



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:35 pm GMT

PDB ID : 7OII  
EMDB ID : EMD-12930  
Title : CspA-70 cotranslational folding intermediate 2  
Authors : Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.;  
Novacek, J.; Valle, M.; Rodnina, M.V.  
Deposited on : 2021-05-11  
Resolution : 3.00 Å(reported)  
Based on initial model : 6ORE

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

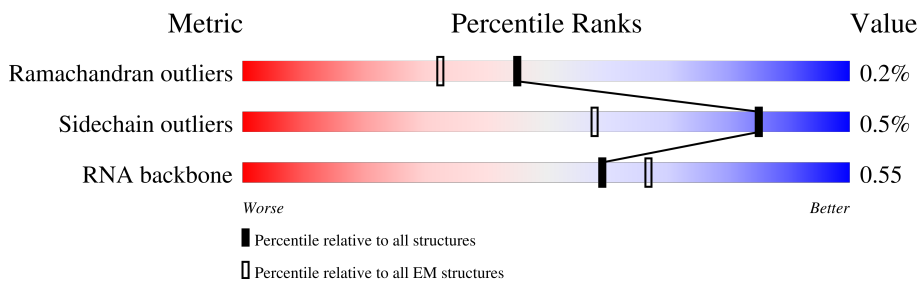
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



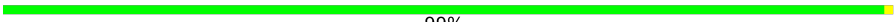
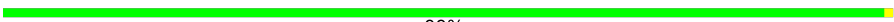












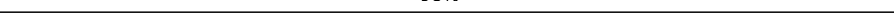
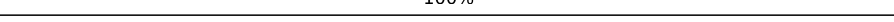
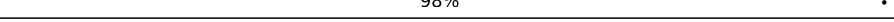
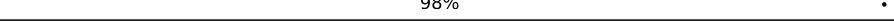
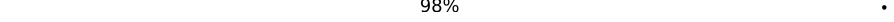
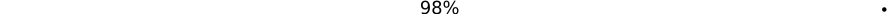
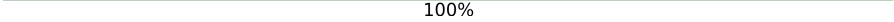
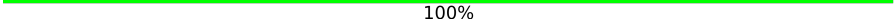
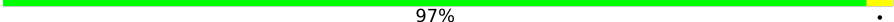
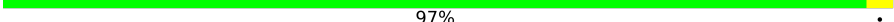

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	2903	71% 27% .
2	2	1534	77% 22% .
3	3	120	82% 17% .
4	C	271	100%
5	D	209	98% .
6	E	201	100%
7	F	177	99% .
8	G	175	99% .
9	H	149	98% .

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Mol	Chain	Length	Quality of chain
10	I	142	 99% .
11	J	123	 99% .
12	K	144	 99% .
13	L	136	 99% .
14	M	119	 99% .
15	N	116	 100%
16	O	114	 100%
17	P	117	 99% .
18	Q	103	 98% .
19	R	110	 99% .
20	S	94	 100%
21	T	103	 99% .
22	U	94	 99% .
23	V	84	 98% .
24	W	77	 100%
25	X	62	 98% .
26	Y	58	 98% .
27	Z	66	 98% .
28	a	56	 98% .
29	b	52	 100%
30	c	46	 100%
31	d	64	 97% .
32	e	38	 97% .
33	f	225	 100%
34	g	208	 99% .

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Mol	Chain	Length	Quality of chain
35	h	205	100%
36	i	156	97% .
37	j	104	100%
38	k	151	100%
39	l	129	100%
40	m	127	98% .
41	n	99	98% ..
42	o	117	99% .
43	p	123	99% .
44	q	116	100%
45	r	100	100%
46	s	88	100%
47	t	82	100%
48	u	80	100%
49	v	66	100%
50	w	83	99% .
51	x	86	100%
52	y	70	97% .
53	4	6	67% 33%
54	z	85	52% 34% 14%
55	B	39	100%

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145171 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	103	Total	C	N	O		
			788	498	148	142	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

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

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	62	Total	C	N	O	S	
			501	308	98	94	1	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	58	Total	C	N	O	S	
			448	281	87	78	2	0

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	66	Total	C	N	O	S	
			522	323	99	94	6	0

- Molecule 28 is a protein called 50S ribosomal protein L32.



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

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	52	Total	C	N	O	S	0	0
			426	275	78	73			

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

- Molecule 31 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	6	Total	C	N	O	P	0	0
			122	55	17	44	6		

- Molecule 54 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	85	Total	C	N	O	P	0	0
			1830	822	328	595	85		

- Molecule 55 is a protein called Cold-shock DNA-binding protein family.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	B	39	Total	C	N	O	0	0
			250	159	43	48		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ILE	VAL	conflict	UNP A0A1H2D2H5

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

Mol	Chain	Residues	Atoms		AltConf
56	1	282	Total 282	Mg 282	0
56	2	119	Total 119	Mg 119	0
56	3	8	Total 8	Mg 8	0
56	C	1	Total 1	Mg 1	0
56	D	1	Total 1	Mg 1	0
56	M	1	Total 1	Mg 1	0
56	P	1	Total 1	Mg 1	0
56	a	2	Total 2	Mg 2	0
56	h	1	Total 1	Mg 1	0
56	q	1	Total 1	Mg 1	0
56	4	1	Total 1	Mg 1	0
56	z	4	Total 4	Mg 4	0

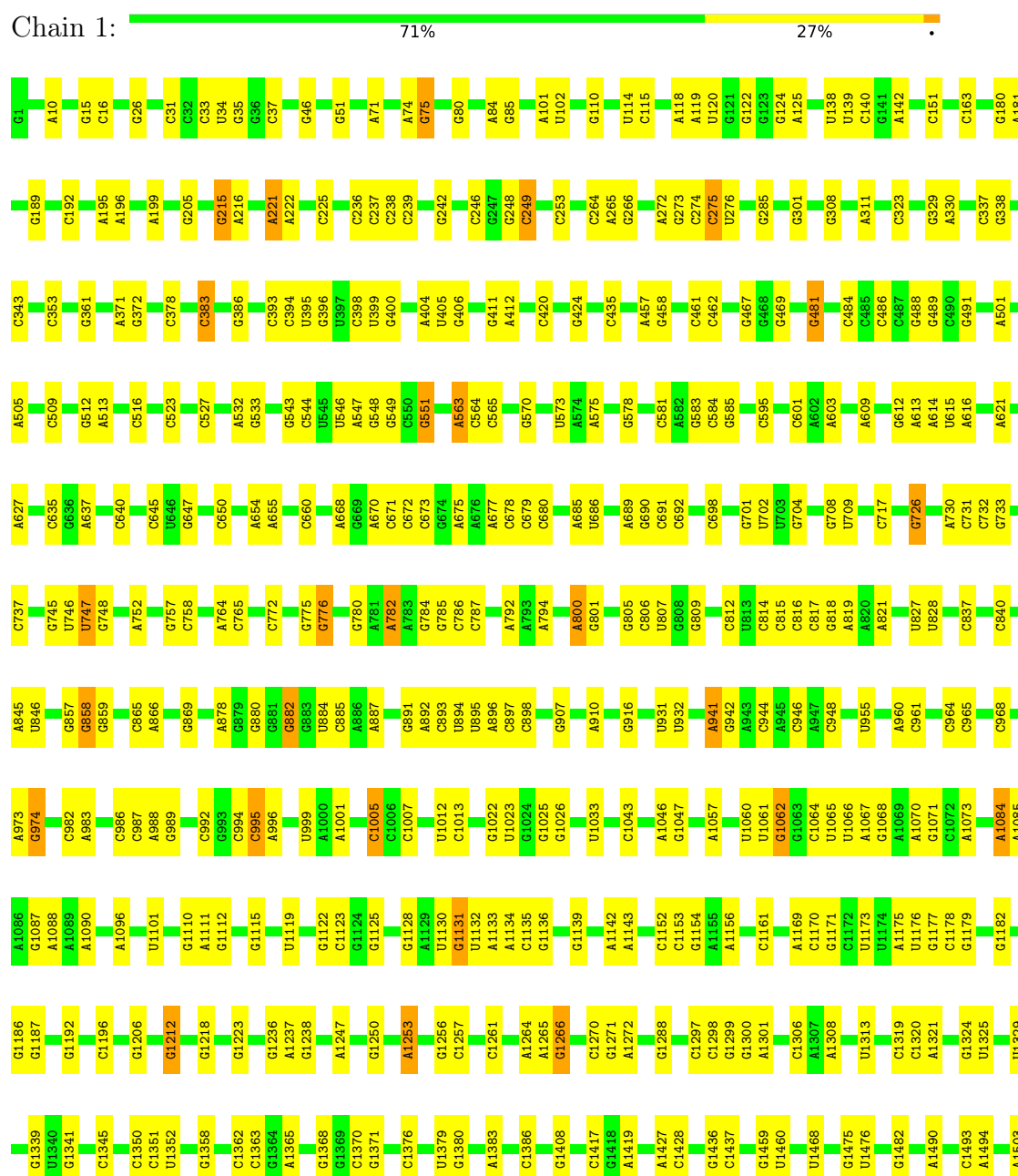
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	Z	1	Total 1	Zn 1	0
57	e	1	Total 1	Zn 1	0

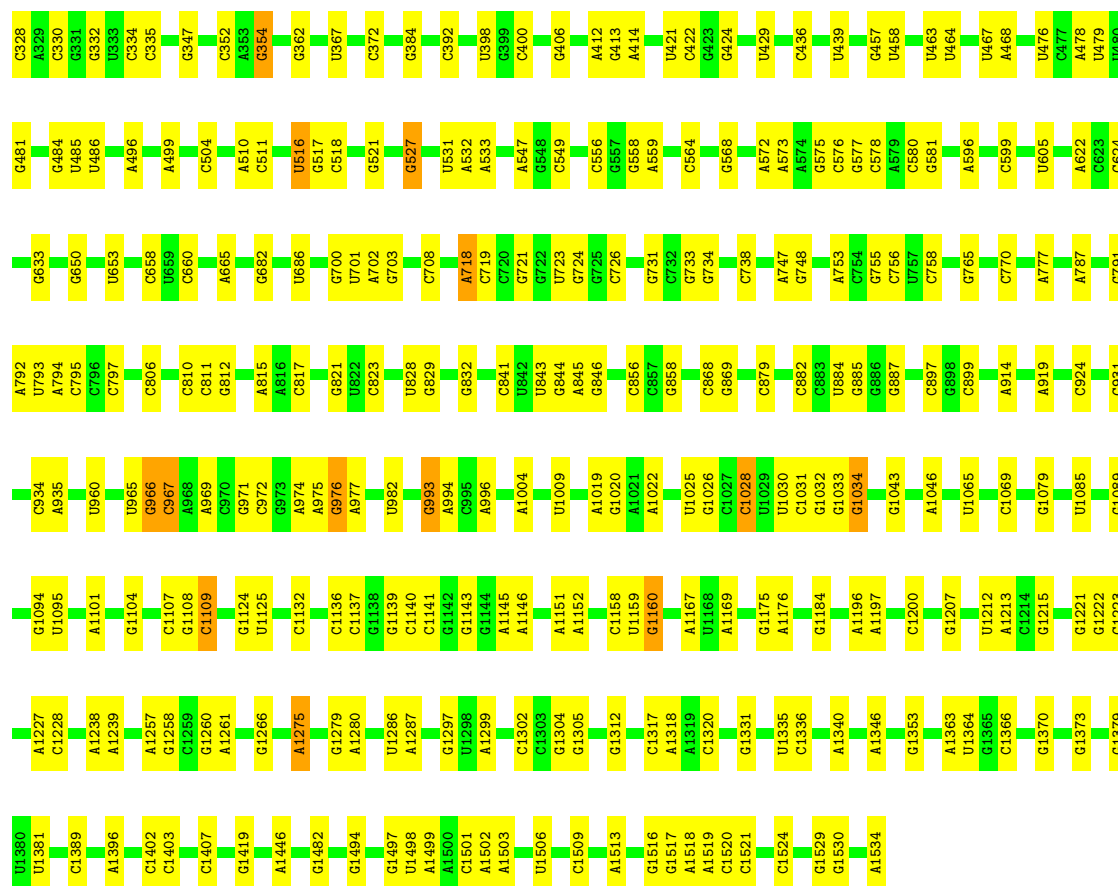
### 3 Residue-property plots [i](#)

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

- Molecule 1: 23S rRNA

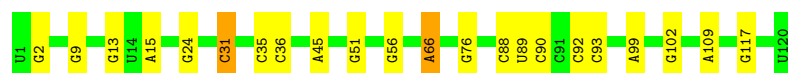


A1504	A1618	C1793	U1923	U2022	A2114	A2225	C2347	A2476	U2586	C2730	A2879
A1508	G1619	A1794	C1924	G2022	G2115	U2229	C2350	U2477	C2591	A2733	C2880
A1509	C1625	C1795	G1929	G2024	G2116	U2239	G2357	U2478	C2592	A2734	A2883
G1510	G1631	C1800	G1930	C2025	A2117	C2232	G2361	C2480	U2593	G2744	U2884
A1515	A1634	A1801	G1939	G2029	A2118	G2238	G2365	U2491	C2594	A2748	G2885
G1521	A1638	A1808	C1934	A2030	G2121	G2239	C2364	C2496	G2597	G2751	C2888
G1524	C1639	G1811	A1936	A2031	G2122	U2243	G2365	A2497	C2601	U2756	U2891
G1529	C1646	A1815	A1937	A2032	G2123	U2244	A2376	C2498	A2502	A2757	G2894
G1530	U1647	C1816	A1938	A2033	G2124	C2248	G2382	G2502	U2605	A2785	U2898
A1531	U1648	C1822	U1939	A2034	G2125	U2249	G2383	A2503	G2607	G2777	U2903
A1532	U1649	G1828	U1940	A2035	U2131	G2250	U2384	U2504	G2608	A2778	G2903
A1535	A1650	A1829	C1941	C2043	U2132	G2251	G2385	U2505	U2609	G2791	G2908
C1536	A1651	G1835	C1947	C2044	U2133	G2252	G2386	U2506	C2611	A2792	U2909
G1537	A1652	C1836	G1950	C2045	A2134	G2253	U2402	C2507	C2612	C2793	G2910
U1554	A1653	C1832	U1955	C2050	U2139	C2260	C2403	C2510	U2613	A2797	G2911
C1557	U1657	U1833	C1958	A2051	G2140	C2263	A2406	U2511	U2629	U2798	A2798
C1558	C1658	U1834	C1961	A2052	G2141	C2264	C2417	A2512	G2645	A2799	G2811
U1559	A1668	C1836	C1962	C2053	C2145	G2271	U2423	U2513	C2646	G2811	G2812
C1564	A1669	A1848	C1967	A2054	C2146	C2275	A2424	C2514	G2647	G2813	U2613
C1565	C1670	A1853	C1970	A2055	A2158	A2278	A2425	A2515	G2648	A2675	U2629
C1566	G1673	G1857	A1971	C2056	G2160	C2283	A2426	U2516	U2675	C2815	C2815
G1567	G1674	G1857	U1971	C2063	C2161	C2284	G2428	C2517	U2676	U2818	U2818
G1568	C1675	A1858	U1972	C2064	G2162	C2285	G2429	C2518	G2677	G2819	G2819
A1569	G1697	U1865	G1973	C2065	C2163	G2286	A2430	G2519	C2678	A2820	A2820
A1570	C1731	C1974	C1974	C2066	A2165	G2287	U2431	G2520	C2681	A2823	A2823
A1571	G1715	C1985	C1985	C2069	C2166	A2288	A2435	G2521	C2682	C2824	G2824
A1572	C1728	C1868	C1986	C2070	A2169	U2305	C2440	C2522	C2683	G2825	G2825
G1573	U1729	G1869	C1986	C2071	G2170	C2308	U2441	C2523	U2688	U2833	U2833
U1578	U1730	C1870	C1990	C2072	A2171	A2309	C2442	C2524	U2689	G2834	G2834
A1579	G1731	A1871	U1991	C2073	U2172	G2332	G2443	C2525	U2690	A2835	A2835
A1580	C1732	A1872	G1992	U2075	A2173	A2334	G2444	C2526	C2704	U2836	U2836
A1583	C1738	C1894	U1993	G2083	C2178	A2335	G2445	C2527	G2709	C2841	C2841
G1587	G1756	C1895	C1996	C2084	A2183	G2339	G2446	U2528	C2710	G2848	G2848
G1588	C1761	G1896	C1997	C2085	U2189	A2342	A2448	G2529	G2711	C2853	C2853
A1590	C1761	A1899	C1999	C2086	G2190	G2323	A2450	C2530	C2712	U2858	U2858
A1590	C1761	C2000	C2000	C2087	A2191	U2324	A2451	C2531	C2713	U2859	U2859
A1603	C1764	G1904	C2001	C2088	U2192	G2325	G2454	C2532	C2714	C2860	C2860
C1604	A1773	C1905	G2002	C2089	G2193	C2326	U2457	C2533	C2715	U2861	U2861
A1608	C1778	G1906	C2006	C2090	U2194	A2327	G2458	C2534	C2716	G2862	G2862
A1612	C1788	U1911	U2007	C2091	U2195	A2333	U2459	C2535	C2717	C2863	C2863
C1615	A1789	A1912	C2008	C2092	A2198	U2334	G2465	C2536	C2718	G2867	G2867
A1616	C1790	A1913	A2009	C2093	G2204	U2335	C2466	C2537	G2719	A2872	A2872
A1617	A1791	C1914	U2011	C2094	U2211	A2336	G2467	C2538	U2720	A2873	A2873
C1617	G1792	3D1915	G2012	C2095	G2212	A2337	G2468	C2539	C2721		
		A2013	A2013	C2096	G2213	A2338	G2469	C2540	C2722		
		U1917	A2014	C2097	G2214	A2339	G2470	C2541	C2723		
				C2098	G2215	A2340		C2542	U2724		
				C2099	G2216	A2341		C2543	A2725		
				C2100	G2217	A2342		C2544	A2726		
				C2101	G2218	A2343		C2545			
				C2102	G2219	A2344		C2546			
				C2103	G2220	A2345		C2547			
				C2104	G2221	A2346		C2548			
				C2105	G2222	A2347		C2549			
				C2106	G2223	A2348		C2550			
				C2107	G2224	A2349		C2551			
				C2108	G2225	A2350		C2552			
				C2109	G2226	A2351		C2553			
				C2110	G2227	A2352		C2554			
				C2111	G2228	A2353		C2555			
				C2112	G2229	A2354		C2556			
				C2113	G2230	A2355		C2557			
				C2114	G2231	A2356		C2558			
				C2115	G2232	A2357		C2559			
				C2116	G2233	A2358		C2560			
				C2117	G2234	A2359		C2561			
				C2118	G2235	A2360		C2562			
				C2119	G2236	A2361		C2563			
				C2120	G2237	A2362		C2564			
				C2121	G2238	A2363		C2565			
				C2122	G2239	A2364		C2566			
				C2123	G2240	A2365		C2567			
				C2124	G2241	A2366		C2568			
				C2125	G2242	A2367		C2569			
				C2126	G2243	A2368		C2570			
				C2127	G2244	A2369		C2571			
				C2128	G2245	A2370		C2572			
				C2129	G2246	A2371		C2573			
				C2130	G2247	A2372		C2574			
				C2131	G2248	A2373		C2575			
				C2132	G2249	A2374		C2576			
				C2133	G2250	A2375		C2577			
				C2134	G2251	A2376		C2578			
				C2135	G2252	A2377		C2579			
				C2136	G2253	A2378		C2580			
				C2137	G2254	A2379		C2581			
				C2138	G2255	A2380		C2582			
				C2139	G2256	A2381		C2583			
				C2140	G2257	A2382		C2584			
				C2141	G2258	A2383		C2585			
				C2142	G2259	A2384		C2586			
				C2143	G2260	A2385		C2587			
				C2144	G2261	A2386		C2588			
				C2145	G2262	A2387		C2589			
				C2146	G2263	A2388		C2590			
				C2147	G2264	A2389		C2591			
				C2148	G2265	A2390		C2592			
				C2149	G2266	A2391		C2593			
				C2150	G2267	A2392		C2594			
				C2151	G2268	A2393		C2595			
				C2152	G2269	A2394		C2596			
				C2153	G2270	A2395		C2597			
				C2154	G2271	A2396		C2598			
				C2155	G2272	A2397		C2599			
				C2156	G2273	A2398		C2600			
				C2157	G2274	A2399		C2601			
				C2158	G2275	A2400		C2602			
				C2159	G2276	A2401		C2603			
				C2160	G2277	A2402		C2604			
				C2161	G2278	A2403		C2605			
				C2162	G2279	A2404		C2606			
				C2163	G2280	A2405		C2607			
				C2164	G2281	A2406		C2608			
				C2165	G2282	A2407		C2609			
				C2166	G2283	A2408		C2610			
				C2167	G2284	A2409		C2611			
				C2168	G2285	A2410		C2612			
				C2169	G2286	A2411		C2613			
				C2170	G2287	A2412		C2614			
				C2171	G2288	A2413		C2615			
				C2172	G2289	A2414		C2616			
				C2173	G2290	A2415		C2617			
				C2174	G2291	A2416		C2618			
				C2175	G2292	A2417		C2619			
				C2176	G2293	A2418		C2620			
				C2177	G2294	A2419		C2621			
				C2178	G2295	A2420		C2622			
				C2179	G2296	A2421		C2623			
				C2180	G2297	A2422		C2624			
				C2181	G2298	A2423		C2625			
				C2182	G2299	A2424		C2626			
				C2183	G2300	A2425		C2627			
				C2184	G2301	A2426		C2628			
				C2185	G2302	A2427		C2629			
				C2186	G2303	A2428		C2630			
				C2187	G2304	A2429		C2631			
				C2188	G2305	A2430		C2632			
				C2189	G2306	A2431		C2633			
				C2190	G2307	A2432		C2634			
				C2191	G2308	A2433		C2635			
				C2192	G2309	A2434		C2636			
				C2193	G2310	A2435	</				



