



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 12:05 PM BST

PDB ID : 5F8K  
Title : Crystal structure of the Bac7(1-16) antimicrobial peptide bound to the *Thermus thermophilus* 70S ribosome  
Authors : Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian, M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.  
Deposited on : 2015-12-09  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

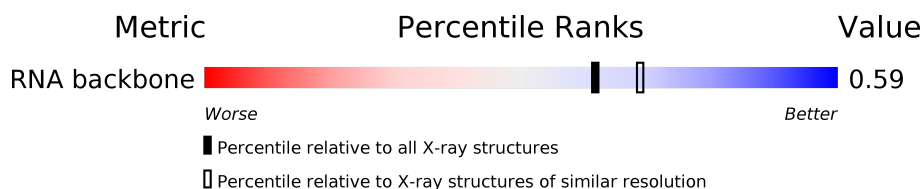
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
RNA backbone	3102	1227 (3.10-2.50)
















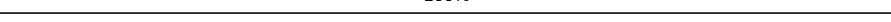
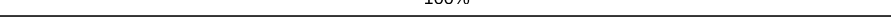
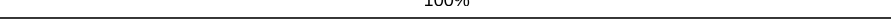
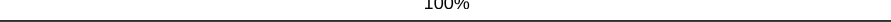
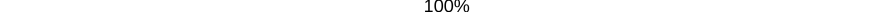
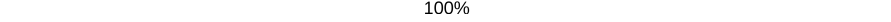
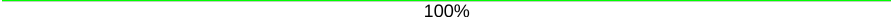
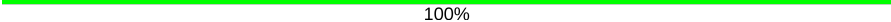

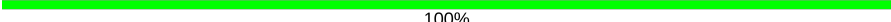
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1A	2915	 82% 16% ..
1	2A	2915	 83% 15% ..
2	1B	120	 93% 8%
2	2B	120	 94% 5% .
3	1D	275	 100%
3	2D	275	 100%
4	1E	204	 100%
4	2E	204	 100%
5	1F	203	 100%
5	2F	203	 100%
















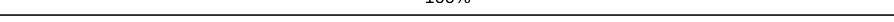
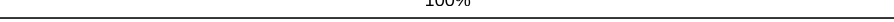
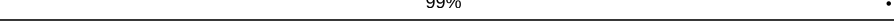
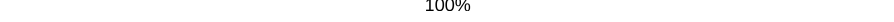
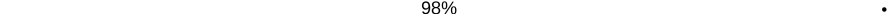
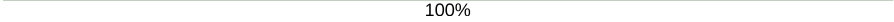
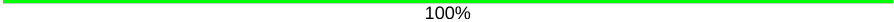

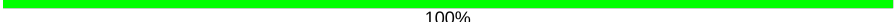
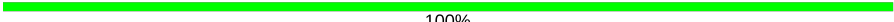
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Mol	Chain	Length	Quality of chain
6	1G	181	 100%
6	2G	181	 100%
7	1H	174	 100%
7	2H	174	 99%
8	1I	147	 100%
8	2I	147	 99%
9	1N	140	 100%
9	2N	140	 100%
10	1O	122	 100%
10	2O	122	 100%
11	1P	149	 100%
11	2P	149	 100%
12	1Q	141	 99%
12	2Q	141	 100%
13	1R	118	 100%
13	2R	118	 100%
14	1S	110	 100%
14	2S	110	 100%
15	1T	131	 100%
15	2T	131	 100%
16	1U	116	 100%
16	2U	116	 100%
17	1V	101	 100%
17	2V	101	 100%
18	1W	112	 100%
















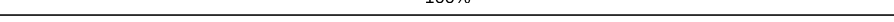
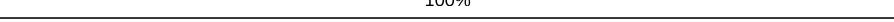
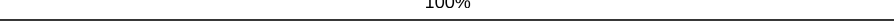
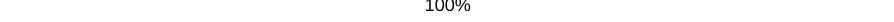
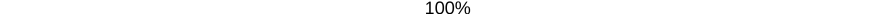
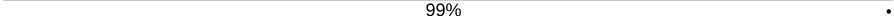
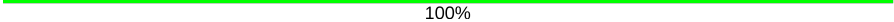
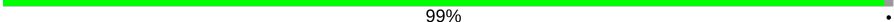
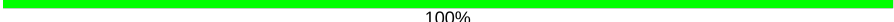
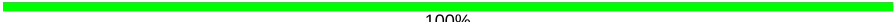
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Mol	Chain	Length	Quality of chain
18	2W	112	 100%
19	1X	95	 100%
19	2X	95	 99%
20	1Y	107	 100%
20	2Y	107	 100%
21	1Z	203	 100%
21	2Z	203	 99%
22	10	77	 100%
22	20	77	 100%
23	11	97	 100%
23	21	97	 100%
24	12	70	 99%
24	22	70	 100%
25	13	59	 100%
25	23	59	 100%
26	14	69	 100%
26	24	69	 99%
27	15	59	 100%
27	25	59	 98%
28	16	53	 100%
28	26	53	 100%
29	17	48	 100%
29	27	48	 100%
30	18	64	 100%
30	28	64	 100%

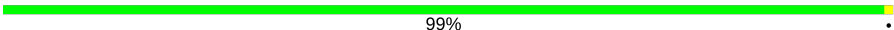

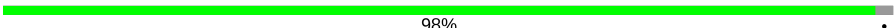

















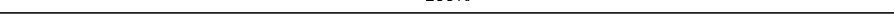
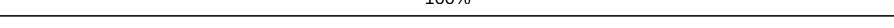
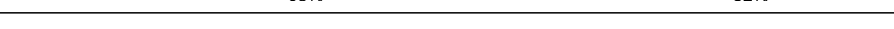
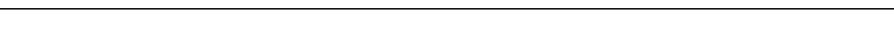

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Mol	Chain	Length	Quality of chain
31	19	37	 100%
31	29	37	 100%
32	1a	1520	 83% 14% ..
32	2a	1520	 82% 15% ..
33	1b	231	 100%
33	2b	231	 100%
34	1c	206	 100%
34	2c	206	 100%
35	1d	208	 100%
35	2d	208	 100%
36	1e	148	 100%
36	2e	148	 100%
37	1f	100	 100%
37	2f	100	 100%
38	1g	155	 100%
38	2g	155	 100%
39	1h	137	 100%
39	2h	137	 100%
40	1i	127	 100%
40	2i	127	 99% .
41	1j	97	 100%
41	2j	97	 99% .
42	1k	114	 100%
42	2k	114	 100%
43	1l	122	 99% .

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Mol	Chain	Length	Quality of chain
43	2l	122	 99%
44	1m	116	 100%
44	2m	116	 98%
45	1n	60	 100%
45	2n	60	 100%
46	1o	88	 100%
46	2o	88	 100%
47	1p	82	 100%
47	2p	82	 100%
48	1q	99	 100%
48	2q	99	 100%
49	1r	68	 100%
49	2r	68	 100%
50	1s	83	 100%
50	2s	83	 100%
51	1t	98	 98%
51	2t	98	 100%
52	1u	23	 100%
52	2u	23	 100%
53	1v	3	 100%
53	2v	3	 100%
54	1x	76	 68% 32%
54	2x	76	 78% 22%
55	1y	16	 94% 6%
55	2y	16	 94% 6%

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 296108 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61872	27540	11574	19886	2872			
1	2A	2867	Total	C	N	O	P	0	0	0
			61761	27491	11552	19852	2866			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2571	1146	476	831	118			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	0	0	0
			1091	680	225	185			
15	2T	131	Total	C	N	O	0	0	0
			1083	675	224	183			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
53	2v	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			

- Molecule 54 is a RNA chain called tRNAiMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
54	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 55 is a protein called Cathelicidin-3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1y	16	Total	C	N	O	0	0	0
			147	90	40	17			
55	2y	16	Total	C	N	O	0	0	0
			147	90	40	17			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	6	Total	Mg	0	0
			6	6		
56	17	2	Total	Mg	0	0
			2	2		
56	2d	4	Total	Mg	0	0
			4	4		
56	1T	1	Total	Mg	0	0
			1	1		
56	1N	4	Total	Mg	0	0
			4	4		
56	20	5	Total	Mg	0	0
			5	5		
56	18	1	Total	Mg	0	0
			1	1		
56	1o	2	Total	Mg	0	0
			2	2		
56	2W	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	2h	2	Total 2	Mg 2	0	0
56	1P	4	Total 4	Mg 4	0	0
56	2B	25	Total 25	Mg 25	0	0
56	1q	1	Total 1	Mg 1	0	0
56	2a	221	Total 221	Mg 221	0	0
56	1E	7	Total 7	Mg 7	0	0
56	1b	1	Total 1	Mg 1	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2F	9	Total 9	Mg 9	0	0
56	28	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	3	Total 3	Mg 3	0	0
56	1A	973	Total 973	Mg 973	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	2P	3	Total 3	Mg 3	0	0
56	1X	1	Total 1	Mg 1	0	0
56	2i	1	Total 1	Mg 1	0	0
56	1S	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	25	3	Total 3	Mg 3	0	0
56	2b	1	Total 1	Mg 1	0	0
56	1D	14	Total 14	Mg 14	0	0
56	2N	3	Total 3	Mg 3	0	0
56	1e	1	Total 1	Mg 1	0	0
56	2G	3	Total 3	Mg 3	0	0
56	29	2	Total 2	Mg 2	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	3	Total 3	Mg 3	0	0
56	2X	2	Total 2	Mg 2	0	0
56	1a	240	Total 240	Mg 240	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	15	7	Total 7	Mg 7	0	0
56	1x	13	Total 13	Mg 13	0	0
56	2j	1	Total 1	Mg 1	0	0
56	1R	4	Total 4	Mg 4	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	1	Total 1	Mg 1	0	0
56	2U	7	Total 7	Mg 7	0	0
56	1G	3	Total 3	Mg 3	0	0
56	11	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1d	5	Total 5	Mg 5	0	0
56	2n	1	Total 1	Mg 1	0	0
56	1H	2	Total 2	Mg 2	0	0
56	2g	1	Total 1	Mg 1	0	0
56	1i	1	Total 1	Mg 1	0	0
56	2Y	2	Total 2	Mg 2	0	0
56	23	2	Total 2	Mg 2	0	0
56	2x	12	Total 12	Mg 12	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2D	17	Total 17	Mg 17	0	0
56	1U	3	Total 3	Mg 3	0	0
56	27	2	Total 2	Mg 2	0	0
56	19	3	Total 3	Mg 3	0	0
56	1l	3	Total 3	Mg 3	0	0
56	2V	1	Total 1	Mg 1	0	0
56	1F	10	Total 10	Mg 10	0	0
56	2H	2	Total 2	Mg 2	0	0
56	10	8	Total 8	Mg 8	0	0
56	1g	1	Total 1	Mg 1	0	0
56	2o	1	Total 1	Mg 1	0	0
56	1Q	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2A	986	Total 986	Mg 986	0	0
56	1h	1	Total 1	Mg 1	0	0
56	1B	27	Total 27	Mg 27	0	0
56	2S	1	Total 1	Mg 1	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	29	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	26	1	Total 1	Zn 1	0	0
57	25	1	Total 1	Zn 1	0	0
57	24	1	Total 1	Zn 1	0	0
57	2n	1	Total 1	Zn 1	0	0
57	2Y	1	Total 1	Zn 1	0	0
57	16	1	Total 1	Zn 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1x	1	Total	K	0	0
			1	1		
59	2A	1	Total	K	0	0
			1	1		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1795	Total	O	0	0
			1795	1795		
60	1B	49	Total	O	0	0
			49	49		
60	1D	23	Total	O	0	0
			23	23		
60	1E	16	Total	O	0	0
			16	16		
60	1F	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1G	2	Total 2	O 2	0	0
60	1H	4	Total 4	O 4	0	0
60	1N	8	Total 8	O 8	0	0
60	1P	14	Total 14	O 14	0	0
60	1Q	6	Total 6	O 6	0	0
60	1R	6	Total 6	O 6	0	0
60	1T	5	Total 5	O 5	0	0
60	1U	3	Total 3	O 3	0	0
60	1V	6	Total 6	O 6	0	0
60	1W	1	Total 1	O 1	0	0
60	1X	6	Total 6	O 6	0	0
60	1Y	4	Total 4	O 4	0	0
60	10	5	Total 5	O 5	0	0
60	11	5	Total 5	O 5	0	0
60	13	1	Total 1	O 1	0	0
60	15	3	Total 3	O 3	0	0
60	16	1	Total 1	O 1	0	0
60	17	2	Total 2	O 2	0	0
60	18	8	Total 8	O 8	0	0
60	19	2	Total 2	O 2	0	0
60	1a	408	Total 408	O 408	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1d	8	Total 8	O 8	0	0
60	1e	3	Total 3	O 3	0	0
60	1f	1	Total 1	O 1	0	0
60	1h	1	Total 1	O 1	0	0
60	1j	1	Total 1	O 1	0	0
60	1l	4	Total 4	O 4	0	0
60	1m	1	Total 1	O 1	0	0
60	1o	2	Total 2	O 2	0	0
60	1p	1	Total 1	O 1	0	0
60	1t	2	Total 2	O 2	0	0
60	1v	2	Total 2	O 2	0	0
60	1x	5	Total 5	O 5	0	0
60	1y	2	Total 2	O 2	0	0
60	2A	1787	Total 1787	O 1787	0	0
60	2B	46	Total 46	O 46	0	0
60	2D	20	Total 20	O 20	0	0
60	2E	15	Total 15	O 15	0	0
60	2F	11	Total 11	O 11	0	0
60	2G	2	Total 2	O 2	0	0
60	2H	4	Total 4	O 4	0	0
60	2N	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2P	17	Total 17	O 17	0	0
60	2Q	4	Total 4	O 4	0	0
60	2R	6	Total 6	O 6	0	0
60	2T	4	Total 4	O 4	0	0
60	2U	5	Total 5	O 5	0	0
60	2V	3	Total 3	O 3	0	0
60	2W	1	Total 1	O 1	0	0
60	2X	5	Total 5	O 5	0	0
60	2Y	8	Total 8	O 8	0	0
60	20	9	Total 9	O 9	0	0
60	21	2	Total 2	O 2	0	0
60	23	2	Total 2	O 2	0	0
60	25	2	Total 2	O 2	0	0
60	26	1	Total 1	O 1	0	0
60	27	2	Total 2	O 2	0	0
60	28	9	Total 9	O 9	0	0
60	29	4	Total 4	O 4	0	0
60	2a	408	Total 408	O 408	0	0
60	2d	7	Total 7	O 7	0	0
60	2e	4	Total 4	O 4	0	0
60	2f	1	Total 1	O 1	0	0

