



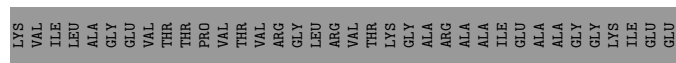
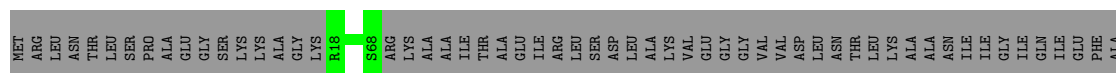
- Molecule 40: 50S ribosomal protein L34

Chain l2:  98% •



- Molecule 41: 50S ribosomal protein L15

Chain o2:  35% 65%



- Molecule 42: Nascent chain

Chain p:  60% 40%




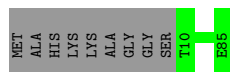
- Molecule 43: 50S ribosomal protein L18

Chain r2:  99% .



- Molecule 44: 50S ribosomal protein L27

Chain z2:  89% 11%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OMG, 6MZ, UR3, 3TD, MA6, MG, H2U, 4OC, PSU, OMC, 5MU, G7M, CM0, MIA, 2MG, 5MC, OMU, 7MG, 1MG, PUT, 4SU, SPD, 2MA

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	12	0.25	0/635	0.63	0/848
2	32	0.22	0/453	0.53	0/605
3	4	0.25	0/543	0.60	1/726 (0.1%)
3	41	0.25	0/120	0.59	0/158
4	62	0.24	0/513	0.55	0/676
5	71	0.15	0/429	0.69	0/664
5	72	0.18	1/69306 (0.0%)	0.70	15/108116 (0.0%)
6	82	0.18	0/2872	0.74	2/4478 (0.0%)
7	A1	0.22	0/36794	0.76	1/57392 (0.0%)
7	A2	0.22	0/36681	0.75	9/57217 (0.0%)
8	B	0.24	0/1846	0.53	0/2488
8	B2	0.25	0/1807	0.50	0/2435
9	C1	0.25	0/1692	0.56	0/2280
9	C2	0.27	0/1685	0.59	0/2270
10	D1	0.26	0/1665	0.54	0/2227
10	D2	0.24	0/1665	0.54	0/2227
11	E1	0.26	0/1179	0.52	0/1584
11	E2	0.26	0/1179	0.52	0/1584
12	F1	0.24	0/881	0.51	0/1189
12	F2	0.26	0/881	0.50	0/1189
13	G1	0.24	0/1246	0.53	0/1672
13	G2	0.25	0/1230	0.56	0/1649
14	H1	0.25	0/989	0.53	0/1326
14	H2	0.25	0/989	0.52	0/1326
15	I1	0.25	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.26	0/827	0.63	0/1117
16	J2	0.25	0/813	0.63	0/1100
17	K1	0.26	0/873	0.55	0/1180
17	K2	0.26	0/900	0.56	0/1215
18	L1	0.26	0/969	0.60	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
18	L2	0.26	0/969	0.61	0/1300
19	M1	0.24	0/900	0.57	0/1204
19	M2	0.24	0/919	0.58	0/1226
20	N1	0.25	0/817	0.59	0/1088
20	N2	0.25	0/817	0.58	0/1088
21	O1	0.23	0/722	0.55	0/964
21	O2	0.24	0/722	0.57	0/964
22	P1	0.25	0/659	0.61	0/884
23	Q1	0.27	0/657	0.58	0/881
23	Q2	0.25	0/657	0.56	0/881
24	R1	0.24	0/635	0.57	0/849
24	R2	0.24	0/637	0.61	0/851
25	S1	0.25	0/680	0.52	0/915
25	S2	0.25	0/680	0.53	0/915
26	T1	0.25	0/676	0.54	0/895
27	U1	0.25	0/598	0.61	0/792
27	U2	0.24	0/598	0.58	0/792
28	V2	0.31	0/1427	0.91	5/2224 (0.2%)
29	W	0.39	1/1604 (0.1%)	1.29	5/2496 (0.2%)
30	W1	0.27	0/747	0.88	0/1161
31	Y	0.34	1/1725 (0.1%)	0.78	0/2687
32	Y1	0.20	0/786	0.79	0/1216
33	Z1	0.26	0/76	0.34	0/101
34	a2	0.25	0/1676	0.49	0/2259
35	b2	0.25	0/2121	0.59	0/2852
36	e2	0.25	0/1444	0.52	0/1937
37	g2	0.25	0/434	0.51	0/576
38	h2	0.24	0/1104	0.57	0/1474
39	i2	0.31	0/1122	0.57	0/1515
40	l2	0.24	0/380	0.62	0/498
41	o2	0.26	0/383	0.67	0/501
42	p	0.59	0/77	0.66	0/104
43	r2	0.25	0/901	0.58	0/1209
44	z2	0.26	0/589	0.54	0/779
All	All	0.22	3/202683 (0.0%)	0.70	38/305085 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	12	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	1
10	D1	0	1
10	D2	0	1
13	G2	0	3
16	J1	0	1
16	J2	0	2
17	K1	0	1
21	O2	0	1
22	P1	0	1
34	a2	0	1
39	i2	0	3
42	p	0	1
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	1	G	OP3-P	-10.61	1.48	1.61
5	72	1	G	OP3-P	-10.59	1.48	1.61
29	W	1	A	OP3-P	-10.57	1.48	1.61

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	43	G	O5'-P-OP2	-28.04	77.05	110.70
29	W	43	G	OP1-P-OP2	-27.57	78.24	119.60
29	W	43	G	O5'-P-OP1	15.99	129.89	110.70
29	W	42	G	OP1-P-O3'	-14.69	72.88	105.20
29	W	42	G	OP2-P-O3'	14.47	137.04	105.20
5	72	1916	A	P-O3'-C3'	-9.21	108.65	119.70
5	72	1913	A	P-O3'-C3'	-9.08	108.80	119.70
5	72	2176	A	C5'-C4'-O4'	8.26	119.01	109.10
7	A2	1492	A	P-O3'-C3'	-8.20	109.86	119.70
7	A2	1491	G	P-O3'-C3'	-8.06	110.03	119.70
5	72	1939	5MU	P-O3'-C3'	-7.03	111.27	119.70
7	A2	531	U	P-O3'-C3'	-6.54	111.85	119.70
28	V2	32	U	N1-C2-O2	6.28	127.19	122.80
28	V2	48	C	N1-C2-O2	6.25	122.65	118.90
5	72	1313	U	C2-N1-C1'	6.17	125.10	117.70
7	A2	1030	U	C2-N1-C1'	6.11	125.03	117.70
28	V2	32	U	C2-N1-C1'	6.06	124.97	117.70
5	72	1912	A	P-O3'-C3'	6.05	126.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	1313	U	N1-C2-O2	6.02	127.01	122.80
28	V2	32	U	N3-C2-O2	-5.83	118.12	122.20
5	72	1211	C	OP2-P-O3'	5.82	118.01	105.20
7	A2	532	A	P-O3'-C3'	-5.75	112.80	119.70
6	82	3	C	OP1-P-O3'	5.75	117.85	105.20
5	72	1020	A	P-O3'-C3'	5.74	126.59	119.70
5	72	1675	C	C2-N1-C1'	5.74	125.11	118.80
7	A2	1030	U	N3-C2-O2	-5.72	118.20	122.20
7	A2	1535	C	P-O3'-C3'	5.63	126.46	119.70
28	V2	48	C	C2-N1-C1'	5.62	124.98	118.80
6	82	3	C	P-O3'-C3'	5.58	126.40	119.70
7	A1	1536	C	OP2-P-O3'	5.55	117.40	105.20
5	72	1313	U	N3-C2-O2	-5.53	118.33	122.20
5	72	2176	A	C2'-C3'-O3'	5.53	122.55	113.70
7	A2	1030	U	N1-C2-O2	5.48	126.64	122.80
7	A2	754	C	C2-N1-C1'	5.21	124.53	118.80
5	72	1020	A	OP2-P-O3'	5.14	116.51	105.20
5	72	1675	C	N1-C2-O2	5.12	121.97	118.90
5	72	1130	U	P-O3'-C3'	5.09	125.80	119.70
3	4	22	MET	CA-CB-CG	5.05	121.89	113.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	12	74	ARG	Sidechain
3	4	56	ARG	Sidechain
10	D1	104	ARG	Sidechain
10	D2	104	ARG	Sidechain
13	G2	3	ARG	Sidechain
13	G2	5	ARG	Sidechain
13	G2	78	ARG	Sidechain
16	J1	31	ARG	Sidechain
16	J2	37	ARG	Sidechain
16	J2	48	ARG	Sidechain
17	K1	98	ARG	Sidechain
21	O2	84	ARG	Sidechain
22	P1	51	ARG	Sidechain
34	a2	71	ARG	Sidechain
39	i2	116	ARG	Sidechain
39	i2	50	ARG	Sidechain
39	i2	51	ARG	Sidechain

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Mol	Chain	Res	Type	Group
42	p	31	ARG	Sidechain

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

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

## 5.3 Torsion angles [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	12	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	33
3	4	66/70 (94%)	57 (86%)	9 (14%)	0	100	100
3	41	12/70 (17%)	10 (83%)	2 (17%)	0	100	100
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	B	231/241 (96%)	193 (84%)	34 (15%)	4 (2%)	7	35
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100	100
9	C1	211/233 (91%)	178 (84%)	26 (12%)	7 (3%)	3	20
9	C2	210/233 (90%)	185 (88%)	25 (12%)	0	100	100
10	D1	203/206 (98%)	183 (90%)	19 (9%)	1 (0%)	25	64
10	D2	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
11	E1	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
11	E2	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
12	F1	104/135 (77%)	104 (100%)	0	0	100	100
12	F2	104/135 (77%)	80 (77%)	23 (22%)	1 (1%)	13	49
13	G1	153/179 (86%)	151 (99%)	2 (1%)	0	100	100
13	G2	152/179 (85%)	121 (80%)	24 (16%)	7 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	H1	127/130 (98%)	127 (100%)	0	0	100	100
14	H2	127/130 (98%)	127 (100%)	0	0	100	100
15	I1	125/130 (96%)	103 (82%)	22 (18%)	0	100	100
15	I2	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
16	J1	100/103 (97%)	92 (92%)	8 (8%)	0	100	100
16	J2	98/103 (95%)	86 (88%)	9 (9%)	3 (3%)	3	21
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	14	51
17	K2	116/129 (90%)	101 (87%)	14 (12%)	1 (1%)	14	51
18	L1	121/124 (98%)	115 (95%)	5 (4%)	1 (1%)	16	54
18	L2	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M1	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	M2	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
20	N1	98/101 (97%)	84 (86%)	14 (14%)	0	100	100
20	N2	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
21	O1	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	O2	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P1	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
23	Q1	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
23	Q2	78/84 (93%)	75 (96%)	2 (3%)	1 (1%)	10	41
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9	39
24	R2	72/75 (96%)	53 (74%)	17 (24%)	2 (3%)	4	24
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
25	S2	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	5	26
27	U1	68/71 (96%)	58 (85%)	10 (15%)	0	100	100
27	U2	68/71 (96%)	60 (88%)	8 (12%)	0	100	100
33	Z1	7/557 (1%)	7 (100%)	0	0	100	100
34	a2	221/234 (94%)	201 (91%)	15 (7%)	5 (2%)	5	27
35	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
36	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
37	g2	50/55 (91%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	h2	135/136 (99%)	135 (100%)	0	0	100	100
39	i2	147/149 (99%)	115 (78%)	26 (18%)	6 (4%)	2	17
40	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
41	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100
42	p	8/10 (80%)	5 (62%)	2 (25%)	1 (12%)	0	4
43	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
44	z2	74/85 (87%)	74 (100%)	0	0	100	100
All	All	6206/7310 (85%)	5700 (92%)	461 (7%)	45 (1%)	21	56

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
13	G2	18	PHE
13	G2	35	LYS
13	G2	54	SER
13	G2	146	GLU
23	Q2	12	VAL
34	a2	157	LYS
34	a2	158	ALA
42	p	30	VAL
9	C1	78	GLY
10	D1	175	ALA
12	F2	38	ARG
13	G2	17	LYS
13	G2	81	GLY
16	J2	94	ALA
34	a2	156	ALA
39	i2	115	VAL
8	B	102	THR
13	G2	145	ALA
16	J2	89	ARG
17	K1	80	LYS
17	K2	80	LYS
18	L1	43	LYS
34	a2	204	ALA
39	i2	90	LEU
39	i2	91	PHE
39	i2	116	ARG
8	B	103	ASN

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Mol	Chain	Res	Type
26	T1	55	GLN
39	i2	107	GLY
9	C1	129	MET
9	C1	208	LEU
24	R1	21	ILE
34	a2	201	PRO
2	32	33	HIS
8	B	90	PHE
9	C1	71	ALA
9	C1	75	ILE
24	R2	5	PHE
24	R2	71	THR
39	i2	88	GLY
9	C1	73	PRO
8	B	38	VAL
16	J2	79	PRO
26	T1	56	PRO