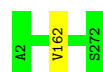
- Molecule 3: 5S rRNA

Chain 3: 82% 17%



- Molecule 4: 50S ribosomal protein L2

Chain C: 100%



- Molecule 5: 50S ribosomal protein L3

Chain D: 98%



- Molecule 6: 50S ribosomal protein L4

Chain E: 100%





- Molecule 7: 50S ribosomal protein L5

Chain F:  99%



- Molecule 8: 50S ribosomal protein L6

Chain G:  99%



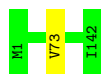
- Molecule 9: 50S ribosomal protein L9

Chain H:  98%



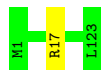
- Molecule 10: 50S ribosomal protein L13

Chain I:  99%



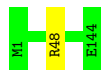
- Molecule 11: 50S ribosomal protein L14

Chain J:  99%



- Molecule 12: 50S ribosomal protein L15

Chain K:  99%



- Molecule 13: 50S ribosomal protein L16

Chain L:  99%



- Molecule 14: 50S ribosomal protein L17

Chain M:  99%



- Molecule 15: 50S ribosomal protein L18

Chain N:  100%

There are no outlier residues recorded for this chain.

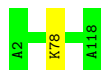
- Molecule 16: 50S ribosomal protein L19

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L20

Chain P:  99%



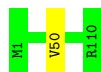
- Molecule 18: 50S ribosomal protein L21

Chain Q:  98%



- Molecule 19: 50S ribosomal protein L22

Chain R:  99%



- Molecule 20: 50S ribosomal protein L23

Chain S:  100%

There are no outlier residues recorded for this chain.

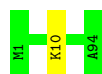
- Molecule 21: 50S ribosomal protein L24

Chain T:  99%



- Molecule 22: 50S ribosomal protein L25

Chain U:  99%



- Molecule 23: 50S ribosomal protein L27

Chain V:  98%



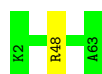
- Molecule 24: 50S ribosomal protein L28

Chain W:  100%

There are no outlier residues recorded for this chain.

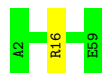
- Molecule 25: 50S ribosomal protein L29

Chain X:  98%



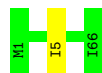
- Molecule 26: 50S ribosomal protein L30

Chain Y:  98%



- Molecule 27: 50S ribosomal protein L31

Chain Z:  98%



- Molecule 28: 50S ribosomal protein L32

Chain a:  98%



- Molecule 29: 50S ribosomal protein L33

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L34

Chain c:  100%

There are no outlier residues recorded for this chain.

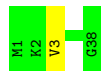
- Molecule 31: 50S ribosomal protein L35

Chain d:  97%



- Molecule 32: 50S ribosomal protein L36

Chain e:  97%



- Molecule 33: 30S ribosomal protein S2

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 30S ribosomal protein S3

Chain g:  99%



- Molecule 35: 30S ribosomal protein S4

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 36: 30S ribosomal protein S5

Chain i:  97%



- Molecule 37: 30S ribosomal protein S6

Chain j: 100%

There are no outlier residues recorded for this chain.

- Molecule 38: 30S ribosomal protein S7

Chain k: 100%

There are no outlier residues recorded for this chain.

- Molecule 39: 30S ribosomal protein S8

Chain l: 100%

There are no outlier residues recorded for this chain.

- Molecule 40: 30S ribosomal protein S9

Chain m: 98%



- Molecule 41: 30S ribosomal protein S10

Chain n: 98%



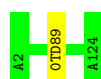
- Molecule 42: 30S ribosomal protein S11

Chain o: 99%



- Molecule 43: 30S ribosomal protein S12

Chain p: 99%



- Molecule 44: 30S ribosomal protein S13

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: 30S ribosomal protein S14

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 46: 30S ribosomal protein S15

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 30S ribosomal protein S16

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 30S ribosomal protein S17

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 49: 30S ribosomal protein S18

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 50: 30S ribosomal protein S19

Chain w:  99%



- Molecule 51: 30S ribosomal protein S20

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 52: 30S ribosomal protein S21

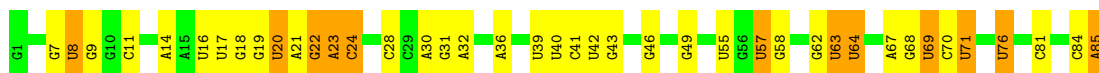
Chain y:  97%



- Molecule 53: mRNA



- Molecule 54: tRNA-Leu



- Molecule 55: Cold-shock DNA-binding protein family



There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23782	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 5MC, OMU, OMC, MG, 5MU, ZN, 0TD, UR3, 3TD, 2MG, 1MG, PSU, 4OC, 2MA, MA6, 6MZ, OMG

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	1	1.63	238/69286 (0.3%)	1.27	240/108087 (0.2%)
2	2	1.45	60/36590 (0.2%)	1.19	59/57074 (0.1%)
3	3	1.39	3/2872 (0.1%)	1.16	8/4478 (0.2%)
4	C	1.06	1/2121 (0.0%)	0.71	0/2852
5	D	1.07	1/1586 (0.1%)	0.72	1/2134 (0.0%)
6	E	0.96	0/1571	0.69	1/2113 (0.0%)
7	F	0.75	0/1434	0.68	0/1926
8	G	0.71	0/1333	0.64	0/1805
9	H	0.51	0/1122	0.79	0/1515
10	I	1.03	1/1152 (0.1%)	0.67	0/1551
11	J	0.98	0/955	0.74	0/1279
12	K	0.98	0/1062	0.76	0/1413
13	L	1.01	0/1093	0.69	0/1460
14	M	1.00	0/964	0.73	0/1289
15	N	0.89	0/902	0.68	0/1209
16	O	1.03	0/929	0.68	0/1242
17	P	1.19	0/960	0.75	0/1278
18	Q	1.02	0/829	0.70	0/1107
19	R	1.02	1/864 (0.1%)	0.73	0/1156
20	S	0.98	0/752	0.65	0/1005
21	T	0.89	0/796	0.66	0/1062
22	U	0.88	0/766	0.66	0/1025
23	V	1.04	0/642	0.70	0/848
24	W	0.99	0/635	0.71	0/848
25	X	0.76	0/502	0.74	1/667 (0.1%)
26	Y	0.93	0/452	0.73	1/605 (0.2%)
27	Z	0.64	1/531 (0.2%)	0.67	0/709
28	a	1.02	1/450 (0.2%)	0.74	0/599
29	b	0.83	0/433	0.62	0/576
30	c	1.03	0/380	0.78	0/498
31	d	1.05	0/513	0.74	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	e	1.05	1/303 (0.3%)	0.75	0/397
33	f	0.65	0/1791	0.66	0/2413
34	g	0.82	0/1663	0.66	0/2241
35	h	0.80	0/1665	0.64	0/2227
36	i	0.95	2/1165 (0.2%)	0.73	0/1568
37	j	0.76	0/867	0.67	0/1171
38	k	0.73	0/1195	0.68	0/1602
39	l	0.93	0/989	0.70	0/1326
40	m	0.82	0/1034	0.71	0/1375
41	n	0.74	0/800	0.79	1/1082 (0.1%)
42	o	0.80	0/893	0.68	0/1205
43	p	0.94	0/960	0.72	0/1286
44	q	0.71	0/909	0.69	0/1215
45	r	0.80	0/817	0.66	0/1088
46	s	0.80	0/722	0.68	0/964
47	t	0.90	0/659	0.67	0/884
48	u	0.81	0/657	0.71	0/881
49	v	0.84	0/553	0.69	0/743
50	w	0.69	0/680	0.62	0/915
51	x	0.78	0/675	0.69	0/895
52	y	0.71	0/597	0.66	0/792
53	4	1.64	1/134 (0.7%)	1.42	0/205
54	z	1.47	9/1768 (0.5%)	1.33	14/2759 (0.5%)
55	B	0.55	0/255	0.62	0/347
All	All	1.40	320/156228 (0.2%)	1.13	326/233667 (0.1%)

All (320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	32	A	N9-C4	-8.67	1.32	1.37
1	1	2442	C	N1-C6	-7.47	1.32	1.37
54	z	84	C	N1-C6	-7.46	1.32	1.37
1	1	1999	C	N1-C6	-7.20	1.32	1.37
1	1	673	C	N1-C6	-7.17	1.32	1.37
1	1	786	C	N1-C6	-7.13	1.32	1.37
1	1	565	C	N1-C6	-7.02	1.32	1.37
1	1	964	C	N1-C6	-6.92	1.32	1.37
1	1	787	C	N1-C6	-6.91	1.33	1.37
1	1	691	C	N1-C6	-6.87	1.33	1.37
1	1	581	C	N1-C6	-6.87	1.33	1.37
1	1	2512	C	N1-C6	-6.81	1.33	1.37
53	4	4	C	N1-C6	-6.70	1.33	1.37