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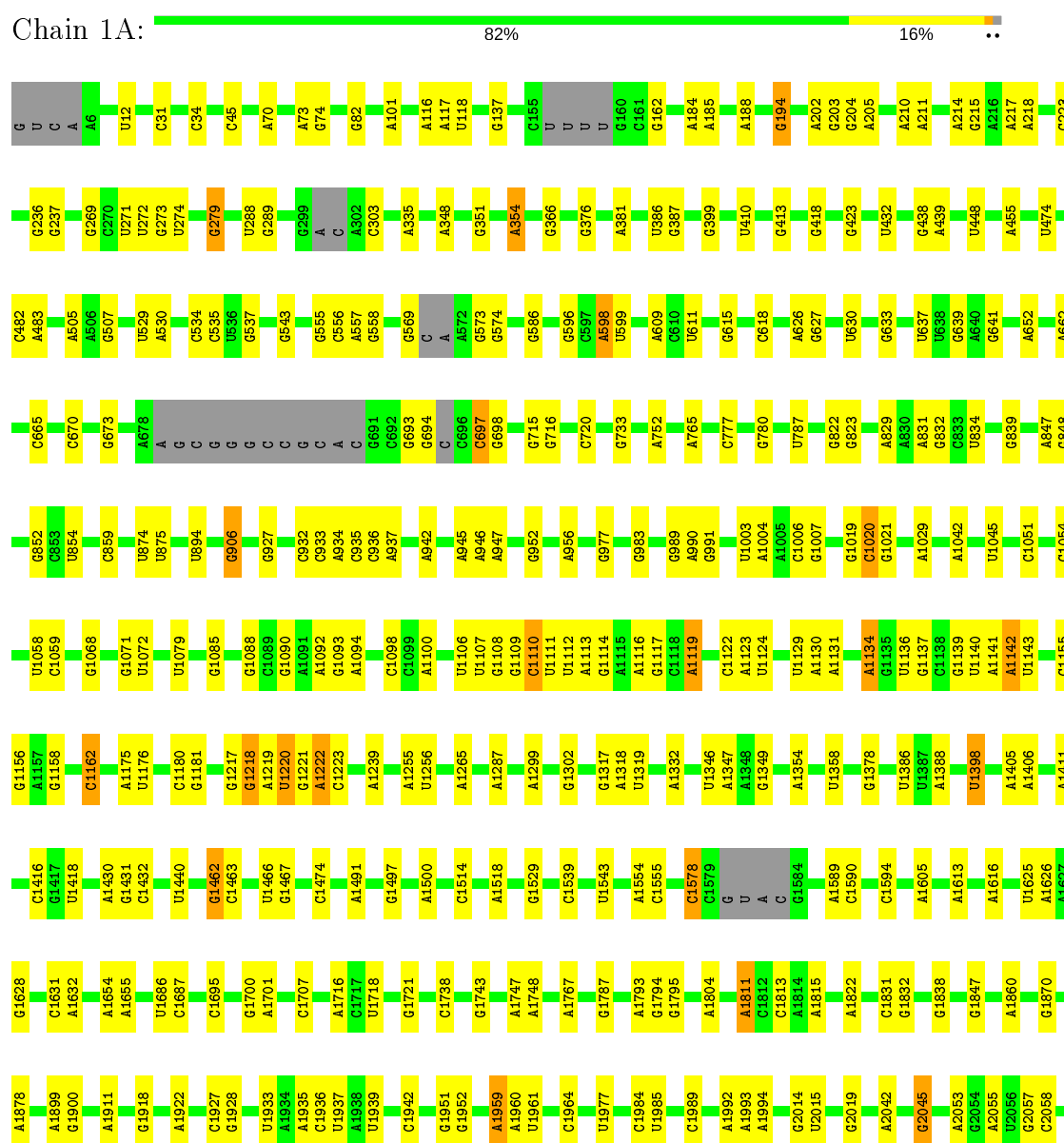
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			1	1		
60	2j	2	Total	O	0	0
			2	2		
60	2l	7	Total	O	0	0
			7	7		
60	2m	1	Total	O	0	0
			1	1		
60	2n	1	Total	O	0	0
			1	1		
60	2t	1	Total	O	0	0
			1	1		
60	2v	3	Total	O	0	0
			3	3		
60	2x	4	Total	O	0	0
			4	4		
60	2y	4	Total	O	0	0
			4	4		

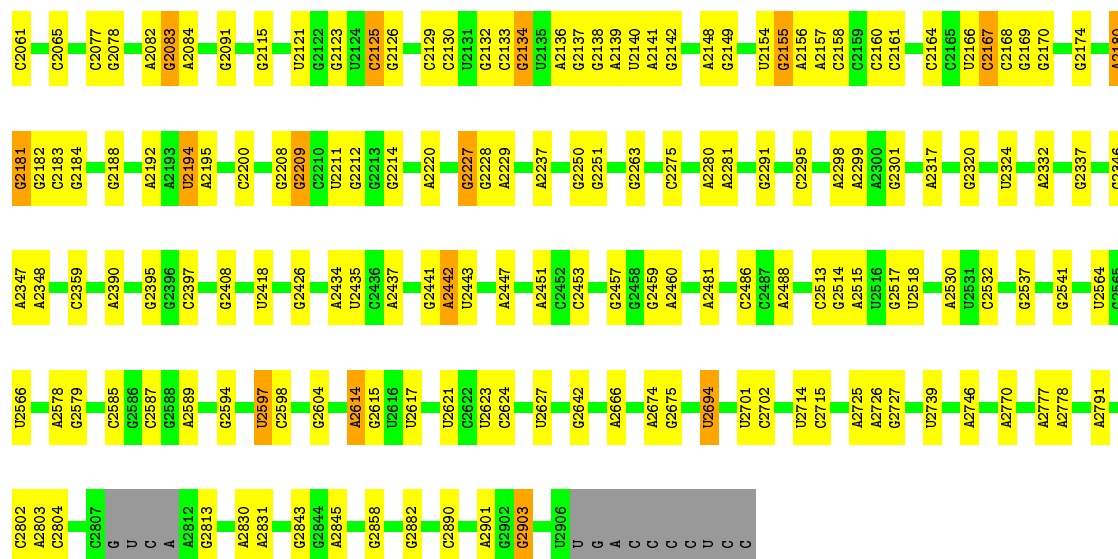
### 3 Residue-property plots

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.

Note EDS failed to run properly.

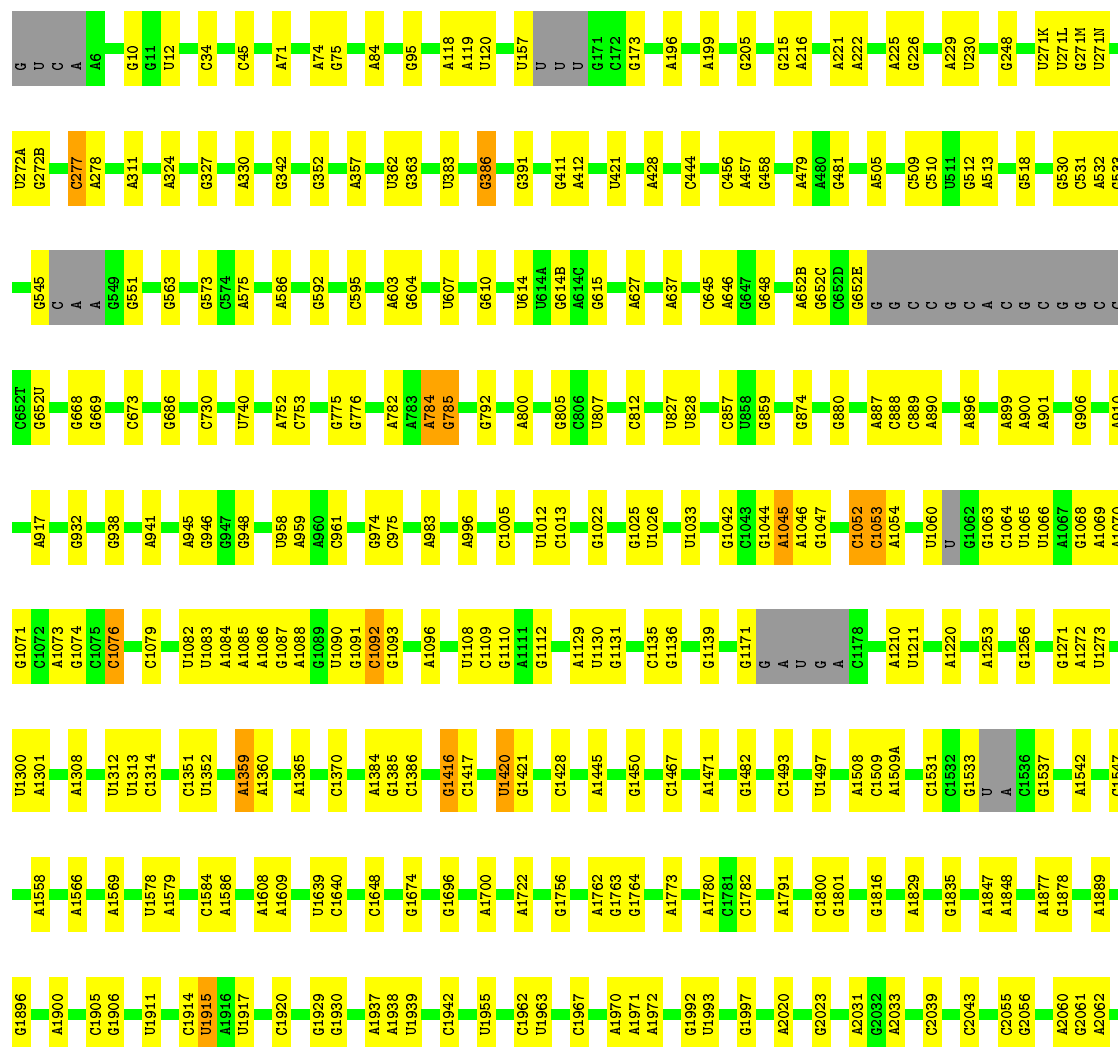
- Molecule 1: 23S ribosomal RNA

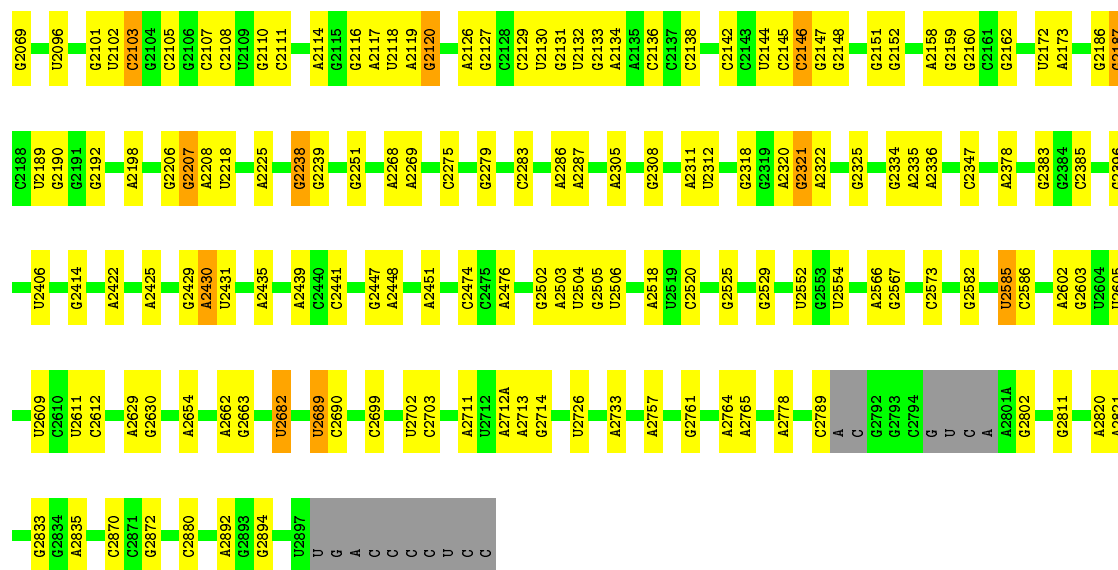




### ● Molecule 1: 23S ribosomal RNA

Chain 2A: 83% 15% ..





- Molecule 2: 5S ribosomal RNA



- Molecule 2: 5S ribosomal RNA



- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



There are no outlier residues recorded for this chain.

- Molecule 4: 50S ribosomal protein L3



There are no outlier residues recorded for this chain.

- Molecule 4: 50S ribosomal protein L3

Chain 2E:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: 50S ribosomal protein L4

Chain 1F:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: 50S ribosomal protein L4

Chain 2F:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: 50S ribosomal protein L5

Chain 1G:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: 50S ribosomal protein L5

Chain 2G:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: 50S ribosomal protein L6

Chain 1H:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: 50S ribosomal protein L6

Chain 2H:  99%



- Molecule 8: 50S ribosomal protein L9

Chain 1I:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: 50S ribosomal protein L9

Chain 2I:  99%



- Molecule 9: 50S ribosomal protein L13

Chain 1N:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: 50S ribosomal protein L13

Chain 2N:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: 50S ribosomal protein L14

Chain 1O:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: 50S ribosomal protein L14

Chain 2O:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: 50S ribosomal protein L15

Chain 1P:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: 50S ribosomal protein L15

Chain 2P:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  99%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 50S ribosomal protein L17

Chain 1R:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 50S ribosomal protein L17

Chain 2R:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: 50S ribosomal protein L18

Chain 1S:  100%

There are no outlier residues recorded for this chain.

- Molecule 14: 50S ribosomal protein L18

Chain 2S:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: 50S ribosomal protein L19

Chain 1T:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: 50S ribosomal protein L19

Chain 2T:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 50S ribosomal protein L20

Chain 1U:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: 50S ribosomal protein L20

Chain 2U:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L21

Chain 1V:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L21

Chain 2V:  100%



There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L22

Chain 1W:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L22

Chain 2W:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L23

Chain 1X:  100%

There are no outlier residues recorded for this chain.

- Molecule 19: 50S ribosomal protein L23

Chain 2X:  99%



- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  100%

There are no outlier residues recorded for this chain.

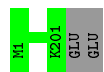
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  99%



- Molecule 22: 50S ribosomal protein L27

Chain 10:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: 50S ribosomal protein L27

Chain 20:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: 50S ribosomal protein L28

Chain 11:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: 50S ribosomal protein L28

Chain 21:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L29

Chain 12:  99%



- Molecule 24: 50S ribosomal protein L29

Chain 22:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L30

Chain 13:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L30

Chain 23:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L31

Chain 14:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L31

Chain 24:  99% .



- Molecule 27: 50S ribosomal protein L32

Chain 15:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L32

Chain 25:  98% .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: 50S ribosomal protein L33

Chain 26:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L34

Chain 17:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L34

Chain 27:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L35

Chain 18:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L35

Chain 28:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

Chain 19:  100%


There are no outlier residues recorded for this chain.