### 5.3.2 Protein sidechains [i](#)

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	12	67/68 (98%)	66 (98%)	1 (2%)	60	75
2	32	48/49 (98%)	48 (100%)	0	100	100
3	4	60/62 (97%)	60 (100%)	0	100	100
3	41	12/62 (19%)	12 (100%)	0	100	100
4	62	51/52 (98%)	51 (100%)	0	100	100
8	B	192/199 (96%)	192 (100%)	0	100	100
8	B2	189/199 (95%)	188 (100%)	1 (0%)	86	89
9	C1	173/190 (91%)	172 (99%)	1 (1%)	84	88
9	C2	172/190 (90%)	172 (100%)	0	100	100
10	D1	172/173 (99%)	170 (99%)	2 (1%)	67	79
10	D2	172/173 (99%)	170 (99%)	2 (1%)	67	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	E1	120/126 (95%)	120 (100%)	0	100	100
11	E2	120/126 (95%)	120 (100%)	0	100	100
12	F1	92/116 (79%)	92 (100%)	0	100	100
12	F2	92/116 (79%)	92 (100%)	0	100	100
13	G1	128/147 (87%)	128 (100%)	0	100	100
13	G2	127/147 (86%)	127 (100%)	0	100	100
14	H1	104/105 (99%)	104 (100%)	0	100	100
14	H2	104/105 (99%)	104 (100%)	0	100	100
15	I1	105/107 (98%)	105 (100%)	0	100	100
15	I2	106/107 (99%)	106 (100%)	0	100	100
16	J1	89/90 (99%)	89 (100%)	0	100	100
16	J2	88/90 (98%)	88 (100%)	0	100	100
17	K1	88/99 (89%)	88 (100%)	0	100	100
17	K2	91/99 (92%)	91 (100%)	0	100	100
18	L1	103/104 (99%)	103 (100%)	0	100	100
18	L2	103/104 (99%)	103 (100%)	0	100	100
19	M1	93/96 (97%)	93 (100%)	0	100	100
19	M2	95/96 (99%)	95 (100%)	0	100	100
20	N1	83/84 (99%)	83 (100%)	0	100	100
20	N2	83/84 (99%)	83 (100%)	0	100	100
21	O1	76/77 (99%)	76 (100%)	0	100	100
21	O2	76/77 (99%)	76 (100%)	0	100	100
22	P1	65/65 (100%)	65 (100%)	0	100	100
23	Q1	74/78 (95%)	74 (100%)	0	100	100
23	Q2	74/78 (95%)	74 (100%)	0	100	100
24	R1	64/65 (98%)	64 (100%)	0	100	100
24	R2	64/65 (98%)	63 (98%)	1 (2%)	58	74
25	S1	72/79 (91%)	72 (100%)	0	100	100
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	63 (97%)	2 (3%)	35	55
27	U1	60/61 (98%)	59 (98%)	1 (2%)	56	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	U2	60/61 (98%)	60 (100%)	0	100	100
33	Z1	8/461 (2%)	8 (100%)	0	100	100
34	a2	174/181 (96%)	174 (100%)	0	100	100
35	b2	216/218 (99%)	216 (100%)	0	100	100
36	e2	149/150 (99%)	148 (99%)	1 (1%)	81	87
37	g2	47/49 (96%)	47 (100%)	0	100	100
38	h2	110/109 (101%)	110 (100%)	0	100	100
39	i2	114/114 (100%)	114 (100%)	0	100	100
40	l2	38/38 (100%)	37 (97%)	1 (3%)	41	60
41	o2	35/103 (34%)	35 (100%)	0	100	100
42	p	5/5 (100%)	3 (60%)	2 (40%)	0	0
43	r2	86/87 (99%)	86 (100%)	0	100	100
44	z2	58/63 (92%)	58 (100%)	0	100	100
All	All	5184/5994 (86%)	5169 (100%)	15 (0%)	90	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12	72	ARG
8	B2	128	LYS
9	C1	135	LYS
10	D1	15	GLU
10	D1	58	LYS
10	D2	44	ARG
10	D2	63	ARG
24	R2	7	ARG
26	T1	49	LYS
26	T1	85	LYS
27	U1	66	ARG
36	e2	3	LYS
40	l2	3	ARG
42	p	34	ARG
42	p	35	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:



Mol	Chain	Res	Type
8	B	93	ASN
8	B	94	HIS
8	B2	89	GLN
12	F2	46	GLN
13	G2	148	ASN
14	H1	18	GLN
15	I1	75	GLN
15	I2	75	GLN
17	K2	119	ASN
18	L2	29	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	58/59 (98%)	40 (68%)	9 (15%)
29	W	74/76 (97%)	28 (37%)	3 (4%)
30	W1	34/76 (44%)	10 (29%)	2 (5%)
31	Y	75/76 (98%)	21 (28%)	2 (2%)
32	Y1	32/76 (42%)	5 (15%)	2 (6%)
5	71	17/2904 (0%)	1 (5%)	0
5	72	2899/2904 (99%)	460 (15%)	38 (1%)
6	82	119/120 (99%)	21 (17%)	3 (2%)
7	A1	1538/1542 (99%)	447 (29%)	36 (2%)
7	A2	1533/1542 (99%)	393 (25%)	30 (1%)
All	All	6379/9375 (68%)	1426 (22%)	125 (1%)

All (1426) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1907	G
5	72	10	A
5	72	15	G
5	72	34	U
5	72	44	A
5	72	46	G
5	72	55	G
5	72	71	A
5	72	74	A
5	72	75	G
5	72	101	A
5	72	102	U
5	72	103	A

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Mol	Chain	Res	Type
5	72	110	G
5	72	118	A
5	72	119	A
5	72	120	U
5	72	125	A
5	72	135	U
5	72	139	U
5	72	141	G
5	72	142	A
5	72	159	G
5	72	163	C
5	72	174	U
5	72	177	G
5	72	178	G
5	72	181	A
5	72	196	A
5	72	199	A
5	72	215	G
5	72	216	A
5	72	221	A
5	72	222	A
5	72	248	G
5	72	252	G
5	72	275	C
5	72	277	G
5	72	278	A
5	72	279	A
5	72	283	G
5	72	284	U
5	72	285	G
5	72	286	U
5	72	311	A
5	72	330	A
5	72	345	A
5	72	353	C
5	72	359	G
5	72	361	G
5	72	362	A
5	72	386	G
5	72	395	U
5	72	396	G
5	72	401	A

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Mol	Chain	Res	Type
5	72	405	U
5	72	412	A
5	72	455	C
5	72	456	C
5	72	457	A
5	72	470	A
5	72	473	G
5	72	481	G
5	72	491	G
5	72	505	A
5	72	506	G
5	72	509	C
5	72	513	A
5	72	527	C
5	72	532	A
5	72	547	A
5	72	549	G
5	72	563	A
5	72	573	U
5	72	575	A
5	72	578	G
5	72	603	A
5	72	613	A
5	72	614	A
5	72	615	U
5	72	637	A
5	72	645	C
5	72	646	U
5	72	647	G
5	72	654	A
5	72	655	A
5	72	686	U
5	72	717	C
5	72	726	G
5	72	729	G
5	72	730	A
5	72	747	5MU
5	72	748	G
5	72	749	A
5	72	764	A
5	72	765	C
5	72	775	G

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Mol	Chain	Res	Type
5	72	776	G
5	72	782	A
5	72	784	G
5	72	785	G
5	72	789	A
5	72	805	G
5	72	812	C
5	72	819	A
5	72	827	U
5	72	830	G
5	72	845	A
5	72	846	U
5	72	847	U
5	72	858	G
5	72	859	G
5	72	869	G
5	72	878	A
5	72	883	G
5	72	887	U
5	72	888	C
5	72	890	C
5	72	896	A
5	72	897	C
5	72	898	C
5	72	900	A
5	72	902	C
5	72	907	G
5	72	910	A
5	72	917	A
5	72	919	U
5	72	931	U
5	72	932	U
5	72	941	A
5	72	946	C
5	72	961	C
5	72	962	G
5	72	974	G
5	72	983	A
5	72	995	C
5	72	996	A
5	72	999	U
5	72	1005	C

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Mol	Chain	Res	Type
5	72	1012	U
5	72	1013	C
5	72	1021	A
5	72	1026	G
5	72	1033	U
5	72	1046	A
5	72	1047	G
5	72	1055	G
5	72	1060	U
5	72	1070	A
5	72	1081	U
5	72	1083	U
5	72	1084	A
5	72	1085	A
5	72	1087	G
5	72	1088	A
5	72	1090	A
5	72	1097	U
5	72	1112	G
5	72	1130	U
5	72	1131	G
5	72	1132	U
5	72	1133	A
5	72	1134	A
5	72	1135	C
5	72	1136	G
5	72	1142	A
5	72	1149	G
5	72	1161	C
5	72	1169	A
5	72	1172	C
5	72	1173	U
5	72	1174	U
5	72	1176	U
5	72	1178	C
5	72	1179	G
5	72	1180	U
5	72	1212	G
5	72	1235	G
5	72	1236	G
5	72	1247	A
5	72	1249	U

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Mol	Chain	Res	Type
5	72	1250	G
5	72	1253	A
5	72	1256	G
5	72	1262	A
5	72	1271	G
5	72	1272	A
5	72	1273	U
5	72	1300	G
5	72	1301	A
5	72	1321	A
5	72	1329	U
5	72	1345	C
5	72	1352	U
5	72	1365	A
5	72	1368	G
5	72	1379	U
5	72	1380	G
5	72	1383	A
5	72	1395	A
5	72	1396	U
5	72	1416	G
5	72	1417	C
5	72	1419	A
5	72	1420	A
5	72	1421	G
5	72	1428	C
5	72	1434	A
5	72	1452	G
5	72	1453	A
5	72	1461	C
5	72	1476	U
5	72	1482	G
5	72	1488	C
5	72	1490	A
5	72	1491	G
5	72	1493	C
5	72	1494	A
5	72	1497	U
5	72	1503	A
5	72	1508	A
5	72	1509	A
5	72	1515	A

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Mol	Chain	Res	Type
5	72	1524	G
5	72	1532	A
5	72	1539	U
5	72	1566	A
5	72	1569	A
5	72	1578	U
5	72	1581	G
5	72	1583	A
5	72	1584	U
5	72	1608	A
5	72	1610	A
5	72	1619	G
5	72	1647	U
5	72	1648	U
5	72	1649	G
5	72	1674	G
5	72	1715	G
5	72	1727	C
5	72	1729	U
5	72	1730	C
5	72	1731	G
5	72	1738	G
5	72	1764	C
5	72	1773	A
5	72	1782	U
5	72	1784	A
5	72	1786	A
5	72	1791	A
5	72	1799	G
5	72	1800	C
5	72	1801	A
5	72	1807	G
5	72	1808	A
5	72	1816	C
5	72	1848	A
5	72	1870	C
5	72	1872	A
5	72	1873	G
5	72	1901	A
5	72	1913	A
5	72	1914	C
5	72	1919	A

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Mol	Chain	Res	Type
5	72	1920	C
5	72	1921	G
5	72	1927	A
5	72	1928	A
5	72	1929	G
5	72	1930	G
5	72	1937	A
5	72	1938	A
5	72	1939	5MU
5	72	1940	U
5	72	1941	C
5	72	1955	U
5	72	1956	U
5	72	1960	A
5	72	1963	U
5	72	1964	G
5	72	1966	A
5	72	1967	C
5	72	1970	A
5	72	1971	U
5	72	1972	G
5	72	1975	G
5	72	1982	U
5	72	1991	U
5	72	1993	U
5	72	1997	C
5	72	2022	U
5	72	2023	C
5	72	2032	G
5	72	2033	A
5	72	2043	C
5	72	2055	C
5	72	2056	G
5	72	2059	A
5	72	2060	A
5	72	2061	G
5	72	2062	A
5	72	2069	G7M
5	72	2072	C
5	72	2098	U
5	72	2100	G
5	72	2101	A

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Mol	Chain	Res	Type
5	72	2103	C
5	72	2104	C
5	72	2110	G
5	72	2111	U
5	72	2112	G
5	72	2113	U
5	72	2117	A
5	72	2118	U
5	72	2119	A
5	72	2120	G
5	72	2121	G
5	72	2126	A
5	72	2130	U
5	72	2131	U
5	72	2132	U
5	72	2133	G
5	72	2134	A
5	72	2137	U
5	72	2141	G
5	72	2146	C
5	72	2152	G
5	72	2153	C
5	72	2161	C
5	72	2164	C
5	72	2165	C
5	72	2166	U
5	72	2167	U
5	72	2170	A
5	72	2172	U
5	72	2173	A
5	72	2175	C
5	72	2176	A
5	72	2177	C
5	72	2182	U
5	72	2190	G
5	72	2195	U
5	72	2196	C
5	72	2198	A
5	72	2204	G
5	72	2211	A
5	72	2225	A
5	72	2238	G

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Mol	Chain	Res	Type
5	72	2239	G
5	72	2243	U
5	72	2251	OMG
5	72	2268	A
5	72	2278	A
5	72	2279	G
5	72	2283	C
5	72	2287	A
5	72	2305	U
5	72	2308	G
5	72	2309	A
5	72	2311	A
5	72	2312	U
5	72	2319	G
5	72	2321	U
5	72	2322	A
5	72	2325	G
5	72	2333	A
5	72	2336	A
5	72	2345	G
5	72	2347	C
5	72	2350	C
5	72	2361	G
5	72	2372	U
5	72	2375	G
5	72	2379	G
5	72	2383	G
5	72	2385	C
5	72	2391	G
5	72	2402	U
5	72	2403	C
5	72	2406	A
5	72	2410	G
5	72	2423	U
5	72	2425	A
5	72	2429	G
5	72	2430	A
5	72	2431	U
5	72	2441	U
5	72	2448	A
5	72	2457	PSU
5	72	2464	G

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Mol	Chain	Res	Type
5	72	2475	C
5	72	2476	A
5	72	2478	A
5	72	2482	A
5	72	2484	G
5	72	2491	U
5	72	2494	G
5	72	2498	OMC
5	72	2502	G
5	72	2504	PSU
5	72	2505	G
5	72	2507	C
5	72	2514	U
5	72	2518	A
5	72	2529	G
5	72	2535	G
5	72	2537	U
5	72	2547	A
5	72	2549	G
5	72	2554	U
5	72	2556	C
5	72	2566	A
5	72	2567	G
5	72	2571	U
5	72	2572	A
5	72	2573	C
5	72	2581	G
5	72	2582	G
5	72	2586	U
5	72	2602	A
5	72	2608	G
5	72	2609	U
5	72	2613	U
5	72	2614	A
5	72	2615	U
5	72	2629	U
5	72	2630	G
5	72	2663	G
5	72	2689	U
5	72	2690	U
5	72	2714	G
5	72	2726	A

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Mol	Chain	Res	Type
5	72	2732	G
5	72	2733	A
5	72	2743	U
5	72	2744	G
5	72	2748	A
5	72	2751	G
5	72	2757	A
5	72	2765	A
5	72	2778	A
5	72	2779	U
5	72	2798	U
5	72	2800	A
5	72	2818	U
5	72	2820	A
5	72	2821	A
5	72	2832	U
5	72	2835	A
5	72	2861	U
5	72	2867	G
5	72	2873	A
5	72	2879	A
5	72	2880	C
5	72	2883	A
5	72	2884	U
5	72	2885	G
5	72	2886	A
5	72	2891	U
5	72	2904	U
6	82	4	C
6	82	9	G
6	82	13	G
6	82	33	G
6	82	34	A
6	82	35	C
6	82	37	C
6	82	40	U
6	82	41	G
6	82	45	A
6	82	48	U
6	82	50	A
6	82	51	G
6	82	66	A

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Mol	Chain	Res	Type
6	82	67	G
6	82	87	U
6	82	89	U
6	82	90	C
6	82	91	C
6	82	99	A
6	82	109	A
7	A1	4	U
7	A1	5	U
7	A1	6	G
7	A1	7	A
7	A1	8	A
7	A1	9	G
7	A1	26	A
7	A1	28	A
7	A1	32	A
7	A1	33	A
7	A1	39	G
7	A1	47	C
7	A1	48	C
7	A1	50	A
7	A1	51	A
7	A1	52	C
7	A1	54	C
7	A1	58	C
7	A1	70	U
7	A1	71	A
7	A1	72	A
7	A1	75	G
7	A1	76	G
7	A1	78	A
7	A1	79	G
7	A1	80	A
7	A1	82	G
7	A1	84	U
7	A1	85	U
7	A1	86	G
7	A1	88	U
7	A1	89	U
7	A1	90	C
7	A1	91	U
7	A1	92	U