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	672	C	N1-C6	-6.68	1.33	1.37
1	1	584	C	N1-C6	-6.64	1.33	1.37
1	1	2066	C	N1-C6	-6.63	1.33	1.37
1	1	671	C	N1-C6	-6.60	1.33	1.37
1	1	2515	C	N1-C6	-6.60	1.33	1.37
1	1	944	C	N1-C6	-6.59	1.33	1.37
1	1	987	C	N1-C6	-6.54	1.33	1.37
1	1	1376	C	N1-C6	-6.53	1.33	1.37
1	1	1985	C	N1-C6	-6.51	1.33	1.37
54	z	85	A	N9-C4	-6.42	1.33	1.37
1	1	679	C	N1-C6	-6.42	1.33	1.37
1	1	772	C	N1-C6	-6.40	1.33	1.37
1	1	2065	C	N1-C6	-6.36	1.33	1.37
1	1	2264	C	N1-C6	-6.35	1.33	1.37
2	2	18	C	N1-C6	-6.34	1.33	1.37
1	1	2841	C	N1-C6	-6.34	1.33	1.37
1	1	523	C	N1-C6	-6.29	1.33	1.37
1	1	2443	C	N1-C6	-6.29	1.33	1.37
1	1	2540	C	N1-C6	-6.26	1.33	1.37
1	1	2681	C	N1-C6	-6.26	1.33	1.37
1	1	2064	C	N1-C6	-6.26	1.33	1.37
1	1	1370	C	N1-C6	-6.23	1.33	1.37
1	1	1656	C	N1-C6	-6.23	1.33	1.37
1	1	1084	A	O3'-P	-6.21	1.53	1.61
1	1	1363	C	N1-C6	-6.21	1.33	1.37
1	1	782	A	N9-C4	-6.19	1.34	1.37
1	1	1270	C	N1-C6	-6.19	1.33	1.37
1	1	2601	C	N1-C6	-6.19	1.33	1.37
1	1	968	C	N1-C6	-6.18	1.33	1.37
1	1	678	C	N1-C6	-6.18	1.33	1.37
1	1	31	C	N1-C6	-6.17	1.33	1.37
1	1	1604	C	N1-C6	-6.16	1.33	1.37
1	1	1298	C	N1-C6	-6.15	1.33	1.37
1	1	800	A	N9-C4	-6.12	1.34	1.37
2	2	758	C	N1-C6	-6.11	1.33	1.37
1	1	1638	C	N1-C6	-6.10	1.33	1.37
1	1	1257	C	N1-C6	-6.08	1.33	1.37
2	2	1520	C	N1-C6	-6.07	1.33	1.37
2	2	879	C	N1-C6	-6.07	1.33	1.37
1	1	2683	C	N1-C6	-6.06	1.33	1.37
1	1	817	C	N1-C6	-6.04	1.33	1.37
2	2	719	C	N1-C6	-6.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2050	C	N1-C6	-6.03	1.33	1.37
1	1	2499	C	N1-C6	-6.03	1.33	1.37
1	1	806	C	N3-C4	-6.03	1.29	1.33
1	1	239	C	N1-C6	-6.00	1.33	1.37
1	1	2260	C	N1-C6	-5.98	1.33	1.37
1	1	2073	C	N1-C6	-5.96	1.33	1.37
1	1	635	C	N1-C6	-5.96	1.33	1.37
2	2	756	C	N1-C6	-5.96	1.33	1.37
1	1	1790	C	N1-C6	-5.95	1.33	1.37
36	i	137	VAL	CB-CG1	-5.93	1.40	1.52
1	1	2521	C	N1-C6	-5.92	1.33	1.37
1	1	2417	C	N1-C6	-5.90	1.33	1.37
1	1	2591	C	N1-C6	-5.90	1.33	1.37
1	1	1007	C	N1-C6	-5.88	1.33	1.37
1	1	815	C	N1-C6	-5.88	1.33	1.37
1	1	398	C	N1-C6	-5.87	1.33	1.37
1	1	816	C	N1-C6	-5.87	1.33	1.37
1	1	692	C	N1-C6	-5.87	1.33	1.37
1	1	680	C	N1-C6	-5.86	1.33	1.37
1	1	2676	C	N1-C6	-5.86	1.33	1.37
1	1	660	C	N1-C6	-5.85	1.33	1.37
1	1	1958	C	N1-C6	-5.85	1.33	1.37
1	1	2466	C	N1-C6	-5.83	1.33	1.37
2	2	919	A	N9-C4	-5.83	1.34	1.37
1	1	1005	C	N1-C6	-5.82	1.33	1.37
1	1	698	C	N1-C6	-5.81	1.33	1.37
1	1	585	G	N9-C8	-5.81	1.33	1.37
1	1	1557	C	N1-C6	-5.80	1.33	1.37
1	1	1905	C	N1-C6	-5.80	1.33	1.37
1	1	337	C	N1-C6	-5.79	1.33	1.37
1	1	806	C	N1-C6	-5.78	1.33	1.37
1	1	1795	C	N1-C6	-5.78	1.33	1.37
2	2	549	C	N1-C6	-5.77	1.33	1.37
1	1	2036	C	C4-C5	-5.77	1.38	1.43
54	z	36	A	N9-C4	-5.77	1.34	1.37
1	1	516	C	N1-C6	-5.76	1.33	1.37
1	1	988	A	N9-C4	-5.76	1.34	1.37
2	2	23	C	N1-C6	-5.75	1.33	1.37
1	1	840	C	N1-C6	-5.74	1.33	1.37
1	1	965	C	N1-C6	-5.74	1.33	1.37
1	1	1658	C	N1-C6	-5.72	1.33	1.37
1	1	737	C	N1-C6	-5.71	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1639	C	N1-C6	-5.71	1.33	1.37
36	i	136	VAL	CB-CG1	-5.69	1.40	1.52
1	1	2051	A	N9-C4	-5.69	1.34	1.37
1	1	564	C	N1-C6	-5.69	1.33	1.37
1	1	2091	C	N1-C6	-5.68	1.33	1.37
1	1	948	C	N1-C6	-5.66	1.33	1.37
1	1	2263	C	N1-C6	-5.66	1.33	1.37
1	1	1261	C	N1-C6	-5.66	1.33	1.37
1	1	2008	C	N1-C6	-5.66	1.33	1.37
1	1	2559	C	N1-C6	-5.66	1.33	1.37
2	2	924	C	N1-C6	-5.64	1.33	1.37
54	z	41	C	N1-C6	-5.63	1.33	1.37
1	1	2009	A	N9-C4	-5.62	1.34	1.37
2	2	1223	C	N1-C6	-5.62	1.33	1.37
1	1	2710	C	N1-C6	-5.62	1.33	1.37
1	1	2538	C	N1-C6	-5.62	1.33	1.37
1	1	2248	C	N1-C6	-5.61	1.33	1.37
1	1	994	C	N1-C6	-5.61	1.33	1.37
54	z	84	C	C4-C5	-5.60	1.38	1.43
1	1	2539	C	N1-C6	-5.60	1.33	1.37
1	1	2716	C	N1-C6	-5.58	1.33	1.37
1	1	1153	C	N1-C6	-5.58	1.33	1.37
2	2	295	C	N1-C6	-5.57	1.33	1.37
1	1	814	C	N1-C6	-5.57	1.33	1.37
2	2	109	A	N9-C4	-5.56	1.34	1.37
3	3	93	C	N1-C6	-5.55	1.33	1.37
1	1	809	G	N9-C8	-5.55	1.33	1.37
1	1	1612	C	N1-C6	-5.55	1.33	1.37
1	1	758	C	N1-C6	-5.54	1.33	1.37
1	1	1319	C	N1-C6	-5.54	1.33	1.37
1	1	1833	C	N1-C6	-5.54	1.33	1.37
1	1	1605	C	N1-C6	-5.53	1.33	1.37
1	1	668	A	N9-C4	-5.53	1.34	1.37
1	1	2055	C	N1-C6	-5.53	1.33	1.37
2	2	52	C	N1-C6	-5.53	1.33	1.37
1	1	1668	A	N9-C4	-5.52	1.34	1.37
1	1	237	C	N1-C6	-5.52	1.33	1.37
2	2	1389	C	N1-C6	-5.51	1.33	1.37
1	1	1001	A	N9-C4	-5.51	1.34	1.37
2	2	726	C	N1-C6	-5.51	1.33	1.37
1	1	2717	C	N1-C6	-5.50	1.33	1.37
1	1	2063	C	N1-C6	-5.50	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1221	G	N9-C4	-5.49	1.33	1.38
1	1	2427	C	N1-C6	-5.49	1.33	1.37
1	1	2730	C	N1-C6	-5.48	1.33	1.37
2	2	36	C	N1-C6	-5.48	1.33	1.37
2	2	16	A	N9-C4	-5.47	1.34	1.37
1	1	2551	C	N1-C6	-5.47	1.33	1.37
2	2	578	C	N1-C6	-5.47	1.33	1.37
2	2	1509	C	N1-C6	-5.47	1.33	1.37
2	2	811	C	N1-C6	-5.47	1.33	1.37
1	1	2507	C	N1-C6	-5.46	1.33	1.37
1	1	2364	C	N1-C6	-5.46	1.33	1.37
1	1	1832	C	N1-C6	-5.45	1.33	1.37
1	1	2606	C	N1-C6	-5.45	1.33	1.37
2	2	622	A	N9-C4	-5.45	1.34	1.37
1	1	992	C	N1-C6	-5.45	1.33	1.37
1	1	1670	C	C4-C5	-5.45	1.38	1.43
19	R	50	VAL	CB-CG1	-5.44	1.41	1.52
1	1	527	C	N1-C6	-5.44	1.33	1.37
1	1	2006	C	N1-C6	-5.44	1.33	1.37
32	e	3	VAL	CB-CG1	-5.44	1.41	1.52
1	1	2014	A	N9-C4	-5.43	1.34	1.37
1	1	486	C	N1-C6	-5.43	1.33	1.37
1	1	601	C	N1-C6	-5.43	1.33	1.37
1	1	1815	A	N9-C4	-5.43	1.34	1.37
1	1	1997	C	N1-C6	-5.43	1.33	1.37
2	2	599	C	N1-C6	-5.43	1.33	1.37
1	1	757	G	N9-C4	-5.42	1.33	1.38
2	2	1513	A	N9-C4	-5.42	1.34	1.37
2	2	1109	C	N1-C6	-5.42	1.33	1.37
2	2	897	C	N1-C6	-5.41	1.33	1.37
1	1	393	C	N1-C6	-5.41	1.33	1.37
1	1	195	A	N9-C4	-5.41	1.34	1.37
1	1	2072	C	N1-C6	-5.39	1.33	1.37
1	1	1571	A	N9-C4	-5.39	1.34	1.37
1	1	1986	C	N1-C6	-5.39	1.33	1.37
1	1	1990	C	N1-C6	-5.39	1.33	1.37
1	1	2450	A	N9-C4	-5.39	1.34	1.37
54	z	32	A	N3-C4	-5.39	1.31	1.34
1	1	2612	C	N1-C6	-5.38	1.33	1.37
1	1	1822	C	N1-C6	-5.38	1.33	1.37
1	1	672	C	C4-C5	-5.38	1.38	1.43
2	2	792	A	N9-C4	-5.38	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2010	G	N9-C4	-5.38	1.33	1.38
1	1	1670	C	N1-C6	-5.36	1.33	1.37
1	1	1947	C	N1-C6	-5.36	1.33	1.37
2	2	931	C	N1-C6	-5.36	1.33	1.37
2	2	504	C	N1-C6	-5.36	1.33	1.37
1	1	640	C	N1-C6	-5.36	1.33	1.37
1	1	1899	A	N9-C4	-5.36	1.34	1.37
1	1	2719	G	C2-N2	-5.36	1.29	1.34
1	1	115	C	N1-C6	-5.35	1.33	1.37
1	1	1625	C	N1-C6	-5.34	1.33	1.37
3	3	76	G	N9-C4	-5.34	1.33	1.38
1	1	2497	A	N9-C4	-5.34	1.34	1.37
1	1	2010	G	N9-C8	-5.34	1.34	1.37
1	1	794	A	N9-C4	-5.34	1.34	1.37
1	1	246	C	N1-C6	-5.34	1.33	1.37
1	1	1297	C	N1-C6	-5.33	1.33	1.37
2	2	1524	C	N1-C6	-5.33	1.33	1.37
2	2	708	C	N1-C6	-5.33	1.33	1.37
1	1	2001	C	N1-C6	-5.33	1.33	1.37
1	1	2499	C	C5-C6	-5.33	1.30	1.34
1	1	151	C	N1-C6	-5.33	1.33	1.37
2	2	556	C	N1-C6	-5.32	1.33	1.37
2	2	810	C	N1-C6	-5.32	1.33	1.37
1	1	2688	G	N9-C4	-5.32	1.33	1.38
1	1	2815	C	N1-C6	-5.32	1.33	1.37
2	2	882	C	N1-C6	-5.31	1.33	1.37
1	1	1615	C	N1-C6	-5.31	1.33	1.37
1	1	1934	C	N1-C6	-5.31	1.33	1.37
1	1	1123	C	N1-C6	-5.30	1.33	1.37
1	1	378	C	N1-C6	-5.30	1.33	1.37
1	1	1362	C	N1-C6	-5.29	1.33	1.37
1	1	704	G	N9-C4	-5.29	1.33	1.38
54	z	30	A	N9-C4	-5.29	1.34	1.37
1	1	394	C	N1-C6	-5.29	1.33	1.37
1	1	2594	C	N1-C6	-5.29	1.33	1.37
2	2	795	C	N1-C6	-5.29	1.33	1.37
1	1	1152	C	N1-C6	-5.28	1.33	1.37
2	2	335	C	N1-C6	-5.28	1.33	1.37
1	1	192	C	N1-C6	-5.28	1.33	1.37
1	1	1196	C	N1-C6	-5.28	1.33	1.37
1	1	238	C	C4-C5	-5.27	1.38	1.43
1	1	1264	A	N9-C4	-5.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1996	C	N1-C6	-5.26	1.33	1.37
1	1	732	C	N1-C6	-5.26	1.33	1.37
1	1	1670	C	C4-N4	-5.26	1.29	1.33
2	2	400	C	N1-C6	-5.26	1.33	1.37
1	1	2496	C	N1-C6	-5.25	1.33	1.37
2	2	868	C	N1-C6	-5.25	1.33	1.37
1	1	383	C	N1-C6	-5.25	1.34	1.37
1	1	2502	G	N9-C4	-5.25	1.33	1.38
1	1	2440	C	N1-C6	-5.25	1.34	1.37
2	2	1501	C	N1-C6	-5.24	1.34	1.37
1	1	986	C	N1-C6	-5.24	1.34	1.37
1	1	2000	C	N1-C6	-5.24	1.34	1.37
1	1	2719	G	N9-C4	-5.24	1.33	1.38
1	1	2232	C	N1-C6	-5.23	1.34	1.37
1	1	2510	C	N1-C6	-5.23	1.34	1.37
2	2	797	C	N1-C6	-5.23	1.34	1.37
4	C	162	VAL	CB-CG1	-5.22	1.41	1.52
1	1	2036	C	N1-C6	-5.22	1.34	1.37
1	1	2465	C	N1-C6	-5.22	1.34	1.37
1	1	1265	A	N9-C4	-5.22	1.34	1.37
1	1	1974	C	N1-C6	-5.21	1.34	1.37
1	1	731	C	N1-C6	-5.21	1.34	1.37
1	1	1564	C	N1-C6	-5.20	1.34	1.37
1	1	780	G	N9-C4	-5.20	1.33	1.38
1	1	2678	C	N1-C6	-5.20	1.34	1.37
1	1	1192	G	N9-C4	-5.20	1.33	1.38
1	1	1161	C	N1-C6	-5.19	1.34	1.37
1	1	236	C	N1-C6	-5.19	1.34	1.37
1	1	690	G	N9-C8	-5.18	1.34	1.37
2	2	312	C	N1-C6	-5.18	1.34	1.37
2	2	624	C	N1-C6	-5.18	1.34	1.37
1	1	1257	C	C4-C5	-5.17	1.38	1.43
5	D	155	VAL	CB-CG2	-5.16	1.42	1.52
1	1	1237	A	N9-C4	-5.16	1.34	1.37
2	2	658	C	N1-C6	-5.16	1.34	1.37
2	2	334	C	N1-C6	-5.16	1.34	1.37
1	1	2033	A	N9-C4	-5.15	1.34	1.37
1	1	37	C	N1-C6	-5.15	1.34	1.37
1	1	1603	A	N9-C4	-5.15	1.34	1.37
1	1	1617	C	N1-C6	-5.15	1.34	1.37
54	z	85	A	C6-N6	-5.15	1.29	1.33
1	1	1961	C	N1-C6	-5.14	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1253	A	N9-C4	-5.14	1.34	1.37
1	1	253	C	N1-C6	-5.14	1.34	1.37
1	1	1646	C	N1-C6	-5.14	1.34	1.37
1	1	2451	A	N9-C4	-5.14	1.34	1.37
10	I	73	VAL	CB-CG1	-5.13	1.42	1.52
2	2	290	C	N1-C6	-5.13	1.34	1.37
1	1	2675	A	N9-C4	-5.13	1.34	1.37
1	1	2715	C	N1-C6	-5.13	1.34	1.37
2	2	1318	A	N9-C4	-5.13	1.34	1.37
1	1	461	C	N1-C6	-5.13	1.34	1.37
1	1	249	C	N1-C6	-5.12	1.34	1.37
1	1	2053	G	N9-C8	-5.12	1.34	1.37
1	1	2045	C	N1-C6	-5.12	1.34	1.37
2	2	580	C	N1-C6	-5.11	1.34	1.37
28	a	3	VAL	CB-CG1	-5.11	1.42	1.52
1	1	462	C	N1-C6	-5.11	1.34	1.37
1	1	2558	C	N1-C6	-5.11	1.34	1.37
1	1	1351	C	N1-C6	-5.10	1.34	1.37
1	1	1764	C	N1-C6	-5.10	1.34	1.37
2	2	823	C	N1-C6	-5.10	1.34	1.37
1	1	995	C	N1-C6	-5.09	1.34	1.37
1	1	865	C	N1-C6	-5.08	1.34	1.37
2	2	106	C	N1-C6	-5.08	1.34	1.37
1	1	2863	C	N1-C6	-5.08	1.34	1.37
1	1	578	G	C6-N1	-5.08	1.35	1.39
1	1	677	A	N9-C4	-5.08	1.34	1.37
1	1	16	C	N1-C6	-5.07	1.34	1.37
1	1	501	A	N9-C4	-5.07	1.34	1.37
2	2	856	C	N1-C6	-5.07	1.34	1.37
2	2	1521	C	N1-C6	-5.06	1.34	1.37
1	1	2575	C	N1-C6	-5.06	1.34	1.37
1	1	595	C	N1-C6	-5.05	1.34	1.37
1	1	2499	C	C4-C5	-5.05	1.39	1.43
2	2	330	C	N1-C6	-5.05	1.34	1.37
1	1	2704	C	N1-C6	-5.05	1.34	1.37
2	2	899	C	N1-C6	-5.05	1.34	1.37
1	1	1652	A	N9-C4	-5.04	1.34	1.37
27	Z	5	ILE	C-N	-5.04	1.22	1.34
1	1	420	C	N1-C6	-5.04	1.34	1.37
1	1	1152	C	N3-C4	-5.04	1.30	1.33
1	1	1793	C	N1-C6	-5.04	1.34	1.37
2	2	806	C	N1-C6	-5.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2611	C	N1-C6	-5.03	1.34	1.37
2	2	578	C	C4-C5	-5.03	1.39	1.43
1	1	2025	C	N1-C6	-5.03	1.34	1.37
2	2	1069	C	N1-C6	-5.03	1.34	1.37
1	1	1853	A	N9-C4	-5.02	1.34	1.37
1	1	821	A	N9-C4	-5.02	1.34	1.37
1	1	2853	C	N1-C6	-5.02	1.34	1.37
3	3	92	C	N1-C6	-5.02	1.34	1.37
1	1	1308	A	C6-N6	-5.02	1.29	1.33
2	2	765	G	N9-C4	-5.01	1.33	1.38
1	1	2285	C	N1-C6	-5.01	1.34	1.37
2	2	738	C	N1-C6	-5.01	1.34	1.37
2	2	718	A	N9-C4	-5.01	1.34	1.37