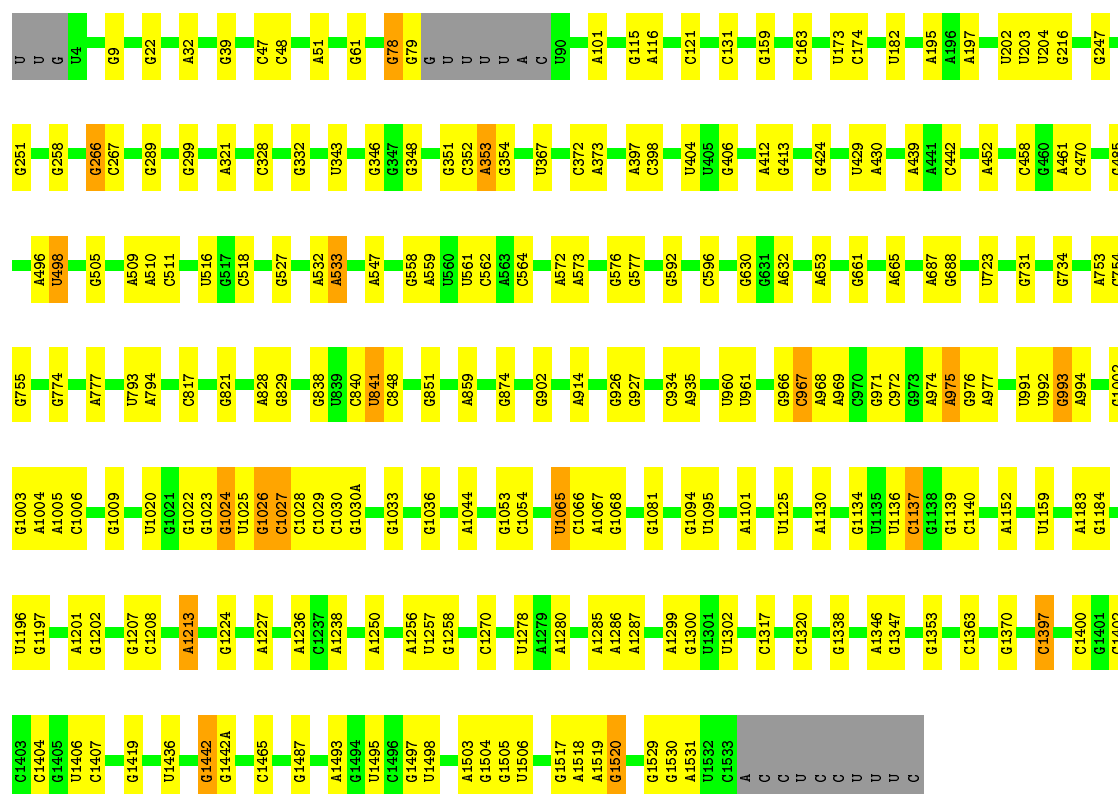
- Molecule 31: 50S ribosomal protein L36

Chain 29:  100%


There are no outlier residues recorded for this chain.

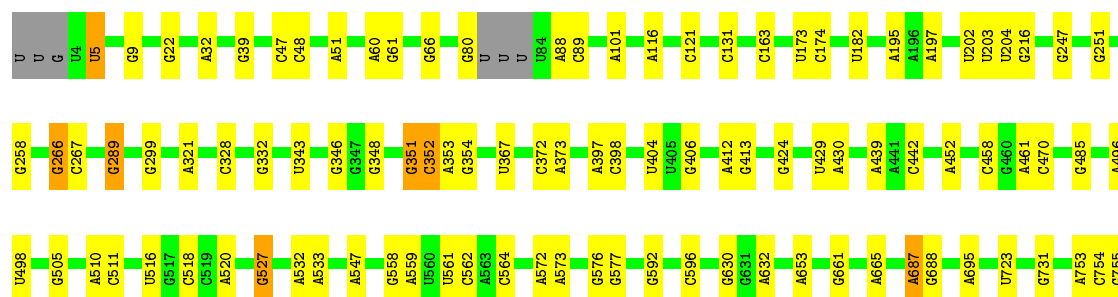
- Molecule 32: 16S ribosomal RNA

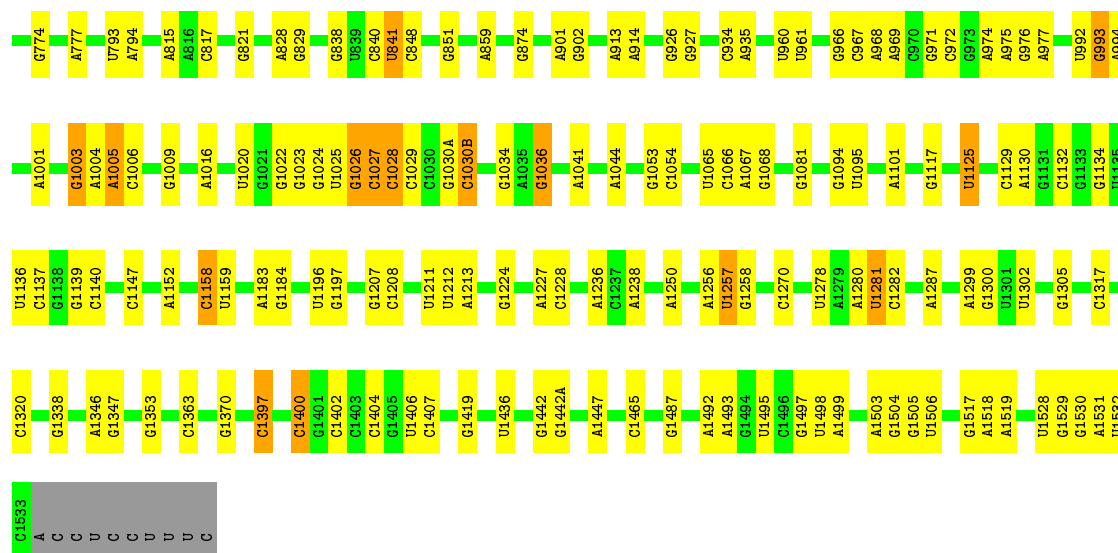
Chain 1a:  83% 14% ..



- Molecule 32: 16S ribosomal RNA

Chain 2a:  82% 15% ..





- Molecule 33: 30S ribosomal protein S2

Chain 1b:  100%



- Molecule 33: 30S ribosomal protein S2

Chain 2b:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 30S ribosomal protein S3

Chain 1c:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 30S ribosomal protein S3

Chain 2c:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: 30S ribosomal protein S4

Chain 1d:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: 30S ribosomal protein S4

Chain 2d:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: 30S ribosomal protein S5

Chain 1e:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: 30S ribosomal protein S5

Chain 2e:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: 30S ribosomal protein S6

Chain 1f:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: 30S ribosomal protein S6

Chain 2f:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: 30S ribosomal protein S7

Chain 1g:  100%

There are no outlier residues recorded for this chain.

- Molecule 38: 30S ribosomal protein S7

Chain 2g:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 30S ribosomal protein S8

Chain 1h:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 30S ribosomal protein S8

Chain 2h:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 30S ribosomal protein S9

Chain 1i:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 30S ribosomal protein S9

Chain 2i:  99%



- Molecule 41: 30S ribosomal protein S10

Chain 1j:  100%

There are no outlier residues recorded for this chain.

- Molecule 41: 30S ribosomal protein S10

Chain 2j:  99%



- Molecule 42: 30S ribosomal protein S11

Chain 1k:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 30S ribosomal protein S11

Chain 2k:  100%

There are no outlier residues recorded for this chain.

- Molecule 43: 30S ribosomal protein S12

Chain 1l:  99%



- Molecule 43: 30S ribosomal protein S12

Chain 2l:  99%



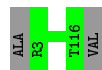
- Molecule 44: 30S ribosomal protein S13

Chain 1m:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 30S ribosomal protein S13

Chain 2m:  98%



- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 30S ribosomal protein S15

Chain 1o:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 30S ribosomal protein S15

Chain 2o:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 30S ribosomal protein S16

Chain 1p:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 30S ribosomal protein S16

Chain 2p:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S17

Chain 1q:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S17



Chain 2q:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S18

Chain 1r:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S18

Chain 2r:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 30S ribosomal protein S19

Chain 1s:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 30S ribosomal protein S19

Chain 2s:  100%

There are no outlier residues recorded for this chain.

- Molecule 51: 30S ribosomal protein S20

Chain 1t:  98%



- Molecule 51: 30S ribosomal protein S20

Chain 2t:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein Thx

Chain 1u:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein Thx

Chain 2u:  100%

There are no outlier residues recorded for this chain.

- Molecule 53: mRNA

Chain 1v:  100%

There are no outlier residues recorded for this chain.

- Molecule 53: mRNA

Chain 2v:  100%


There are no outlier residues recorded for this chain.

- Molecule 54: tRNAiMet

Chain 1x:  68% 32%



- Molecule 54: tRNAiMet

Chain 2x:  78% 22%



- Molecule 55: Cathelicidin-3

Chain 1y:  94% 6%



- Molecule 55: Cathelicidin-3

Chain 2y:  94% 6%



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.96Å 450.13Å 622.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 2.80	Depositor
% Data completeness (in resolution range)	99.5 (48.62-2.80)	Depositor
$R_{merge}$	0.51	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.249 , 0.292	Depositor
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.182	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	296108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, M2G, OMG, OMU, MA6, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, K, PSU

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	1A	0.54	0/69034	1.07	167/107758 (0.2%)
1	2A	0.44	0/68906	0.97	77/107556 (0.1%)
2	1B	0.46	0/2879	1.03	11/4490 (0.2%)
2	2B	0.41	0/2874	0.97	2/4482 (0.0%)
3	1D	0.39	0/2181	0.64	1/2940 (0.0%)
3	2D	0.34	0/2186	0.61	0/2944
4	1E	0.38	0/1592	0.61	0/2149
4	2E	0.34	0/1592	0.62	0/2149
5	1F	0.36	0/1619	0.60	0/2193
5	2F	0.32	0/1615	0.56	0/2188
6	1G	0.33	0/1451	0.61	0/1961
6	2G	0.31	0/1449	0.60	0/1957
7	1H	0.34	0/1356	0.55	0/1834
7	2H	0.31	0/1350	0.54	0/1826
8	1I	0.31	0/1109	0.62	0/1512
8	2I	0.29	0/1091	0.58	0/1490
9	1N	0.36	0/1148	0.60	0/1547
9	2N	0.30	0/1144	0.55	0/1543
10	1O	0.41	0/943	0.61	0/1269
10	2O	0.35	0/943	0.58	0/1269
11	1P	0.35	0/1152	0.62	0/1533
11	2P	0.31	0/1152	0.57	0/1533
12	1Q	0.44	1/1143 (0.1%)	0.64	2/1527 (0.1%)
12	2Q	0.32	0/1143	0.54	0/1527
13	1R	0.37	0/982	0.61	0/1312
13	2R	0.32	0/982	0.57	0/1312
14	1S	0.32	0/887	0.59	0/1180
14	2S	0.31	0/880	0.58	0/1172
15	1T	0.34	0/1105	0.60	0/1477
15	2T	0.32	0/1097	0.58	0/1468
16	1U	0.37	0/977	0.58	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.31	0/977	0.53	0/1301
17	1V	0.37	0/786	0.60	0/1053
17	2V	0.32	0/782	0.60	0/1049
18	1W	0.39	0/897	0.60	0/1205
18	2W	0.32	0/897	0.55	0/1205
19	1X	0.39	0/764	0.60	0/1025
19	2X	0.34	0/764	0.63	1/1025 (0.1%)
20	1Y	0.38	0/823	0.62	0/1099
20	2Y	0.33	0/823	0.63	0/1100
21	1Z	0.33	0/1620	0.57	0/2200
21	2Z	0.32	0/1590	0.58	0/2162
22	10	0.36	0/616	0.61	0/821
22	20	0.33	0/616	0.58	0/821
23	11	0.36	0/761	0.57	0/1013
23	21	0.33	0/766	0.56	0/1018
24	12	0.35	0/590	0.63	1/781 (0.1%)
24	22	0.31	0/594	0.53	0/785
25	13	0.35	0/474	0.57	0/635
25	23	0.30	0/469	0.53	0/630
26	14	0.35	0/559	0.68	0/754
26	24	0.37	0/549	0.67	0/741
27	15	0.39	0/473	0.63	0/639
27	25	0.31	0/469	0.61	1/635 (0.2%)
28	16	0.36	0/460	0.59	0/613
28	26	0.34	0/456	0.57	0/608
29	17	0.41	0/426	0.65	0/561
29	27	0.36	0/426	0.55	0/561
30	18	0.38	0/525	0.61	0/691
30	28	0.34	0/525	0.57	0/691
31	19	0.36	0/310	0.61	0/407
31	29	0.31	0/310	0.58	0/407
32	1a	0.41	0/35795	0.99	69/55864 (0.1%)
32	2a	0.40	1/35890 (0.0%)	1.00	91/56012 (0.2%)
33	1b	0.34	0/1876	0.63	0/2533
33	2b	0.33	0/1860	0.59	0/2518
34	1c	0.31	0/1582	0.57	0/2137
34	2c	0.31	0/1566	0.58	0/2119
35	1d	0.32	0/1695	0.60	0/2274
35	2d	0.29	0/1698	0.55	0/2277
36	1e	0.32	0/1149	0.58	0/1548
36	2e	0.32	0/1149	0.58	0/1548
37	1f	0.32	0/827	0.57	0/1120
37	2f	0.31	0/829	0.57	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.32	0/1254	0.55	0/1683
38	2g	0.29	0/1248	0.52	0/1676
39	1h	0.30	0/1118	0.58	0/1506
39	2h	0.30	0/1108	0.56	0/1494
40	1i	0.30	0/1005	0.58	0/1351
40	2i	0.32	0/985	0.57	0/1329
41	1j	0.32	0/732	0.58	0/993
41	2j	0.32	0/723	0.60	0/984
42	1k	0.33	0/849	0.59	0/1150
42	2k	0.36	0/848	0.61	0/1149
43	1l	0.31	0/937	0.56	0/1260
43	2l	0.31	0/937	0.61	0/1260
44	1m	0.29	0/924	0.60	0/1242
44	2m	0.31	0/905	0.58	0/1217
45	1n	0.31	0/501	0.55	0/664
45	2n	0.33	0/501	0.55	0/664
46	1o	0.31	0/739	0.58	0/985
46	2o	0.29	0/739	0.52	0/985
47	1p	0.30	0/697	0.56	0/939
47	2p	0.31	0/693	0.55	0/935
48	1q	0.32	0/836	0.60	0/1117
48	2q	0.31	0/836	0.56	0/1117
49	1r	0.30	0/560	0.56	0/746
49	2r	0.31	0/560	0.56	0/746
50	1s	0.30	0/663	0.61	0/895
50	2s	0.29	0/660	0.60	0/893
51	1t	0.31	0/734	0.57	0/969
51	2t	0.29	0/736	0.54	0/976
52	1u	0.28	0/203	0.57	0/266
52	2u	0.30	0/203	0.57	0/266
53	1v	0.45	0/72	0.91	0/110
53	2v	0.48	0/72	1.04	0/110
54	1x	0.42	0/1725	0.94	0/2689
54	2x	0.40	0/1725	0.96	3/2689 (0.1%)
55	1y	0.37	0/152	0.83	1/203 (0.5%)
55	2y	0.33	0/152	0.87	1/203 (0.5%)
All	All	0.43	2/312307 (0.0%)	0.92	428/467169 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	24	0	1
33	1b	0	1
55	1y	0	1
55	2y	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1Q	41	TRP	NE1-CE2	6.34	1.45	1.37
32	2a	1034	G	N9-C4	5.00	1.42	1.38