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Mol	Chain	Res	Type
7	A1	94	G
7	A1	95	C
7	A1	100	G
7	A1	120	A
7	A1	121	U
7	A1	122	G
7	A1	129	A
7	A1	131	A
7	A1	136	C
7	A1	137	U
7	A1	138	G
7	A1	141	G
7	A1	142	G
7	A1	143	A
7	A1	144	G
7	A1	145	G
7	A1	146	G
7	A1	150	U
7	A1	156	C
7	A1	163	C
7	A1	164	G
7	A1	169	C
7	A1	173	U
7	A1	174	A
7	A1	176	C
7	A1	182	A
7	A1	183	C
7	A1	184	G
7	A1	185	U
7	A1	191	G
7	A1	192	A
7	A1	193	C
7	A1	194	C
7	A1	197	A
7	A1	198	G
7	A1	201	G
7	A1	204	G
7	A1	205	A
7	A1	208	U
7	A1	209	U
7	A1	210	C
7	A1	211	G

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Mol	Chain	Res	Type
7	A1	212	G
7	A1	215	C
7	A1	222	C
7	A1	239	U
7	A1	240	G
7	A1	245	U
7	A1	247	G
7	A1	251	G
7	A1	252	U
7	A1	253	A
7	A1	259	G
7	A1	261	U
7	A1	264	C
7	A1	266	G
7	A1	267	C
7	A1	275	G
7	A1	281	G
7	A1	289	G
7	A1	294	U
7	A1	298	A
7	A1	301	G
7	A1	306	A
7	A1	315	A
7	A1	316	C
7	A1	323	U
7	A1	328	C
7	A1	329	A
7	A1	330	C
7	A1	345	C
7	A1	351	G
7	A1	352	C
7	A1	354	G
7	A1	363	A
7	A1	367	U
7	A1	372	C
7	A1	373	A
7	A1	384	G
7	A1	387	U
7	A1	388	G
7	A1	406	G
7	A1	407	U
7	A1	411	A

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Mol	Chain	Res	Type
7	A1	412	A
7	A1	413	G
7	A1	415	A
7	A1	421	U
7	A1	422	C
7	A1	423	G
7	A1	424	G
7	A1	428	G
7	A1	429	U
7	A1	438	U
7	A1	442	G
7	A1	446	G
7	A1	451	A
7	A1	457	G
7	A1	458	U
7	A1	459	A
7	A1	460	A
7	A1	464	U
7	A1	465	A
7	A1	468	A
7	A1	470	C
7	A1	471	U
7	A1	474	G
7	A1	475	C
7	A1	476	U
7	A1	479	U
7	A1	484	G
7	A1	486	U
7	A1	496	A
7	A1	509	A
7	A1	511	C
7	A1	517	G
7	A1	518	C
7	A1	521	G
7	A1	522	C
7	A1	527	G7M
7	A1	530	G
7	A1	531	U
7	A1	532	A
7	A1	536	C
7	A1	547	A
7	A1	559	A

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Mol	Chain	Res	Type
7	A1	562	U
7	A1	566	G
7	A1	572	A
7	A1	573	A
7	A1	575	G
7	A1	576	C
7	A1	577	G
7	A1	582	C
7	A1	596	A
7	A1	611	C
7	A1	633	G
7	A1	639	G
7	A1	640	A
7	A1	643	C
7	A1	649	A
7	A1	650	G
7	A1	652	U
7	A1	653	U
7	A1	654	G
7	A1	661	G
7	A1	664	G
7	A1	665	A
7	A1	668	G
7	A1	672	U
7	A1	674	G
7	A1	675	A
7	A1	684	U
7	A1	686	U
7	A1	687	A
7	A1	690	G
7	A1	693	G
7	A1	694	A
7	A1	702	A
7	A1	703	G
7	A1	704	A
7	A1	705	G
7	A1	709	U
7	A1	712	A
7	A1	717	U
7	A1	720	C
7	A1	721	G
7	A1	723	U

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Mol	Chain	Res	Type
7	A1	724	G
7	A1	725	G
7	A1	731	G
7	A1	734	G
7	A1	736	C
7	A1	746	A
7	A1	748	G
7	A1	755	G
7	A1	763	G
7	A1	774	G
7	A1	777	A
7	A1	782	A
7	A1	787	A
7	A1	790	A
7	A1	793	U
7	A1	794	A
7	A1	799	G
7	A1	806	C
7	A1	808	C
7	A1	815	A
7	A1	817	C
7	A1	828	U
7	A1	831	A
7	A1	835	U
7	A1	837	U
7	A1	841	C
7	A1	842	U
7	A1	843	U
7	A1	844	G
7	A1	845	A
7	A1	846	G
7	A1	848	C
7	A1	849	G
7	A1	850	U
7	A1	860	A
7	A1	864	A
7	A1	870	U
7	A1	871	U
7	A1	874	G
7	A1	876	C
7	A1	884	U
7	A1	885	G

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Mol	Chain	Res	Type
7	A1	887	G
7	A1	889	A
7	A1	890	G
7	A1	899	C
7	A1	902	G
7	A1	914	A
7	A1	922	G
7	A1	926	G
7	A1	933	G
7	A1	934	C
7	A1	935	A
7	A1	939	G
7	A1	940	C
7	A1	942	G
7	A1	943	U
7	A1	947	G
7	A1	958	A
7	A1	960	U
7	A1	961	U
7	A1	966	2MG
7	A1	969	A
7	A1	971	G
7	A1	973	G
7	A1	975	A
7	A1	976	G
7	A1	977	A
7	A1	979	C
7	A1	981	U
7	A1	992	U
7	A1	993	G
7	A1	994	A
7	A1	995	C
7	A1	996	A
7	A1	998	C
7	A1	1003	G
7	A1	1004	A
7	A1	1008	U
7	A1	1009	U
7	A1	1010	U
7	A1	1014	A
7	A1	1017	U
7	A1	1020	G

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Mol	Chain	Res	Type
7	A1	1021	A
7	A1	1027	C
7	A1	1029	U
7	A1	1030	U
7	A1	1031	C
7	A1	1032	G
7	A1	1034	G
7	A1	1036	A
7	A1	1044	A
7	A1	1045	C
7	A1	1046	A
7	A1	1050	G
7	A1	1054	C
7	A1	1055	A
7	A1	1058	G
7	A1	1066	C
7	A1	1068	G
7	A1	1070	U
7	A1	1073	U
7	A1	1078	U
7	A1	1085	U
7	A1	1086	U
7	A1	1094	G
7	A1	1095	U
7	A1	1101	A
7	A1	1103	C
7	A1	1108	G
7	A1	1121	U
7	A1	1124	G
7	A1	1125	U
7	A1	1126	U
7	A1	1127	G
7	A1	1129	C
7	A1	1132	C
7	A1	1133	G
7	A1	1135	U
7	A1	1136	C
7	A1	1137	C
7	A1	1139	G
7	A1	1140	C
7	A1	1141	C
7	A1	1147	C

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Mol	Chain	Res	Type
7	A1	1151	A
7	A1	1152	A
7	A1	1154	G
7	A1	1157	A
7	A1	1159	U
7	A1	1161	C
7	A1	1162	C
7	A1	1168	U
7	A1	1169	A
7	A1	1170	A
7	A1	1174	G
7	A1	1182	G
7	A1	1183	U
7	A1	1191	A
7	A1	1196	A
7	A1	1197	A
7	A1	1201	A
7	A1	1202	U
7	A1	1206	G
7	A1	1211	U
7	A1	1212	U
7	A1	1213	A
7	A1	1214	C
7	A1	1215	G
7	A1	1221	G
7	A1	1224	U
7	A1	1225	A
7	A1	1226	C
7	A1	1227	A
7	A1	1228	C
7	A1	1235	U
7	A1	1236	A
7	A1	1239	A
7	A1	1240	U
7	A1	1241	G
7	A1	1243	C
7	A1	1250	A
7	A1	1253	G
7	A1	1256	A
7	A1	1257	A
7	A1	1258	G
7	A1	1260	G

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Mol	Chain	Res	Type
7	A1	1270	G
7	A1	1272	G
7	A1	1279	G
7	A1	1280	A
7	A1	1281	C
7	A1	1287	A
7	A1	1298	U
7	A1	1300	G
7	A1	1301	U
7	A1	1302	C
7	A1	1308	U
7	A1	1309	G
7	A1	1310	G
7	A1	1317	C
7	A1	1320	C
7	A1	1328	C
7	A1	1331	G
7	A1	1335	U
7	A1	1336	C
7	A1	1338	G
7	A1	1345	U
7	A1	1346	A
7	A1	1347	G
7	A1	1348	U
7	A1	1352	C
7	A1	1356	G
7	A1	1363	A
7	A1	1364	U
7	A1	1365	G
7	A1	1368	A
7	A1	1369	C
7	A1	1379	G
7	A1	1383	C
7	A1	1399	C
7	A1	1418	A
7	A1	1419	G
7	A1	1424	U
7	A1	1425	U
7	A1	1426	G
7	A1	1429	A
7	A1	1430	A
7	A1	1432	G

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Mol	Chain	Res	Type
7	A1	1433	A
7	A1	1439	G
7	A1	1440	U
7	A1	1441	A
7	A1	1442	G
7	A1	1446	A
7	A1	1450	U
7	A1	1451	U
7	A1	1452	C
7	A1	1454	G
7	A1	1455	G
7	A1	1460	C
7	A1	1461	G
7	A1	1462	C
7	A1	1464	U
7	A1	1475	G
7	A1	1476	A
7	A1	1486	G
7	A1	1487	G
7	A1	1492	A
7	A1	1493	A
7	A1	1499	A
7	A1	1503	A
7	A1	1505	G
7	A1	1506	U
7	A1	1507	A
7	A1	1517	G
7	A1	1529	G
7	A1	1530	G
7	A1	1536	C
7	A1	1537	U
7	A1	1539	C
7	A1	1541	U
7	A1	1542	A
7	A2	3	A
7	A2	4	U
7	A2	7	A
7	A2	8	A
7	A2	9	G
7	A2	16	A
7	A2	26	A
7	A2	30	U

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Mol	Chain	Res	Type
7	A2	31	G
7	A2	32	A
7	A2	39	G
7	A2	40	C
7	A2	47	C
7	A2	48	C
7	A2	51	A
7	A2	64	G
7	A2	70	U
7	A2	71	A
7	A2	72	A
7	A2	73	C
7	A2	74	A
7	A2	75	G
7	A2	76	G
7	A2	78	A
7	A2	82	G
7	A2	85	U
7	A2	86	G
7	A2	88	U
7	A2	90	C
7	A2	91	U
7	A2	94	G
7	A2	95	C
7	A2	97	G
7	A2	98	A
7	A2	116	A
7	A2	120	A
7	A2	121	U
7	A2	129	A
7	A2	131	A
7	A2	137	U
7	A2	138	G
7	A2	141	G
7	A2	143	A
7	A2	148	G
7	A2	150	U
7	A2	155	A
7	A2	163	C
7	A2	164	G
7	A2	173	U
7	A2	174	A

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Mol	Chain	Res	Type
7	A2	176	C
7	A2	177	G
7	A2	182	A
7	A2	183	C
7	A2	186	C
7	A2	187	G
7	A2	188	C
7	A2	193	C
7	A2	195	A
7	A2	197	A
7	A2	199	A
7	A2	202	G
7	A2	204	G
7	A2	205	A
7	A2	207	C
7	A2	208	U
7	A2	209	U
7	A2	210	C
7	A2	215	C
7	A2	216	U
7	A2	218	U
7	A2	224	U
7	A2	240	G
7	A2	245	U
7	A2	247	G
7	A2	250	A
7	A2	251	G
7	A2	252	U
7	A2	253	A
7	A2	257	G
7	A2	262	A
7	A2	263	A
7	A2	266	G
7	A2	267	C
7	A2	269	C
7	A2	275	G
7	A2	276	G
7	A2	278	G
7	A2	279	A
7	A2	281	G
7	A2	282	A
7	A2	289	G

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Mol	Chain	Res	Type
7	A2	301	G
7	A2	305	G
7	A2	316	C
7	A2	323	U
7	A2	328	C
7	A2	329	A
7	A2	330	C
7	A2	331	G
7	A2	347	G
7	A2	351	G
7	A2	352	C
7	A2	354	G
7	A2	355	C
7	A2	356	A
7	A2	361	G
7	A2	367	U
7	A2	368	U
7	A2	370	C
7	A2	372	C
7	A2	373	A
7	A2	374	A
7	A2	375	U
7	A2	387	U
7	A2	388	G
7	A2	391	G
7	A2	393	A
7	A2	397	A
7	A2	398	U
7	A2	405	U
7	A2	406	G
7	A2	408	A
7	A2	409	U
7	A2	411	A
7	A2	412	A
7	A2	413	G
7	A2	414	A
7	A2	415	A
7	A2	416	G
7	A2	422	C
7	A2	423	G
7	A2	424	G
7	A2	426	U

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Mol	Chain	Res	Type
7	A2	428	G
7	A2	429	U
7	A2	431	A
7	A2	437	U
7	A2	439	U
7	A2	440	C
7	A2	442	G
7	A2	443	C
7	A2	444	G
7	A2	445	G
7	A2	448	A
7	A2	450	G
7	A2	452	A
7	A2	456	A
7	A2	457	G
7	A2	458	U
7	A2	459	A
7	A2	460	A
7	A2	461	A
7	A2	462	G
7	A2	464	U
7	A2	465	A
7	A2	466	A
7	A2	467	U
7	A2	468	A
7	A2	469	C
7	A2	472	U
7	A2	473	U
7	A2	474	G
7	A2	475	C
7	A2	478	A
7	A2	479	U
7	A2	480	U
7	A2	481	G
7	A2	482	A
7	A2	484	G
7	A2	492	C
7	A2	495	A
7	A2	496	A
7	A2	497	G
7	A2	498	A
7	A2	499	A