All (326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1670	C	C5-C4-N4	-9.67	113.43	120.20
1	1	1670	C	N3-C4-C5	9.66	125.76	121.90
1	1	2719	G	C2-N3-C4	-9.16	107.32	111.90
1	1	2193	G	C4-N9-C1'	9.01	138.21	126.50
1	1	1509	A	O4'-C1'-N9	8.55	115.04	108.20
1	1	2193	G	C8-N9-C1'	-8.22	116.31	127.00
1	1	1871	A	O4'-C1'-N9	8.00	114.60	108.20
1	1	512	G	O4'-C1'-N9	7.92	114.53	108.20
1	1	2499	C	C5-C4-N4	-7.91	114.66	120.20
1	1	1923	U	O4'-C1'-N1	7.88	114.50	108.20
1	1	221	A	O4'-C1'-N9	7.58	114.26	108.20
1	1	481	G	O4'-C1'-N9	7.50	114.20	108.20
41	n	87	LEU	CA-CB-CG	7.47	132.48	115.30
54	z	32	A	C2-N3-C4	-7.42	106.89	110.60
1	1	275	C	C2-N1-C1'	-7.35	110.72	118.80
1	1	2799	A	N9-C4-C5	-7.30	102.88	105.80
1	1	2193	G	C6-C5-N7	-7.29	126.02	130.40
1	1	75	G	N3-C4-N9	-7.12	121.73	126.00
1	1	1857	G	O4'-C1'-N9	6.98	113.79	108.20
1	1	274	C	N1-C2-O2	6.97	123.08	118.90
1	1	801	G	C2-N3-C4	-6.97	108.42	111.90
1	1	1670	C	C6-N1-C2	6.94	123.07	120.30
1	1	982	C	N3-C4-C5	6.80	124.62	121.90
1	1	1905	C	N3-C4-C5	6.76	124.61	121.90
1	1	1187	G	C2-N3-C4	-6.75	108.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	84	C	N3-C4-C5	6.75	124.60	121.90
1	1	308	G	C2-N3-C4	-6.74	108.53	111.90
1	1	752	A	N1-C6-N6	6.74	122.64	118.60
1	1	2688	G	C2-N3-C4	-6.73	108.53	111.90
1	1	323	C	C2-N1-C1'	6.72	126.19	118.80
1	1	1615	C	C5-C4-N4	-6.71	115.51	120.20
1	1	1697	G	C2-N3-C4	-6.71	108.55	111.90
2	2	1221	G	N3-C4-C5	6.70	131.95	128.60
1	1	1728	C	N1-C2-O2	-6.70	114.88	118.90
2	2	581	G	C2-N3-C4	-6.67	108.57	111.90
1	1	2365	G	C2-N3-C4	-6.66	108.57	111.90
1	1	2430	A	N1-C6-N6	6.64	122.58	118.60
2	2	74	A	O4'-C1'-N9	6.63	113.51	108.20
2	2	1200	C	C5-C4-N4	-6.62	115.57	120.20
1	1	2719	G	N1-C2-N3	6.60	127.86	123.90
1	1	806	C	N1-C2-O2	6.59	122.85	118.90
2	2	686	U	O4'-C1'-N1	6.58	113.47	108.20
1	1	675	A	N1-C6-N6	6.57	122.54	118.60
1	1	2799	A	C4-C5-N7	6.55	113.97	110.70
1	1	818	G	C2-N3-C4	-6.46	108.67	111.90
1	1	2161	C	N3-C2-O2	-6.46	117.38	121.90
6	E	153	LEU	CA-CB-CG	6.44	130.12	115.30
1	1	2314	A	O4'-C1'-N9	6.43	113.35	108.20
2	2	976	G	N3-C2-N2	-6.42	115.40	119.90
1	1	469	G	C2-N3-C4	-6.41	108.70	111.90
1	1	1358	G	C2-N3-C4	-6.40	108.70	111.90
1	1	1313	U	C2-N1-C1'	6.35	125.32	117.70
1	1	2848	G	O4'-C1'-N9	6.32	113.26	108.20
1	1	2765	A	O4'-C1'-N9	6.32	113.26	108.20
1	1	733	G	C2-N3-C4	-6.29	108.75	111.90
1	1	916	G	C2-N3-C4	-6.29	108.75	111.90
1	1	757	G	N3-C4-C5	6.26	131.73	128.60
2	2	1403	C	C5-C4-N4	-6.26	115.81	120.20
2	2	575	G	N3-C4-N9	-6.26	122.24	126.00
2	2	792	A	O4'-C1'-N9	6.26	113.20	108.20
1	1	2158	A	O4'-C1'-N9	6.24	113.19	108.20
1	1	1670	C	C2-N3-C4	-6.23	116.78	119.90
2	2	1221	G	N3-C4-N9	-6.22	122.27	126.00
2	2	354	G	C2-N3-C4	-6.21	108.79	111.90
1	1	2454	G	C2-N3-C4	-6.20	108.80	111.90
2	2	1033	G	N3-C4-C5	6.20	131.70	128.60
1	1	1143	A	C5-C6-N6	-6.17	118.76	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	76	G	C2-N3-C4	-6.17	108.82	111.90
2	2	31	G	N3-C4-N9	-6.16	122.30	126.00
1	1	974	G	O4'-C1'-N9	6.14	113.11	108.20
1	1	275	C	C6-N1-C1'	6.13	128.15	120.80
54	z	84	C	C5-C4-N4	-6.13	115.91	120.20
1	1	308	G	N1-C2-N2	-6.10	110.71	116.20
1	1	323	C	C6-N1-C1'	-6.10	113.48	120.80
54	z	81	C	C6-N1-C2	6.07	122.73	120.30
2	2	1482	G	C2-N3-C4	-6.07	108.86	111.90
1	1	786	C	C6-N1-C2	6.06	122.72	120.30
2	2	765	G	C2-N3-C4	-6.04	108.88	111.90
1	1	1530	G	N9-C4-C5	-6.02	102.99	105.40
1	1	2799	A	N1-C6-N6	6.01	122.21	118.60
2	2	976	G	N3-C4-N9	-6.00	122.40	126.00
2	2	1160	G	N3-C4-N9	-6.00	122.40	126.00
1	1	1625	C	N1-C2-O2	6.00	122.50	118.90
2	2	791	G	C2-N3-C4	-6.00	108.90	111.90
2	2	993	G	O4'-C1'-N9	6.00	113.00	108.20
1	1	1459	G	N3-C4-C5	5.99	131.59	128.60
1	1	807	U	O4'-C1'-N1	5.97	112.98	108.20
3	3	76	G	N3-C4-C5	5.97	131.58	128.60
1	1	585	G	C2-N3-C4	-5.94	108.93	111.90
1	1	1062	G	C4-N9-C1'	5.93	134.21	126.50
1	1	2799	A	C6-C5-N7	-5.92	128.16	132.30
1	1	982	C	C5-C4-N4	-5.92	116.06	120.20
1	1	2714	G	C2-N3-C4	-5.92	108.94	111.90
1	1	1941	C	C5-C4-N4	-5.91	116.06	120.20
1	1	2036	C	N1-C2-O2	5.89	122.44	118.90
1	1	400	G	C2-N3-C4	-5.89	108.95	111.90
1	1	2164	C	P-O3'-C3'	-5.89	112.63	119.70
1	1	1788	C	N1-C2-O2	5.88	122.43	118.90
2	2	1502	A	N1-C6-N6	5.88	122.13	118.60
2	2	1033	G	N3-C4-N9	-5.87	122.48	126.00
1	1	942	G	C5-C6-O6	5.86	132.12	128.60
2	2	1396	A	C5-C6-N6	-5.86	119.01	123.70
1	1	1261	C	N3-C4-C5	5.86	124.24	121.90
1	1	2572	A	O4'-C1'-N9	5.86	112.88	108.20
1	1	1154	G	C2-N3-C4	-5.85	108.98	111.90
2	2	1109	C	O4'-C1'-N1	5.85	112.88	108.20
1	1	180	G	N3-C4-N9	-5.84	122.49	126.00
1	1	2382	G	C2-N3-C4	-5.84	108.98	111.90
1	1	780	G	C2-N3-C4	-5.83	108.99	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1339	G	C2-N3-C4	-5.82	108.99	111.90
1	1	26	G	C2-N3-C4	-5.80	109.00	111.90
1	1	2715	C	C2-N1-C1'	5.79	125.17	118.80
1	1	551	G	C8-N9-C1'	-5.79	119.47	127.00
1	1	189	G	C2-N3-C4	-5.78	109.01	111.90
1	1	708	G	O3'-P-O5'	-5.78	93.01	104.00
1	1	1062	G	C8-N9-C1'	-5.78	119.48	127.00
1	1	565	C	C6-N1-C2	5.76	122.61	120.30
1	1	704	G	O4'-C1'-N9	5.76	112.81	108.20
1	1	1062	G	C6-C5-N7	-5.76	126.95	130.40
1	1	882	G	C8-N9-C1'	-5.75	119.53	127.00
1	1	2722	G	C2-N3-C4	-5.74	109.03	111.90
1	1	395	U	O4'-C1'-N1	5.74	112.79	108.20
1	1	458	G	O4'-C1'-N9	5.73	112.78	108.20
1	1	2688	G	N3-C4-C5	5.71	131.46	128.60
1	1	2244	U	N3-C4-O4	5.71	123.40	119.40
54	z	43	G	N3-C4-N9	-5.71	122.58	126.00
1	1	180	G	N3-C4-C5	5.70	131.45	128.60
2	2	81	A	C8-N9-C4	-5.70	103.52	105.80
1	1	837	C	N3-C2-O2	-5.70	117.91	121.90
1	1	1131	G	C2-N3-C4	-5.69	109.06	111.90
1	1	2012	G	C2-N3-C4	-5.69	109.06	111.90
1	1	1115	G	O4'-C1'-N9	5.69	112.75	108.20
1	1	1790	C	C6-N1-C2	5.68	122.57	120.30
3	3	31	C	C2-N1-C1'	5.68	125.05	118.80
1	1	1143	A	N1-C6-N6	5.68	122.01	118.60
1	1	1261	C	C6-N1-C2	5.67	122.57	120.30
2	2	1028	C	C2-N1-C1'	-5.67	112.57	118.80
1	1	124	G	C2-N3-C4	-5.66	109.07	111.90
1	1	2715	C	C6-N1-C1'	-5.66	114.00	120.80
1	1	114	U	C2-N1-C1'	5.66	124.48	117.70
1	1	2248	C	C6-N1-C1'	-5.66	114.01	120.80
2	2	31	G	N3-C4-C5	5.65	131.43	128.60
1	1	726	G	N3-C4-C5	5.65	131.42	128.60
54	z	23	A	O4'-C1'-N9	5.65	112.72	108.20
1	1	2365	G	N1-C2-N2	-5.64	111.12	116.20
1	1	2075	U	N3-C4-O4	5.63	123.34	119.40
1	1	1950	G	N3-C4-N9	-5.63	122.62	126.00
1	1	672	C	N1-C2-O2	5.63	122.28	118.90
1	1	858	G	C2-N3-C4	-5.62	109.09	111.90
1	1	672	C	C2-N1-C1'	5.62	124.98	118.80
1	1	801	G	N3-C4-C5	5.61	131.40	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1905	C	C6-N1-C2	5.60	122.54	120.30
1	1	987	C	C6-N1-C2	5.58	122.53	120.30
1	1	2608	G	C2-N3-C4	-5.58	109.11	111.90
1	1	551	G	C4-N9-C1'	5.56	133.72	126.50
1	1	1828	G	C2-N3-C4	-5.55	109.12	111.90
3	3	31	C	C6-N1-C1'	-5.55	114.13	120.80
54	z	22	G	C2-N3-C4	-5.55	109.12	111.90
1	1	565	C	N3-C4-C5	5.55	124.12	121.90
1	1	2194	U	C2-N1-C1'	-5.54	111.05	117.70
1	1	2275	C	N1-C2-O2	5.53	122.22	118.90
1	1	1306	C	N3-C4-C5	5.52	124.11	121.90
1	1	2888	C	N1-C2-O2	5.51	122.21	118.90
1	1	675	A	C5-C6-N6	-5.51	119.29	123.70
1	1	2502	G	N3-C4-N9	-5.51	122.70	126.00
2	2	558	G	C2-N3-C4	-5.50	109.15	111.90
2	2	770	C	N3-C4-C5	5.50	124.10	121.90
1	1	2723	C	C6-N1-C1'	-5.50	114.20	120.80
2	2	271	C	C6-N1-C2	5.49	122.50	120.30
1	1	1564	C	N1-C2-O2	5.49	122.19	118.90
1	1	2253	G	C2-N3-C4	-5.49	109.16	111.90
1	1	2195	U	O4'-C1'-N1	5.47	112.58	108.20
2	2	1275	A	N1-C6-N6	5.47	121.88	118.60
2	2	73	C	C6-N1-C2	-5.47	118.11	120.30
25	X	48	ARG	CA-CB-CG	5.46	125.42	113.40
1	1	274	C	N3-C2-O2	-5.45	118.08	121.90
1	1	2308	G	C8-N9-C1'	5.45	134.08	127.00
1	1	1568	G	N3-C4-C5	5.45	131.32	128.60
2	2	1396	A	C4-C5-N7	5.45	113.42	110.70
1	1	748	G	O4'-C1'-N9	5.45	112.56	108.20
5	D	152	PRO	CA-N-CD	-5.44	103.89	111.50
2	2	1107	C	N3-C4-C5	5.43	124.07	121.90
1	1	780	G	N3-C4-C5	5.43	131.31	128.60
3	3	102	G	N3-C4-N9	-5.43	122.75	126.00
1	1	1371	G	C2-N3-C4	-5.42	109.19	111.90
1	1	33	C	O4'-C1'-N1	5.42	112.54	108.20
1	1	2308	G	C4-N9-C1'	-5.42	119.45	126.50
1	1	2193	G	N3-C4-N9	5.42	129.25	126.00
1	1	570	G	C2-N3-C4	-5.42	109.19	111.90
1	1	960	A	C5-C6-N1	5.42	120.41	117.70
1	1	1192	G	N3-C4-C5	5.41	131.31	128.60
1	1	2430	A	C5-C6-N6	-5.41	119.37	123.70
2	2	869	G	C2-N3-C4	-5.41	109.20	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2248	C	C2-N1-C1'	5.40	124.74	118.80
1	1	205	G	O4'-C1'-N9	5.40	112.52	108.20
54	z	32	A	N3-C4-C5	5.40	130.58	126.80
2	2	1222	G	N3-C4-N9	-5.40	122.76	126.00
1	1	2597	G	C2-N3-C4	-5.40	109.20	111.90
2	2	1304	G	C2-N3-C4	-5.39	109.20	111.90
1	1	2719	G	C5-C6-N1	-5.39	108.81	111.50
1	1	689	A	C5-C6-N6	-5.38	119.39	123.70
1	1	2035	G	O4'-C1'-N9	5.38	112.51	108.20
2	2	1079	G	C2-N3-C4	-5.38	109.21	111.90
2	2	322	C	N3-C4-C5	5.37	124.05	121.90
1	1	2499	C	C6-N1-C1'	-5.37	114.36	120.80
2	2	207	C	N1-C2-O2	-5.36	115.68	118.90
1	1	2271	G	C2-N3-C4	-5.36	109.22	111.90
2	2	1373	G	C2-N3-C4	-5.35	109.22	111.90
1	1	2894	G	N3-C4-N9	-5.35	122.79	126.00
1	1	2440	C	C5-C4-N4	-5.35	116.46	120.20
1	1	563	A	N1-C6-N6	-5.34	115.40	118.60
1	1	2190	G	C6-C5-N7	-5.34	127.20	130.40
1	1	484	C	C5-C4-N4	-5.34	116.46	120.20
1	1	1905	C	C2-N3-C4	-5.33	117.23	119.90
2	2	682	G	N3-C4-C5	5.33	131.26	128.60
1	1	726	G	N3-C4-N9	-5.33	122.80	126.00
54	z	24	C	C2-N1-C1'	5.33	124.66	118.80
1	1	338	G	C2-N3-C4	-5.33	109.24	111.90
1	1	1761	C	N3-C4-C5	5.31	124.03	121.90
1	1	2715	C	N1-C2-O2	5.31	122.08	118.90
1	1	2124	G	N3-C4-N9	-5.30	122.82	126.00
2	2	1366	C	N1-C2-O2	5.30	122.08	118.90
2	2	1034	G	O4'-C1'-N9	5.29	112.44	108.20
1	1	680	C	N1-C2-O2	5.29	122.07	118.90
1	1	882	G	C4-N9-C1'	5.29	133.38	126.50
1	1	2193	G	C4-C5-N7	5.29	112.92	110.80
1	1	1996	C	C5-C4-N4	-5.29	116.50	120.20
2	2	66	A	C4-C5-N7	5.29	113.34	110.70
2	2	770	C	C6-N1-C2	5.29	122.41	120.30
54	z	9	G	OP1-P-OP2	5.29	127.53	119.60
1	1	1212	G	N3-C4-C5	5.28	131.24	128.60
1	1	2720	U	N3-C4-O4	5.27	123.09	119.40
1	1	2323	G	C2-N3-C4	-5.27	109.26	111.90
1	1	1788	C	C2-N1-C1'	5.27	124.60	118.80
1	1	2592	G	C2-N3-C4	-5.27	109.27	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1299	G	C2-N3-C4	-5.26	109.27	111.90
2	2	1502	A	C5-C6-N6	-5.26	119.49	123.70
1	1	2083	G	C2-N3-C4	-5.26	109.27	111.90
1	1	215	G	C2-N3-C4	-5.25	109.28	111.90
1	1	1894	C	N1-C2-O2	5.23	122.04	118.90
1	1	488	G	C2-N3-C4	-5.23	109.28	111.90
1	1	2709	G	C2-N3-C4	-5.23	109.29	111.90
54	z	28	C	N1-C2-O2	5.23	122.04	118.90
1	1	581	C	C6-N1-C1'	-5.22	114.54	120.80
1	1	1266	G	N3-C4-N9	-5.22	122.87	126.00
1	1	1673	G	C2-N3-C4	-5.21	109.30	111.90
1	1	1350	C	C6-N1-C2	5.20	122.38	120.30
1	1	1143	A	C4-C5-N7	5.20	113.30	110.70
1	1	726	G	C2-N3-C4	-5.20	109.30	111.90
3	3	117	G	N3-C4-C5	5.20	131.20	128.60
1	1	2858	C	C5-C4-N4	-5.19	116.57	120.20
54	z	31	G	N1-C6-O6	5.19	123.01	119.90
1	1	2123	G	O4'-C1'-N9	5.19	112.35	108.20
2	2	15	G	C2-N3-C4	-5.19	109.31	111.90
1	1	2325	G	C2-N3-C4	-5.18	109.31	111.90
2	2	879	C	C6-N1-C2	5.18	122.37	120.30
2	2	858	G	C2-N3-C4	-5.18	109.31	111.90
1	1	37	C	N3-C4-C5	5.18	123.97	121.90
1	1	1339	G	N3-C4-N9	-5.17	122.90	126.00
1	1	1631	G	C2-N3-C4	-5.17	109.32	111.90
1	1	1223	G	C2-N3-C4	-5.16	109.32	111.90
1	1	1761	C	C5-C4-N4	-5.16	116.59	120.20
1	1	1904	G	C2-N3-C4	-5.16	109.32	111.90
3	3	66	A	N1-C6-N6	5.16	121.69	118.60
3	3	15	A	N1-C6-N6	5.15	121.69	118.60
1	1	583	G	C2-N3-C4	-5.15	109.33	111.90
1	1	1257	C	C6-N1-C2	5.15	122.36	120.30
1	1	801	G	N3-C4-N9	-5.15	122.91	126.00
1	1	2502	G	C2-N3-C4	-5.15	109.33	111.90
1	1	585	G	N1-C2-N3	5.14	126.99	123.90
1	1	383	C	C5-C4-N4	-5.14	116.60	120.20
1	1	794	A	C5-N7-C8	-5.13	101.33	103.90
1	1	2458	G	C2-N3-C4	-5.13	109.33	111.90
1	1	2723	C	C2-N1-C1'	5.13	124.44	118.80
1	1	1521	G	C2-N3-C4	-5.12	109.34	111.90
1	1	704	G	N3-C4-C5	5.12	131.16	128.60
1	1	242	G	N3-C4-N9	-5.12	122.93	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1459	G	N3-C4-N9	-5.11	122.93	126.00
1	1	1675	C	C5-C4-N4	-5.11	116.62	120.20
1	1	2029	G	C2-N3-C4	-5.11	109.34	111.90
2	2	21	G	C2-N3-C4	-5.11	109.34	111.90
26	Y	16	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	1	1935	G	C2-N3-C4	-5.11	109.34	111.90
1	1	2447	G	C2-N3-C4	-5.10	109.35	111.90
2	2	580	C	N1-C2-O2	5.10	121.96	118.90
1	1	748	G	N3-C4-N9	-5.09	122.94	126.00
1	1	1653	G	C2-N3-C4	-5.09	109.36	111.90
1	1	2443	C	N1-C2-O2	5.09	121.95	118.90
1	1	941	A	C5-C6-N6	-5.09	119.63	123.70
1	1	757	G	N3-C4-N9	-5.08	122.95	126.00
1	1	1436	G	C2-N3-C4	-5.08	109.36	111.90
1	1	581	C	N3-C4-C5	5.08	123.93	121.90
1	1	704	G	N3-C4-N9	-5.07	122.96	126.00
1	1	1530	G	C8-N9-C1'	-5.07	120.42	127.00
1	1	2502	G	N3-C4-C5	5.07	131.13	128.60
1	1	1836	C	N3-C4-C5	5.06	123.93	121.90
54	z	11	C	C6-N1-C2	5.06	122.33	120.30
1	1	601	C	O4'-C1'-N1	5.06	112.25	108.20
1	1	2440	C	N3-C4-C5	5.06	123.92	121.90
1	1	2194	U	O4'-C1'-N1	5.06	112.25	108.20
54	z	31	G	C2-N3-C4	-5.06	109.37	111.90
1	1	709	U	C6-N1-C2	-5.06	117.97	121.00
1	1	1313	U	C6-N1-C1'	-5.06	114.12	121.20
1	1	1573	G	C2-N3-C4	-5.06	109.37	111.90
1	1	2417	C	N1-C2-O2	5.05	121.93	118.90
1	1	1288	G	C2-N3-C4	-5.05	109.38	111.90
1	1	701	G	C2-N3-C4	-5.05	109.38	111.90
1	1	857	G	C2-N3-C4	-5.05	109.38	111.90
2	2	1331	G	O4'-C1'-N9	5.04	112.23	108.20
1	1	2834	G	C2-N3-C4	-5.04	109.38	111.90
2	2	1266	G	N3-C4-N9	-5.04	122.98	126.00
1	1	1320	C	O4'-C1'-N1	5.03	112.23	108.20
1	1	2110	G	N9-C1'-C2'	5.03	120.54	114.00
2	2	812	G	C2-N3-C4	-5.03	109.39	111.90
2	2	765	G	N3-C4-N9	-5.03	122.98	126.00
1	1	2676	C	N1-C2-O2	5.02	121.91	118.90
2	2	733	G	O4'-C1'-N9	5.02	112.22	108.20
1	1	776	G	C2-N3-C4	-5.01	109.39	111.90
1	1	1568	G	N3-C4-N9	-5.01	122.99	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	650	C	N1-C2-O2	5.01	121.91	118.90
2	2	169	C	O4'-C1'-N1	5.01	112.21	108.20
2	2	580	C	C2-N1-C1'	5.01	124.31	118.80
1	1	1125	G	C2-N3-C4	-5.00	109.40	111.90
1	1	2723	C	N1-C2-O2	5.00	121.90	118.90
2	2	335	C	N3-C4-C5	5.00	123.90	121.90
1	1	1728	C	C2-N1-C1'	-5.00	113.30	118.80