All (428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP1	-31.64	72.74	110.70
32	1a	1520	G	O5'-P-OP1	-30.14	74.54	110.70
32	2a	1208	C	OP1-P-OP2	-27.27	78.69	119.60
32	1a	1520	G	OP1-P-OP2	-26.36	80.06	119.60
32	1a	1520	G	O5'-P-OP2	19.44	134.03	110.70
32	2a	1208	C	O5'-P-OP2	17.89	132.16	110.70
32	2a	1207	2MG	OP1-P-O3'	13.62	135.16	105.20
32	2a	1207	2MG	OP2-P-O3'	-12.53	77.64	105.20
1	1A	720	C	C2-N3-C4	-12.23	113.79	119.90
1	1A	787	U	O5'-P-OP2	-11.63	95.24	105.70
1	1A	834	U	O5'-P-OP1	-11.59	95.27	105.70
32	1a	558	G	O5'-P-OP1	-11.56	95.29	105.70
1	2A	1639	U	O5'-P-OP2	-10.79	95.99	105.70
32	1a	1495	U	N1-C2-O2	10.76	130.33	122.80
1	1A	1686	U	O5'-P-OP2	-10.56	96.19	105.70
32	2a	351	G	OP1-P-O3'	-10.39	82.33	105.20
32	2a	404	U	N1-C2-O2	10.16	129.91	122.80
1	1A	2694	U	O5'-P-OP2	-10.05	96.65	105.70
1	2A	2711	A	O5'-P-OP1	-9.70	96.97	105.70
2	1B	75	G	C6-N1-C2	-9.56	119.36	125.10
1	1A	1045	U	O5'-P-OP2	-9.54	97.12	105.70
1	1A	2227	G	C4-N9-C1'	-9.53	114.12	126.50
1	2A	673	C	C2-N3-C4	-9.51	115.15	119.90
1	2A	2682	U	O5'-P-OP2	-9.46	97.18	105.70
1	1A	2188	G	N3-C4-N9	-9.08	120.55	126.00
32	2a	1495	U	N1-C2-O2	8.97	129.08	122.80
1	1A	2083	G	O5'-P-OP2	-8.90	97.69	105.70
32	2a	352	C	OP1-P-OP2	8.89	132.94	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	948	G	O5'-P-OP1	-8.85	97.73	105.70
1	1A	854	U	C2-N3-C4	-8.73	121.76	127.00
32	1a	343	U	C2-N1-C1'	-8.67	107.30	117.70
32	2a	351	G	OP2-P-O3'	-8.63	86.20	105.20
1	1A	2227	G	C8-N9-C1'	8.63	138.22	127.00
1	1A	2442	A	O5'-P-OP2	-8.53	98.03	105.70
1	1A	932	C	C6-N1-C2	-8.49	116.90	120.30
32	2a	299	G	C5-C6-O6	-8.40	123.56	128.60
32	2a	558	G	O5'-P-OP1	-8.39	98.14	105.70
32	1a	404	U	N1-C2-O2	8.39	128.67	122.80
32	1a	841	U	C5-C6-N1	8.28	126.84	122.70
1	1A	354	A	C2-N3-C4	-8.24	106.48	110.60
32	1a	1137	C	C6-N1-C2	-8.22	117.01	120.30
32	1a	1436	U	C2-N3-C4	-8.19	122.08	127.00
32	1a	1465	C	C2-N3-C4	-8.19	115.81	119.90
1	1A	82	G	N9-C4-C5	-8.16	102.14	105.40
32	2a	1034	G	C5-C6-N1	8.03	115.51	111.50
32	2a	1034	G	N3-C4-C5	-8.00	124.60	128.60
32	2a	343	U	C5-C4-O4	7.98	130.69	125.90
1	2A	785	G	O5'-P-OP2	-7.92	98.57	105.70
1	1A	354	A	N1-C2-N3	7.90	133.25	129.30
1	1A	2058	C	O5'-P-OP1	-7.89	98.60	105.70
32	2a	343	U	N3-C4-O4	-7.86	113.90	119.40
32	2a	343	U	C2-N1-C1'	-7.77	108.38	117.70
1	1A	952	G	C5-C6-O6	7.75	133.25	128.60
1	2A	807	U	C2-N3-C4	-7.74	122.36	127.00
32	2a	1465	C	C2-N3-C4	-7.54	116.13	119.90
32	2a	1034	G	C6-N1-C2	-7.54	120.58	125.10
32	1a	1495	U	N3-C2-O2	-7.53	116.93	122.20
32	1a	299	G	C5-C6-O6	-7.46	124.12	128.60
55	2y	15	PRO	O-C-N	-7.46	110.76	122.70
1	1A	1700	G	P-O3'-C3'	7.46	128.65	119.70
1	2A	906	G	C5-C6-O6	7.46	133.07	128.60
32	1a	1397	C	N1-C2-O2	7.45	123.37	118.90
32	2a	1027	C	C6-N1-C2	-7.43	117.33	120.30
32	1a	1495	U	C2-N1-C1'	7.42	126.60	117.70
1	1A	1358	U	C5-C4-O4	7.41	130.35	125.90
1	1A	952	G	N3-C4-N9	-7.39	121.57	126.00
1	1A	2858	G	O4'-C1'-N9	7.29	114.03	108.20
2	1B	102	A	C6-N1-C2	-7.28	114.23	118.60
32	1a	343	U	O4'-C1'-N1	7.24	114.00	108.20
32	2a	1001	A	O4'-C1'-N9	7.18	113.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1034	G	N3-C4-N9	7.15	130.29	126.00
1	1A	2604	G	O5'-P-OP1	-7.15	99.27	105.70
1	2A	740	U	O5'-P-OP2	-7.12	99.29	105.70
1	1A	2227	G	N3-C4-N9	-7.08	121.75	126.00
32	2a	1125	U	C2-N1-C1'	7.06	126.17	117.70
2	1B	59	A	C6-N1-C2	-7.04	114.38	118.60
2	1B	24	G	N3-C4-C5	-7.03	125.09	128.60
32	2a	1034	G	C2-N3-C4	6.99	115.39	111.90
1	1A	2188	G	C8-N9-C1'	6.96	136.05	127.00
1	1A	720	C	N3-C4-C5	6.94	124.68	121.90
1	1A	1378	G	O5'-P-OP1	-6.93	99.47	105.70
1	1A	932	C	C5-C6-N1	6.91	124.46	121.00
32	2a	1436	U	C2-N3-C4	-6.88	122.87	127.00
1	1A	2188	G	C6-C5-N7	6.87	134.52	130.40
1	1A	194	G	O5'-P-OP2	-6.84	99.54	105.70
1	1A	2802	C	C2-N1-C1'	-6.84	111.28	118.80
1	1A	2188	G	C4-N9-C1'	-6.83	117.63	126.50
1	1A	2188	G	N9-C4-C5	6.81	108.12	105.40
1	1A	101	A	N1-C6-N6	6.79	122.67	118.60
32	2a	993	G	N3-C4-N9	6.79	130.07	126.00
19	2X	57	LEU	CA-CB-CG	6.78	130.88	115.30
32	1a	1397	C	C2-N1-C1'	6.77	126.24	118.80
1	2A	1092	C	N1-C2-O2	6.76	122.96	118.90
32	1a	1137	C	C5-C6-N1	6.75	124.38	121.00
32	2a	404	U	C2-N1-C1'	6.73	125.77	117.70
1	1A	848	G	O5'-P-OP2	-6.72	99.65	105.70
32	2a	1003	G	C8-N9-C4	-6.72	103.71	106.40
1	1A	2459	G	C6-N1-C2	-6.71	121.07	125.10
1	2A	383	U	N1-C2-O2	6.69	127.48	122.80
1	1A	215	G	C2-N3-C4	6.68	115.24	111.90
1	2A	1416	G	O4'-C1'-N9	6.67	113.54	108.20
32	2a	299	G	N1-C6-O6	6.66	123.90	119.90
32	2a	993	G	N3-C4-C5	-6.64	125.28	128.60
1	1A	952	G	N9-C4-C5	6.62	108.05	105.40
32	1a	343	U	C6-N1-C1'	6.62	130.47	121.20
1	1A	537	G	O4'-C1'-N9	6.62	113.50	108.20
1	1A	418	G	C6-N1-C2	-6.62	121.13	125.10
32	2a	993	G	C4-N9-C1'	6.59	135.07	126.50
1	2A	2130	U	C5-C6-N1	6.54	125.97	122.70
1	1A	1140	U	O4'-C1'-N1	6.52	113.41	108.20
32	1a	1436	U	C5-C4-O4	-6.49	122.01	125.90
32	2a	1397	C	C2-N1-C1'	6.49	125.94	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2188	G	C5-C6-O6	6.48	132.49	128.60
32	2a	1030(B)	C	C2-N1-C1'	6.47	125.92	118.80
32	2a	404	U	N3-C2-O2	-6.47	117.67	122.20
32	2a	299	G	C4-C5-N7	6.46	113.38	110.80
55	1y	15	PRO	O-C-N	-6.45	112.38	122.70
1	2A	807	U	C5-C4-O4	-6.41	122.05	125.90
32	1a	78	G	C8-N9-C1'	6.40	135.32	127.00
1	1A	215	G	N1-C2-N2	6.38	121.94	116.20
1	1A	720	C	N1-C2-N3	6.36	123.65	119.20
1	1A	2227	G	N3-C4-C5	6.36	131.78	128.60
32	2a	1003	G	N3-C4-C5	-6.36	125.42	128.60
1	2A	2102	U	N1-C2-O2	6.34	127.24	122.80
1	2A	1835	G	C4-N9-C1'	6.34	134.74	126.50
1	1A	1462	G	O4'-C1'-N9	6.33	113.26	108.20
1	1A	2180	A	O4'-C1'-N9	6.32	113.25	108.20
1	2A	2689	U	N3-C2-O2	-6.30	117.79	122.20
32	2a	1003	G	C4-N9-C1'	6.29	134.68	126.50
1	2A	1076	C	O4'-C1'-N1	6.28	113.23	108.20
1	2A	2447	G	C6-N1-C2	-6.28	121.33	125.10
1	1A	2136	A	N1-C6-N6	-6.28	114.83	118.60
1	1A	2390	A	C4-C5-C6	6.28	120.14	117.00
1	1A	410	U	N1-C2-O2	6.28	127.19	122.80
1	1A	1134	A	O4'-C1'-N9	6.28	113.22	108.20
32	2a	299	G	C6-C5-N7	-6.28	126.64	130.40
32	1a	343	U	C5-C4-O4	6.25	129.65	125.90
1	1A	2802	C	C6-N1-C1'	6.25	128.30	120.80
32	1a	533	A	N1-C6-N6	6.25	122.35	118.60
32	1a	1406	U	C2-N3-C4	-6.23	123.26	127.00
2	2B	59	A	C6-N1-C2	-6.22	114.87	118.60
32	2a	5	U	C2-N1-C1'	6.22	125.17	117.70
1	1A	1398	U	O5'-P-OP1	-6.21	100.11	105.70
1	2A	1052	C	C2-N1-C1'	6.20	125.62	118.80
32	2a	346	G	C6-N1-C2	-6.20	121.38	125.10
1	2A	2699	C	C6-N1-C2	6.19	122.78	120.30
1	1A	2903	G	N3-C4-N9	-6.19	122.29	126.00
1	2A	1835	G	C8-N9-C1'	-6.19	118.96	127.00
1	2A	2187	G	C6-C5-N7	-6.18	126.69	130.40
32	2a	1030(B)	C	N1-C2-O2	6.18	122.61	118.90
1	1A	1386	U	C2-N3-C4	-6.16	123.30	127.00
32	1a	1465	C	N3-C4-C5	6.15	124.36	121.90
1	1A	82	G	C2-N3-C4	-6.14	108.83	111.90
32	2a	1228	C	N1-C2-O2	6.14	122.59	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1087	G	N3-C4-N9	-6.10	122.34	126.00
1	1A	1110	C	C5-C6-N1	6.09	124.05	121.00
32	2a	1036	G	N7-C8-N9	6.08	116.14	113.10
2	1B	24	G	C6-N1-C2	-6.07	121.46	125.10
1	2A	1053	C	P-O3'-C3'	6.07	126.98	119.70
32	2a	343	U	C6-N1-C1'	6.07	129.69	121.20
32	1a	1024	G	N3-C4-N9	6.06	129.64	126.00
1	1A	598	A	O5'-P-OP1	-6.06	100.25	105.70
32	1a	78	G	C4-N9-C1'	-6.06	118.63	126.50
32	2a	1028	C	C6-N1-C2	-6.05	117.88	120.30
1	1A	2188	G	C4-C5-N7	-6.03	108.39	110.80
1	1A	720	C	N1-C2-O2	-6.02	115.29	118.90
32	1a	1024	G	C8-N9-C1'	-6.02	119.17	127.00
32	1a	1024	G	C4-N9-C1'	6.02	134.32	126.50
1	1A	1418	U	C2-N1-C1'	6.01	124.91	117.70
32	1a	498	U	C5-C4-O4	6.00	129.50	125.90
32	1a	1495	U	C5-C6-N1	6.00	125.70	122.70
1	1A	2161	C	C5-C6-N1	5.99	124.00	121.00
1	2A	2103	C	C6-N1-C2	-5.99	117.90	120.30
32	2a	5	U	N3-C2-O2	-5.99	118.01	122.20
1	1A	2125	C	N1-C2-O2	5.98	122.48	118.90
1	1A	2227	G	C6-C5-N7	5.97	133.99	130.40
1	1A	1578	C	C6-N1-C2	-5.96	117.92	120.30
32	2a	1005	A	C8-N9-C4	-5.96	103.42	105.80
32	1a	299	G	C4-C5-N7	5.96	113.18	110.80
2	1B	75	G	C5-C6-O6	-5.96	125.03	128.60
1	2A	1087	G	C8-N9-C1'	5.94	134.72	127.00
1	1A	215	G	C6-C5-N7	5.93	133.96	130.40
1	1A	637	U	O4'-C1'-N1	5.93	112.94	108.20
32	1a	1285	A	P-O3'-C3'	5.93	126.81	119.70
32	2a	1495	U	C2-N1-C1'	5.91	124.79	117.70
1	1A	952	G	C4-C5-N7	-5.91	108.44	110.80
32	1a	1495	U	C2-N3-C4	5.90	130.54	127.00
32	2a	1495	U	N3-C2-O2	-5.87	118.09	122.20
1	1A	952	G	C6-C5-N7	5.86	133.92	130.40
32	2a	346	G	C5-C6-N1	5.84	114.42	111.50
1	1A	1959	A	N1-C6-N6	-5.84	115.09	118.60
1	2A	277	C	N1-C2-O2	5.84	122.40	118.90
2	1B	75	G	N3-C4-C5	-5.84	125.68	128.60
1	1A	2136	A	C8-N9-C4	-5.83	103.47	105.80
32	2a	1465	C	C5-C4-N4	-5.82	116.12	120.20
1	2A	2430	A	O5'-P-OP2	-5.82	100.46	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	5	U	N1-C2-O2	5.82	126.88	122.80
32	1a	841	U	C6-N1-C2	-5.82	117.51	121.00
1	2A	1992	G	P-O3'-C3'	5.82	126.68	119.70
32	2a	1228	C	N3-C2-O2	-5.81	117.83	121.90
32	1a	1397	C	N3-C2-O2	-5.80	117.84	121.90
32	2a	1026	G	N7-C8-N9	5.79	116.00	113.10
1	1A	217	A	C5-N7-C8	-5.78	101.01	103.90
1	2A	752	A	P-O3'-C3'	5.78	126.63	119.70
32	1a	78	G	O4'-C1'-N9	5.77	112.81	108.20
32	2a	266	G	P-O3'-C3'	5.77	126.62	119.70
1	1A	1440	U	O5'-P-OP1	-5.76	100.51	105.70
1	1A	2157	A	N1-C6-N6	5.76	122.06	118.60
32	2a	1024	G	C2-N3-C4	5.75	114.78	111.90
32	2a	754	C	C2-N1-C1'	5.75	125.12	118.80
32	1a	343	U	C5-C6-N1	-5.75	119.83	122.70
32	2a	346	G	C5-C6-O6	-5.74	125.16	128.60
1	2A	1313	U	C2-N1-C1'	5.73	124.58	117.70
32	1a	533	A	C5-C6-N6	-5.71	119.13	123.70
1	2A	673	C	N3-C4-C5	5.71	124.18	121.90