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Mol	Chain	Res	Type
7	A2	501	C
7	A2	506	G
7	A2	511	C
7	A2	512	U
7	A2	513	C
7	A2	516	U
7	A2	518	C
7	A2	520	A
7	A2	521	G
7	A2	524	G
7	A2	527	G7M
7	A2	529	G
7	A2	530	G
7	A2	531	U
7	A2	533	A
7	A2	534	U
7	A2	536	C
7	A2	538	G
7	A2	539	A
7	A2	542	G
7	A2	547	A
7	A2	549	C
7	A2	551	U
7	A2	558	G
7	A2	559	A
7	A2	562	U
7	A2	572	A
7	A2	573	A
7	A2	575	G
7	A2	576	C
7	A2	577	G
7	A2	633	G
7	A2	653	U
7	A2	665	A
7	A2	703	G
7	A2	718	A
7	A2	721	G
7	A2	723	U
7	A2	724	G
7	A2	731	G
7	A2	733	G
7	A2	734	G

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Mol	Chain	Res	Type
7	A2	735	C
7	A2	748	G
7	A2	755	G
7	A2	777	A
7	A2	788	U
7	A2	790	A
7	A2	793	U
7	A2	794	A
7	A2	815	A
7	A2	817	C
7	A2	821	G
7	A2	828	U
7	A2	829	G
7	A2	841	C
7	A2	842	U
7	A2	843	U
7	A2	844	G
7	A2	845	A
7	A2	846	G
7	A2	902	G
7	A2	914	A
7	A2	926	G
7	A2	933	G
7	A2	934	C
7	A2	935	A
7	A2	945	G
7	A2	953	G
7	A2	960	U
7	A2	961	U
7	A2	966	2MG
7	A2	968	A
7	A2	969	A
7	A2	974	A
7	A2	975	A
7	A2	976	G
7	A2	977	A
7	A2	989	U
7	A2	991	U
7	A2	992	U
7	A2	993	G
7	A2	994	A
7	A2	996	A

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Mol	Chain	Res	Type
7	A2	1004	A
7	A2	1006	G
7	A2	1008	U
7	A2	1009	U
7	A2	1011	C
7	A2	1014	A
7	A2	1017	U
7	A2	1018	G
7	A2	1019	A
7	A2	1020	G
7	A2	1021	A
7	A2	1022	A
7	A2	1023	U
7	A2	1029	U
7	A2	1030	U
7	A2	1031	C
7	A2	1032	G
7	A2	1033	G
7	A2	1034	G
7	A2	1044	A
7	A2	1046	A
7	A2	1056	U
7	A2	1063	C
7	A2	1064	G
7	A2	1065	U
7	A2	1067	A
7	A2	1074	G
7	A2	1081	A
7	A2	1085	U
7	A2	1086	U
7	A2	1094	G
7	A2	1095	U
7	A2	1098	C
7	A2	1101	A
7	A2	1108	G
7	A2	1113	C
7	A2	1124	G
7	A2	1125	U
7	A2	1127	G
7	A2	1128	C
7	A2	1129	C
7	A2	1130	A

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Mol	Chain	Res	Type
7	A2	1131	G
7	A2	1133	G
7	A2	1134	G
7	A2	1136	C
7	A2	1137	C
7	A2	1138	G
7	A2	1139	G
7	A2	1140	C
7	A2	1141	C
7	A2	1146	A
7	A2	1152	A
7	A2	1157	A
7	A2	1158	C
7	A2	1159	U
7	A2	1160	G
7	A2	1168	U
7	A2	1169	A
7	A2	1182	G
7	A2	1184	G
7	A2	1185	G
7	A2	1191	A
7	A2	1196	A
7	A2	1197	A
7	A2	1201	A
7	A2	1202	U
7	A2	1206	G
7	A2	1212	U
7	A2	1213	A
7	A2	1215	G
7	A2	1217	C
7	A2	1218	C
7	A2	1225	A
7	A2	1226	C
7	A2	1227	A
7	A2	1238	A
7	A2	1241	G
7	A2	1248	A
7	A2	1249	C
7	A2	1253	G
7	A2	1256	A
7	A2	1257	A
7	A2	1268	G

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Mol	Chain	Res	Type
7	A2	1270	G
7	A2	1271	A
7	A2	1280	A
7	A2	1281	C
7	A2	1282	C
7	A2	1286	U
7	A2	1287	A
7	A2	1291	U
7	A2	1297	G
7	A2	1298	U
7	A2	1300	G
7	A2	1305	G
7	A2	1317	C
7	A2	1318	A
7	A2	1320	C
7	A2	1332	A
7	A2	1336	C
7	A2	1338	G
7	A2	1340	A
7	A2	1346	A
7	A2	1348	U
7	A2	1351	U
7	A2	1353	G
7	A2	1360	A
7	A2	1363	A
7	A2	1364	U
7	A2	1368	A
7	A2	1370	G
7	A2	1375	A
7	A2	1379	G
7	A2	1397	C
7	A2	1398	A
7	A2	1429	A
7	A2	1441	A
7	A2	1446	A
7	A2	1448	C
7	A2	1454	G
7	A2	1487	G
7	A2	1492	A
7	A2	1499	A
7	A2	1503	A
7	A2	1506	U

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Mol	Chain	Res	Type
7	A2	1517	G
7	A2	1529	G
7	A2	1530	G
7	A2	1533	C
7	A2	1534	A
7	A2	1535	C
7	A2	1536	C
28	V2	6	A
28	V2	8	A
28	V2	9	A
28	V2	10	G
28	V2	11	G
28	V2	14	G
28	V2	15	G
28	V2	16	U
28	V2	17	G
28	V2	18	A
28	V2	19	G
28	V2	20	C
28	V2	21	U
28	V2	23	C
28	V2	24	G
28	V2	30	A
28	V2	32	U
28	V2	33	A
28	V2	34	A
28	V2	35	A
28	V2	36	A
28	V2	37	A
28	V2	38	A
28	V2	39	A
28	V2	40	A
28	V2	41	G
28	V2	42	G
28	V2	43	U
28	V2	45	U
28	V2	46	C
28	V2	47	G
28	V2	48	C
28	V2	49	G
28	V2	51	U
28	V2	53	G

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Mol	Chain	Res	Type
28	V2	54	G
28	V2	58	A
28	V2	61	U
28	V2	62	C
28	V2	63	G
29	W	2	G
29	W	12	U
29	W	15	A
29	W	16	H2U
29	W	17	H2U
29	W	18	G
29	W	19	G
29	W	20	H2U
29	W	21	A
29	W	22	G
29	W	25	C
29	W	32	PSU
29	W	44	G
29	W	46	G7M
29	W	47	U
29	W	48	U
29	W	49	G
29	W	54	5MU
29	W	57	G
29	W	58	A
29	W	60	U
29	W	64	U
29	W	65	C
29	W	69	C
29	W	72	U
29	W	73	G
29	W	75	C
29	W	76	A
30	W1	9	A
30	W1	10	G
30	W1	11	C
30	W1	15	G
30	W1	22	G
30	W1	35	A
30	W1	44	G
30	W1	46	G7M
30	W1	47	U

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Mol	Chain	Res	Type
30	W1	48	C
31	Y	15	G
31	Y	16	C
31	Y	17	H2U
31	Y	18	G
31	Y	19	G
31	Y	20	G
31	Y	21	A
31	Y	22	G
31	Y	34	G
31	Y	36	C
31	Y	39	G
31	Y	45	G
31	Y	46	G7M
31	Y	48	C
31	Y	49	A
31	Y	53	G
31	Y	56	C
31	Y	64	C
31	Y	71	C
31	Y	73	A
31	Y	76	A
32	Y1	10	G
32	Y1	11	C
32	Y1	22	G
32	Y1	46	7MG
32	Y1	47	U

All (125) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	72	43	G
5	72	134	G
5	72	158	U
5	72	277	G
5	72	285	G
5	72	352	A
5	72	404	A
5	72	504	A
5	72	613	A
5	72	747	5MU
5	72	748	G

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Mol	Chain	Res	Type
5	72	784	G
5	72	827	U
5	72	1020	A
5	72	1046	A
5	72	1130	U
5	72	1211	C
5	72	1266	G
5	72	1416	G
5	72	1419	A
5	72	1420	A
5	72	1475	G
5	72	1490	A
5	72	1580	A
5	72	1847	A
5	72	1927	A
5	72	1940	U
5	72	2061	G
5	72	2117	A
5	72	2120	G
5	72	2151	U
5	72	2169	A
5	72	2175	C
5	72	2176	A
5	72	2198	A
5	72	2430	A
5	72	2581	G
5	72	2756	U
6	82	3	C
6	82	39	A
6	82	88	C
7	A1	5	U
7	A1	7	A
7	A1	51	A
7	A1	70	U
7	A1	129	A
7	A1	173	U
7	A1	197	A
7	A1	209	U
7	A1	251	G
7	A1	274	A
7	A1	372	C
7	A1	421	U

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Mol	Chain	Res	Type
7	A1	428	G
7	A1	438	U
7	A1	535	A
7	A1	559	A
7	A1	575	G
7	A1	653	U
7	A1	686	U
7	A1	870	U
7	A1	884	U
7	A1	992	U
7	A1	993	G
7	A1	1054	C
7	A1	1067	A
7	A1	1085	U
7	A1	1182	G
7	A1	1190	G
7	A1	1201	A
7	A1	1302	C
7	A1	1335	U
7	A1	1432	G
7	A1	1440	U
7	A1	1452	C
7	A1	1463	U
7	A1	1536	C
7	A2	7	A
7	A2	30	U
7	A2	70	U
7	A2	183	C
7	A2	208	U
7	A2	209	U
7	A2	251	G
7	A2	367	U
7	A2	411	A
7	A2	428	G
7	A2	438	U
7	A2	537	G
7	A2	717	U
7	A2	845	A
7	A2	992	U
7	A2	993	G
7	A2	1085	U
7	A2	1101	A

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Mol	Chain	Res	Type
7	A2	1129	C
7	A2	1136	C
7	A2	1140	C
7	A2	1168	U
7	A2	1190	G
7	A2	1201	A
7	A2	1256	A
7	A2	1281	C
7	A2	1297	G
7	A2	1319	A
7	A2	1534	A
7	A2	1535	C
28	V2	8	A
28	V2	23	C
28	V2	31	U
28	V2	35	A
28	V2	36	A
28	V2	37	A
28	V2	39	A
28	V2	46	C
28	V2	53	G
29	W	9	A
29	W	43	G
29	W	48	U
30	W1	21	A
30	W1	43	C
31	Y	17	H2U
31	Y	63	G
32	Y1	10	G
32	Y1	46	7MG

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

64 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
5	PSU	72	2504	5	18,21,22	4.69	8 (44%)	22,30,33	1.83	5 (22%)
7	UR3	A2	1498	7	19,22,23	2.79	8 (42%)	26,32,35	1.32	3 (11%)
7	5MC	A2	1407	7	18,22,23	4.04	7 (38%)	26,32,35	0.97	2 (7%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.69	5 (19%)
29	H2U	W	16	29	18,21,22	3.04	5 (27%)	21,30,33	1.99	5 (23%)
31	H2U	Y	17	31	18,21,22	3.08	5 (27%)	21,30,33	2.02	5 (23%)
7	4OC	A1	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.89	1 (3%)
30	G7M	W1	46	30	20,26,27	2.82	7 (35%)	17,39,42	1.13	1 (5%)
29	MIA	W	37	29	24,31,32	2.32	3 (12%)	26,44,47	3.04	8 (30%)
30	MIA	W1	37	30	24,31,32	2.36	3 (12%)	26,44,47	2.76	7 (26%)
7	5MC	A1	967	7	18,22,23	4.06	7 (38%)	26,32,35	1.02	2 (7%)
5	5MC	72	1962	5	18,22,23	4.03	7 (38%)	26,32,35	1.07	2 (7%)
29	5MU	W	54	29	19,22,23	4.09	14 (73%)	28,32,35	4.01	13 (46%)
32	CM0	Y1	34	32	23,26,27	3.71	6 (26%)	27,37,40	1.58	3 (11%)
7	MA6	A2	1519	7	18,26,27	1.06	2 (11%)	19,38,41	3.35	3 (15%)
30	PSU	W1	32	30	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
5	H2U	72	2449	5,48	18,21,22	3.06	5 (27%)	21,30,33	2.04	5 (23%)
5	3TD	71	1915	5	19,22,23	4.08	7 (36%)	21,32,35	1.69	2 (9%)
5	5MU	72	747	5	19,22,23	0.27	0	28,32,35	0.52	0
5	PSU	72	746	5	18,21,22	0.89	1 (5%)	22,30,33	0.61	0
7	4OC	A2	1402	7	20,23,24	3.26	8 (40%)	26,32,35	0.90	1 (3%)
7	5MC	A2	967	7	18,22,23	4.03	7 (38%)	26,32,35	0.99	2 (7%)
7	G7M	A2	527	7	20,26,27	2.79	8 (40%)	17,39,42	1.01	1 (5%)
7	G7M	A1	527	7	20,26,27	2.79	8 (40%)	17,39,42	1.02	1 (5%)
7	2MG	A2	966	7	18,26,27	2.85	7 (38%)	16,38,41	1.34	3 (18%)
32	7MG	Y1	46	32	22,26,27	3.90	10 (45%)	29,39,42	2.04	9 (31%)
31	G7M	Y	46	31	20,26,27	2.82	8 (40%)	17,39,42	1.08	1 (5%)
5	PSU	72	955	5	18,21,22	4.67	8 (44%)	22,30,33	1.86	5 (22%)
5	2MA	72	2503	5,48	19,25,26	3.63	6 (31%)	21,37,40	3.73	3 (14%)
29	PSU	W	32	29	18,21,22	4.67	8 (44%)	22,30,33	1.91	5 (22%)
29	4SU	W	8	29	18,21,22	3.81	7 (38%)	26,30,33	2.26	4 (15%)
29	G7M	W	46	29	20,26,27	2.81	8 (40%)	17,39,42	1.11	1 (5%)
5	PSU	72	2604	5	18,21,22	4.66	8 (44%)	22,30,33	1.86	5 (22%)
7	2MG	A2	1207	7	18,26,27	2.86	7 (38%)	16,38,41	1.36	3 (18%)
31	5MU	Y	54	31	19,22,23	4.14	14 (73%)	28,32,35	4.14	12 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	6MZ	Y1	37	32	18,25,26	2.06	3 (16%)	16,36,39	2.45	4 (25%)
7	5MC	A1	1407	7	18,22,23	4.06	7 (38%)	26,32,35	0.96	2 (7%)
7	UR3	A1	1498	7	19,22,23	2.78	8 (42%)	26,32,35	1.28	2 (7%)
5	2MG	72	1835	5	18,26,27	2.85	6 (33%)	16,38,41	1.43	4 (25%)
7	MA6	A2	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.34	3 (15%)
5	PSU	72	2605	5	18,21,22	4.66	8 (44%)	22,30,33	1.81	5 (22%)
7	2MG	A2	1516	7	18,26,27	2.84	7 (38%)	16,38,41	1.34	3 (18%)
30	PSU	W1	39	30	18,21,22	4.68	8 (44%)	22,30,33	1.82	5 (22%)
5	OMC	72	2498	5,48	19,22,23	3.30	8 (42%)	26,31,34	0.77	0
5	PSU	72	2580	5	18,21,22	4.66	8 (44%)	22,30,33	1.84	6 (27%)
5	6MZ	72	1618	5	18,25,26	2.03	3 (16%)	16,36,39	2.24	4 (25%)
29	PSU	W	55	29	18,21,22	0.87	1 (5%)	22,30,33	0.58	0
5	3TD	72	1915	5	19,22,23	0.82	1 (5%)	21,32,35	0.66	0
5	2MG	72	2445	5	18,26,27	2.85	7 (38%)	16,38,41	1.39	3 (18%)
7	MA6	A1	1519	7	18,26,27	1.06	2 (11%)	19,38,41	3.41	3 (15%)
5	5MU	72	1939	5	19,22,23	4.14	15 (78%)	28,32,35	4.12	12 (42%)
5	OMG	72	2251	5,31	18,26,27	2.85	7 (38%)	19,38,41	1.53	4 (21%)
5	6MZ	72	2030	5	18,25,26	2.06	4 (22%)	16,36,39	2.33	3 (18%)
5	1MG	72	745	5	18,26,27	2.75	6 (33%)	19,39,42	1.43	3 (15%)
29	H2U	W	20	29	18,21,22	3.07	5 (27%)	21,30,33	2.02	5 (23%)
7	2MG	A1	1516	7	18,26,27	2.88	7 (38%)	16,38,41	1.35	3 (18%)
30	4SU	W1	8	30	18,21,22	3.81	7 (38%)	26,30,33	2.24	4 (15%)
7	2MG	A1	1207	7	18,26,27	2.86	6 (33%)	16,38,41	1.34	3 (18%)
31	PSU	Y	55	31	18,21,22	0.87	1 (5%)	22,30,33	0.58	0
5	PSU	72	2457	5	18,21,22	4.67	8 (44%)	22,30,33	1.87	5 (22%)
7	2MG	A1	966	7	18,26,27	2.85	6 (33%)	16,38,41	1.40	4 (25%)
7	MA6	A1	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.37	3 (15%)
29	H2U	W	17	29	18,21,22	3.06	5 (27%)	21,30,33	2.02	5 (23%)
5	G7M	72	2069	5	20,26,27	2.80	8 (40%)	17,39,42	1.04	1 (5%)