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	269/271 (99%)	256 (95%)	13 (5%)	0	100	100
5	D	207/209 (99%)	201 (97%)	3 (1%)	3 (1%)	9	37
6	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
7	F	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	22	57
8	G	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
9	H	147/149 (99%)	135 (92%)	10 (7%)	2 (1%)	9	37
10	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
11	J	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
12	K	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
13	L	134/136 (98%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	M	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
15	N	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
16	O	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
17	P	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
18	Q	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	6	29
19	R	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
20	S	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
21	T	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
22	U	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	V	82/84 (98%)	73 (89%)	7 (8%)	2 (2%)	5	25
24	W	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
25	X	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	Z	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
28	a	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	b	50/52 (96%)	50 (100%)	0	0	100	100
30	c	44/46 (96%)	44 (100%)	0	0	100	100
31	d	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
32	e	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
33	f	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
34	g	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
35	h	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
36	i	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
37	j	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
38	k	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
39	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
40	m	125/127 (98%)	117 (94%)	8 (6%)	0	100	100
41	n	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
42	o	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
43	p	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
44	q	114/116 (98%)	109 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	r	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
46	s	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
47	t	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
48	u	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
49	v	64/66 (97%)	64 (100%)	0	0	100	100
50	w	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
51	x	84/86 (98%)	84 (100%)	0	0	100	100
52	y	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
55	B	37/39 (95%)	29 (78%)	8 (22%)	0	100	100
All	All	5653/5754 (98%)	5440 (96%)	203 (4%)	10 (0%)	45	77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	152	PRO
5	D	153	GLY
5	D	154	LYS
9	H	90	LEU
23	V	5	LYS
23	V	11	ARG
18	Q	52	PRO
18	Q	53	PHE
9	H	89	LYS
7	F	124	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	216/216 (100%)	216 (100%)	0	100	100
5	D	164/164 (100%)	163 (99%)	1 (1%)	84	93
6	E	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	148/148 (100%)	148 (100%)	0	100	100
8	G	136/136 (100%)	135 (99%)	1 (1%)	81	91
9	H	114/114 (100%)	113 (99%)	1 (1%)	75	89
10	I	116/116 (100%)	116 (100%)	0	100	100
11	J	104/104 (100%)	103 (99%)	1 (1%)	73	88
12	K	103/103 (100%)	102 (99%)	1 (1%)	73	88
13	L	109/109 (100%)	108 (99%)	1 (1%)	75	89
14	M	99/99 (100%)	98 (99%)	1 (1%)	73	88
15	N	86/86 (100%)	86 (100%)	0	100	100
16	O	99/99 (100%)	99 (100%)	0	100	100
17	P	89/89 (100%)	88 (99%)	1 (1%)	70	87
18	Q	84/84 (100%)	84 (100%)	0	100	100
19	R	93/93 (100%)	93 (100%)	0	100	100
20	S	81/81 (100%)	81 (100%)	0	100	100
21	T	84/84 (100%)	83 (99%)	1 (1%)	67	86
22	U	78/78 (100%)	77 (99%)	1 (1%)	65	85
23	V	62/62 (100%)	62 (100%)	0	100	100
24	W	67/67 (100%)	67 (100%)	0	100	100
25	X	54/54 (100%)	54 (100%)	0	100	100
26	Y	48/48 (100%)	48 (100%)	0	100	100
27	Z	59/59 (100%)	59 (100%)	0	100	100
28	a	47/47 (100%)	47 (100%)	0	100	100
29	b	47/47 (100%)	47 (100%)	0	100	100
30	c	38/38 (100%)	38 (100%)	0	100	100
31	d	51/51 (100%)	49 (96%)	2 (4%)	27	61
32	e	34/34 (100%)	34 (100%)	0	100	100
33	f	187/187 (100%)	187 (100%)	0	100	100
34	g	171/171 (100%)	169 (99%)	2 (1%)	67	86
35	h	172/172 (100%)	172 (100%)	0	100	100
36	i	119/119 (100%)	117 (98%)	2 (2%)	56	81
37	j	91/91 (100%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	k	124/124 (100%)	124 (100%)	0	100	100
39	l	104/104 (100%)	104 (100%)	0	100	100
40	m	105/105 (100%)	103 (98%)	2 (2%)	52	79
41	n	86/86 (100%)	84 (98%)	2 (2%)	45	75
42	o	90/90 (100%)	89 (99%)	1 (1%)	70	87
43	p	102/102 (100%)	102 (100%)	0	100	100
44	q	94/94 (100%)	94 (100%)	0	100	100
45	r	83/83 (100%)	83 (100%)	0	100	100
46	s	76/76 (100%)	76 (100%)	0	100	100
47	t	65/65 (100%)	65 (100%)	0	100	100
48	u	74/74 (100%)	74 (100%)	0	100	100
49	v	57/57 (100%)	57 (100%)	0	100	100
50	w	72/72 (100%)	71 (99%)	1 (1%)	62	83
51	x	65/65 (100%)	65 (100%)	0	100	100
52	y	60/60 (100%)	58 (97%)	2 (3%)	33	67
55	B	16/28 (57%)	16 (100%)	0	100	100
All	All	4688/4700 (100%)	4664 (100%)	24 (0%)	85	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	151	THR
8	G	47	ASP
9	H	122	LEU
11	J	17	ARG
12	K	48	ARG
13	L	59	ARG
14	M	80	PHE
17	P	78	LYS
21	T	68	SER
22	U	10	LYS
31	d	31	HIS
31	d	51	SER
34	g	118	ASP
34	g	164	ARG
36	i	29	ARG

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Mol	Chain	Res	Type
36	i	93	ARG
40	m	25	ASN
40	m	106	ARG
41	n	5	ARG
41	n	87	LEU
42	o	56	ARG
50	w	78	ARG
52	y	5	LYS
52	y	13	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
8	G	38	ASN
9	H	128	HIS
31	d	31	HIS
33	f	36	ASN
50	w	69	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2898/2903 (99%)	494 (17%)	10 (0%)
2	2	1529/1534 (99%)	255 (16%)	5 (0%)
3	3	119/120 (99%)	16 (13%)	0
53	4	5/6 (83%)	1 (20%)	0
54	z	84/85 (98%)	26 (30%)	0
All	All	4635/4648 (99%)	792 (17%)	15 (0%)

All (792) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	15	G
1	1	34	U
1	1	35	G
1	1	46	G
1	1	51	G
1	1	71	A
1	1	74	A

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Mol	Chain	Res	Type
1	1	75	G
1	1	80	G
1	1	84	A
1	1	85	G
1	1	101	A
1	1	102	U
1	1	110	G
1	1	118	A
1	1	119	A
1	1	120	U
1	1	122	G
1	1	125	A
1	1	138	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	181	A
1	1	196	A
1	1	199	A
1	1	215	G
1	1	216	A
1	1	221	A
1	1	222	A
1	1	225	C
1	1	248	G
1	1	249	C
1	1	264	C
1	1	265	A
1	1	266	G
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	285	G
1	1	301	G
1	1	311	A
1	1	329	G
1	1	330	A
1	1	343	C
1	1	353	C
1	1	361	G

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Mol	Chain	Res	Type
1	1	371	A
1	1	372	G
1	1	383	C
1	1	386	G
1	1	396	G
1	1	399	U
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	424	G
1	1	435	C
1	1	457	A
1	1	467	G
1	1	481	G
1	1	489	G
1	1	491	G
1	1	505	A
1	1	509	C
1	1	513	A
1	1	532	A
1	1	533	G
1	1	543	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	551	G
1	1	563	A
1	1	573	U
1	1	575	A
1	1	603	A
1	1	609	A
1	1	612	G
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	627	A
1	1	637	A

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Mol	Chain	Res	Type
1	1	645	C
1	1	647	G
1	1	654	A
1	1	655	A
1	1	670	A
1	1	685	A
1	1	686	U
1	1	702	U
1	1	717	C
1	1	726	G
1	1	730	A
1	1	747	5MU
1	1	764	A
1	1	765	C
1	1	775	G
1	1	776	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	792	A
1	1	800	A
1	1	805	G
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	845	A
1	1	846	U
1	1	858	G
1	1	859	G
1	1	866	A
1	1	869	G
1	1	878	A
1	1	880	G
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U

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Mol	Chain	Res	Type
1	1	896	A
1	1	897	C
1	1	898	C
1	1	907	G
1	1	910	A
1	1	931	U
1	1	932	U
1	1	941	A
1	1	946	C
1	1	961	C
1	1	973	A
1	1	974	G
1	1	983	A
1	1	989	G
1	1	995	C
1	1	996	A
1	1	999	U
1	1	1005	C
1	1	1012	U
1	1	1013	C
1	1	1022	G
1	1	1023	U
1	1	1025	G
1	1	1026	G
1	1	1033	U
1	1	1043	C
1	1	1046	A
1	1	1047	G
1	1	1057	A
1	1	1060	U
1	1	1061	U
1	1	1062	G
1	1	1064	C
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1084	A
1	1	1085	A

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Mol	Chain	Res	Type
1	1	1087	G
1	1	1088	A
1	1	1090	A
1	1	1096	A
1	1	1101	U
1	1	1110	G
1	1	1111	A
1	1	1112	G
1	1	1119	U
1	1	1122	G
1	1	1128	G
1	1	1130	U
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1134	A
1	1	1135	C
1	1	1136	G
1	1	1139	G
1	1	1142	A
1	1	1156	A
1	1	1169	A
1	1	1170	C
1	1	1171	G
1	1	1173	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1179	G
1	1	1182	G
1	1	1186	G
1	1	1206	G
1	1	1212	G
1	1	1218	G
1	1	1236	G
1	1	1238	G
1	1	1247	A
1	1	1250	G
1	1	1253	A
1	1	1256	G
1	1	1266	G

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Mol	Chain	Res	Type
1	1	1271	G
1	1	1272	A
1	1	1300	G
1	1	1301	A
1	1	1321	A
1	1	1324	G
1	1	1325	U
1	1	1329	U
1	1	1341	G
1	1	1345	C
1	1	1352	U
1	1	1365	A
1	1	1368	G
1	1	1379	U
1	1	1380	G
1	1	1383	A
1	1	1386	C
1	1	1408	G
1	1	1417	C
1	1	1419	A
1	1	1427	A
1	1	1428	C
1	1	1437	C
1	1	1460	U
1	1	1468	U
1	1	1476	U
1	1	1482	G
1	1	1490	A
1	1	1493	C
1	1	1494	A
1	1	1503	A
1	1	1504	A
1	1	1508	A
1	1	1509	A
1	1	1510	G
1	1	1515	A
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1532	A
1	1	1535	A
1	1	1536	C

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Mol	Chain	Res	Type
1	1	1537	G
1	1	1554	U
1	1	1559	U
1	1	1566	A
1	1	1569	A
1	1	1578	U
1	1	1580	A
1	1	1583	A
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1608	A
1	1	1619	G
1	1	1634	A
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1651	G
1	1	1674	G
1	1	1715	G
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1738	G
1	1	1756	G
1	1	1764	C
1	1	1773	A
1	1	1782	U
1	1	1791	A
1	1	1800	C
1	1	1801	A
1	1	1808	A
1	1	1811	G
1	1	1816	C
1	1	1829	A
1	1	1833	C
1	1	1835	2MG
1	1	1847	A
1	1	1848	A
1	1	1858	A
1	1	1865	U
1	1	1868	C

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Mol	Chain	Res	Type
1	1	1869	G
1	1	1870	C
1	1	1871	A
1	1	1872	A
1	1	1873	G
1	1	1896	G
1	1	1906	G
1	1	1907	G
1	1	1912	A
1	1	1914	C
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1936	A
1	1	1937	A
1	1	1938	A
1	1	1955	U
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1991	U
1	1	1992	G
1	1	1993	U
1	1	1997	C
1	1	2002	G
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2033	A
1	1	2043	C
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2069	G7M
1	1	2093	G
1	1	2095	A
1	1	2100	G

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Mol	Chain	Res	Type
1	1	2102	G
1	1	2107	G
1	1	2110	G
1	1	2112	G
1	1	2113	U
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2121	G
1	1	2122	U
1	1	2125	G
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2145	C
1	1	2146	C
1	1	2147	A
1	1	2158	A
1	1	2159	G
1	1	2162	G
1	1	2163	A
1	1	2164	C
1	1	2165	C
1	1	2169	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2178	C
1	1	2183	A
1	1	2189	U
1	1	2190	G
1	1	2191	A
1	1	2194	U
1	1	2198	A
1	1	2204	G
1	1	2211	A