1	2A	2144	U	O4'-C1'-N1	5.71	112.76	108.20
32	1a	343	U	N3-C4-O4	-5.70	115.41	119.40
1	1A	529	U	C2-N1-C1'	5.70	124.54	117.70
32	1a	533	A	C6-C5-N7	-5.69	128.32	132.30
1	2A	2451	A	C5-N7-C8	-5.68	101.06	103.90
1	1A	989	G	N7-C8-N9	5.68	115.94	113.10
1	1A	2209	G	C5-C6-O6	-5.67	125.20	128.60
1	2A	1052	C	N1-C2-O2	5.67	122.30	118.90
54	2x	22	G	C5-N7-C8	-5.67	101.47	104.30
1	1A	780	G	C5-N7-C8	5.66	107.13	104.30
32	1a	1067	A	P-O3'-C3'	5.66	126.49	119.70
1	1A	215	G	N1-C2-N3	-5.66	120.51	123.90
32	2a	1406	U	C2-N3-C4	-5.66	123.61	127.00
32	2a	1067	A	P-O3'-C3'	5.64	126.47	119.70
1	1A	2123	G	O4'-C1'-N9	5.64	112.71	108.20
1	1A	1718	U	O5'-P-OP2	-5.63	100.63	105.70
1	2A	383	U	N3-C2-O2	-5.63	118.26	122.20
2	1B	75	G	C5-C6-N1	5.63	114.31	111.50
32	2a	1281	U	C2-N1-C1'	5.63	124.45	117.70
32	2a	993	G	C8-N9-C1'	-5.62	119.69	127.00
1	1A	2275	C	N1-C2-O2	-5.61	115.53	118.90
2	1B	24	G	N3-C4-N9	5.61	129.37	126.00
1	2A	1087	G	C4-N9-C1'	-5.60	119.22	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1397	C	C6-N1-C2	-5.58	118.07	120.30
32	2a	299	G	N9-C4-C5	-5.58	103.17	105.40
1	1A	2136	A	N9-C4-C5	5.57	108.03	105.80
1	1A	2802	C	O4'-C1'-N1	5.57	112.66	108.20
1	2A	512	G	O4'-C1'-N9	5.57	112.66	108.20
32	2a	1034	G	C5-C6-O6	-5.57	125.26	128.60
2	2B	8	U	C5-C6-N1	5.57	125.48	122.70
1	1A	1838	G	C2-N3-C4	-5.56	109.12	111.90
1	2A	2102	U	N3-C2-O2	-5.56	118.31	122.20
1	1A	1811	A	O5'-P-OP1	-5.56	100.70	105.70
1	2A	673	C	C5-C4-N4	-5.56	116.31	120.20
1	1A	2903	G	N9-C4-C5	5.55	107.62	105.40
2	1B	102	A	N1-C2-N3	5.55	132.07	129.30
1	1A	215	G	N9-C4-C5	5.55	107.62	105.40
1	2A	1092	C	C2-N1-C1'	5.54	124.89	118.80
32	1a	1065	U	P-O3'-C3'	5.54	126.34	119.70
1	1A	31	C	O5'-P-OP1	-5.53	100.72	105.70
1	1A	2589	A	O5'-P-OP1	-5.53	100.72	105.70
1	1A	2903	G	C6-C5-N7	5.53	133.72	130.40
1	1A	1054	C	C6-N1-C2	-5.53	118.09	120.30
1	2A	226	G	C4-N9-C1'	-5.52	119.32	126.50
32	1a	1465	C	C5-C4-N4	-5.52	116.33	120.20
32	2a	1158	C	C6-N1-C2	-5.52	118.09	120.30
32	2a	1005	A	N7-C8-N9	5.52	116.56	113.80
1	1A	215	G	O4'-C1'-N9	5.52	112.61	108.20
1	1A	2181	G	O4'-C1'-N9	5.51	112.61	108.20
32	2a	841	U	C5-C6-N1	5.51	125.45	122.70
32	1a	266	G	P-O3'-C3'	5.50	126.31	119.70
32	1a	993	G	C4-N9-C1'	5.50	133.65	126.50
32	1a	991	U	P-O3'-C3'	5.49	126.28	119.70
27	25	58	LEU	CA-CB-CG	5.49	127.92	115.30
32	2a	1026	G	C5-N7-C8	-5.49	101.56	104.30
1	1A	1398	U	O5'-P-OP2	5.48	117.28	110.70
32	1a	1442	G	N3-C4-C5	-5.47	125.86	128.60
1	2A	2870	C	C6-N1-C2	-5.47	118.11	120.30
32	2a	299	G	N3-C4-N9	5.46	129.28	126.00
1	1A	952	G	C8-N9-C1'	5.46	134.10	127.00
1	1A	1222	A	O5'-P-OP1	-5.46	100.78	105.70
1	1A	2167	C	C5-C6-N1	5.46	123.73	121.00
32	2a	289	G	O5'-P-OP2	5.45	117.24	110.70
32	2a	520	A	N9-C4-C5	5.45	107.98	105.80
32	2a	1436	U	C5-C4-O4	-5.45	122.63	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	101	A	C4-C5-C6	5.44	119.72	117.00
1	1A	215	G	C8-N9-C1'	5.44	134.07	127.00
1	2A	1312	U	C5-C4-O4	5.44	129.16	125.90
54	2x	47	U	C5-C6-N1	5.44	125.42	122.70
1	2A	2207	G	N7-C8-N9	5.42	115.81	113.10
32	2a	1158	C	C2-N1-C1'	5.42	124.76	118.80
1	2A	2321	G	P-O3'-C3'	5.41	126.19	119.70
1	1A	2183	C	C5-C6-N1	5.41	123.70	121.00
1	2A	513	A	N1-C6-N6	5.39	121.83	118.60
1	1A	215	G	N3-C4-N9	-5.39	122.77	126.00
1	1A	223	C	N1-C2-O2	5.38	122.13	118.90
1	1A	184	A	P-O3'-C3'	5.38	126.16	119.70
1	1A	2057	G	O5'-P-OP1	-5.37	100.86	105.70
32	2a	404	U	C5-C6-N1	5.37	125.39	122.70
1	1A	2390	A	N1-C6-N6	5.37	121.82	118.60
1	2A	2120	G	N3-C4-N9	5.36	129.22	126.00
32	2a	901	A	N1-C6-N6	5.36	121.82	118.60
1	1A	854	U	N1-C2-N3	5.36	118.12	114.90
1	1A	82	G	C8-N9-C4	5.36	108.54	106.40
1	1A	2459	G	C5-C6-N1	5.35	114.18	111.50
1	1A	1418	U	C5-C4-O4	-5.35	122.69	125.90
1	2A	784	A	P-O3'-C3'	5.34	126.11	119.70
32	1a	1201	A	P-O3'-C3'	5.34	126.11	119.70
1	1A	2627	U	O5'-P-OP1	-5.33	100.90	105.70
1	1A	1020	C	O5'-P-OP1	-5.33	100.90	105.70
1	1A	1815	A	O5'-P-OP2	-5.33	100.90	105.70
32	1a	299	G	N9-C4-C5	-5.33	103.27	105.40
32	1a	404	U	N3-C2-O2	-5.33	118.47	122.20
1	1A	2188	G	N3-C4-C5	5.33	131.26	128.60
32	1a	754	C	C2-N1-C1'	5.32	124.65	118.80
32	2a	343	U	O4'-C1'-N1	5.32	112.45	108.20
1	2A	1992	G	N3-C4-C5	-5.30	125.95	128.60
1	2A	1351	C	OP1-P-O3'	5.29	116.85	105.20
32	2a	1030(B)	C	C5-C6-N1	5.29	123.65	121.00
32	1a	404	U	C2-N1-C1'	5.29	124.05	117.70
1	1A	906	G	C8-N9-C4	5.29	108.52	106.40
1	2A	2144	U	C2-N1-C1'	5.29	124.04	117.70
1	1A	697	C	C5-C6-N1	5.28	123.64	121.00
1	2A	1359	A	C2-N3-C4	5.28	113.24	110.60
32	1a	1024	G	C6-C5-N7	-5.28	127.23	130.40
1	1A	2587	C	O5'-P-OP2	-5.27	100.95	105.70
32	2a	60	A	P-O3'-C3'	5.27	126.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	854	U	C5-C4-O4	-5.26	122.74	125.90
1	1A	2457	G	N1-C6-O6	-5.26	116.74	119.90
1	1A	2134	G	N3-C4-C5	-5.26	125.97	128.60
1	1A	1162	C	C2-N1-C1'	5.25	124.58	118.80
32	1a	975	A	O4'-C1'-N9	-5.25	104.00	108.20
1	1A	236	G	C8-N9-C4	5.25	108.50	106.40
1	1A	2045	G	O5'-P-OP1	-5.25	100.98	105.70
1	1A	1220	U	P-O3'-C3'	5.25	125.99	119.70
32	1a	346	G	C5-C6-O6	-5.24	125.45	128.60
1	2A	2318	G	C4-N9-C1'	5.24	133.31	126.50
1	2A	1045	A	C2-N3-C4	5.23	113.22	110.60
1	2A	2146	C	O4'-C1'-N1	5.23	112.38	108.20
32	2a	404	U	C2-N3-C4	5.23	130.14	127.00
1	1A	1716	A	C8-N9-C4	-5.23	103.71	105.80
1	2A	386	G	C6-N1-C2	-5.22	121.97	125.10
12	1Q	41	TRP	CD2-CE2-CZ2	5.22	128.56	122.30
1	1A	82	G	C4-C5-N7	5.22	112.89	110.80
1	1A	697	C	N1-C2-O2	5.21	122.03	118.90
32	1a	353	A	OP2-P-O3'	5.21	116.67	105.20
32	2a	1027	C	N3-C2-O2	-5.21	118.25	121.90
1	1A	1119	A	C2-N3-C4	5.21	113.21	110.60
1	2A	2114	A	C8-N9-C4	-5.21	103.72	105.80
1	1A	2194	U	C5-C4-O4	5.20	129.02	125.90
32	2a	1026	G	C8-N9-C4	-5.20	104.32	106.40
54	2x	46	G	C6-N1-C2	-5.20	121.98	125.10
32	2a	1036	G	C8-N9-C4	-5.20	104.32	106.40
1	1A	1687	C	O4'-C1'-N1	5.20	112.36	108.20
1	1A	847	A	N1-C6-N6	-5.20	115.48	118.60
32	1a	1213	A	N1-C6-N6	-5.19	115.48	118.60
1	1A	1239	A	N1-C6-N6	-5.19	115.49	118.60
32	1a	1067	A	C8-N9-C4	-5.19	103.72	105.80
1	1A	2155	G	O4'-C1'-N9	5.18	112.35	108.20
1	1A	1110	C	C2-N1-C1'	5.18	124.50	118.80
1	1A	215	G	C4-N9-C1'	-5.18	119.77	126.50
1	1A	599	U	O5'-P-OP1	-5.18	101.04	105.70
1	1A	1388	A	O5'-P-OP2	-5.17	101.04	105.70
1	1A	665	C	C6-N1-C2	-5.17	118.23	120.30
1	1A	1707	C	N3-C4-N4	-5.17	114.38	118.00
32	1a	1442	G	P-O3'-C3'	5.17	125.90	119.70
1	1A	752	A	N1-C6-N6	5.16	121.70	118.60
32	2a	1397	C	C6-N1-C1'	-5.16	114.61	120.80
1	1A	1220	U	OP1-P-O3'	5.15	116.54	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	952	G	O4'-C1'-N9	5.14	112.31	108.20
1	1A	2192	A	O4'-C1'-N9	5.14	112.31	108.20
32	2a	266	G	C4-N9-C1'	5.14	133.18	126.50
32	1a	533	A	C4-C5-C6	5.13	119.57	117.00
1	2A	2378	A	N1-C6-N6	5.13	121.68	118.60
1	1A	101	A	N9-C4-C5	-5.13	103.75	105.80
32	2a	1257	U	O4'-C1'-N1	5.13	112.30	108.20
1	1A	1255	A	P-O3'-C3'	5.13	125.85	119.70
12	1Q	41	TRP	CE2-CD2-CG	5.13	111.40	107.30
1	2A	458	G	O4'-C1'-N9	5.12	112.29	108.20
1	2A	277	C	C2-N1-C1'	5.11	124.42	118.80
1	2A	1416	G	C4-N9-C1'	-5.11	119.86	126.50
32	2a	520	A	C8-N9-C4	-5.11	103.76	105.80
32	1a	1026	G	O4'-C1'-N9	5.11	112.29	108.20
1	1A	1142	A	O4'-C1'-N9	5.10	112.28	108.20
32	1a	1027	C	C5-C6-N1	5.10	123.55	121.00
1	2A	2187	G	N3-C4-N9	5.10	129.06	126.00
1	1A	1134	A	C4-N9-C1'	5.09	135.47	126.30
3	1D	155	LEU	CA-CB-CG	5.09	127.02	115.30
32	1a	78	G	N3-C4-N9	-5.09	122.95	126.00
32	1a	1036	G	C4-N9-C1'	5.09	133.12	126.50
1	1A	203	G	O4'-C1'-N9	5.08	112.27	108.20
1	1A	2597	U	OP1-P-O3'	5.08	116.37	105.20
1	2A	2318	G	C8-N9-C4	-5.08	104.37	106.40
1	1A	637	U	C2-N1-C1'	5.08	123.79	117.70
1	1A	1218	G	O4'-C1'-N9	5.08	112.26	108.20
1	1A	1738	C	N3-C2-O2	-5.08	118.35	121.90
1	1A	2155	G	C4-N9-C1'	-5.07	119.91	126.50
32	2a	1016	A	N1-C6-N6	5.07	121.64	118.60
2	1B	24	G	C4-N9-C1'	5.07	133.09	126.50
32	1a	115	G	P-O3'-C3'	5.07	125.78	119.70
1	2A	614	U	C2-N1-C1'	5.06	123.78	117.70
1	2A	2585	U	OP1-P-O3'	5.06	116.34	105.20
32	1a	533	A	C6-N1-C2	-5.06	115.56	118.60
1	2A	2238	G	N3-C4-C5	-5.06	126.07	128.60
32	2a	913	A	P-O3'-C3'	5.06	125.77	119.70
1	1A	137	G	C8-N9-C1'	-5.06	120.43	127.00
1	1A	2014	G	O5'-P-OP1	-5.05	101.15	105.70
32	2a	687	A	P-O3'-C3'	5.05	125.76	119.70
1	1A	2513	C	C2-N1-C1'	-5.05	113.25	118.80
1	1A	2903	G	N3-C2-N2	-5.05	116.37	119.90
1	1A	101	A	C8-N9-C1'	-5.05	118.61	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1835	G	O4'-C1'-N9	-5.05	104.16	108.20
32	2a	1465	C	N3-C4-C5	5.04	123.92	121.90
1	1A	1007	G	OP1-P-O3'	5.04	116.29	105.20
1	1A	1098	C	C6-N1-C2	-5.04	118.28	120.30
1	2A	1420	U	P-O3'-C3'	5.04	125.75	119.70
1	1A	2614	A	P-O3'-C3'	5.04	125.74	119.70
32	2a	1004	A	O4'-C1'-N9	5.03	112.23	108.20
1	1A	894	U	C2-N1-C1'	5.03	123.73	117.70
24	12	69	ARG	N-CA-C	5.03	124.58	111.00
1	1A	1332	A	C8-N9-C4	5.02	107.81	105.80
1	1A	611	U	O5'-P-OP2	-5.02	101.18	105.70
1	1A	279	G	O4'-C1'-N9	-5.02	104.19	108.20
1	1A	765	A	N1-C6-N6	5.01	121.61	118.60
1	2A	906	G	N9-C4-C5	5.01	107.41	105.40
1	2A	1131	G	O4'-C1'-N9	5.01	112.21	108.20
1	1A	399	G	O4'-C1'-N9	5.01	112.21	108.20
1	2A	226	G	C8-N9-C1'	5.01	133.51	127.00
1	2A	800	A	O5'-P-OP1	-5.01	101.19	105.70
1	2A	2114	A	N7-C8-N9	5.01	116.30	113.80
1	2A	391	G	C6-N1-C2	-5.00	122.10	125.10
32	1a	993	G	N3-C4-N9	5.00	129.00	126.00
1	2A	1210	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	231	GLU	Peptide
55	1y	15	PRO	Mainchain
26	24	59	PHE	Peptide
55	2y	15	PRO	Mainchain