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
5	PSU	72	2504	5	-	0/7/25/26	0/2/2/2
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
31	H2U	Y	17	31	-	7/7/38/39	0/2/2/2
7	4OC	A1	1402	7	-	1/9/29/30	0/2/2/2
30	G7M	W1	46	30	-	2/3/25/26	0/3/3/3
29	MIA	W	37	29	-	6/11/33/34	0/3/3/3
30	MIA	W1	37	30	-	4/11/33/34	0/3/3/3
7	5MC	A1	967	7	-	1/7/25/26	0/2/2/2
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2
32	CM0	Y1	34	32	-	4/12/30/31	0/2/2/2
7	MA6	A2	1519	7	-	2/7/29/30	0/3/3/3
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
5	H2U	72	2449	5,48	-	0/7/38/39	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
5	5MU	72	747	5	-	2/7/25/26	0/2/2/2
5	PSU	72	746	5	-	4/7/25/26	0/2/2/2
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
7	G7M	A2	527	7	-	3/3/25/26	0/3/3/3
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
31	G7M	Y	46	31	-	2/3/25/26	0/3/3/3
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
5	2MA	72	2503	5,48	-	0/3/25/26	0/3/3/3
29	PSU	W	32	29	-	5/7/25/26	0/2/2/2
29	4SU	W	8	29	-	0/7/25/26	0/2/2/2
29	G7M	W	46	29	-	1/3/25/26	0/3/3/3
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
31	5MU	Y	54	31	-	0/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MA6	A2	1518	7	-	2/7/29/30	0/3/3/3
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
5	OMC	72	2498	5,48	-	2/9/27/28	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
29	PSU	W	55	29	-	0/7/25/26	0/2/2/2
5	3TD	72	1915	5	-	0/7/25/26	0/2/2/2
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
7	MA6	A1	1519	7	-	3/7/29/30	0/3/3/3
5	5MU	72	1939	5	-	3/7/25/26	0/2/2/2
5	OMG	72	2251	5,31	-	3/5/27/28	0/3/3/3
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
29	H2U	W	20	29	-	3/7/38/39	0/2/2/2
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
31	PSU	Y	55	31	-	0/7/25/26	0/2/2/2
5	PSU	72	2457	5	-	0/7/25/26	0/2/2/2
7	2MG	A1	966	7	-	0/5/27/28	0/3/3/3
7	MA6	A1	1518	7	-	3/7/29/30	0/3/3/3
29	H2U	W	17	29	-	2/7/38/39	0/2/2/2
5	G7M	72	2069	5	-	2/3/25/26	0/3/3/3