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Mol	Chain	Res	Type
1	1	2225	A
1	1	2229	U
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2250	G
1	1	2278	A
1	1	2283	C
1	1	2286	G
1	1	2287	A
1	1	2288	A
1	1	2305	U
1	1	2309	A
1	1	2319	G
1	1	2322	A
1	1	2325	G
1	1	2327	A
1	1	2333	A
1	1	2334	U
1	1	2336	A
1	1	2345	G
1	1	2347	C
1	1	2350	C
1	1	2357	G
1	1	2361	G
1	1	2376	A
1	1	2383	G
1	1	2385	C
1	1	2402	U
1	1	2403	C
1	1	2406	A
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2435	A
1	1	2441	U
1	1	2445	2MG
1	1	2448	A
1	1	2470	G

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Mol	Chain	Res	Type
1	1	2476	A
1	1	2478	A
1	1	2480	C
1	1	2491	U
1	1	2498	OMC
1	1	2502	G
1	1	2504	PSU
1	1	2505	G
1	1	2506	U
1	1	2507	C
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2529	G
1	1	2535	G
1	1	2547	A
1	1	2554	U
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2586	U
1	1	2602	A
1	1	2609	U
1	1	2613	U
1	1	2629	U
1	1	2646	C
1	1	2663	G
1	1	2689	U
1	1	2690	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2725	A
1	1	2726	A
1	1	2733	A
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2757	A
1	1	2765	A
1	1	2777	G

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Mol	Chain	Res	Type
1	1	2778	A
1	1	2791	G
1	1	2793	C
1	1	2797	U
1	1	2799	A
1	1	2811	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2825	G
1	1	2833	U
1	1	2835	A
1	1	2836	U
1	1	2861	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2891	U
1	1	2898	U
2	2	7	A
2	2	8	A
2	2	9	G
2	2	22	G
2	2	32	A
2	2	39	G
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	54	C
2	2	66	A
2	2	68	G
2	2	69	G
2	2	70	U
2	2	72	A
2	2	73	C

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Mol	Chain	Res	Type
2	2	74	A
2	2	75	G
2	2	76	G
2	2	81	A
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	92	U
2	2	120	A
2	2	121	U
2	2	130	A
2	2	131	A
2	2	141	G
2	2	144	G
2	2	149	A
2	2	160	A
2	2	163	C
2	2	164	G
2	2	177	G
2	2	181	A
2	2	182	A
2	2	197	A
2	2	204	G
2	2	210	C
2	2	211	G
2	2	212	G
2	2	226	G
2	2	245	U
2	2	247	G
2	2	251	G
2	2	266	G
2	2	267	C
2	2	279	A
2	2	289	G
2	2	306	A
2	2	319	G
2	2	321	A
2	2	328	C
2	2	332	G
2	2	347	G

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Mol	Chain	Res	Type
2	2	352	C
2	2	354	G
2	2	362	G
2	2	367	U
2	2	372	C
2	2	384	G
2	2	392	C
2	2	398	U
2	2	406	G
2	2	412	A
2	2	413	G
2	2	414	A
2	2	421	U
2	2	422	C
2	2	424	G
2	2	429	U
2	2	436	C
2	2	439	U
2	2	457	G
2	2	458	U
2	2	463	U
2	2	464	U
2	2	467	U
2	2	468	A
2	2	476	U
2	2	478	A
2	2	479	U
2	2	481	G
2	2	484	G
2	2	485	U
2	2	486	U
2	2	496	A
2	2	499	A
2	2	510	A
2	2	511	C
2	2	517	G
2	2	518	C
2	2	521	G
2	2	527	G7M
2	2	531	U
2	2	532	A
2	2	533	A

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Mol	Chain	Res	Type
2	2	547	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	596	A
2	2	605	U
2	2	633	G
2	2	650	G
2	2	653	U
2	2	660	C
2	2	665	A
2	2	700	G
2	2	701	U
2	2	702	A
2	2	703	G
2	2	718	A
2	2	721	G
2	2	723	U
2	2	724	G
2	2	731	G
2	2	734	G
2	2	747	A
2	2	748	G
2	2	753	A
2	2	755	G
2	2	777	A
2	2	787	A
2	2	793	U
2	2	794	A
2	2	815	A
2	2	817	C
2	2	821	G
2	2	828	U
2	2	829	G
2	2	832	G
2	2	841	C
2	2	843	U
2	2	844	G

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Mol	Chain	Res	Type
2	2	845	A
2	2	846	G
2	2	884	U
2	2	885	G
2	2	887	G
2	2	914	A
2	2	934	C
2	2	935	A
2	2	960	U
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	972	C
2	2	974	A
2	2	975	A
2	2	976	G
2	2	977	A
2	2	982	U
2	2	993	G
2	2	994	A
2	2	996	A
2	2	1004	A
2	2	1009	U
2	2	1019	A
2	2	1020	G
2	2	1022	A
2	2	1025	U
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1032	G
2	2	1034	G
2	2	1043	G
2	2	1046	A
2	2	1065	U
2	2	1085	U
2	2	1089	G
2	2	1094	G
2	2	1095	U

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Mol	Chain	Res	Type
2	2	1101	A
2	2	1104	G
2	2	1108	G
2	2	1124	G
2	2	1125	U
2	2	1132	C
2	2	1136	C
2	2	1137	C
2	2	1139	G
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1146	A
2	2	1151	A
2	2	1152	A
2	2	1158	C
2	2	1159	U
2	2	1160	G
2	2	1167	A
2	2	1169	A
2	2	1175	G
2	2	1176	A
2	2	1184	G
2	2	1196	A
2	2	1197	A
2	2	1212	U
2	2	1213	A
2	2	1215	G
2	2	1227	A
2	2	1228	C
2	2	1238	A
2	2	1239	A
2	2	1257	A
2	2	1258	G
2	2	1260	G
2	2	1261	A
2	2	1275	A
2	2	1279	G
2	2	1280	A
2	2	1286	U
2	2	1287	A
2	2	1297	G

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Mol	Chain	Res	Type
2	2	1299	A
2	2	1302	C
2	2	1305	G
2	2	1312	G
2	2	1317	C
2	2	1320	C
2	2	1335	U
2	2	1336	C
2	2	1340	A
2	2	1346	A
2	2	1353	G
2	2	1363	A
2	2	1364	U
2	2	1370	G
2	2	1379	G
2	2	1381	U
2	2	1419	G
2	2	1446	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1503	A
2	2	1506	U
2	2	1517	G
2	2	1529	G
2	2	1530	G
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	13	G
3	3	24	G
3	3	31	C
3	3	35	C
3	3	36	C
3	3	45	A
3	3	51	G
3	3	56	G
3	3	66	A
3	3	88	C
3	3	89	U
3	3	90	C
3	3	99	A

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Mol	Chain	Res	Type
3	3	109	A
53	4	6	A
54	z	7	G
54	z	8	5MU
54	z	14	A
54	z	16	U
54	z	17	U
54	z	18	G
54	z	19	G
54	z	20	5MU
54	z	21	A
54	z	22	G
54	z	23	A
54	z	24	C
54	z	46	G
54	z	49	G
54	z	57	5MU
54	z	58	G
54	z	62	G
54	z	63	5MU
54	z	64	5MU
54	z	67	A
54	z	68	G
54	z	69	5MU
54	z	70	C
54	z	71	5MU
54	z	76	5MU
54	z	85	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	372	G
1	1	404	A
1	1	613	A
1	1	784	G
1	1	891	G
1	1	894	U
1	1	1379	U
1	1	1475	G
1	1	2189	U
1	1	2756	U

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Mol	Chain	Res	Type
2	2	85	U
2	2	86	G
2	2	516	PSU
2	2	1109	C
2	2	1145	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1	2457	1	18,21,22	1.18	2 (11%)	22,30,33	2.20	5 (22%)
1	6MZ	1	2030	1	18,25,26	1.89	4 (22%)	16,36,39	3.27	3 (18%)
1	5MC	1	1962	1	18,22,23	3.04	7 (38%)	26,32,35	1.26	5 (19%)
2	2MG	2	1516	2	18,26,27	2.21	7 (38%)	16,38,41	1.47	4 (25%)
1	PSU	1	1911	1	18,21,22	0.90	0	22,30,33	1.87	3 (13%)
2	MA6	2	1518	2	18,26,27	1.31	1 (5%)	19,38,41	3.44	2 (10%)
54	5MU	z	40	54	19,22,23	1.38	5 (26%)	28,32,35	2.27	11 (39%)
1	PSU	1	1917	1	18,21,22	1.01	1 (5%)	22,30,33	2.13	5 (22%)
54	5MU	z	57	54	19,22,23	4.54	7 (36%)	28,32,35	3.71	9 (32%)
1	PSU	1	955	1	18,21,22	1.08	1 (5%)	22,30,33	1.99	5 (22%)
1	2MG	1	1835	1	18,26,27	2.04	7 (38%)	16,38,41	1.45	3 (18%)
2	2MG	2	1207	2	18,26,27	2.22	7 (38%)	16,38,41	1.35	3 (18%)
2	G7M	2	527	2	20,26,27	2.23	9 (45%)	17,39,42	1.11	1 (5%)
2	4OC	2	1402	2	20,23,24	2.69	8 (40%)	26,32,35	1.08	1 (3%)
2	2MG	2	966	2	18,26,27	2.27	7 (38%)	16,38,41	1.32	3 (18%)
1	OMC	1	2498	56,1	19,22,23	2.51	6 (31%)	26,31,34	0.96	0
1	G7M	1	2069	1	20,26,27	2.17	8 (40%)	17,39,42	1.29	2 (11%)
1	6MZ	1	1618	1	18,25,26	1.89	5 (27%)	16,36,39	3.26	3 (18%)
1	5MU	1	1939	56,1	19,22,23	4.39	7 (36%)	28,32,35	3.71	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5MC	2	967	2	18,22,23	3.27	7 (38%)	26,32,35	1.12	2 (7%)
54	5MU	z	20	56,54	19,22,23	4.78	7 (36%)	28,32,35	3.73	9 (32%)
1	PSU	1	2504	1	18,21,22	0.98	1 (5%)	22,30,33	1.85	4 (18%)
54	5MU	z	39	54	19,22,23	1.44	5 (26%)	28,32,35	2.17	9 (32%)
2	MA6	2	1519	2	18,26,27	1.37	1 (5%)	19,38,41	3.65	2 (10%)
54	5MU	z	71	54	19,22,23	1.34	5 (26%)	28,32,35	2.21	9 (32%)
1	OMU	1	2552	1	19,22,23	2.74	6 (31%)	26,31,34	1.67	6 (23%)
1	PSU	1	2580	56,1	18,21,22	1.14	1 (5%)	22,30,33	2.23	6 (27%)
54	5MU	z	69	54	19,22,23	6.60	6 (31%)	28,32,35	28.78	14 (50%)
54	5MU	z	42	54,2	19,22,23	4.34	7 (36%)	28,32,35	3.84	11 (39%)
54	5MU	z	63	54	19,22,23	1.45	6 (31%)	28,32,35	2.45	13 (46%)
54	5MU	z	55	54	19,22,23	4.68	7 (36%)	28,32,35	3.48	9 (32%)
1	5MU	1	747	1	19,22,23	4.50	7 (36%)	28,32,35	3.78	9 (32%)
1	1MG	1	745	1	18,26,27	2.61	5 (27%)	19,39,42	1.62	4 (21%)
2	PSU	2	516	56,2	18,21,22	0.97	1 (5%)	22,30,33	1.88	3 (13%)
54	5MU	z	76	54	19,22,23	1.43	6 (31%)	28,32,35	2.14	9 (32%)
1	2MG	1	2445	1	18,26,27	2.15	7 (38%)	16,38,41	1.25	4 (25%)
54	5MU	z	8	54	19,22,23	4.51	7 (36%)	28,32,35	3.93	9 (32%)
1	OMG	1	2251	54,1	18,26,27	2.01	7 (38%)	19,38,41	1.44	4 (21%)
1	2MA	1	2503	56,1	19,25,26	2.87	7 (36%)	21,37,40	1.64	4 (19%)
1	3TD	1	1915	1	18,22,23	4.04	7 (38%)	22,32,35	1.54	3 (13%)
1	PSU	1	746	56,1	18,21,22	1.04	2 (11%)	22,30,33	1.74	3 (13%)
2	UR3	2	1498	2	19,22,23	2.41	6 (31%)	26,32,35	1.04	2 (7%)
43	0TD	p	89	43	7,9,10	1.49	1 (14%)	6,11,13	1.92	2 (33%)
54	5MU	z	64	54	19,22,23	1.44	6 (31%)	28,32,35	2.32	7 (25%)
2	5MC	2	1407	2	18,22,23	3.12	7 (38%)	26,32,35	0.90	1 (3%)
1	PSU	1	2605	1	18,21,22	1.05	1 (5%)	22,30,33	1.92	4 (18%)

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
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	3/7/29/30	0/3/3/3
54	5MU	z	40	54	-	2/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	z	57	54	-	2/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
2	G7M	2	527	2	-	3/3/25/26	0/3/3/3
2	4OC	2	1402	2	-	2/9/29/30	0/2/2/2
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3
1	OMC	1	2498	56,1	-	0/9/27/28	0/2/2/2
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
1	6MZ	1	1618	1	-	3/5/27/28	0/3/3/3
1	5MU	1	1939	56,1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	2/7/25/26	0/2/2/2
54	5MU	z	20	56,54	-	4/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
54	5MU	z	39	54	-	4/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	5/7/29/30	0/3/3/3
54	5MU	z	71	54	-	3/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2580	56,1	-	0/7/25/26	0/2/2/2
54	5MU	z	69	54	-	2/7/25/26	1/2/2/2
54	5MU	z	42	54,2	-	0/7/25/26	0/2/2/2
54	5MU	z	63	54	-	2/7/25/26	0/2/2/2
54	5MU	z	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	PSU	2	516	56,2	-	2/7/25/26	0/2/2/2
54	5MU	z	76	54	-	2/7/25/26	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
54	5MU	z	8	54	-	2/7/25/26	0/2/2/2
1	OMG	1	2251	54,1	-	0/5/27/28	0/3/3/3
1	2MA	1	2503	56,1	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	3TD	1	1915	1	-	3/7/25/26	0/2/2/2
1	PSU	1	746	56,1	-	1/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	1/7/25/26	0/2/2/2
43	0TD	p	89	43	-	3/7/12/14	-
54	5MU	z	64	54	-	2/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2