## 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](#)

There are no protein backbone outliers to report in this entry.

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	407 (14%)	0
1	2A	2857/2915 (98%)	408 (14%)	0
2	1B	119/120 (99%)	5 (4%)	0
2	2B	118/120 (98%)	6 (5%)	0
32	1a	1494/1520 (98%)	208 (13%)	0
32	2a	1498/1520 (98%)	220 (14%)	0
53	1v	2/3 (66%)	0	0
53	2v	2/3 (66%)	0	0
54	1x	75/76 (98%)	20 (26%)	0
54	2x	75/76 (98%)	10 (13%)	0
All	All	9103/9268 (98%)	1284 (14%)	0

All (1284) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	162	G
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	202	A
1	1A	204	G
1	1A	205	A
1	1A	210	A
1	1A	211	A
1	1A	214	A
1	1A	218	A
1	1A	237	G

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Mol	Chain	Res	Type
1	1A	269	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	279	G
1	1A	288	U
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	348	A
1	1A	351	G
1	1A	354	A
1	1A	366	G
1	1A	376	G
1	1A	381	A
1	1A	386	U
1	1A	387	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	455	A
1	1A	474	U
1	1A	482	C
1	1A	483	A
1	1A	505	A
1	1A	507	G
1	1A	530	A
1	1A	534	C
1	1A	535	C
1	1A	543	G
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	574	G
1	1A	586	G

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Mol	Chain	Res	Type
1	1A	596	G
1	1A	598	A
1	1A	609	A
1	1A	615	G
1	1A	618	C
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	633	G
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	673	G
1	1A	693	G
1	1A	694	G
1	1A	697	C
1	1A	698	G
1	1A	715	G
1	1A	716	G
1	1A	733	G
1	1A	777	C
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	927	G
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	942	A
1	1A	945	A

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Mol	Chain	Res	Type
1	1A	946	A
1	1A	947	A
1	1A	956	A
1	1A	977	G
1	1A	983	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1021	G
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1079	U
1	1A	1085	G
1	1A	1088	G
1	1A	1090	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1106	U
1	1A	1107	U
1	1A	1108	G
1	1A	1109	G
1	1A	1110	C
1	1A	1111	U
1	1A	1112	U
1	1A	1113	A
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1122	C

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Mol	Chain	Res	Type
1	1A	1123	A
1	1A	1124	U
1	1A	1129	U
1	1A	1130	A
1	1A	1131	A
1	1A	1134	A
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1141	A
1	1A	1142	A
1	1A	1143	U
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1265	A
1	1A	1287	A
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1354	A
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1411	A
1	1A	1416	C
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1500	A
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1543	U
1	1A	1554	A
1	1A	1555	C
1	1A	1578	C
1	1A	1589	A
1	1A	1590	C
1	1A	1594	C
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1767	A
1	1A	1787	G

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Mol	Chain	Res	Type
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1918	G
1	1A	1922	A
1	1A	1927	C
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G

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Mol	Chain	Res	Type
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2115	G
1	1A	2121	U
1	1A	2125	C
1	1A	2126	G
1	1A	2129	C
1	1A	2130	C
1	1A	2132	G
1	1A	2133	C
1	1A	2134	G
1	1A	2137	G
1	1A	2138	G
1	1A	2139	A
1	1A	2140	U
1	1A	2141	A
1	1A	2142	G
1	1A	2148	A
1	1A	2149	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2158	C
1	1A	2160	C
1	1A	2164	C
1	1A	2166	U
1	1A	2167	C
1	1A	2168	C
1	1A	2169	G
1	1A	2170	G
1	1A	2174	G
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2194	U
1	1A	2195	A
1	1A	2200	C
1	1A	2208	G
1	1A	2209	G

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Mol	Chain	Res	Type
1	1A	2211	U
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2291	G
1	1A	2295	C
1	1A	2298	A
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2324	U
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2347	A
1	1A	2348	A
1	1A	2359	C
1	1A	2395	G
1	1A	2397	C
1	1A	2408	G
1	1A	2418	U
1	1A	2426	G
1	1A	2434	A
1	1A	2435	U
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2481	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2486	C
1	1A	2488	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2537	G
1	1A	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2594	G
1	1A	2597	U
1	1A	2598	C
1	1A	2614	A
1	1A	2615	G
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2642	G
1	1A	2666	A
1	1A	2674	A
1	1A	2675	G
1	1A	2694	U
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2777	A
1	1A	2778	A
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G

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Mol	Chain	Res	Type
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	30	C
2	1B	56	G
2	1B	73	A
2	1B	110	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	159	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	630	G
32	1a	632	A
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	753	A
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	838	G
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	859	A
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	967	5MC

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Mol	Chain	Res	Type
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	1002	G
32	1a	1003	G
32	1a	1004	A
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1033	G
32	1a	1044	A
32	1a	1053	G
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1125	U
32	1a	1130	A
32	1a	1134	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1317	C
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1487	G

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Mol	Chain	Res	Type
32	1a	1493	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
54	1x	3	C
54	1x	6	G
54	1x	9	G
54	1x	14	A
54	1x	16	C
54	1x	19	G
54	1x	20	U
54	1x	21	A
54	1x	30	G
54	1x	34	C
54	1x	42	G
54	1x	44	A
54	1x	47	U
54	1x	50	U
54	1x	60	U
54	1x	63	G
54	1x	69	C
54	1x	72	A
54	1x	75	C
54	1x	76	A
1	2A	10	G
1	2A	12	U
1	2A	34	C
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	95	G
1	2A	118	A
1	2A	119	A

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Mol	Chain	Res	Type
1	2A	120	U
1	2A	157	U
1	2A	173	G
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	357	A
1	2A	362	U
1	2A	363	G
1	2A	386	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	428	A
1	2A	444	C
1	2A	456	C
1	2A	457	A
1	2A	479	A
1	2A	481	G
1	2A	505	A

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Mol	Chain	Res	Type
1	2A	509	C
1	2A	510	C
1	2A	518	G
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	592	G
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	610	G
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	648	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(E)	G
1	2A	652(U)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	730	C
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G

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Mol	Chain	Res	Type
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	880	G
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	896	A
1	2A	899	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1042	G
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1052	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1053	C
1	2A	1054	A
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1096	A
1	2A	1108	U
1	2A	1109	C
1	2A	1110	G
1	2A	1112	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1171	G
1	2A	1211	U
1	2A	1220	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A

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Mol	Chain	Res	Type
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1308	A
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1533	G
1	2A	1537	G
1	2A	1542	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1579	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A

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Mol	Chain	Res	Type
1	2A	1640	C
1	2A	1648	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1722	A
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1896	G
1	2A	1900	A
1	2A	1905	C
1	2A	1906	G
1	2A	1914	C
1	2A	1915	5MU
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A

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Mol	Chain	Res	Type
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2039	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2101	G
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2138	C
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2151	G
1	2A	2152	G
1	2A	2158	A
1	2A	2159	G

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Mol	Chain	Res	Type
1	2A	2160	G
1	2A	2162	G
1	2A	2172	U
1	2A	2173	A
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2286	A
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2347	C
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2406	U
1	2A	2414	G
1	2A	2422	A

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Mol	Chain	Res	Type
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2431	U
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2474	C
1	2A	2476	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2585	U
1	2A	2586	C
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2662	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A

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Mol	Chain	Res	Type
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2802	G
1	2A	2811	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
2	2B	8	U
2	2B	30	C
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	61	G
32	2a	66	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C

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Mol	Chain	Res	Type
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	348	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	485	G

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Mol	Chain	Res	Type
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	7MG
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	592	G
32	2a	596	C
32	2a	630	G
32	2a	632	A
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	753	A
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	838	G

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Mol	Chain	Res	Type
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1036	G
32	2a	1041	A
32	2a	1044	A

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Mol	Chain	Res	Type
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1152	A
32	2a	1158	C
32	2a	1159	U
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1270	C
32	2a	1278	U
32	2a	1280	A
32	2a	1281	U

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Mol	Chain	Res	Type
32	2a	1282	C
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1305	G
32	2a	1317	C
32	2a	1320	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1400	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1487	G
32	2a	1492	A
32	2a	1493	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1517	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
54	2x	9	G
54	2x	13	C
54	2x	20	U
54	2x	21	A
54	2x	48	C
54	2x	50	U
54	2x	62	C

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Mol	Chain	Res	Type
54	2x	63	G
54	2x	65	C
54	2x	76	A

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
32	5MC	1a	1400	32	15,22,23	0.78	0	19,32,35	1.04	2 (10%)
1	2MA	2A	2503	1,56	17,25,26	2.76	6 (35%)	19,37,40	2.63	5 (26%)
32	4OC	2a	1402	32	16,23,24	2.38	7 (43%)	17,32,35	3.18	3 (17%)
54	4SU	1x	8	54	14,21,22	1.65	2 (14%)	15,30,33	2.21	2 (13%)
1	5MC	2A	1962	1,56	15,22,23	0.85	0	19,32,35	0.90	1 (5%)
1	PSU	2A	1911	1	17,21,22	2.08	6 (35%)	20,30,33	4.47	7 (35%)
54	5MC	2x	32	54	15,22,23	0.80	0	19,32,35	0.93	1 (5%)
1	PSU	1A	1933	1	17,21,22	2.05	5 (29%)	20,30,33	4.43	8 (40%)
1	5MU	2A	1915	1	15,22,23	1.35	2 (13%)	16,32,35	2.66	1 (6%)
32	MA6	1a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	4.93	3 (16%)
32	2MG	2a	1207	32	19,26,27	3.15	7 (36%)	21,38,41	2.25	8 (38%)
32	4OC	1a	1402	32	16,23,24	2.43	7 (43%)	17,32,35	1.80	2 (11%)
1	5MU	2A	1939	1	15,22,23	1.51	2 (13%)	16,32,35	2.47	1 (6%)
1	5MC	2A	1942	1	15,22,23	0.90	0	19,32,35	0.97	1 (5%)
1	PSU	1A	2617	1	17,21,22	1.82	4 (23%)	20,30,33	4.42	5 (25%)
1	5MU	1A	1961	1	15,22,23	1.27	1 (6%)	16,32,35	2.57	1 (6%)
54	5MC	1x	32	54	15,22,23	0.94	0	19,32,35	0.93	2 (10%)
32	5MC	1a	1404	32	15,22,23	0.90	0	19,32,35	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	5MC	2a	967	32	15,22,23	0.72	0	19,32,35	1.09	2 (10%)
54	PSU	1x	55	54	17,21,22	2.09	5 (29%)	20,30,33	4.59	6 (30%)
1	OMC	2A	1920	1	15,22,23	2.32	6 (40%)	17,31,34	1.43	2 (11%)
32	M2G	1a	966	32	20,27,28	3.08	7 (35%)	22,40,43	1.54	6 (27%)
1	OMU	2A	2552	1,56	14,22,23	8.04	8 (57%)	14,31,34	0.77	0
32	MA6	2a	1519	32	19,26,27	0.97	1 (5%)	18,38,41	5.18	3 (16%)
1	PSU	1A	1939	1,56	17,21,22	2.09	7 (41%)	20,30,33	4.54	7 (35%)
1	PSU	2A	2605	1	17,21,22	2.05	5 (29%)	20,30,33	4.52	6 (30%)
1	5MC	1A	1984	1,56	15,22,23	0.85	0	19,32,35	1.08	1 (5%)
32	M2G	2a	966	32	20,27,28	3.21	7 (35%)	22,40,43	1.73	5 (22%)
1	OMU	1A	2564	1,56	14,22,23	8.00	8 (57%)	14,31,34	0.71	0
32	7MG	2a	527	32	22,26,27	3.19	6 (27%)	28,39,42	1.68	7 (25%)
32	5MC	2a	1407	32	15,22,23	0.95	0	19,32,35	0.94	1 (5%)
32	5MC	1a	1407	32	15,22,23	0.96	1 (6%)	19,32,35	1.11	3 (15%)
32	5MC	1a	967	32	15,22,23	0.86	0	19,32,35	0.93	1 (5%)
43	0TD	2l	92	43	4,9,10	1.77	1 (25%)	3,11,13	2.34	2 (66%)
1	5MU	1A	1937	1	15,22,23	1.31	1 (6%)	16,32,35	2.53	1 (6%)
32	7MG	1a	527	32,56	22,26,27	2.99	6 (27%)	28,39,42	1.69	8 (28%)
54	PSU	2x	55	54,56	17,21,22	2.20	4 (23%)	20,30,33	4.46	5 (25%)
32	PSU	1a	516	32	17,21,22	2.36	5 (29%)	20,30,33	4.37	8 (40%)
43	0TD	1l	92	43	4,9,10	1.99	2 (50%)	3,11,13	2.92	2 (66%)
1	PSU	2A	1917	1	17,21,22	1.96	4 (23%)	20,30,33	4.47	7 (35%)
32	MA6	1a	1519	32	19,26,27	0.98	2 (10%)	18,38,41	5.30	3 (16%)
54	5MU	2x	54	54	15,22,23	1.45	1 (6%)	16,32,35	2.61	1 (6%)
32	UR3	2a	1498	32	14,22,23	2.07	3 (21%)	15,32,35	0.77	0
1	5MC	1A	1964	1,56	15,22,23	0.80	0	19,32,35	0.99	2 (10%)
32	5MC	2a	1400	32	15,22,23	0.83	0	19,32,35	1.00	1 (5%)
32	MA6	2a	1518	32	19,26,27	1.04	1 (5%)	18,38,41	5.11	3 (16%)
32	5MC	2a	1404	32	15,22,23	1.02	1 (6%)	19,32,35	0.99	2 (10%)
32	UR3	1a	1498	32	14,22,23	1.88	3 (21%)	15,32,35	0.76	1 (6%)
1	OMG	1A	2263	1,54	18,26,27	2.73	7 (38%)	20,38,41	2.20	8 (40%)
54	5MU	1x	54	54	15,22,23	1.27	1 (6%)	16,32,35	2.62	1 (6%)
54	4SU	2x	8	54	14,21,22	1.48	3 (21%)	15,30,33	2.67	2 (13%)
1	OMG	2A	2251	1,54	18,26,27	2.65	5 (27%)	20,38,41	2.34	6 (30%)
32	2MG	1a	1207	32	19,26,27	3.32	6 (31%)	21,38,41	2.55	9 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MA	1A	2515	1,56	17,25,26	2.73	6 (35%)	19,37,40	2.97	5 (26%)
1	OMC	1A	1942	1	15,22,23	2.36	6 (40%)	17,31,34	1.43	2 (11%)
32	PSU	2a	516	32	17,21,22	2.02	5 (29%)	20,30,33	4.35	8 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	2/3/25/26	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
54	4SU	1x	8	54	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/5/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	4/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	2A	1939	1	-	2/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/5/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/5/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/7/27/28	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	OMU	2A	2552	1,56	-	1/7/27/28	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
1	PSU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1,56	-	2/5/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	OMU	1A	2564	1,56	-	0/7/27/28	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/3/12/14	-
1	5MU	1A	1937	1	-	2/5/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	2/7/37/38	0/3/3/3
54	PSU	2x	55	54,56	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
54	5MU	2x	54	54	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1964	1,56	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
1	OMG	1A	2263	1,54	-	2/5/27/28	0/3/3/3
54	5MU	1x	54	54	-	0/5/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/5/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	1/5/27/28	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,56	-	1/3/25/26	0/3/3/3
1	OMC	1A	1942	1	-	1/7/27/28	0/2/2/2
32	PSU	2a	516	32	-	1/7/25/26	0/2/2/2