All (407) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	71	1915	3TD	C6-C5	12.66	1.50	1.35
32	Y1	34	CM0	C6-C5	12.62	1.48	1.34
5	72	2504	PSU	C6-C5	12.23	1.49	1.35
5	72	955	PSU	C6-C5	12.20	1.49	1.35
30	W1	39	PSU	C6-C5	12.20	1.49	1.35
5	72	2457	PSU	C6-C5	12.18	1.49	1.35
29	W	32	PSU	C6-C5	12.18	1.49	1.35
5	72	2580	PSU	C6-C5	12.17	1.49	1.35
5	72	2604	PSU	C6-C5	12.15	1.49	1.35
5	72	2605	PSU	C6-C5	12.11	1.49	1.35
30	W1	32	PSU	C6-C5	12.09	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y1	46	7MG	C8-N9	10.05	1.51	1.46
29	W	54	5MU	C3'-C2'	-10.03	1.25	1.53
7	A1	967	5MC	C6-C5	10.00	1.51	1.34
7	A1	1407	5MC	C6-C5	9.92	1.50	1.34
5	72	1939	5MU	C3'-C2'	-9.92	1.26	1.53
5	72	1962	5MC	C6-C5	9.88	1.50	1.34
7	A2	1407	5MC	C6-C5	9.88	1.50	1.34
7	A2	967	5MC	C6-C5	9.84	1.50	1.34
31	Y	54	5MU	C3'-C2'	-9.77	1.26	1.53
5	72	2504	PSU	C2-N1	9.65	1.49	1.36
5	72	2457	PSU	C2-N1	9.64	1.49	1.36
29	W	32	PSU	C2-N1	9.64	1.49	1.36
5	72	2605	PSU	C2-N1	9.59	1.49	1.36
5	72	2604	PSU	C2-N1	9.58	1.49	1.36
5	72	955	PSU	C2-N1	9.57	1.49	1.36
30	W1	39	PSU	C2-N1	9.57	1.49	1.36
30	W1	32	PSU	C2-N1	9.55	1.49	1.36
5	72	2580	PSU	C2-N1	9.52	1.49	1.36
5	72	2449	H2U	C2-N1	9.46	1.49	1.35
29	W	20	H2U	C2-N1	9.44	1.49	1.35
31	Y	17	H2U	C2-N1	9.41	1.49	1.35
29	W	17	H2U	C2-N1	9.40	1.49	1.35
29	W	16	H2U	C2-N1	9.33	1.48	1.35
5	72	2503	2MA	C4-N3	9.21	1.50	1.35
30	W1	8	4SU	C4-N3	9.00	1.47	1.37
29	W	8	4SU	C4-N3	8.99	1.47	1.37
5	71	1915	3TD	C2-N1	8.87	1.48	1.37
30	W1	39	PSU	C2-N3	8.32	1.51	1.37
5	72	2504	PSU	C2-N3	8.32	1.51	1.37
30	W1	32	PSU	C2-N3	8.31	1.51	1.37
5	72	2604	PSU	C2-N3	8.29	1.51	1.37
5	72	2605	PSU	C2-N3	8.27	1.51	1.37
29	W	32	PSU	C2-N3	8.26	1.51	1.37
5	72	2457	PSU	C2-N3	8.25	1.51	1.37
5	72	2580	PSU	C2-N3	8.23	1.51	1.37
5	72	955	PSU	C2-N3	8.21	1.51	1.37
5	72	2503	2MA	C2-N3	8.05	1.48	1.34
29	W	37	MIA	C2-S10	8.02	1.82	1.75
32	Y1	46	7MG	C5-N7	7.96	1.44	1.35
30	W1	37	MIA	C2-S10	7.80	1.82	1.75
32	Y1	34	CM0	C2-N1	7.52	1.50	1.38
7	A2	967	5MC	C4-N3	7.50	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	1962	5MC	C4-N3	7.48	1.46	1.34
7	A1	967	5MC	C4-N3	7.46	1.46	1.34
7	A1	1407	5MC	C4-N3	7.46	1.46	1.34
7	A2	1407	5MC	C4-N3	7.42	1.46	1.34
5	72	2030	6MZ	C6-N6	7.40	1.47	1.35
32	Y1	37	6MZ	C6-N6	7.39	1.47	1.35
7	A2	1498	UR3	C2-N1	7.25	1.48	1.38
5	72	1618	6MZ	C6-N6	7.25	1.46	1.35
5	72	2251	OMG	C2-N2	7.22	1.51	1.34
7	A2	1402	4OC	C4-N3	7.20	1.45	1.32
7	A1	1498	UR3	C2-N1	7.19	1.48	1.38
7	A1	1402	4OC	C4-N3	7.08	1.45	1.32
5	72	2552	OMU	C2-N3	7.05	1.50	1.38
32	Y1	34	CM0	C2-N3	7.03	1.50	1.38
29	W	8	4SU	C2-N3	7.02	1.50	1.38
5	72	1962	5MC	C2-N3	7.01	1.50	1.36
30	W1	37	MIA	C6-N6	6.99	1.47	1.34
7	A1	1407	5MC	C2-N3	6.99	1.50	1.36
5	72	2498	OMC	C2-N3	6.99	1.50	1.36
7	A1	967	5MC	C2-N3	6.97	1.50	1.36
7	A2	967	5MC	C2-N3	6.96	1.50	1.36
7	A2	1407	5MC	C2-N3	6.96	1.50	1.36
30	W1	8	4SU	C2-N3	6.94	1.50	1.38
5	72	745	1MG	C2-N3	6.89	1.47	1.34
30	W1	46	G7M	C2-N2	6.60	1.49	1.34
31	Y	46	G7M	C2-N2	6.59	1.49	1.34
5	72	2069	G7M	C2-N2	6.57	1.49	1.34
7	A1	1516	2MG	C2-N2	6.56	1.48	1.33
29	W	46	G7M	C2-N2	6.56	1.49	1.34
7	A1	527	G7M	C2-N2	6.55	1.49	1.34
5	72	2552	OMU	C2-N1	6.54	1.48	1.38
7	A2	527	G7M	C2-N2	6.54	1.49	1.34
7	A2	966	2MG	C2-N2	6.52	1.47	1.33
29	W	20	H2U	C2-N3	6.52	1.49	1.38
7	A1	1207	2MG	C2-N2	6.52	1.47	1.33
7	A2	1516	2MG	C2-N2	6.50	1.47	1.33
31	Y	17	H2U	C2-N3	6.50	1.49	1.38
7	A2	1207	2MG	C2-N2	6.47	1.47	1.33
29	W	17	H2U	C2-N3	6.47	1.49	1.38
5	72	2449	H2U	C2-N3	6.47	1.49	1.38
5	72	2445	2MG	C2-N2	6.46	1.47	1.33
29	W	37	MIA	C6-N6	6.46	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A1	1402	4OC	C6-C5	6.45	1.50	1.35
29	W	16	H2U	C2-N3	6.44	1.49	1.38
7	A1	966	2MG	C2-N2	6.44	1.47	1.33
5	72	1835	2MG	C2-N2	6.40	1.47	1.33
5	72	745	1MG	C2-N2	6.38	1.45	1.34
7	A2	1402	4OC	C6-C5	6.36	1.49	1.35
31	Y	54	5MU	C2-N1	-6.33	1.28	1.38
7	A2	1402	4OC	C2-N3	6.29	1.49	1.36
7	A1	1402	4OC	C2-N3	6.28	1.49	1.36
7	A2	1498	UR3	C6-C5	6.19	1.49	1.35
5	72	2503	2MA	C2-N1	6.17	1.45	1.34
7	A1	1498	UR3	C6-C5	6.17	1.49	1.35
5	72	2498	OMC	C6-C5	6.16	1.49	1.35
5	72	2503	2MA	C6-N1	6.07	1.44	1.33
5	72	1939	5MU	C2-N1	-6.04	1.28	1.38
29	W	8	4SU	C4-S4	-5.99	1.57	1.68
30	W1	8	4SU	C4-S4	-5.97	1.57	1.68
31	Y	46	G7M	C2-N3	5.87	1.47	1.33
29	W	8	4SU	C2-N1	5.87	1.47	1.38
30	W1	8	4SU	C6-C5	5.84	1.48	1.35
5	72	2504	PSU	C6-N1	5.84	1.45	1.36
30	W1	46	G7M	C2-N3	5.84	1.47	1.33
30	W1	39	PSU	C6-N1	5.84	1.45	1.36
32	Y1	46	7MG	C2-N3	5.83	1.47	1.33
5	72	2580	PSU	C6-N1	5.82	1.45	1.36
30	W1	8	4SU	C2-N1	5.81	1.47	1.38
5	72	2604	PSU	C6-N1	5.81	1.45	1.36
30	W1	32	PSU	C6-N1	5.80	1.45	1.36
5	72	2457	PSU	C6-N1	5.79	1.45	1.36
7	A2	527	G7M	C2-N3	5.79	1.47	1.33
29	W	46	G7M	C2-N3	5.79	1.47	1.33
29	W	32	PSU	C6-N1	5.78	1.45	1.36
5	72	2605	PSU	C6-N1	5.78	1.45	1.36
7	A1	527	G7M	C2-N3	5.78	1.47	1.33
29	W	54	5MU	C2-N1	-5.76	1.29	1.38
5	72	955	PSU	C6-N1	5.75	1.45	1.36
5	72	2069	G7M	C2-N3	5.75	1.47	1.33
29	W	8	4SU	C6-C5	5.73	1.48	1.35
7	A1	967	5MC	C4-N4	5.70	1.48	1.34
7	A1	1407	5MC	C4-N4	5.70	1.48	1.34
7	A2	1407	5MC	C6-N1	5.68	1.47	1.38
7	A2	967	5MC	C4-N4	5.67	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	1407	5MC	C4-N4	5.67	1.48	1.34
7	A1	1407	5MC	C6-N1	5.66	1.47	1.38
32	Y1	46	7MG	C4-N3	5.65	1.47	1.34
5	72	1962	5MC	C4-N4	5.63	1.48	1.34
32	Y1	46	7MG	C4-N9	5.63	1.44	1.37
7	A1	967	5MC	C6-N1	5.60	1.47	1.38
7	A1	1516	2MG	C4-N3	5.60	1.50	1.37
5	72	2445	2MG	C4-N3	5.59	1.50	1.37
5	72	2498	OMC	C4-N3	5.55	1.45	1.34
5	71	1915	3TD	C6-N1	5.53	1.45	1.36
7	A2	967	5MC	C6-N1	5.53	1.47	1.38
7	A2	966	2MG	C4-N3	5.52	1.50	1.37
7	A2	1207	2MG	C4-N3	5.51	1.50	1.37
5	72	2552	OMU	C6-C5	5.49	1.47	1.35
5	72	1835	2MG	C4-N3	5.49	1.50	1.37
7	A1	1207	2MG	C2-N1	5.47	1.45	1.36
7	A1	966	2MG	C4-N3	5.46	1.50	1.37
7	A2	1516	2MG	C4-N3	5.46	1.50	1.37
7	A1	1207	2MG	C4-N3	5.46	1.50	1.37
5	72	1962	5MC	C6-N1	5.45	1.47	1.38
7	A1	966	2MG	C2-N1	5.45	1.45	1.36
5	72	1835	2MG	C2-N1	5.45	1.45	1.36
7	A2	1207	2MG	C2-N1	5.43	1.45	1.36
7	A2	966	2MG	C2-N1	5.41	1.45	1.36
5	72	1939	5MU	O4'-C1'	-5.41	1.29	1.42
7	A2	1516	2MG	C2-N1	5.41	1.45	1.36
31	Y	54	5MU	O4'-C1'	-5.39	1.29	1.42
7	A1	1516	2MG	C2-N1	5.37	1.45	1.36
30	W1	46	G7M	C4-N3	5.36	1.50	1.37
5	72	2445	2MG	C2-N1	5.35	1.45	1.36
29	W	46	G7M	C4-N3	5.31	1.50	1.37
5	72	2251	OMG	C2-N3	5.25	1.46	1.33
7	A1	1498	UR3	C2-N3	5.24	1.49	1.39
5	72	2498	OMC	C4-N4	5.22	1.46	1.33
31	Y	46	G7M	C4-N3	5.21	1.50	1.37
7	A2	1498	UR3	C2-N3	5.20	1.49	1.39
5	72	2069	G7M	C4-N3	5.19	1.50	1.37
7	A1	527	G7M	C4-N3	5.18	1.49	1.37
7	A2	1402	4OC	C4-N4	5.12	1.46	1.35
7	A2	527	G7M	C4-N3	5.12	1.49	1.37
7	A1	1402	4OC	C4-N4	5.10	1.46	1.35
5	72	745	1MG	C4-N3	5.09	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	54	5MU	O4'-C1'	-5.01	1.30	1.42
29	W	17	H2U	C4-N3	4.94	1.46	1.37
31	Y	17	H2U	C4-N3	4.94	1.46	1.37
29	W	20	H2U	C4-N3	4.93	1.46	1.37
5	72	2449	H2U	C4-N3	4.90	1.45	1.37
29	W	16	H2U	C4-N3	4.88	1.45	1.37
5	72	1939	5MU	C2-N3	-4.75	1.29	1.38
32	Y1	46	7MG	C2-N2	4.74	1.45	1.34
31	Y	54	5MU	C2-N3	-4.66	1.29	1.38
5	72	1962	5MC	C2-N1	4.64	1.50	1.40
5	72	2552	OMU	C4-N3	4.64	1.46	1.38
29	W	54	5MU	C2-N3	-4.63	1.29	1.38
5	72	2251	OMG	C4-N3	4.62	1.48	1.37
7	A1	967	5MC	C2-N1	4.60	1.50	1.40
7	A1	1407	5MC	C2-N1	4.59	1.49	1.40
31	Y	54	5MU	C2'-C1'	4.57	1.68	1.53
29	W	54	5MU	C2'-C1'	4.57	1.68	1.53
7	A2	1407	5MC	C2-N1	4.55	1.49	1.40
7	A2	967	5MC	C2-N1	4.54	1.49	1.40
29	W	54	5MU	O4'-C4'	4.52	1.55	1.45
5	72	1939	5MU	O4'-C4'	4.52	1.55	1.45
31	Y	46	G7M	C6-N1	4.50	1.44	1.37
31	Y	54	5MU	C5'-C4'	-4.49	1.37	1.51
5	72	2498	OMC	C2-N1	4.48	1.49	1.40
29	W	54	5MU	C5'-C4'	-4.48	1.37	1.51
30	W1	46	G7M	C6-N1	4.45	1.44	1.37
31	Y	54	5MU	C6-N1	-4.44	1.30	1.38
5	72	2069	G7M	C6-N1	4.43	1.44	1.37
5	72	2504	PSU	C4-N3	4.43	1.47	1.38
5	72	955	PSU	C4-N3	4.42	1.47	1.38
30	W1	32	PSU	C4-N3	4.41	1.47	1.38
5	72	1939	5MU	C6-N1	-4.40	1.30	1.38
7	A2	527	G7M	C6-N1	4.40	1.44	1.37
5	72	2552	OMU	O4-C4	-4.39	1.16	1.24
5	72	2580	PSU	C4-N3	4.37	1.46	1.38
32	Y1	34	CM0	C6-N1	4.36	1.45	1.38
7	A2	1402	4OC	C2-N1	4.36	1.49	1.40
30	W1	39	PSU	C4-N3	4.35	1.46	1.38
5	72	2605	PSU	C4-N3	4.35	1.46	1.38
5	72	2457	PSU	C4-N3	4.34	1.46	1.38
7	A1	527	G7M	C6-N1	4.33	1.44	1.37
29	W	54	5MU	C6-N1	-4.33	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	46	G7M	C6-N1	4.32	1.44	1.37
29	W	32	PSU	C4-N3	4.31	1.46	1.38
5	72	2604	PSU	C4-N3	4.30	1.46	1.38
5	72	1939	5MU	C5'-C4'	-4.30	1.38	1.51
7	A1	1402	4OC	C2-N1	4.29	1.49	1.40
5	71	1915	3TD	C2-N3	4.25	1.48	1.38
5	72	1939	5MU	C2'-C1'	4.24	1.67	1.53
7	A1	1516	2MG	C6-N1	4.21	1.44	1.37
31	Y	54	5MU	O4'-C4'	4.21	1.54	1.45
5	72	1835	2MG	C6-N1	4.20	1.44	1.37
7	A1	966	2MG	C6-N1	4.16	1.44	1.37
5	72	2498	OMC	O2-C2	-4.15	1.16	1.23
7	A1	1207	2MG	C6-N1	4.11	1.44	1.37
5	72	2445	2MG	C6-N1	4.10	1.44	1.37
7	A2	1516	2MG	C6-N1	4.08	1.43	1.37
7	A2	966	2MG	C6-N1	4.05	1.43	1.37
7	A2	1207	2MG	C6-N1	4.04	1.43	1.37
7	A1	1402	4OC	C5-C4	4.00	1.49	1.40
7	A2	1402	4OC	C5-C4	3.95	1.49	1.40
5	72	2445	2MG	C5-C6	3.92	1.55	1.47
7	A1	1516	2MG	C5-C6	3.92	1.55	1.47
7	A2	1207	2MG	C5-C6	3.90	1.55	1.47
7	A1	966	2MG	C5-C6	3.88	1.55	1.47
5	72	2498	OMC	C6-N1	3.87	1.47	1.38
5	72	1835	2MG	C5-C6	3.86	1.55	1.47
32	Y1	34	CM0	C4-N3	3.85	1.46	1.38
7	A2	1516	2MG	C5-C6	3.84	1.55	1.47
7	A1	1207	2MG	C5-C6	3.84	1.55	1.47
32	Y1	46	7MG	C2-N1	3.83	1.47	1.37
7	A2	966	2MG	C5-C6	3.81	1.55	1.47
5	72	2552	OMU	C6-N1	3.73	1.47	1.38
31	Y	54	5MU	C6-C5	3.56	1.40	1.34
5	72	2552	OMU	O2-C2	-3.54	1.16	1.23
30	W1	8	4SU	C5-C4	3.54	1.47	1.42
32	Y1	46	7MG	C5-C6	3.54	1.52	1.43
31	Y	46	G7M	C5-C6	3.49	1.54	1.45
30	W1	46	G7M	C5-C6	3.49	1.54	1.45
29	W	46	G7M	C5-C6	3.46	1.54	1.45
5	72	1939	5MU	C6-C5	3.45	1.40	1.34
7	A2	527	G7M	C5-C6	3.45	1.54	1.45
7	A1	527	G7M	C5-C6	3.45	1.54	1.45
5	72	746	PSU	C6-C5	3.44	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2069	G7M	C5-C6	3.43	1.54	1.45
29	W	54	5MU	C6-C5	3.43	1.40	1.34
32	Y1	46	7MG	C6-N1	3.42	1.45	1.38
30	W1	8	4SU	C6-N1	3.42	1.46	1.38
29	W	55	PSU	C6-C5	3.42	1.39	1.35
29	W	8	4SU	C5-C4	3.41	1.47	1.42
29	W	8	4SU	C6-N1	3.39	1.46	1.38
7	A1	1402	4OC	C6-N1	3.38	1.46	1.38
5	72	2503	2MA	C6-C5	3.37	1.55	1.43
31	Y	55	PSU	C6-C5	3.35	1.39	1.35
5	72	2251	OMG	C2-N1	3.35	1.46	1.37
5	72	1915	3TD	C6-C5	3.35	1.39	1.35
5	72	1939	5MU	C4-N3	-3.30	1.32	1.38
7	A2	1402	4OC	C6-N1	3.29	1.45	1.38
31	Y	54	5MU	C4-N3	-3.23	1.32	1.38
29	W	54	5MU	C4-N3	-3.21	1.32	1.38
5	72	955	PSU	O4-C4	-3.20	1.17	1.23
5	72	2580	PSU	O4-C4	-3.16	1.17	1.23
5	72	2605	PSU	O4-C4	-3.15	1.17	1.23
29	W	32	PSU	O4-C4	-3.15	1.17	1.23
30	W1	39	PSU	O4-C4	-3.13	1.17	1.23
5	72	2604	PSU	O4-C4	-3.13	1.17	1.23
5	72	2457	PSU	O4-C4	-3.13	1.17	1.23
31	Y	54	5MU	O3'-C3'	3.12	1.50	1.43
30	W1	32	PSU	O4-C4	-3.11	1.17	1.23
7	A1	1498	UR3	C6-N1	3.10	1.45	1.38
7	A2	1498	UR3	C6-N1	3.10	1.45	1.38
5	72	1939	5MU	O3'-C3'	3.10	1.50	1.43
5	72	2504	PSU	O4-C4	-3.08	1.17	1.23
29	W	54	5MU	O3'-C3'	3.07	1.50	1.43
7	A2	527	G7M	C2-N1	3.06	1.45	1.37
7	A1	527	G7M	C2-N1	3.06	1.45	1.37
31	Y	46	G7M	C2-N1	3.04	1.45	1.37
5	72	2069	G7M	C2-N1	3.04	1.45	1.37
5	72	2251	OMG	C6-N1	3.03	1.42	1.37
29	W	46	G7M	C2-N1	3.00	1.45	1.37
30	W1	46	G7M	C2-N1	3.00	1.45	1.37
5	72	2251	OMG	C5-C6	2.94	1.53	1.47
5	72	2498	OMC	C5-C4	2.85	1.49	1.42
5	72	2580	PSU	C1'-C5	2.82	1.56	1.50
5	72	2504	PSU	C1'-C5	2.81	1.56	1.50
5	72	2605	PSU	C1'-C5	2.80	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	W1	39	PSU	C1'-C5	2.77	1.56	1.50
30	W1	32	PSU	C1'-C5	2.76	1.56	1.50
5	72	955	PSU	C1'-C5	2.76	1.56	1.50
5	72	2457	PSU	C1'-C5	2.73	1.56	1.50
5	72	1939	5MU	C3'-C4'	2.72	1.59	1.53
7	A1	1519	MA6	C2-N3	2.71	1.36	1.32
5	72	2604	PSU	C1'-C5	2.71	1.56	1.50
7	A2	1402	4OC	O2-C2	-2.71	1.18	1.23
7	A1	1402	4OC	O2-C2	-2.69	1.18	1.23
29	W	32	PSU	C1'-C5	2.68	1.56	1.50
7	A1	1518	MA6	C2-N3	2.67	1.36	1.32
7	A2	1518	MA6	C2-N3	2.67	1.36	1.32
5	72	1939	5MU	O4-C4	-2.66	1.18	1.23
7	A2	1519	MA6	C2-N3	2.65	1.36	1.32
5	71	1915	3TD	C1'-C5	2.63	1.56	1.50
5	71	1915	3TD	C4-N3	2.63	1.46	1.40
32	Y1	34	CM0	O5-C7	-2.61	1.38	1.44
5	72	2605	PSU	O2-C2	-2.60	1.17	1.23
5	72	2604	PSU	O2-C2	-2.59	1.18	1.23
29	W	54	5MU	O4-C4	-2.59	1.18	1.23
29	W	32	PSU	O2-C2	-2.58	1.18	1.23
5	72	2504	PSU	O2-C2	-2.58	1.18	1.23
30	W1	39	PSU	O2-C2	-2.58	1.18	1.23
5	72	955	PSU	O2-C2	-2.57	1.18	1.23
30	W1	32	PSU	O2-C2	-2.56	1.18	1.23
5	72	2457	PSU	O2-C2	-2.56	1.18	1.23
5	72	2580	PSU	O2-C2	-2.54	1.18	1.23
29	W	37	MIA	C5-C4	-2.54	1.34	1.40
7	A1	1207	2MG	C5-C4	-2.54	1.36	1.43
31	Y	54	5MU	O4-C4	-2.53	1.18	1.23
7	A1	966	2MG	C5-C4	-2.53	1.36	1.43
31	Y	54	5MU	O2-C2	-2.52	1.18	1.23
7	A2	1516	2MG	C5-C4	-2.52	1.36	1.43
32	Y1	46	7MG	O6-C6	-2.50	1.18	1.23
5	72	745	1MG	C6-N1	2.49	1.43	1.39
7	A2	1207	2MG	C5-C4	-2.47	1.36	1.43
7	A1	1516	2MG	C5-C4	-2.46	1.36	1.43
7	A2	966	2MG	C5-C4	-2.45	1.36	1.43
5	72	1835	2MG	C5-C4	-2.42	1.36	1.43
5	72	2445	2MG	C5-C4	-2.41	1.36	1.43
30	W1	37	MIA	C5-C4	-2.40	1.34	1.40
5	72	2251	OMG	C5-C4	-2.38	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2552	OMU	C5-C4	2.37	1.48	1.43
31	Y	54	5MU	C3'-C4'	2.31	1.58	1.53
5	72	745	1MG	C5-C6	2.31	1.54	1.47
7	A1	1518	MA6	C5-C4	-2.30	1.34	1.40
7	A2	1518	MA6	C5-C4	-2.30	1.34	1.40
5	72	745	1MG	C5-C4	-2.30	1.37	1.43
7	A2	1519	MA6	C5-C4	-2.29	1.34	1.40
7	A1	1498	UR3	C5-C4	2.29	1.49	1.43
5	72	1939	5MU	O2-C2	-2.28	1.18	1.23
5	72	2449	H2U	O2-C2	-2.27	1.18	1.23
7	A1	1407	5MC	O2-C2	-2.27	1.19	1.23
31	Y	17	H2U	O2-C2	-2.27	1.18	1.23
5	71	1915	3TD	O4-C4	-2.26	1.18	1.23
7	A2	1498	UR3	C5-C4	2.26	1.49	1.43
7	A1	1498	UR3	C4-N3	2.26	1.45	1.40
29	W	54	5MU	O2-C2	-2.26	1.18	1.23
29	W	20	H2U	O2-C2	-2.25	1.18	1.23
7	A2	967	5MC	O2-C2	-2.24	1.19	1.23
32	Y1	37	6MZ	C5-C4	-2.23	1.35	1.40
7	A1	1519	MA6	C5-C4	-2.23	1.35	1.40
5	72	1962	5MC	O2-C2	-2.23	1.19	1.23
29	W	16	H2U	O2-C2	-2.23	1.19	1.23
7	A2	1407	5MC	O2-C2	-2.22	1.19	1.23
7	A2	1498	UR3	C4-N3	2.20	1.45	1.40
5	72	1618	6MZ	C5-C4	-2.19	1.35	1.40
29	W	17	H2U	O2-C2	-2.19	1.19	1.23
7	A1	967	5MC	O2-C2	-2.19	1.19	1.23
5	72	2030	6MZ	C5-C4	-2.18	1.35	1.40
29	W	46	G7M	O6-C6	-2.17	1.18	1.23
29	W	20	H2U	O4-C4	-2.17	1.18	1.23
29	W	54	5MU	O5'-C5'	-2.15	1.39	1.44
5	72	2069	G7M	O6-C6	-2.15	1.18	1.23
5	72	1939	5MU	C1'-N1	-2.15	1.41	1.47
7	A2	1498	UR3	O2-C2	-2.13	1.18	1.22
7	A1	527	G7M	O6-C6	-2.13	1.19	1.23
29	W	16	H2U	O4-C4	-2.13	1.18	1.23
31	Y	46	G7M	O6-C6	-2.12	1.19	1.23
29	W	17	H2U	O4-C4	-2.12	1.19	1.23
7	A2	1498	UR3	O4-C4	-2.12	1.19	1.23
31	Y	17	H2U	O4-C4	-2.12	1.19	1.23
30	W1	46	G7M	O6-C6	-2.12	1.19	1.23
7	A2	527	G7M	C8-N7	2.11	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A1	1498	UR3	O4-C4	-2.11	1.19	1.23
31	Y	46	G7M	C8-N7	2.10	1.37	1.33
7	A1	527	G7M	C8-N7	2.10	1.36	1.33
7	A2	527	G7M	O6-C6	-2.10	1.19	1.23
32	Y1	37	6MZ	C2-N3	2.09	1.35	1.32
5	72	2449	H2U	O4-C4	-2.09	1.19	1.23
5	72	2030	6MZ	C2-N3	2.08	1.35	1.32
5	72	2069	G7M	C8-N7	2.06	1.36	1.33
5	72	2445	2MG	O6-C6	-2.06	1.19	1.23
5	72	2503	2MA	C5-N7	-2.05	1.32	1.39
5	72	1618	6MZ	C2-N3	2.05	1.35	1.32
5	72	2030	6MZ	C2-N1	2.05	1.37	1.33
7	A1	1516	2MG	O6-C6	-2.05	1.19	1.23
7	A1	1498	UR3	O2-C2	-2.03	1.18	1.22
7	A2	1516	2MG	O6-C6	-2.03	1.19	1.23
7	A2	1207	2MG	O6-C6	-2.02	1.19	1.23
7	A2	966	2MG	O6-C6	-2.02	1.19	1.23
29	W	46	G7M	C8-N7	2.01	1.36	1.33