All (235) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	z	69	5MU	C6-C5	23.78	1.73	1.34
1	1	1915	3TD	C6-C5	11.71	1.49	1.35
54	z	57	5MU	C2-N1	11.02	1.56	1.38
54	z	20	5MU	C2-N1	10.76	1.55	1.38
54	z	20	5MU	C6-N1	10.47	1.55	1.38
54	z	42	5MU	C2-N1	10.46	1.55	1.38
54	z	55	5MU	C2-N1	10.34	1.55	1.38
54	z	20	5MU	C4-C5	10.30	1.61	1.44
54	z	55	5MU	C6-N1	10.22	1.55	1.38
1	1	747	5MU	C2-N1	10.12	1.54	1.38
1	1	1939	5MU	C2-N1	9.97	1.54	1.38
54	z	69	5MU	C4-C5	-9.95	1.28	1.44
54	z	8	5MU	C2-N1	9.91	1.54	1.38
1	1	747	5MU	C6-N1	9.67	1.54	1.38
54	z	55	5MU	C4-C5	9.54	1.60	1.44
54	z	8	5MU	C6-N1	9.25	1.53	1.38
54	z	57	5MU	C6-N1	9.21	1.53	1.38
54	z	8	5MU	C4-C5	9.20	1.60	1.44
54	z	69	5MU	C6-N1	9.20	1.53	1.38
1	1	1939	5MU	C6-N1	9.01	1.53	1.38
1	1	1915	3TD	C2-N1	8.95	1.48	1.37
1	1	1939	5MU	C4-C5	8.85	1.59	1.44
1	1	747	5MU	C4-C5	8.50	1.58	1.44
54	z	42	5MU	C6-N1	8.50	1.52	1.38
54	z	42	5MU	C4-N3	-8.42	1.23	1.38
54	z	57	5MU	C4-C5	8.37	1.58	1.44
2	2	1407	5MC	C6-C5	8.23	1.48	1.34
54	z	57	5MU	C4-N3	-8.16	1.23	1.38
54	z	42	5MU	C4-C5	8.05	1.58	1.44
1	1	747	5MU	C4-N3	-7.99	1.24	1.38
2	2	967	5MC	C6-C5	7.97	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1939	5MU	C4-N3	-7.86	1.24	1.38
54	z	8	5MU	C4-N3	-7.86	1.24	1.38
1	1	2503	2MA	C4-N3	7.69	1.47	1.35
54	z	55	5MU	C4-N3	-7.64	1.24	1.38
1	1	745	1MG	C2-N2	7.49	1.47	1.34
1	1	1962	5MC	C6-C5	7.07	1.46	1.34
54	z	69	5MU	C4-N3	6.96	1.51	1.38
54	z	20	5MU	C4-N3	-6.96	1.25	1.38
2	2	1402	4OC	C4-N3	6.27	1.43	1.32
1	1	1962	5MC	C4-N3	6.24	1.44	1.34
2	2	967	5MC	C4-N3	6.19	1.44	1.34
1	1	2552	OMU	C2-N3	6.10	1.48	1.38
54	z	55	5MU	C6-C5	6.04	1.44	1.34
54	z	20	5MU	C6-C5	5.96	1.44	1.34
2	2	1498	UR3	C6-C5	5.95	1.48	1.35
2	2	967	5MC	C2-N3	5.85	1.48	1.36
1	1	2552	OMU	C2-N1	5.76	1.47	1.38
1	1	1915	3TD	C6-N1	5.70	1.45	1.36
1	1	1618	6MZ	C6-N6	5.70	1.44	1.35
1	1	2503	2MA	C2-N3	5.63	1.44	1.34
1	1	2498	OMC	C2-N3	5.50	1.47	1.36
1	1	2030	6MZ	C6-N6	5.38	1.43	1.35
1	1	1962	5MC	C2-N3	5.32	1.47	1.36
1	1	747	5MU	C6-C5	5.30	1.43	1.34
54	z	8	5MU	C6-C5	5.22	1.43	1.34
2	2	1402	4OC	C2-N3	5.22	1.46	1.36
1	1	2552	OMU	C6-C5	5.20	1.47	1.35
2	2	1407	5MC	C4-N3	5.17	1.42	1.34
2	2	1407	5MC	C2-N3	5.08	1.46	1.36
54	z	57	5MU	C6-C5	5.08	1.42	1.34
2	2	1402	4OC	C6-C5	5.07	1.46	1.35
2	2	966	2MG	C2-N2	5.04	1.44	1.33
2	2	527	G7M	C2-N3	4.98	1.45	1.33
2	2	966	2MG	C4-N3	4.93	1.49	1.37
2	2	1498	UR3	C2-N1	4.92	1.45	1.38
1	1	2498	OMC	C6-C5	4.74	1.46	1.35
2	2	1207	2MG	C2-N2	4.66	1.43	1.33
1	1	1915	3TD	C2-N3	4.60	1.48	1.38
1	1	1939	5MU	C6-C5	4.57	1.42	1.34
1	1	2503	2MA	C6-N1	4.47	1.42	1.33
2	2	527	G7M	C2-N2	4.46	1.44	1.34
1	1	2503	2MA	C2-N1	4.45	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2251	OMG	C2-N3	4.40	1.43	1.33
2	2	1207	2MG	C4-N3	4.35	1.47	1.37
2	2	527	G7M	C4-N3	4.34	1.47	1.37
1	1	2445	2MG	C2-N2	4.32	1.43	1.33
1	1	2069	G7M	C2-N3	4.30	1.43	1.33
1	1	2498	OMC	C4-N3	4.27	1.43	1.34
1	1	1835	2MG	C4-N3	4.22	1.47	1.37
2	2	967	5MC	C4-N4	4.17	1.44	1.34
1	1	745	1MG	C2-N3	4.12	1.41	1.34
2	2	1516	2MG	C2-N2	4.08	1.42	1.33
1	1	1835	2MG	C2-N2	4.07	1.42	1.33
54	z	42	5MU	C6-C5	4.05	1.41	1.34
2	2	1498	UR3	C2-N3	4.05	1.46	1.39
2	2	1516	2MG	C2-N1	4.02	1.43	1.36
1	1	745	1MG	C4-N3	4.00	1.47	1.37
1	1	2498	OMC	C4-N4	4.00	1.43	1.33
2	2	1516	2MG	C4-N3	4.00	1.47	1.37
54	z	69	5MU	C2-N1	3.99	1.44	1.38
1	1	2445	2MG	C4-N3	3.98	1.47	1.37
2	2	1407	5MC	C6-N1	3.97	1.44	1.38
1	1	745	1MG	O6-C6	-3.95	1.14	1.22
1	1	2069	G7M	C4-N3	3.94	1.46	1.37
1	1	2069	G7M	C2-N2	3.90	1.43	1.34
1	1	2552	OMU	C4-N3	3.85	1.45	1.38
2	2	1402	4OC	C4-N4	3.76	1.43	1.35
2	2	1207	2MG	C2-N1	3.75	1.42	1.36
1	1	1962	5MC	C4-N4	3.74	1.43	1.34
2	2	1407	5MC	C4-N4	3.70	1.43	1.34
1	1	1962	5MC	C2-N1	3.66	1.47	1.40
2	2	1519	MA6	C5-C4	-3.63	1.31	1.40
2	2	966	2MG	C2-N1	3.60	1.42	1.36
54	z	42	5MU	O4-C4	-3.55	1.16	1.23
1	1	2251	OMG	C4-N3	3.55	1.46	1.37
1	1	747	5MU	O4-C4	-3.53	1.16	1.23
2	2	967	5MC	C2-N1	3.50	1.47	1.40
54	z	8	5MU	O4-C4	-3.48	1.17	1.23
1	1	2498	OMC	C2-N1	3.41	1.47	1.40
2	2	967	5MC	C6-N1	3.39	1.43	1.38
54	z	8	5MU	O2-C2	-3.39	1.16	1.23
1	1	2030	6MZ	C5-C4	-3.36	1.32	1.40
1	1	2445	2MG	C2-N1	3.34	1.42	1.36
2	2	1402	4OC	C2-N1	3.31	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1407	5MC	O2-C2	-3.29	1.17	1.23
2	2	1518	MA6	C5-C4	-3.29	1.32	1.40
2	2	1407	5MC	C2-N1	3.27	1.47	1.40
1	1	2251	OMG	C5-C4	-3.25	1.34	1.43
54	z	57	5MU	O4-C4	-3.23	1.17	1.23
1	1	1835	2MG	C2-N1	3.23	1.41	1.36
1	1	2445	2MG	C5-C4	-3.22	1.34	1.43
2	2	1498	UR3	C3U-N3	-3.18	1.41	1.47
2	2	967	5MC	O2-C2	-3.18	1.17	1.23
1	1	1962	5MC	O2-C2	-3.18	1.17	1.23
1	1	1618	6MZ	C5-C4	-3.16	1.32	1.40
1	1	2069	G7M	C6-N1	3.16	1.42	1.37
1	1	1939	5MU	O4-C4	-3.16	1.17	1.23
1	1	2498	OMC	O2-C2	-3.12	1.17	1.23
2	2	1402	4OC	O2-C2	-3.11	1.17	1.23
54	z	55	5MU	O4-C4	-2.96	1.18	1.23
54	z	20	5MU	O4-C4	-2.96	1.18	1.23
2	2	1516	2MG	C5-C4	-2.95	1.35	1.43
1	1	1962	5MC	C6-N1	2.94	1.43	1.38
2	2	1207	2MG	C5-C4	-2.93	1.35	1.43
1	1	2552	OMU	O4-C4	-2.92	1.18	1.24
2	2	1516	2MG	C6-N1	2.88	1.42	1.37
1	1	1939	5MU	O2-C2	-2.87	1.17	1.23
1	1	2552	OMU	O2-C2	-2.82	1.17	1.23
1	1	1835	2MG	C5-C4	-2.82	1.35	1.43
2	2	1402	4OC	C5-C4	2.81	1.46	1.40
1	1	2251	OMG	O6-C6	-2.80	1.17	1.23
2	2	966	2MG	C5-C4	-2.78	1.36	1.43
1	1	747	5MU	O2-C2	-2.77	1.18	1.23
1	1	2503	2MA	C6-N6	-2.76	1.23	1.34
54	z	64	5MU	C4-N3	-2.76	1.33	1.38
2	2	1207	2MG	C5-C6	2.75	1.53	1.47
1	1	745	1MG	C5-C4	-2.75	1.36	1.43
54	z	57	5MU	O2-C2	-2.75	1.18	1.23
54	z	39	5MU	C4-N3	-2.72	1.33	1.38
54	z	39	5MU	C6-C5	2.70	1.39	1.34
2	2	1516	2MG	C5-C6	2.70	1.52	1.47
54	z	42	5MU	O2-C2	-2.68	1.18	1.23
54	z	76	5MU	C4-N3	-2.68	1.33	1.38
54	z	69	5MU	O2-C2	-2.66	1.18	1.23
54	z	63	5MU	C4-N3	-2.63	1.34	1.38
1	1	1915	3TD	O4-C4	-2.60	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1207	2MG	C6-N1	2.60	1.41	1.37
54	z	55	5MU	O2-C2	-2.59	1.18	1.23
54	z	64	5MU	C6-C5	2.57	1.38	1.34
1	1	2445	2MG	O6-C6	-2.55	1.18	1.23
54	z	76	5MU	C6-C5	2.55	1.38	1.34
54	z	63	5MU	C6-C5	2.55	1.38	1.34
2	2	1498	UR3	O2-C2	-2.55	1.17	1.22
1	1	2580	PSU	C4-C5	-2.53	1.36	1.44
1	1	1835	2MG	O6-C6	-2.52	1.18	1.23
1	1	2069	G7M	O6-C6	-2.52	1.18	1.23
2	2	527	G7M	O6-C6	-2.51	1.18	1.23
54	z	63	5MU	C4-C5	2.51	1.48	1.44
2	2	966	2MG	O6-C6	-2.51	1.18	1.23
1	1	2069	G7M	CN7-N7	-2.50	1.41	1.47
1	1	1915	3TD	O2-C2	-2.48	1.18	1.23
54	z	76	5MU	C4-C5	2.48	1.48	1.44
54	z	64	5MU	C6-N1	-2.48	1.33	1.38
54	z	39	5MU	C2-N1	2.48	1.42	1.38
54	z	71	5MU	C4-N3	-2.47	1.34	1.38
1	1	2069	G7M	C5-C4	-2.46	1.34	1.39
2	2	527	G7M	C6-N1	2.46	1.41	1.37
54	z	40	5MU	C6-C5	2.45	1.38	1.34
1	1	1835	2MG	C5-C6	2.44	1.52	1.47
54	z	40	5MU	C4-N3	-2.43	1.34	1.38
2	2	516	PSU	C4-C5	-2.41	1.37	1.44
1	1	1618	6MZ	C6-N1	-2.40	1.30	1.34
54	z	40	5MU	C6-N1	-2.39	1.34	1.38
54	z	76	5MU	C6-N1	-2.39	1.34	1.38
54	z	40	5MU	C4-C5	2.38	1.48	1.44
1	1	2503	2MA	C5-C4	-2.37	1.34	1.40
1	1	2457	PSU	C4-C5	-2.37	1.37	1.44
2	2	966	2MG	C6-N1	2.36	1.41	1.37
2	2	1207	2MG	O6-C6	-2.34	1.18	1.23
54	z	20	5MU	O2-C2	-2.34	1.18	1.23
2	2	527	G7M	C5-C6	2.33	1.51	1.45
54	z	71	5MU	C6-C5	2.32	1.38	1.34
1	1	955	PSU	C4-C5	-2.32	1.37	1.44
2	2	1516	2MG	O6-C6	-2.30	1.18	1.23
54	z	64	5MU	C4-C5	2.30	1.48	1.44
2	2	1498	UR3	C6-N1	2.30	1.43	1.38
54	z	39	5MU	C4-C5	2.29	1.48	1.44
54	z	71	5MU	C2-N1	2.29	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2251	OMG	C2-N2	2.28	1.39	1.34
1	1	2069	G7M	C5-C6	2.28	1.51	1.45
1	1	2445	2MG	C2'-C1'	-2.27	1.50	1.53
54	z	40	5MU	C2-N1	2.27	1.42	1.38
2	2	966	2MG	C5-C6	2.25	1.52	1.47
54	z	39	5MU	C6-N1	-2.25	1.34	1.38
1	1	2251	OMG	C6-N1	2.25	1.41	1.37
54	z	63	5MU	C6-N1	-2.24	1.34	1.38
1	1	1917	PSU	C4-C5	-2.24	1.37	1.44
1	1	2030	6MZ	C5-N7	-2.23	1.31	1.39
1	1	2503	2MA	C6-C5	2.22	1.51	1.43
43	p	89	0TD	CSB-SB	-2.20	1.75	1.79
2	2	1402	4OC	C6-N1	2.20	1.43	1.38
54	z	64	5MU	C2-N1	2.20	1.42	1.38
1	1	2030	6MZ	C6-N1	-2.19	1.30	1.34
54	z	71	5MU	C6-N1	-2.19	1.34	1.38
1	1	2605	PSU	C4-C5	-2.14	1.38	1.44
54	z	76	5MU	C2-N3	-2.12	1.34	1.38
54	z	63	5MU	C2-N1	2.12	1.41	1.38
54	z	63	5MU	C2-N3	-2.12	1.34	1.38
2	2	527	G7M	C2-N1	2.11	1.42	1.37
1	1	746	PSU	C4-C5	-2.10	1.38	1.44
54	z	64	5MU	C2-N3	-2.10	1.34	1.38
2	2	527	G7M	C5-C4	-2.10	1.34	1.39
1	1	1618	6MZ	C4-N3	-2.09	1.32	1.35
54	z	76	5MU	C2-N1	2.09	1.41	1.38
1	1	746	PSU	C6-C5	2.08	1.37	1.35
1	1	2251	OMG	C5-C6	2.08	1.51	1.47
1	1	2504	PSU	C4-C5	-2.08	1.38	1.44
2	2	527	G7M	CN7-N7	-2.08	1.42	1.47
1	1	1618	6MZ	C5-N7	-2.07	1.32	1.39
1	1	1835	2MG	C6-N1	2.06	1.40	1.37
54	z	71	5MU	C4-C5	2.06	1.48	1.44
1	1	2457	PSU	C6-N1	-2.05	1.32	1.36
1	1	2445	2MG	CM2-N2	-2.05	1.41	1.45
1	1	1915	3TD	O4'-C1'	-2.02	1.41	1.43