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C6-N1	18.60	1.58	1.35
1	2A	2552	OMU	C6-N1	18.43	1.58	1.35
1	2A	2552	OMU	C6-C5	-12.22	1.11	1.38
1	1A	2564	OMU	C6-C5	-12.14	1.11	1.38
1	2A	2552	OMU	C4-N3	-11.94	1.12	1.33
1	1A	2564	OMU	C4-N3	-11.74	1.12	1.33
1	2A	2552	OMU	O4'-C1'	11.64	1.57	1.41
1	1A	2564	OMU	O4'-C1'	11.15	1.56	1.41
32	1a	1207	2MG	C2-N2	10.58	1.43	1.34
32	2a	1207	2MG	C2-N2	9.91	1.42	1.34
32	2a	527	7MG	C4-N3	8.63	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C3'-C2'	-8.56	1.33	1.52
1	2A	2552	OMU	C3'-C2'	-8.32	1.34	1.52
32	1a	527	7MG	C4-N3	7.85	1.44	1.34
32	1a	527	7MG	C6-C5	7.58	1.51	1.41
32	2a	527	7MG	C6-C5	7.50	1.51	1.41
32	2a	966	M2G	C4-N3	7.49	1.47	1.35
32	1a	516	PSU	C5-C1'	-7.42	1.45	1.52
54	2x	55	PSU	C4-N3	6.76	1.44	1.33
32	1a	966	M2G	C4-N3	6.75	1.46	1.35
1	2A	2251	OMG	C4-N3	6.58	1.46	1.35
1	2A	2552	OMU	O4'-C4'	-6.38	1.30	1.45
1	2A	1911	PSU	C4-N3	6.34	1.44	1.33
54	1x	55	PSU	C4-N3	6.28	1.44	1.33
1	1A	2564	OMU	O4'-C4'	-6.21	1.31	1.45
32	2a	966	M2G	C6-C5	6.14	1.51	1.41
1	1A	1939	PSU	C4-N3	6.08	1.43	1.33
32	1a	966	M2G	C6-C5	6.08	1.51	1.41
32	1a	1207	2MG	C4-N3	5.95	1.45	1.35
32	2a	966	M2G	C2-N2	5.94	1.44	1.34
1	1A	2263	OMG	C4-N3	5.81	1.44	1.35
1	2A	1917	PSU	C4-N3	5.64	1.42	1.33
32	1a	966	M2G	C2-N2	5.63	1.44	1.34
32	2a	1207	2MG	C4-N3	5.60	1.44	1.35
1	2A	2605	PSU	C4-N3	5.59	1.42	1.33
1	1A	1933	PSU	C4-N3	5.58	1.42	1.33
1	2A	2503	2MA	C6-C5	5.55	1.49	1.41
1	1A	2515	2MA	C6-C5	5.52	1.49	1.41
1	1A	2515	2MA	C2-N1	5.50	1.43	1.34
1	1A	2263	OMG	C6-C5	5.46	1.50	1.41
1	2A	2503	2MA	C4-N3	5.45	1.44	1.35
32	2a	1498	UR3	C6-N1	5.45	1.42	1.35
1	2A	2503	2MA	C2-N1	5.24	1.43	1.34
32	1a	966	M2G	C2-N1	5.15	1.43	1.34
1	1A	2263	OMG	C6-N1	5.10	1.41	1.33
32	2a	527	7MG	C2-N1	5.04	1.44	1.35
32	2a	966	M2G	C2-N1	4.96	1.43	1.34
1	1A	2515	2MA	C4-N3	4.93	1.43	1.35
32	2a	527	7MG	C2-N3	4.91	1.44	1.35
32	1a	1402	4OC	C4-N4	4.89	1.46	1.36
1	1A	2617	PSU	C4-N3	4.87	1.41	1.33
32	2a	1402	4OC	C4-N4	4.86	1.46	1.36
32	2a	516	PSU	C4-N3	4.84	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C2-N3	4.81	1.42	1.34
32	2a	966	M2G	C2-N3	4.79	1.45	1.33
1	2A	2251	OMG	C6-C5	4.78	1.49	1.41
32	2a	1207	2MG	C6-C5	4.66	1.49	1.41
1	2A	2251	OMG	C6-N1	4.64	1.41	1.33
32	1a	1498	UR3	C6-N1	4.62	1.41	1.35
1	1A	2515	2MA	C2-N3	4.59	1.42	1.34
32	1a	1207	2MG	C6-C5	4.52	1.49	1.41
32	1a	527	7MG	C2-N1	4.51	1.43	1.35
32	2a	527	7MG	C6-N1	4.50	1.40	1.33
32	1a	527	7MG	C2-N3	4.42	1.43	1.35
32	1a	966	M2G	C6-N1	4.42	1.40	1.33
54	2x	54	5MU	C4-N3	4.41	1.40	1.33
1	1A	2263	OMG	C2-N1	4.38	1.43	1.35
1	1A	1942	OMC	C6-N1	4.33	1.41	1.35
32	1a	966	M2G	C2-N3	4.32	1.44	1.33
1	2A	1920	OMC	C4-N4	4.31	1.47	1.35
32	2a	966	M2G	C6-N1	4.31	1.40	1.33
1	2A	1939	5MU	C4-N3	4.28	1.40	1.33
1	1A	2564	OMU	C3'-C4'	4.25	1.63	1.53
32	1a	1402	4OC	C6-N1	4.22	1.41	1.35
32	1a	527	7MG	C6-N1	4.21	1.40	1.33
54	1x	8	4SU	C4-S4	-4.20	1.59	1.67
32	2a	1498	UR3	C6-C5	4.19	1.47	1.38
1	1A	1942	OMC	C4-N4	4.06	1.47	1.35
1	2A	1920	OMC	C6-N1	4.04	1.40	1.35
32	2a	516	PSU	C5-C1'	-4.01	1.48	1.52
32	2a	1402	4OC	C5-C4	3.99	1.48	1.39
32	2a	527	7MG	C2-N2	3.96	1.41	1.33
1	1A	1942	OMC	C2-N3	3.94	1.46	1.38
32	1a	1498	UR3	C6-C5	3.90	1.46	1.38
1	2A	2552	OMU	C3'-C4'	3.89	1.62	1.53
1	2A	2251	OMG	C2-N1	3.88	1.42	1.35
54	2x	8	4SU	C5-C4	3.82	1.42	1.38
1	2A	1920	OMC	C2-N3	3.82	1.45	1.38
32	2a	1402	4OC	C2-N3	3.81	1.45	1.38
1	1A	1933	PSU	C5-C1'	-3.81	1.49	1.52
1	1A	1961	5MU	C4-N3	3.78	1.39	1.33
32	1a	1402	4OC	C5-C4	3.73	1.48	1.39
1	2A	1915	5MU	C4-N3	3.71	1.39	1.33
32	1a	1207	2MG	C6-N1	3.65	1.39	1.33
1	1A	1937	5MU	C4-N3	3.57	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1942	OMC	C6-C5	3.57	1.45	1.38
1	2A	2605	PSU	C5-C1'	-3.56	1.49	1.52
32	2a	1207	2MG	C6-N1	3.56	1.39	1.33
32	1a	527	7MG	C2-N2	3.49	1.40	1.33
32	1a	1402	4OC	C2-N3	3.47	1.45	1.38
1	2A	1920	OMC	C6-C5	3.44	1.45	1.38
54	1x	8	4SU	C5-C4	3.43	1.42	1.38
54	1x	54	5MU	C4-N3	3.42	1.39	1.33
32	2a	1402	4OC	C6-N1	3.38	1.40	1.35
32	1a	1402	4OC	C6-C5	3.35	1.45	1.38
54	2x	55	PSU	C4-C5	3.29	1.48	1.41
1	1A	2617	PSU	C6-C5	-3.22	1.33	1.38
1	2A	2605	PSU	C6-C5	-3.20	1.34	1.38
1	1A	2515	2MA	C6-N1	3.17	1.41	1.35
32	1a	1207	2MG	C2-N1	3.17	1.44	1.34
1	1A	1942	OMC	C5-C4	3.16	1.48	1.41
54	1x	55	PSU	C6-N1	3.11	1.41	1.34
32	2a	1207	2MG	C2-N1	3.10	1.44	1.34
1	2A	1920	OMC	C5-C4	3.05	1.48	1.41
32	1a	516	PSU	C4-N3	3.02	1.38	1.33
32	1a	516	PSU	C6-N1	2.95	1.40	1.34
1	1A	1933	PSU	C6-C5	-2.93	1.34	1.38
32	1a	516	PSU	O4'-C1'	-2.92	1.40	1.44
54	2x	55	PSU	C6-N1	2.92	1.40	1.34
1	2A	1920	OMC	C4-N3	2.91	1.40	1.35
1	2A	2503	2MA	C6-N1	2.91	1.40	1.35
32	2a	1402	4OC	C4-N3	2.90	1.40	1.34
32	1a	1498	UR3	C4-N3	2.89	1.42	1.38
43	1l	92	0TD	CB-SB	-2.86	1.77	1.84
1	2A	2552	OMU	O2'-C2'	2.84	1.49	1.42
1	1A	1942	OMC	C4-N3	2.83	1.40	1.35
32	2a	516	PSU	C6-N1	2.80	1.40	1.34
1	1A	1939	PSU	C6-N1	2.79	1.40	1.34
32	2a	1518	MA6	C2-N3	2.79	1.36	1.32
1	2A	1917	PSU	C4-C5	2.77	1.47	1.41
32	2a	1402	4OC	C6-C5	2.77	1.44	1.38
1	2A	1917	PSU	C6-N1	2.75	1.40	1.34
32	1a	1402	4OC	C4-N3	2.74	1.39	1.34
1	2A	1917	PSU	C6-C5	-2.73	1.34	1.38
1	1A	2263	OMG	C2-N2	2.72	1.39	1.33
1	1A	1939	PSU	C5-C1'	-2.72	1.49	1.52
32	2a	516	PSU	O4'-C1'	-2.70	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1498	UR3	C4-N3	2.70	1.42	1.38
32	2a	1402	4OC	CM4-N4	-2.69	1.40	1.45
1	2A	1911	PSU	C6-N1	2.64	1.40	1.34
32	1a	1519	MA6	C2-N3	2.64	1.36	1.32
32	2a	1519	MA6	C2-N3	2.58	1.36	1.32
1	2A	2251	OMG	C2-N2	2.57	1.39	1.33
32	1a	1207	2MG	C2-N3	2.55	1.42	1.34
32	1a	1402	4OC	CM4-N4	-2.54	1.40	1.45
1	1A	1939	PSU	C6-C5	-2.53	1.34	1.38
43	2l	92	0TD	CB-SB	-2.52	1.78	1.84
54	2x	55	PSU	C6-C5	-2.50	1.35	1.38
32	1a	1518	MA6	C2-N3	2.48	1.36	1.32
32	2a	516	PSU	C6-C5	-2.44	1.35	1.38
1	2A	1911	PSU	C6-C5	-2.43	1.35	1.38
1	2A	1911	PSU	C5-C1'	-2.42	1.50	1.52
54	2x	8	4SU	C2-N3	2.41	1.42	1.38
32	2a	1207	2MG	C2-N3	2.39	1.42	1.34
1	1A	2564	OMU	O2'-C2'	2.38	1.48	1.42
54	1x	55	PSU	C6-C5	-2.33	1.35	1.38
1	2A	2605	PSU	C6-N1	2.32	1.39	1.34
1	2A	2605	PSU	C4-C5	2.31	1.46	1.41
1	1A	1939	PSU	C4-C5	2.29	1.46	1.41
1	1A	2263	OMG	C8-N7	2.29	1.38	1.34
54	2x	8	4SU	C4-S4	-2.27	1.63	1.67
1	1A	1933	PSU	C6-N1	2.26	1.39	1.34
32	1a	516	PSU	C6-C5	-2.26	1.35	1.38
1	1A	2515	2MA	C5-C4	-2.24	1.35	1.40
1	1A	2263	OMG	C5-C4	-2.23	1.35	1.40
1	1A	2617	PSU	C6-N1	2.23	1.39	1.34
1	2A	1911	PSU	C4-C5	2.22	1.46	1.41
54	1x	55	PSU	C4-C5	2.20	1.46	1.41
32	2a	966	M2G	CM2-N2	-2.19	1.40	1.45
1	2A	1939	5MU	C4-C5	2.19	1.46	1.41
1	2A	2503	2MA	C5-C4	-2.19	1.35	1.40
1	1A	1933	PSU	O4'-C1'	-2.18	1.41	1.44
32	1a	1518	MA6	C5-C4	-2.18	1.35	1.40
54	1x	55	PSU	C2-N1	2.17	1.42	1.38
1	1A	2617	PSU	C4-C5	2.14	1.46	1.41
1	1A	1939	PSU	O4'-C1'	-2.08	1.41	1.44
32	2a	1404	5MC	C4-N4	2.07	1.39	1.34
32	1a	1407	5MC	CM5-C5	-2.07	1.46	1.51
32	2a	1207	2MG	CM2-N2	-2.07	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	966	M2G	CM2-N2	-2.06	1.40	1.45
43	1l	92	0TD	CA-N	-2.05	1.41	1.47
32	1a	1519	MA6	C5-C4	-2.04	1.35	1.40
1	1A	1939	PSU	C2-N1	2.03	1.42	1.38
1	2A	1915	5MU	C2-N3	2.03	1.42	1.38
1	2A	1911	PSU	O4'-C1'	-2.02	1.41	1.44