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2503	2MA	C1'-N9-C4	15.31	153.54	126.64
7	A1	1519	MA6	N1-C6-N6	-12.47	103.93	117.06
7	A1	1518	MA6	N1-C6-N6	-12.27	104.14	117.06
7	A2	1519	MA6	N1-C6-N6	-12.21	104.21	117.06
7	A2	1518	MA6	N1-C6-N6	-12.05	104.38	117.06
29	W	37	MIA	C11-S10-C2	11.45	110.82	102.27
30	W1	37	MIA	C11-S10-C2	10.67	110.23	102.27
31	Y	54	5MU	C4-N3-C2	-9.10	115.57	127.35
29	W	54	5MU	C5M-C5-C4	9.07	128.75	118.77
5	72	1939	5MU	C4-N3-C2	-9.06	115.61	127.35
31	Y	54	5MU	N3-C2-N1	8.69	126.42	114.89
31	Y	54	5MU	C5M-C5-C4	8.65	128.28	118.77
5	72	1939	5MU	C5M-C5-C4	8.53	128.16	118.77
5	72	1939	5MU	C5-C6-N1	-8.48	114.61	123.34
29	W	54	5MU	C4-N3-C2	-8.44	116.42	127.35
31	Y	54	5MU	C5-C6-N1	-8.40	114.70	123.34
5	72	1939	5MU	N3-C2-N1	8.26	125.85	114.89
29	W	54	5MU	N3-C2-N1	8.08	125.61	114.89
30	W1	8	4SU	C4-N3-C2	-7.87	119.69	127.34
29	W	8	4SU	C4-N3-C2	-7.77	119.79	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	54	5MU	C5-C6-N1	-7.51	115.61	123.34
29	W	54	5MU	C5M-C5-C6	-7.21	113.22	122.85
31	Y	54	5MU	C5M-C5-C6	-7.21	113.23	122.85
5	72	2449	H2U	C4-N3-C2	-7.15	119.86	125.79
29	W	17	H2U	C4-N3-C2	-7.02	119.97	125.79
29	W	20	H2U	C4-N3-C2	-7.01	119.98	125.79
31	Y	17	H2U	C4-N3-C2	-7.01	119.98	125.79
5	72	1939	5MU	C5M-C5-C6	-6.92	113.61	122.85
29	W	16	H2U	C4-N3-C2	-6.85	120.11	125.79
5	72	1939	5MU	C5-C4-N3	6.78	121.09	115.31
31	Y	54	5MU	C5-C4-N3	6.22	120.62	115.31
29	W	54	5MU	C5-C4-N3	6.14	120.56	115.31
32	Y1	37	6MZ	C1'-N9-C4	-5.92	116.24	126.64
29	W	37	MIA	C1'-N9-C4	-5.81	116.43	126.64
7	A2	1519	MA6	N3-C2-N1	-5.63	119.88	128.68
5	72	1618	6MZ	N3-C2-N1	-5.60	119.92	128.68
7	A2	1518	MA6	C1'-N9-C4	5.60	136.48	126.64
32	Y1	37	6MZ	N3-C2-N1	-5.59	119.94	128.68
7	A1	1519	MA6	N3-C2-N1	-5.56	119.98	128.68
5	72	2503	2MA	C2-N3-C4	5.55	120.03	115.52
30	W1	8	4SU	C5-C4-N3	5.55	119.84	114.69
7	A1	1518	MA6	N3-C2-N1	-5.53	120.03	128.68
7	A2	1518	MA6	N3-C2-N1	-5.52	120.05	128.68
29	W	8	4SU	C5-C4-N3	5.51	119.80	114.69
5	72	2030	6MZ	N3-C2-N1	-5.50	120.08	128.68
5	72	2030	6MZ	C1'-N9-C4	-5.49	116.99	126.64
32	Y1	34	CM0	C4-N3-C2	-5.46	120.28	127.35
7	A1	1519	MA6	C1'-N9-C4	5.46	136.23	126.64
7	A1	1518	MA6	C1'-N9-C4	5.35	136.04	126.64
5	71	1915	3TD	N1-C2-N3	5.30	120.32	116.14
31	Y	54	5MU	O2-C2-N1	-5.29	115.75	122.79
7	A2	1519	MA6	C1'-N9-C4	5.21	135.79	126.64
5	72	2552	OMU	C4-N3-C2	-5.18	119.75	126.58
32	Y1	46	7MG	C5-C6-N1	5.03	119.86	110.99
29	W	32	PSU	C4-N3-C2	-4.74	119.51	126.34
5	72	2604	PSU	C4-N3-C2	-4.65	119.63	126.34
7	A1	1498	UR3	C4-N3-C2	-4.65	120.19	124.56
5	72	955	PSU	C4-N3-C2	-4.63	119.67	126.34
5	72	2457	PSU	C4-N3-C2	-4.60	119.71	126.34
5	72	2504	PSU	C4-N3-C2	-4.60	119.72	126.34
30	W1	32	PSU	C4-N3-C2	-4.59	119.73	126.34
5	72	2580	PSU	C4-N3-C2	-4.59	119.73	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2605	PSU	C4-N3-C2	-4.58	119.74	126.34
30	W1	39	PSU	C4-N3-C2	-4.54	119.79	126.34
7	A2	1498	UR3	C4-N3-C2	-4.52	120.30	124.56
32	Y1	46	7MG	C2-N3-C4	4.48	120.29	112.30
32	Y1	37	6MZ	C2-N1-C6	4.27	120.25	116.59
29	W	32	PSU	N1-C2-N3	4.26	119.96	115.13
5	72	1618	6MZ	C1'-N9-C4	-4.25	119.18	126.64
5	72	1939	5MU	O2-C2-N1	-4.23	117.17	122.79
5	72	2030	6MZ	C2-N1-C6	4.23	120.21	116.59
5	72	955	PSU	N1-C2-N3	4.21	119.90	115.13
5	72	2604	PSU	N1-C2-N3	4.20	119.89	115.13
5	72	1939	5MU	O4-C4-N3	-4.17	112.13	120.12
5	72	2580	PSU	N1-C2-N3	4.14	119.82	115.13
5	72	2457	PSU	N1-C2-N3	4.13	119.81	115.13
30	W1	39	PSU	N1-C2-N3	4.12	119.80	115.13
5	72	2605	PSU	N1-C2-N3	4.10	119.78	115.13
30	W1	32	PSU	N1-C2-N3	4.08	119.76	115.13
5	71	1915	3TD	C4-N3-C2	-4.07	120.19	124.61
5	72	2504	PSU	N1-C2-N3	4.07	119.74	115.13
29	W	54	5MU	O4-C4-N3	-4.05	112.35	120.12
31	Y	54	5MU	O4-C4-N3	-4.03	112.39	120.12
5	72	745	1MG	C5-C6-N1	4.02	119.94	113.90
30	W1	37	MIA	C1'-N9-C4	-4.01	119.59	126.64
32	Y1	46	7MG	C5-C4-N3	-3.99	120.53	128.13
29	W	8	4SU	C5-C4-S4	-3.92	119.41	124.47
5	72	1939	5MU	C4'-O4'-C1'	-3.91	100.83	109.47
29	W	37	MIA	N3-C2-N1	-3.90	119.81	126.98
5	72	1618	6MZ	C2-N1-C6	3.83	119.87	116.59
5	72	2552	OMU	N3-C2-N1	3.77	119.89	114.89
29	W	8	4SU	N3-C2-N1	3.76	119.88	114.89
30	W1	8	4SU	N3-C2-N1	3.73	119.84	114.89
30	W1	37	MIA	N3-C2-N1	-3.73	120.13	126.98
30	W1	37	MIA	C12-C13-C14	-3.64	120.06	127.14
5	72	1835	2MG	C5-C6-N1	3.58	120.28	113.95
29	W	37	MIA	C2-N3-C4	3.56	120.23	115.32
32	Y1	34	CM0	N3-C2-N1	3.55	119.60	114.89
30	W1	37	MIA	C2-N3-C4	3.55	120.21	115.32
29	W	32	PSU	C6-C5-C4	3.54	120.67	118.20
5	72	2445	2MG	C5-C6-N1	3.52	120.18	113.95
29	W	54	5MU	O2-C2-N1	-3.48	118.16	122.79
7	A2	966	2MG	C5-C6-N1	3.48	120.09	113.95
30	W1	8	4SU	C5-C4-S4	-3.47	120.00	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A1	1516	2MG	C5-C6-N1	3.47	120.08	113.95
7	A1	966	2MG	C5-C6-N1	3.47	120.07	113.95
7	A2	1516	2MG	C5-C6-N1	3.43	120.02	113.95
7	A2	1207	2MG	C5-C6-N1	3.42	119.99	113.95
5	72	1618	6MZ	C9-N6-C6	-3.41	119.94	122.87
5	72	2251	OMG	C5-C6-N1	3.37	119.91	113.95
7	A1	967	5MC	C5-C6-N1	-3.37	119.88	123.34
5	72	1962	5MC	C5-C6-N1	-3.37	119.88	123.34
7	A1	1207	2MG	C5-C6-N1	3.36	119.88	113.95
29	W	37	MIA	C12-N6-C6	-3.35	117.58	122.55
5	72	2552	OMU	C5-C4-N3	3.35	119.84	114.84
5	72	2457	PSU	C6-C5-C4	3.28	120.49	118.20
29	W	20	H2U	N3-C2-N1	3.26	120.10	116.65
5	72	1939	5MU	C6-N1-C2	3.25	124.59	121.30
5	72	2449	H2U	N3-C2-N1	3.24	120.08	116.65
32	Y1	46	7MG	C4-C5-N7	3.22	110.00	105.53
29	W	17	H2U	N3-C2-N1	3.21	120.05	116.65
5	72	2604	PSU	C6-C5-C4	3.18	120.42	118.20
31	Y	17	H2U	N3-C2-N1	3.16	119.99	116.65
29	W	54	5MU	C4'-O4'-C1'	-3.14	102.54	109.47
29	W	16	H2U	N3-C2-N1	3.13	119.97	116.65
7	A2	967	5MC	C5-C6-N1	-3.13	120.12	123.34
30	W1	46	G7M	C2-N1-C6	-3.11	119.37	125.10
29	W	37	MIA	C12-C13-C14	-3.10	121.11	127.14
29	W	46	G7M	C2-N1-C6	-3.05	119.47	125.10
5	72	2503	2MA	N3-C2-N1	-3.05	120.16	125.73
5	72	955	PSU	C6-C5-C4	3.03	120.32	118.20
5	72	2580	PSU	C6-C5-C4	3.00	120.30	118.20
30	W1	39	PSU	C6-C5-C4	3.00	120.29	118.20
32	Y1	46	7MG	C5-C4-N9	2.97	110.21	106.35
29	W	37	MIA	S10-C2-N3	2.96	126.37	116.10
5	72	2251	OMG	C8-N7-C5	2.93	108.57	102.99
5	72	955	PSU	C6-N1-C2	-2.93	119.69	122.68
5	72	2504	PSU	C6-C5-C4	2.92	120.24	118.20
30	W1	32	PSU	C6-C5-C4	2.91	120.24	118.20
7	A2	527	G7M	C2-N1-C6	-2.90	119.76	125.10
5	72	2605	PSU	C6-N1-C2	-2.90	119.72	122.68
32	Y1	34	CM0	C7-O5-C5	-2.90	113.78	117.58
31	Y	46	G7M	C2-N1-C6	-2.89	119.77	125.10
5	72	2069	G7M	C2-N1-C6	-2.89	119.77	125.10
30	W1	32	PSU	C6-N1-C2	-2.89	119.73	122.68
30	W1	39	PSU	C6-N1-C2	-2.88	119.74	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	54	5MU	C6-N1-C2	2.87	124.20	121.30
5	72	2604	PSU	C6-N1-C2	-2.86	119.75	122.68
5	72	2251	OMG	C2-N1-C6	-2.86	119.83	125.10
5	72	2552	OMU	O4-C4-C5	-2.86	120.14	125.16
7	A1	527	G7M	C2-N1-C6	-2.85	119.85	125.10
31	Y	17	H2U	C5-C4-N3	2.84	119.84	116.65
29	W	54	5MU	O2-C2-N3	-2.83	116.23	121.50
5	72	2449	H2U	C5-C4-N3	2.83	119.83	116.65
32	Y1	46	7MG	O6-C6-C5	-2.80	120.67	127.54
5	72	2580	PSU	C6-N1-C2	-2.80	119.82	122.68
5	72	2504	PSU	C6-N1-C2	-2.80	119.82	122.68
31	Y	54	5MU	C4'-O4'-C1'	-2.80	103.30	109.47
29	W	16	H2U	C5-C4-N3	2.78	119.78	116.65
5	72	2457	PSU	C6-N1-C2	-2.78	119.84	122.68
7	A1	1407	5MC	C5-C6-N1	-2.78	120.48	123.34
7	A2	1407	5MC	C5-C6-N1	-2.78	120.48	123.34
5	72	2605	PSU	C6-C5-C4	2.78	120.14	118.20
29	W	17	H2U	C5-C4-N3	2.78	119.77	116.65
30	W1	37	MIA	S10-C2-N3	2.77	125.71	116.10
29	W	32	PSU	C6-N1-C2	-2.76	119.86	122.68
32	Y1	46	7MG	C2-N1-C6	-2.74	120.10	125.10
29	W	20	H2U	C5-C4-N3	2.74	119.72	116.65
7	A1	966	2MG	C8-N7-C5	2.73	108.20	102.99
5	72	745	1MG	C8-N7-C5	2.73	108.19	102.99
29	W	16	H2U	C5-C6-N1	2.71	120.55	111.61
29	W	54	5MU	O4'-C4'-C3'	-2.69	99.79	105.11
31	Y	17	H2U	C5-C6-N1	2.66	120.38	111.61
7	A1	1516	2MG	C8-N7-C5	2.66	108.06	102.99
5	72	2445	2MG	C8-N7-C5	2.66	108.05	102.99
7	A2	966	2MG	C8-N7-C5	2.66	108.05	102.99
29	W	20	H2U	C5-C6-N1	2.65	120.33	111.61
29	W	17	H2U	C5-C6-N1	2.64	120.30	111.61
5	72	1835	2MG	C8-N7-C5	2.62	107.98	102.99
7	A2	1516	2MG	C8-N7-C5	2.61	107.97	102.99
7	A1	1207	2MG	C8-N7-C5	2.59	107.92	102.99
5	72	2449	H2U	C5-C6-N1	2.58	120.12	111.61
7	A2	1207	2MG	C8-N7-C5	2.58	107.91	102.99
5	72	955	PSU	O2-C2-N1	-2.56	119.97	122.79
32	Y1	46	7MG	N9-C4-N3	2.54	129.27	125.47
29	W	17	H2U	O2-C2-N1	-2.53	119.92	123.11
32	Y1	37	6MZ	C9-N6-C6	-2.51	120.71	122.87
5	72	2449	H2U	O2-C2-N1	-2.50	119.97	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	20	H2U	O2-C2-N1	-2.50	119.97	123.11
31	Y	17	H2U	O2-C2-N1	-2.46	120.02	123.11
30	W1	39	PSU	O2-C2-N1	-2.45	120.09	122.79
5	72	2604	PSU	O2-C2-N1	-2.45	120.10	122.79
29	W	54	5MU	C6-N1-C2	2.45	123.77	121.30
5	72	2457	PSU	O2-C2-N1	-2.44	120.11	122.79
5	72	2580	PSU	O2-C2-N1	-2.44	120.11	122.79
5	72	1939	5MU	O2-C2-N3	-2.43	116.98	121.50
31	Y	54	5MU	C3'-C2'-C1'	2.43	106.04	101.43
29	W	32	PSU	O2-C2-N1	-2.42	120.12	122.79
30	W1	32	PSU	O2-C2-N1	-2.41	120.13	122.79
5	72	2504	PSU	O2-C2-N1	-2.41	120.14	122.79
7	A2	1498	UR3	C1'-N1-C2	2.41	121.05	116.99
5	72	745	1MG	O6-C6-C5	-2.40	119.95	124.19
29	W	16	H2U	O2-C2-N1	-2.40	120.10	123.11
5	72	1835	2MG	O6-C6-C5	-2.39	119.70	124.37
5	72	2605	PSU	O2-C2-N1	-2.39	120.16	122.79
30	W1	37	MIA	C16-C14-C15	2.37	119.84	114.60
7	A1	1402	4OC	C6-C5-C4	2.35	119.84	116.96
7	A2	1402	4OC	C6-C5-C4	2.35	119.83	116.96
5	72	1835	2MG	CM2-N2-C2	-2.30	118.77	123.86
7	A1	1516	2MG	O6-C6-C5	-2.27	119.93	124.37
7	A2	1498	UR3	C6-N1-C2	-2.27	119.76	121.79
7	A2	1516	2MG	O6-C6-C5	-2.27	119.95	124.37
5	72	2445	2MG	O6-C6-C5	-2.26	119.96	124.37
7	A2	966	2MG	O6-C6-C5	-2.26	119.96	124.37
32	Y1	46	7MG	N9-C8-N7	2.25	106.60	103.38
7	A1	966	2MG	O6-C6-C5	-2.24	120.00	124.37
5	72	1962	5MC	CM5-C5-C6	-2.23	119.87	122.85
7	A1	1207	2MG	O6-C6-C5	-2.22	120.03	124.37
7	A2	1207	2MG	O6-C6-C5	-2.22	120.04	124.37
29	W	37	MIA	C16-C14-C15	2.22	119.50	114.60
7	A2	1407	5MC	CM5-C5-C6	-2.18	119.93	122.85
29	W	54	5MU	O4'-C1'-N1	2.17	113.31	108.36
5	72	1939	5MU	O4'-C1'-N1	2.16	113.31	108.36
5	72	2251	OMG	O6-C6-C5	-2.15	120.17	124.37
7	A1	1407	5MC	CM5-C5-C6	-2.14	119.99	122.85
7	A1	967	5MC	CM5-C5-C6	-2.12	120.02	122.85
7	A1	966	2MG	CM2-N2-C2	-2.11	119.20	123.86
31	Y	54	5MU	O4'-C1'-N1	2.11	113.18	108.36
7	A1	1498	UR3	C6-N1-C2	-2.08	119.93	121.79
5	72	2552	OMU	O2-C2-N1	-2.05	120.06	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2580	PSU	O4'-C1'-C2'	2.05	108.03	105.14
7	A2	967	5MC	CM5-C5-C6	-2.01	120.16	122.85