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	69	5MU	C6-C5-C4	-115.15	21.76	118.03
54	z	69	5MU	C5-C4-N3	-87.09	40.98	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	69	5MU	C6-N1-C2	-29.10	91.84	121.30
54	z	69	5MU	O4-C4-C5	-25.79	95.01	124.90
54	z	69	5MU	N3-C2-N1	-18.31	90.58	114.89
2	2	1519	MA6	N1-C6-N6	-14.61	101.68	117.06
2	2	1518	MA6	N1-C6-N6	-13.91	102.42	117.06
54	z	20	5MU	C5-C4-N3	12.87	126.29	115.31
1	1	747	5MU	C5-C4-N3	12.70	126.15	115.31
54	z	8	5MU	C5-C4-N3	12.60	126.06	115.31
54	z	42	5MU	C5-C4-N3	12.09	125.63	115.31
54	z	55	5MU	C5-C4-N3	11.91	125.48	115.31
1	1	1618	6MZ	C1'-N9-C4	-11.73	106.04	126.64
54	z	57	5MU	C5-C4-N3	11.68	125.28	115.31
1	1	2030	6MZ	C1'-N9-C4	-11.47	106.49	126.64
1	1	1939	5MU	C5-C4-N3	11.44	125.08	115.31
54	z	69	5MU	C1'-N1-C2	10.72	136.98	117.57
54	z	57	5MU	C5-C6-N1	-10.51	112.52	123.34
54	z	42	5MU	C5-C6-N1	-10.27	112.77	123.34
1	1	747	5MU	C5-C6-N1	-9.96	113.09	123.34
1	1	1939	5MU	C5-C6-N1	-9.82	113.24	123.34
54	z	8	5MU	C5-C6-N1	-9.67	113.39	123.34
54	z	69	5MU	O2-C2-N1	9.36	135.23	122.79
54	z	55	5MU	C5-C6-N1	-8.98	114.10	123.34
54	z	20	5MU	C5-C6-N1	-8.81	114.28	123.34
54	z	69	5MU	O4-C4-N3	8.28	135.99	120.12
54	z	69	5MU	C5M-C5-C6	7.90	133.40	122.85
54	z	69	5MU	O2-C2-N3	6.80	134.17	121.50
54	z	20	5MU	C5M-C5-C4	6.62	126.06	118.77
54	z	69	5MU	C5M-C5-C4	-6.47	111.65	118.77
1	1	747	5MU	O4-C4-C5	-6.13	117.79	124.90
54	z	69	5MU	C1'-N1-C6	6.03	131.16	121.12
54	z	8	5MU	C4-N3-C2	-6.02	119.56	127.35
54	z	42	5MU	O4-C4-C5	-6.02	117.93	124.90
1	1	2457	PSU	C4-N3-C2	-5.93	117.80	126.34
2	2	1519	MA6	N3-C2-N1	-5.70	119.77	128.68
54	z	57	5MU	O4-C4-C5	-5.69	118.31	124.90
1	1	2457	PSU	N1-C2-N3	5.65	121.53	115.13
1	1	747	5MU	C4-N3-C2	-5.58	120.13	127.35
54	z	57	5MU	C4-N3-C2	-5.56	120.15	127.35
1	1	1939	5MU	C5M-C5-C6	-5.50	115.50	122.85
54	z	42	5MU	C4-N3-C2	-5.47	120.28	127.35
54	z	8	5MU	O4-C4-C5	-5.44	118.60	124.90
54	z	64	5MU	C4-N3-C2	-5.39	120.37	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2580	PSU	C4-N3-C2	-5.39	118.58	126.34
1	1	1917	PSU	C4-N3-C2	-5.39	118.58	126.34
54	z	69	5MU	C5-C6-N1	-5.36	117.83	123.34
2	2	516	PSU	C4-N3-C2	-5.35	118.63	126.34
1	1	2580	PSU	N1-C2-N3	5.31	121.14	115.13
1	1	2605	PSU	C4-N3-C2	-5.25	118.77	126.34
54	z	63	5MU	C4-N3-C2	-5.25	120.56	127.35
1	1	1939	5MU	C4-N3-C2	-5.23	120.58	127.35
54	z	76	5MU	C4-N3-C2	-5.22	120.60	127.35
54	z	8	5MU	N3-C2-N1	5.19	121.78	114.89
1	1	1911	PSU	C4-N3-C2	-5.13	118.94	126.34
54	z	71	5MU	C4-N3-C2	-5.11	120.73	127.35
1	1	1917	PSU	N1-C2-N3	5.11	120.92	115.13
54	z	8	5MU	C5M-C5-C4	5.11	124.39	118.77
54	z	39	5MU	N3-C2-N1	5.09	121.64	114.89
1	1	1939	5MU	C5M-C5-C4	5.06	124.33	118.77
1	1	746	PSU	C4-N3-C2	-5.04	119.08	126.34
1	1	1939	5MU	O4-C4-C5	-5.04	119.06	124.90
54	z	8	5MU	C5M-C5-C6	-5.00	116.17	122.85
54	z	20	5MU	C5M-C5-C6	-4.99	116.18	122.85
1	1	2504	PSU	C4-N3-C2	-4.99	119.15	126.34
1	1	955	PSU	C4-N3-C2	-4.98	119.16	126.34
54	z	64	5MU	N3-C2-N1	4.97	121.49	114.89
1	1	955	PSU	N1-C2-N3	4.92	120.71	115.13
54	z	39	5MU	C4-N3-C2	-4.91	120.99	127.35
54	z	40	5MU	C4-N3-C2	-4.90	121.01	127.35
2	2	1518	MA6	N3-C2-N1	-4.89	121.03	128.68
1	1	2503	2MA	C1'-N9-C4	4.87	135.19	126.64
1	1	2552	OMU	C4-N3-C2	-4.83	120.21	126.58
54	z	76	5MU	N3-C2-N1	4.81	121.27	114.89
54	z	20	5MU	O4-C4-C5	-4.79	119.35	124.90
54	z	57	5MU	N3-C2-N1	4.78	121.23	114.89
54	z	42	5MU	C5M-C5-C6	-4.77	116.48	122.85
54	z	63	5MU	N3-C2-N1	4.75	121.20	114.89
54	z	71	5MU	N3-C2-N1	4.71	121.14	114.89
54	z	71	5MU	C5-C4-N3	4.69	119.32	115.31
1	1	2605	PSU	N1-C2-N3	4.69	120.44	115.13
54	z	63	5MU	C5-C4-N3	4.65	119.28	115.31
1	1	747	5MU	N3-C2-N1	4.63	121.03	114.89
1	1	1911	PSU	N1-C2-N3	4.60	120.35	115.13
54	z	55	5MU	C5M-C5-C4	4.59	123.82	118.77
54	z	40	5MU	N3-C2-N1	4.59	120.98	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	20	5MU	C4-N3-C2	-4.58	121.42	127.35
1	1	2504	PSU	N1-C2-N3	4.56	120.30	115.13
1	1	1939	5MU	N3-C2-N1	4.56	120.94	114.89
1	1	2030	6MZ	N3-C2-N1	-4.55	121.56	128.68
54	z	71	5MU	O4-C4-C5	-4.50	119.69	124.90
54	z	76	5MU	C5-C4-N3	4.50	119.15	115.31
54	z	64	5MU	C5-C4-N3	4.46	119.12	115.31
54	z	55	5MU	C4-N3-C2	-4.45	121.59	127.35
1	1	1618	6MZ	N3-C2-N1	-4.45	121.72	128.68
54	z	55	5MU	O4-C4-C5	-4.42	119.78	124.90
1	1	1915	3TD	N1-C2-N3	4.38	119.59	116.14
1	1	746	PSU	N1-C2-N3	4.37	120.08	115.13
2	2	516	PSU	N1-C2-N3	4.34	120.05	115.13
54	z	64	5MU	C5-C6-N1	-4.22	118.99	123.34
54	z	55	5MU	N3-C2-N1	4.21	120.47	114.89
1	1	745	1MG	CM1-N1-C2	-4.16	116.40	120.72
1	1	2580	PSU	O2-C2-N1	-4.15	118.22	122.79
54	z	42	5MU	N3-C2-N1	4.14	120.39	114.89
54	z	8	5MU	O2-C2-N1	-4.07	117.38	122.79
54	z	40	5MU	C5-C4-N3	4.06	118.78	115.31
54	z	63	5MU	C5-C6-N1	-4.01	119.21	123.34
54	z	55	5MU	C5M-C5-C6	-4.00	117.51	122.85
54	z	39	5MU	C5-C4-N3	3.99	118.71	115.31
54	z	76	5MU	C5-C6-N1	-3.93	119.29	123.34
54	z	64	5MU	O4-C4-C5	-3.85	120.44	124.90
54	z	57	5MU	C6-C5-C4	3.82	121.22	118.03
54	z	63	5MU	O4-C4-C5	-3.81	120.48	124.90
54	z	69	5MU	C4-N3-C2	-3.77	122.47	127.35
54	z	63	5MU	C2'-C1'-N1	-3.77	102.54	113.22
54	z	40	5MU	O4-C4-C5	-3.73	120.58	124.90
54	z	42	5MU	C5M-C5-C4	3.71	122.85	118.77
1	1	1835	2MG	CM2-N2-C2	-3.68	115.72	123.86
43	p	89	0TD	OD2-CG-CB	3.66	121.06	113.15
54	z	39	5MU	O4-C4-C5	-3.57	120.76	124.90
54	z	76	5MU	O4-C4-C5	-3.55	120.78	124.90
1	1	2552	OMU	N3-C2-N1	3.55	119.60	114.89
1	1	2030	6MZ	C9-N6-C6	-3.53	119.83	122.87
1	1	1917	PSU	C6-C5-C4	3.50	120.65	118.20
1	1	2580	PSU	C6-C5-C4	3.48	120.63	118.20
1	1	2457	PSU	O2-C2-N1	-3.47	118.97	122.79
54	z	20	5MU	N3-C2-N1	3.44	119.45	114.89
1	1	747	5MU	C5M-C5-C6	-3.42	118.28	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2251	OMG	C2-N1-C6	-3.39	118.85	125.10
1	1	1915	3TD	C4-N3-C2	-3.39	120.93	124.61
1	1	2503	2MA	C2-N3-C4	3.38	118.27	115.52
1	1	1917	PSU	O2-C2-N1	-3.32	119.13	122.79
1	1	747	5MU	O2-C2-N1	-3.32	118.38	122.79
2	2	966	2MG	C5-C6-N1	3.31	119.79	113.95
54	z	40	5MU	C5-C6-N1	-3.28	119.97	123.34
54	z	57	5MU	C5M-C5-C6	-3.25	118.50	122.85
2	2	1516	2MG	CM2-N2-C2	-3.21	116.76	123.86
2	2	1207	2MG	C5-C6-N1	3.20	119.61	113.95
1	1	745	1MG	CM1-N1-C6	3.16	121.88	117.55
54	z	42	5MU	C6-C5-C4	3.16	120.67	118.03
54	z	39	5MU	C5-C6-N1	-3.11	120.14	123.34
1	1	955	PSU	O2-C2-N1	-3.11	119.37	122.79
54	z	39	5MU	C1'-N1-C2	3.09	123.17	117.57
2	2	1407	5MC	C5-C6-N1	-3.09	120.16	123.34
1	1	1835	2MG	C5-C6-N1	3.08	119.38	113.95
2	2	1498	UR3	C4-N3-C2	-3.07	121.67	124.56
54	z	64	5MU	C2'-C1'-N1	-3.04	104.62	113.22
1	1	1911	PSU	O2-C2-N1	-3.04	119.45	122.79
1	1	745	1MG	C5-C6-N1	3.03	118.45	113.90
54	z	20	5MU	O4-C4-N3	-3.01	114.35	120.12
54	z	40	5MU	C1'-N1-C2	2.98	122.96	117.57
2	2	1402	4OC	CM4-N4-C4	-2.96	116.66	122.45
1	1	2552	OMU	O4-C4-C5	-2.96	119.95	125.16
54	z	63	5MU	O3'-C3'-C2'	2.96	121.39	111.82
1	1	747	5MU	C5M-C5-C4	2.94	122.01	118.77
2	2	1516	2MG	C5-C6-N1	2.94	119.14	113.95
1	1	2503	2MA	N3-C2-N1	-2.91	120.41	125.73
54	z	40	5MU	O4'-C1'-N1	2.88	114.96	108.36
54	z	40	5MU	C1'-N1-C6	-2.87	116.34	121.12
54	z	71	5MU	C5-C6-N1	-2.87	120.39	123.34
54	z	63	5MU	O3'-C3'-C4'	2.86	119.31	111.05
2	2	527	G7M	C2-N1-C6	-2.83	119.89	125.10
54	z	55	5MU	O4-C4-N3	-2.80	114.74	120.12
1	1	2504	PSU	O2-C2-N1	-2.80	119.71	122.79
1	1	1939	5MU	O2-C2-N1	-2.78	119.09	122.79
1	1	2251	OMG	C5-C6-N1	2.76	118.83	113.95
1	1	2552	OMU	C5-C4-N3	2.76	118.97	114.84
1	1	2445	2MG	C5-C6-N1	2.76	118.82	113.95
54	z	55	5MU	O2-C2-N1	-2.74	119.14	122.79
1	1	2552	OMU	CM2-O2'-C2'	-2.72	107.39	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	z	40	5MU	C5M-C5-C4	2.70	121.74	118.77
1	1	746	PSU	O2-C2-N1	-2.69	119.83	122.79
2	2	1207	2MG	CM2-N2-C2	-2.64	118.02	123.86
54	z	42	5MU	C1'-N1-C2	2.64	122.34	117.57
54	z	63	5MU	O2-C2-N1	-2.62	119.31	122.79
1	1	2069	G7M	C2-N1-C6	-2.61	120.30	125.10
2	2	1498	UR3	C3U-N3-C4	2.61	121.61	117.89
54	z	40	5MU	C2'-C1'-N1	-2.60	105.86	113.22
1	1	1962	5MC	CM5-C5-C6	-2.59	119.39	122.85
1	1	1618	6MZ	C9-N6-C6	-2.58	120.65	122.87
1	1	1939	5MU	C6-C5-C4	2.55	120.16	118.03
54	z	71	5MU	C5'-C4'-C3'	-2.53	105.72	115.18
1	1	955	PSU	C6-N1-C2	-2.52	120.11	122.68
2	2	516	PSU	O2-C2-N1	-2.52	120.02	122.79
1	1	2457	PSU	C6-N1-C2	-2.51	120.12	122.68
54	z	8	5MU	O4-C4-N3	-2.49	115.34	120.12
54	z	39	5MU	O4'-C1'-N1	2.49	114.06	108.36
54	z	63	5MU	O4'-C4'-C3'	-2.48	100.21	105.11
54	z	39	5MU	C1'-N1-C6	-2.47	117.02	121.12
1	1	1962	5MC	C5-C4-N4	-2.47	117.79	121.48
2	2	1207	2MG	C8-N7-C5	2.44	107.64	102.99
54	z	20	5MU	O2-C2-N1	-2.43	119.56	122.79
43	p	89	0TD	OD1-CG-CB	-2.42	117.37	122.44
1	1	1962	5MC	C1'-N1-C6	-2.39	117.14	121.12
54	z	57	5MU	C1'-N1-C2	2.39	121.90	117.57
1	1	2251	OMG	C8-N7-C5	2.39	107.54	102.99
1	1	1962	5MC	C5-C6-N1	-2.39	120.88	123.34
54	z	40	5MU	C5M-C5-C6	-2.38	119.68	122.85
1	1	2504	PSU	C6-C5-C4	2.36	119.85	118.20
1	1	955	PSU	C6-C5-C4	2.36	119.85	118.20
1	1	2580	PSU	O4'-C1'-C2'	2.33	108.43	105.14
2	2	966	2MG	C8-N7-C5	2.32	107.41	102.99
1	1	2069	G7M	N2-C2-N1	2.31	121.64	116.71
54	z	76	5MU	O2-C2-N1	-2.31	119.72	122.79
54	z	76	5MU	C2'-C1'-N1	-2.28	106.75	113.22
54	z	63	5MU	C5M-C5-C4	2.28	121.28	118.77
2	2	966	2MG	O6-C6-C5	-2.28	119.92	124.37
54	z	63	5MU	C3'-C2'-C1'	-2.27	97.11	101.43
1	1	2445	2MG	CM2-N2-C2	-2.27	118.85	123.86
54	z	71	5MU	C2'-C3'-C4'	2.27	107.05	102.64
1	1	2503	2MA	CM2-C2-N1	2.27	120.69	117.15
1	1	2605	PSU	C6-C5-C4	2.26	119.78	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2580	PSU	C6-N1-C2	-2.25	120.38	122.68
54	z	42	5MU	C1'-N1-C6	-2.25	117.38	121.12
1	1	745	1MG	C8-N7-C5	2.25	107.27	102.99
2	2	1516	2MG	C8-N7-C5	2.24	107.26	102.99
54	z	76	5MU	C5M-C5-C4	2.24	121.23	118.77
1	1	1939	5MU	O4-C4-N3	-2.22	115.86	120.12
54	z	39	5MU	O2-C2-N3	-2.22	117.37	121.50
1	1	2552	OMU	O2-C2-N1	-2.20	119.86	122.79
2	2	1516	2MG	O6-C6-C5	-2.20	120.08	124.37
1	1	2605	PSU	O2-C2-N1	-2.17	120.40	122.79
54	z	71	5MU	O2-C2-N1	-2.15	119.93	122.79
1	1	2457	PSU	O4'-C1'-C2'	2.14	108.16	105.14
1	1	1915	3TD	C6-C5-C4	2.14	119.70	118.22
54	z	57	5MU	O2-C2-N1	-2.13	119.95	122.79
1	1	2445	2MG	C8-N7-C5	2.13	107.05	102.99
1	1	747	5MU	O4-C4-N3	-2.12	116.05	120.12
1	1	1917	PSU	C6-N1-C2	-2.10	120.53	122.68
1	1	2251	OMG	CM2-O2'-C2'	-2.10	109.01	114.52
1	1	1835	2MG	C8-N7-C5	2.06	106.92	102.99
1	1	2445	2MG	O6-C6-C5	-2.06	120.35	124.37
2	2	967	5MC	CM5-C5-C6	-2.05	120.11	122.85
54	z	71	5MU	C5M-C5-C4	2.04	121.01	118.77
2	2	967	5MC	C5-C6-N1	-2.04	121.24	123.34
54	z	42	5MU	O2-C2-N1	-2.01	120.11	122.79
54	z	64	5MU	O4'-C1'-N1	2.01	112.95	108.36
1	1	1962	5MC	C1'-N1-C2	2.01	122.90	118.42
54	z	76	5MU	C5M-C5-C6	-2.00	120.17	122.85
54	z	63	5MU	C5M-C5-C6	-2.00	120.17	122.85

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	527	G7M	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C9
2	2	1518	MA6	C5-C6-N6-C10
2	2	1519	MA6	O4'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
2	2	1519	MA6	C5-C6-N6-C10
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1915	3TD	C2'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
54	z	8	5MU	O4'-C4'-C5'-O5'
54	z	39	5MU	O4'-C1'-N1-C2
54	z	39	5MU	O4'-C1'-N1-C6
54	z	40	5MU	O4'-C1'-N1-C2
54	z	40	5MU	O4'-C1'-N1-C6
54	z	64	5MU	O4'-C1'-N1-C2
54	z	64	5MU	O4'-C1'-N1-C6
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
54	z	8	5MU	C3'-C4'-C5'-O5'
54	z	57	5MU	C3'-C4'-C5'-O5'
54	z	57	5MU	O4'-C4'-C5'-O5'
54	z	63	5MU	C3'-C4'-C5'-O5'
54	z	69	5MU	C3'-C4'-C5'-O5'
54	z	69	5MU	O4'-C4'-C5'-O5'
54	z	71	5MU	C3'-C4'-C5'-O5'
54	z	71	5MU	O4'-C4'-C5'-O5'
2	2	527	G7M	O4'-C4'-C5'-O5'
2	2	1519	MA6	C3'-C4'-C5'-O5'
54	z	20	5MU	O4'-C4'-C5'-O5'
2	2	1518	MA6	N1-C6-N6-C10
2	2	1519	MA6	N1-C6-N6-C10
1	1	1835	2MG	C3'-C4'-C5'-O5'
1	1	1835	2MG	O4'-C4'-C5'-O5'
54	z	20	5MU	C3'-C4'-C5'-O5'
2	2	1402	4OC	O4'-C4'-C5'-O5'
54	z	39	5MU	O4'-C4'-C5'-O5'
54	z	63	5MU	O4'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2503	2MA	O4'-C4'-C5'-O5'
43	p	89	0TD	CG-CB-SB-CSB
2	2	527	G7M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
43	p	89	0TD	SB-CB-CG-OD1
54	z	71	5MU	C4'-C5'-O5'-P
54	z	76	5MU	O4'-C4'-C5'-O5'
54	z	39	5MU	C3'-C4'-C5'-O5'
1	1	2503	2MA	C3'-C4'-C5'-O5'
54	z	76	5MU	C3'-C4'-C5'-O5'
43	p	89	0TD	SB-CB-CG-OD2
54	z	20	5MU	C2'-C1'-N1-C2
2	2	1402	4OC	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C4'-C5'-O5'
1	1	746	PSU	O4'-C1'-C5-C6
1	1	2069	G7M	O4'-C4'-C5'-O5'
54	z	20	5MU	C4'-C5'-O5'-P

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	z	69	5MU	C2-C4-C5-C6-N1-N3

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 424 ligands modelled in this entry, 424 are monoatomic - leaving 0 for Mogul analysis.

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.