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1519	MA6	N1-C6-N6	-20.95	95.00	117.06
32	2a	1519	MA6	N1-C6-N6	-20.61	95.36	117.06
32	2a	1518	MA6	N1-C6-N6	-20.06	95.95	117.06
32	1a	1518	MA6	N1-C6-N6	-19.20	96.85	117.06
54	1x	55	PSU	N1-C2-N3	-14.46	116.93	128.43
1	1A	1939	PSU	N1-C2-N3	-14.24	117.11	128.43
1	1A	2617	PSU	N1-C2-N3	-14.21	117.14	128.43
54	2x	55	PSU	N1-C2-N3	-14.16	117.17	128.43
1	2A	1911	PSU	N1-C2-N3	-14.00	117.30	128.43
1	2A	1917	PSU	N1-C2-N3	-13.95	117.34	128.43
1	2A	2605	PSU	N1-C2-N3	-13.92	117.36	128.43
1	1A	1933	PSU	N1-C2-N3	-13.76	117.49	128.43
32	2a	516	PSU	N1-C2-N3	-12.65	118.37	128.43
32	2a	1402	4OC	CM4-N4-C4	-12.48	112.25	122.97
32	1a	516	PSU	N1-C2-N3	-11.95	118.93	128.43
54	1x	55	PSU	C4-N3-C2	10.50	124.01	115.14
1	2A	1915	5MU	C4-N3-C2	10.38	123.90	115.14
1	2A	2605	PSU	C4-N3-C2	10.25	123.80	115.14
1	1A	1939	PSU	C4-N3-C2	10.21	123.76	115.14
54	1x	54	5MU	C4-N3-C2	10.21	123.76	115.14
32	1a	516	PSU	C4-N3-C2	10.16	123.72	115.14
1	2A	1911	PSU	C4-N3-C2	10.11	123.68	115.14
54	2x	54	5MU	C4-N3-C2	10.09	123.66	115.14
1	1A	2515	2MA	C1'-N9-C4	10.03	144.26	126.64
1	2A	1917	PSU	C4-N3-C2	10.02	123.61	115.14
32	2a	516	PSU	C4-N3-C2	9.98	123.56	115.14
1	1A	1933	PSU	C4-N3-C2	9.90	123.50	115.14
1	1A	1937	5MU	C4-N3-C2	9.79	123.41	115.14
54	2x	55	PSU	C4-N3-C2	9.74	123.36	115.14
1	1A	2617	PSU	C4-N3-C2	9.74	123.36	115.14
1	1A	1961	5MU	C4-N3-C2	9.73	123.36	115.14
1	2A	2503	2MA	C1'-N9-C4	9.44	143.23	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	C4-N3-C2	9.44	123.11	115.14
1	2A	1911	PSU	C5-C4-N3	-8.20	114.79	125.36
1	2A	2605	PSU	C5-C4-N3	-8.19	114.81	125.36
1	1A	1933	PSU	C5-C4-N3	-8.10	114.93	125.36
54	2x	55	PSU	C5-C4-N3	-7.97	115.09	125.36
54	1x	55	PSU	C5-C4-N3	-7.94	115.13	125.36
32	2a	516	PSU	C5-C4-N3	-7.87	115.22	125.36
1	1A	1939	PSU	C5-C4-N3	-7.83	115.27	125.36
32	1a	516	PSU	C5-C4-N3	-7.76	115.36	125.36
1	2A	1917	PSU	C5-C4-N3	-7.72	115.41	125.36
1	1A	2617	PSU	C5-C4-N3	-7.32	115.93	125.36
54	2x	8	4SU	C2-N3-C4	7.16	125.53	115.15
54	2x	8	4SU	C5-C4-N3	-7.12	114.31	123.83
1	2A	2251	OMG	C1'-N9-C4	6.56	138.16	126.64
32	1a	1207	2MG	C1'-N9-C4	-6.51	115.20	126.64
32	1a	1402	4OC	CM4-N4-C4	-6.39	117.48	122.97
54	1x	8	4SU	C2-N3-C4	6.30	124.28	115.15
32	1a	1518	MA6	C1'-N9-C4	-6.07	115.98	126.64
32	1a	1519	MA6	C1'-N9-C4	-5.85	116.37	126.64
32	2a	1518	MA6	C1'-N9-C4	-5.79	116.47	126.64
1	1A	2263	OMG	N3-C2-N1	-5.55	119.82	127.22
54	1x	8	4SU	C5-C4-N3	-5.50	116.47	123.83
32	2a	1518	MA6	N3-C2-N1	-5.37	120.29	128.68
32	2a	1207	2MG	C1'-N9-C4	-5.36	117.22	126.64
1	2A	2251	OMG	N3-C2-N1	-5.33	120.11	127.22
32	2a	1519	MA6	N3-C2-N1	-5.25	120.47	128.68
32	1a	1518	MA6	N3-C2-N1	-5.20	120.55	128.68
32	1a	516	PSU	C4-C5-C1'	-5.20	111.31	121.12
32	1a	1519	MA6	N3-C2-N1	-5.18	120.58	128.68
32	2a	1519	MA6	C1'-N9-C4	-5.16	117.58	126.64
1	1A	2515	2MA	CM2-C2-N1	4.61	124.35	117.15
32	2a	966	M2G	N3-C2-N2	4.57	121.81	117.18
32	1a	516	PSU	C5-C6-N1	-4.51	118.89	124.44
32	2a	966	M2G	C2-N3-C4	4.46	120.34	115.28
1	1A	1942	OMC	C2-N3-C4	4.29	120.69	116.34
32	1a	1207	2MG	C2-N3-C4	4.14	119.98	115.28
1	2A	1920	OMC	C2-N3-C4	4.06	120.45	116.34
1	1A	2515	2MA	C2-N3-C4	4.05	118.81	115.52
32	2a	1207	2MG	C2-N3-C4	4.03	119.86	115.28
54	2x	55	PSU	C6-N1-C2	4.01	121.97	115.36
1	1A	2617	PSU	C6-N1-C2	3.94	121.87	115.36
1	2A	2251	OMG	C2-N3-C4	3.91	119.83	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	N3-C2-N1	-3.91	120.05	126.23
1	2A	2605	PSU	C6-N1-C2	3.85	121.71	115.36
1	2A	1917	PSU	C6-N1-C2	3.77	121.57	115.36
32	2a	516	PSU	C4-C5-C1'	-3.74	114.06	121.12
32	2a	516	PSU	C5-C6-N1	-3.73	119.86	124.44
1	1A	1939	PSU	C6-N1-C2	3.71	121.48	115.36
43	1l	92	0TD	CSB-SB-CB	3.70	109.13	101.85
32	2a	1207	2MG	N3-C2-N1	-3.70	120.38	126.23
32	2a	527	7MG	N1-C2-N3	-3.67	119.67	125.42
32	1a	1207	2MG	N2-C2-N3	3.64	120.46	116.96
1	1A	1933	PSU	C6-N1-C2	3.61	121.31	115.36
1	1A	2515	2MA	C5-C6-N1	-3.59	119.30	123.06
1	1A	2263	OMG	C1'-N9-C4	3.57	132.92	126.64
32	1a	527	7MG	C5-C4-N9	3.57	111.44	106.44
54	1x	55	PSU	C6-N1-C2	3.54	121.20	115.36
1	2A	1911	PSU	C6-N1-C2	3.53	121.19	115.36
32	1a	966	M2G	C2-N3-C4	3.49	119.24	115.28
32	2a	527	7MG	C6-N1-C2	3.38	121.30	115.93
32	2a	1207	2MG	N2-C2-N3	3.37	120.19	116.96
1	1A	2263	OMG	N2-C2-N1	3.36	122.48	117.25
1	1A	2263	OMG	C2-N3-C4	3.35	119.18	115.36
32	2a	1207	2MG	C5-C6-N1	-3.33	118.88	123.43
32	1a	516	PSU	C5-C1'-C2'	-3.32	109.40	115.32
32	1a	527	7MG	N1-C2-N3	-3.32	120.22	125.42
1	1A	2617	PSU	C5-C6-N1	-3.19	120.52	124.44
1	1A	2515	2MA	N3-C2-N1	-3.18	119.86	125.72
1	2A	2503	2MA	CM2-C2-N1	3.18	122.11	117.15
32	1a	527	7MG	C5-C4-N3	-3.15	121.34	126.49
1	2A	2503	2MA	C5-C6-N1	-3.12	119.79	123.06
43	2l	92	0TD	CSB-SB-CB	3.10	107.94	101.85
32	1a	527	7MG	C6-N1-C2	3.09	120.84	115.93
32	2a	527	7MG	C6-C5-C4	3.09	118.52	115.20
1	2A	2503	2MA	C2-N3-C4	3.04	118.00	115.52
32	2a	516	PSU	C6-N1-C2	3.04	120.37	115.36
32	2a	527	7MG	C5-C4-N3	-3.02	121.56	126.49
32	1a	966	M2G	C5-C6-N1	-2.96	119.38	123.43
1	1A	1939	PSU	C5-C1'-C2'	-2.96	110.04	115.32
32	2a	527	7MG	C5-C4-N9	2.96	110.59	106.44
1	2A	1917	PSU	C5-C6-N1	-2.95	120.81	124.44
1	1A	1939	PSU	C5-C6-N1	-2.94	120.83	124.44
1	1A	2263	OMG	C6-C5-C4	-2.90	118.03	120.80
43	1l	92	0TD	CB-CA-N	-2.88	102.96	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1207	2MG	C6-N1-C2	2.87	120.32	115.18
32	1a	527	7MG	C6-C5-C4	2.86	118.27	115.20
1	2A	2503	2MA	N3-C2-N1	-2.83	120.52	125.72
32	1a	1207	2MG	C5-C6-N1	-2.82	119.57	123.43
1	2A	1920	OMC	N4-C4-N3	2.80	120.91	116.49
1	1A	1933	PSU	C5-C6-N1	-2.79	121.01	124.44
1	2A	2605	PSU	C5-C6-N1	-2.78	121.03	124.44
32	1a	1207	2MG	C6-N1-C2	2.75	120.11	115.18
54	1x	55	PSU	C5-C6-N1	-2.74	121.07	124.44
1	1A	2263	OMG	C5-C6-N1	-2.74	119.69	123.43
1	1A	1984	5MC	C5-C4-N3	2.73	125.56	121.26
54	2x	55	PSU	C5-C6-N1	-2.72	121.09	124.44
32	1a	527	7MG	N2-C2-N1	2.66	121.39	117.25
32	1a	966	M2G	C6-N1-C2	2.65	119.34	116.18
32	2a	967	5MC	C5-C4-N3	2.65	125.44	121.26
54	1x	55	PSU	C4-C5-C1'	-2.64	116.14	121.12
32	1a	1207	2MG	N2-C2-N1	2.63	119.49	116.96
1	1A	1964	5MC	C5-C4-N3	2.63	125.41	121.26
1	1A	2263	OMG	C6-N1-C2	2.62	120.10	115.93
1	1A	1933	PSU	C5-C1'-C2'	-2.62	110.65	115.32
32	2a	1400	5MC	C5-C4-N3	2.60	125.36	121.26
32	1a	967	5MC	C5-C4-N3	2.58	125.34	121.26
1	2A	1917	PSU	C5-C1'-C2'	-2.58	110.72	115.32
32	2a	516	PSU	C5-C1'-C2'	-2.57	110.73	115.32
32	2a	1207	2MG	N2-C2-N1	2.56	119.42	116.96
32	2a	1402	4OC	N4-C4-N3	2.55	122.88	116.37
32	2a	966	M2G	C6-N1-C2	2.53	119.20	116.18
32	1a	1400	5MC	C5-C4-N3	2.50	125.20	121.26
1	2A	1942	5MC	C5-C4-N3	2.47	125.16	121.26
32	1a	1402	4OC	CM2-O2'-C2'	2.46	120.98	114.52
32	2a	516	PSU	O4'-C1'-C2'	2.46	108.64	104.66
32	2a	966	M2G	C5-C6-N1	-2.45	120.08	123.43
1	2A	1911	PSU	C5-C6-N1	-2.45	121.42	124.44
32	2a	527	7MG	N2-C2-N1	2.43	121.02	117.25
54	2x	32	5MC	C5-C4-N3	2.42	125.08	121.26
32	1a	516	PSU	O4'-C1'-C2'	2.42	108.58	104.66
1	2A	2605	PSU	C5-C1'-C2'	-2.42	111.01	115.32
32	1a	527	7MG	N7-C8-N9	2.41	106.82	103.38
32	1a	1407	5MC	C5-C4-N3	2.38	125.02	121.26
32	1a	1404	5MC	C5-C4-N3	2.37	125.00	121.26
32	1a	1207	2MG	CM2-N2-C2	-2.36	120.74	123.59
32	1a	516	PSU	C6-N1-C2	2.33	119.20	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	966	M2G	N1-C2-N2	2.32	119.54	117.19
54	1x	32	5MC	C5-C4-N3	2.31	124.91	121.26
1	2A	1962	5MC	C5-C4-N3	2.31	124.91	121.26
32	2a	1207	2MG	CM2-N2-C2	-2.29	120.82	123.59
32	1a	966	M2G	CM2-N2-C2	-2.28	119.11	121.29
32	2a	967	5MC	C5-C6-N1	-2.22	119.81	122.19
1	2A	2251	OMG	C6-N1-C2	2.20	119.42	115.93
43	2l	92	0TD	CB-CA-N	-2.19	104.42	109.10
1	1A	1939	PSU	C4-C5-C1'	-2.19	116.98	121.12
32	2a	1404	5MC	C5-C4-N3	2.18	124.70	121.26
32	2a	1407	5MC	C5-C4-N3	2.17	124.69	121.26
32	1a	527	7MG	C2-N3-C4	2.17	119.88	113.89
32	1a	1400	5MC	C5-C6-N1	-2.16	119.87	122.19
32	1a	1407	5MC	N4-C4-N3	-2.14	114.00	117.03
32	1a	1207	2MG	O3'-C3'-C2'	2.14	118.75	111.82
54	1x	32	5MC	C5-C6-N1	-2.14	119.89	122.19
32	2a	1404	5MC	C5-C6-N1	-2.13	119.89	122.19
1	2A	2251	OMG	C5-C6-N1	-2.13	120.52	123.43
32	2a	1402	4OC	C5-C4-N4	-2.12	115.72	122.06
1	1A	1933	PSU	O4'-C1'-C2'	2.11	108.08	104.66
32	2a	527	7MG	C2-N3-C4	2.10	119.70	113.89
1	1A	1942	OMC	N4-C4-N3	2.08	119.78	116.49
1	2A	2251	OMG	N2-C2-N1	2.07	120.48	117.25
32	2a	966	M2G	CM2-N2-C2	-2.07	119.32	121.29
1	1A	1964	5MC	C5-C6-N1	-2.06	119.97	122.19
1	2A	1917	PSU	C4-C5-C1'	-2.05	117.25	121.12
1	1A	2263	OMG	C4-C5-N7	-2.05	107.26	109.40
32	1a	1498	UR3	C3U-N3-C4	2.04	120.83	118.12
32	1a	966	M2G	N3-C2-N2	2.04	119.25	117.18
32	1a	1407	5MC	C5-C6-N1	-2.04	120.00	122.19
1	2A	1911	PSU	O4'-C1'-C2'	2.03	107.94	104.66
1	2A	1911	PSU	C4-C5-C1'	-2.03	117.30	121.12
1	1A	1933	PSU	C4-C5-C1'	-2.02	117.31	121.12

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	2A	1915	5MU	C2'-C1'-N1-C6
1	2A	1915	5MU	C3'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C4'-C5'-O5'
1	2A	1939	5MU	C2'-C1'-N1-C6
1	2A	1939	5MU	O4'-C1'-N1-C6
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
1	1A	1937	5MU	C2'-C1'-N1-C6
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	2263	OMG	C1'-C2'-O2'-CM2
1	1A	1942	OMC	C2'-C1'-N1-C6
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C9
32	2a	1400	5MC	C3'-C4'-C5'-O5'
1	2A	1915	5MU	C4'-C5'-O5'-P
1	1A	2515	2MA	O4'-C4'-C5'-O5'
1	2A	2552	OMU	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
1	2A	2251	OMG	C4'-C5'-O5'-P
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
32	2a	516	PSU	O4'-C4'-C5'-O5'
1	1A	2263	OMG	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 2719 ligands modelled in this entry, 2717 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SF4	2d	501	35	0,12,12	0.00	-	-		
58	SF4	1d	501	35	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	2d	501	35	-	-	0/6/5/5
58	SF4	1d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.