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	1402	4OC	C1'-C2'-O2'-CM2
7	A1	1518	MA6	C5-C6-N6-C9
7	A1	1518	MA6	C5-C6-N6-C10
7	A1	1519	MA6	C3'-C4'-C5'-O5'
7	A2	1402	4OC	C1'-C2'-O2'-CM2
31	Y	17	H2U	O4'-C4'-C5'-O5'
31	Y	17	H2U	C3'-C4'-C5'-O5'
31	Y	17	H2U	O4'-C1'-N1-C6
31	Y	17	H2U	C2'-C1'-N1-C2
31	Y	17	H2U	C2'-C1'-N1-C6
32	Y1	37	6MZ	N1-C6-N6-C9
5	72	746	PSU	C2'-C1'-C5-C4
5	72	746	PSU	C2'-C1'-C5-C6
5	72	747	5MU	C3'-C4'-C5'-O5'
5	72	1618	6MZ	C5-C6-N6-C9
5	72	1618	6MZ	N1-C6-N6-C9
5	72	1618	6MZ	O4'-C4'-C5'-O5'
5	72	1618	6MZ	C3'-C4'-C5'-O5'
5	72	1939	5MU	O4'-C4'-C5'-O5'
5	72	2030	6MZ	N1-C6-N6-C9
5	72	2251	OMG	O4'-C4'-C5'-O5'
5	72	2251	OMG	C1'-C2'-O2'-CM2
29	W	37	MIA	O4'-C4'-C5'-O5'
29	W	37	MIA	C3'-C4'-C5'-O5'
29	W	37	MIA	N1-C2-S10-C11
29	W	37	MIA	N3-C2-S10-C11
29	W	37	MIA	N6-C12-C13-C14
29	W	54	5MU	O4'-C4'-C5'-O5'
30	W1	8	4SU	O4'-C4'-C5'-O5'
30	W1	37	MIA	N1-C2-S10-C11
30	W1	37	MIA	N3-C2-S10-C11
29	W	46	G7M	C4'-C5'-O5'-P
7	A1	1498	UR3	O4'-C4'-C5'-O5'
7	A1	1519	MA6	O4'-C4'-C5'-O5'
7	A2	1498	UR3	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
31	Y	46	G7M	C3'-C4'-C5'-O5'
5	72	747	5MU	O4'-C4'-C5'-O5'
5	72	1939	5MU	C3'-C4'-C5'-O5'
5	72	2251	OMG	C3'-C4'-C5'-O5'
5	72	2498	OMC	O4'-C4'-C5'-O5'
29	W	17	H2U	O4'-C4'-C5'-O5'
29	W	32	PSU	O4'-C4'-C5'-O5'
29	W	54	5MU	C3'-C4'-C5'-O5'
30	W1	8	4SU	C3'-C4'-C5'-O5'
30	W1	37	MIA	O4'-C4'-C5'-O5'
30	W1	37	MIA	C3'-C4'-C5'-O5'
30	W1	46	G7M	O4'-C4'-C5'-O5'
32	Y1	34	CM0	O5-C7-C8-O8
32	Y1	34	CM0	O5-C7-C8-O9
7	A1	1498	UR3	C3'-C4'-C5'-O5'
7	A2	1498	UR3	C3'-C4'-C5'-O5'
7	A2	1519	MA6	O4'-C4'-C5'-O5'
5	72	2498	OMC	C3'-C4'-C5'-O5'
29	W	17	H2U	C3'-C4'-C5'-O5'
30	W1	46	G7M	C3'-C4'-C5'-O5'
32	Y1	34	CM0	C3'-C4'-C5'-O5'
32	Y1	34	CM0	O4'-C4'-C5'-O5'
7	A1	1518	MA6	N1-C6-N6-C10
29	W	32	PSU	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C4'-C5'-O5'-P
7	A2	1518	MA6	C5-C6-N6-C10
31	Y	46	G7M	O4'-C4'-C5'-O5'
32	Y1	37	6MZ	C5-C6-N6-C9
5	72	2030	6MZ	C5-C6-N6-C9
7	A2	1519	MA6	C3'-C4'-C5'-O5'
7	A1	527	G7M	C4'-C5'-O5'-P
29	W	20	H2U	C4'-C5'-O5'-P
29	W	54	5MU	C4'-C5'-O5'-P
29	W	16	H2U	C4'-C5'-O5'-P
29	W	37	MIA	C4'-C5'-O5'-P
7	A2	527	G7M	C3'-C4'-C5'-O5'
7	A2	527	G7M	C4'-C5'-O5'-P
31	Y	17	H2U	C4'-C5'-O5'-P
5	72	2069	G7M	C4'-C5'-O5'-P
29	W	32	PSU	C4'-C5'-O5'-P
29	W	20	H2U	O4'-C4'-C5'-O5'
32	Y1	46	7MG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
5	72	746	PSU	O4'-C1'-C5-C4
29	W	32	PSU	O4'-C1'-C5-C4
31	Y	17	H2U	O4'-C1'-N1-C2
7	A2	1518	MA6	C5-C6-N6-C9
7	A2	527	G7M	O4'-C4'-C5'-O5'
5	72	2069	G7M	O4'-C4'-C5'-O5'
7	A1	967	5MC	O4'-C4'-C5'-O5'
29	W	20	H2U	C3'-C4'-C5'-O5'
5	72	746	PSU	O4'-C1'-C5-C6
29	W	32	PSU	O4'-C1'-C5-C6
5	72	1939	5MU	C4'-C5'-O5'-P
7	A2	967	5MC	O4'-C4'-C5'-O5'
5	72	2030	6MZ	O4'-C4'-C5'-O5'
5	71	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](#)

Of 273 ligands modelled in this entry, 270 are monoatomic - leaving 3 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	$\# Z  > 2$
46	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.52	0
46	PUT	72	3002	-	5,5,5	0.26	0	4,4,4	0.54	0
47	SPD	72	3003	-	9,9,9	0.32	0	8,8,8	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PUT	72	3001	-	-	1/3/3/3	-
46	PUT	72	3002	-	-	0/3/3/3	-
47	SPD	72	3003	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.