



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 06:39 pm GMT

PDB ID : 7PJT
EMDB ID : EMD-13459
Title : Structure of the 70S ribosome with tRNAs in hybrid state 1 (H1)
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.;
Fischer, N.
Deposited on : 2021-08-24
Resolution : 6.00 Å (reported)
Based on initial models : 5LZD, 6YSS, 4AQY

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

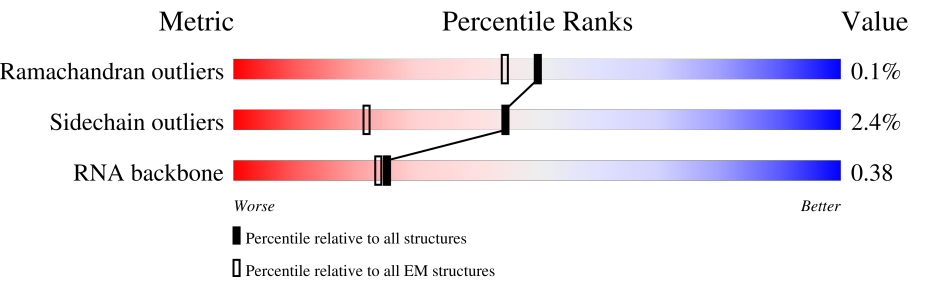
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 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.



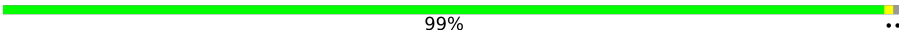
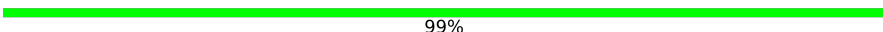
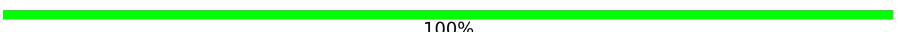
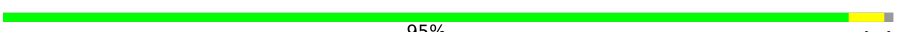
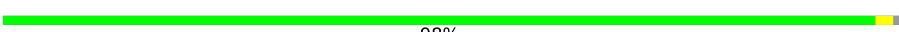
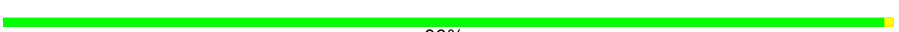






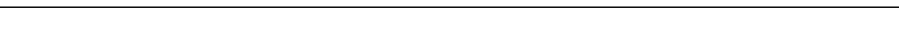

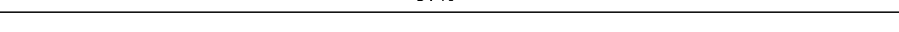
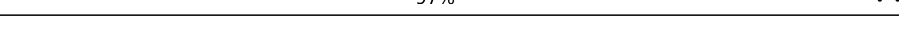
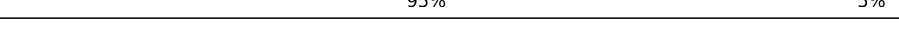
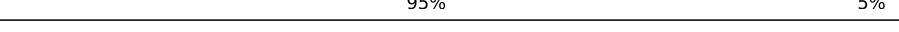

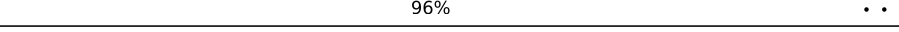
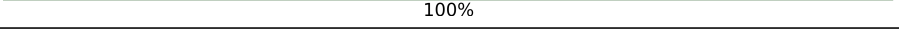

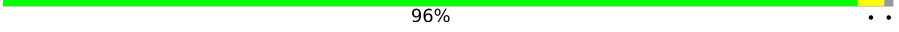

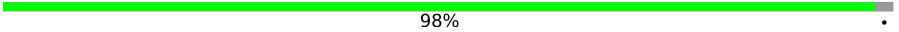
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	57	95% . .
2	1	55	91% 9%
3	2	46	98% .
4	3	65	89% 9% .
5	4	38	95% 5%
6	5	165	79% 21%
7	6	70	84% 10% 6%
8	A	2903	57% 40% .
9	B	120	60% 39% .



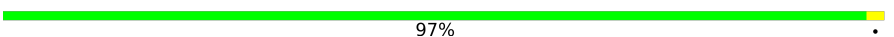
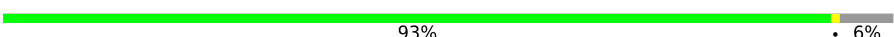


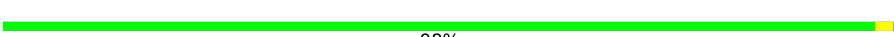



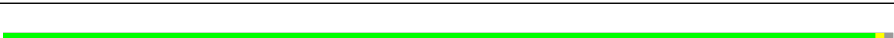

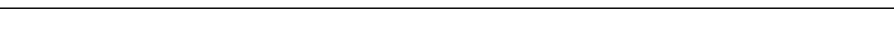
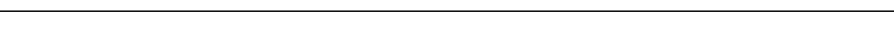
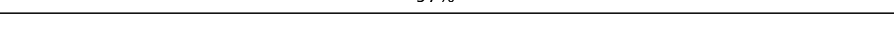
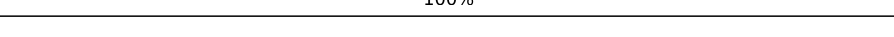
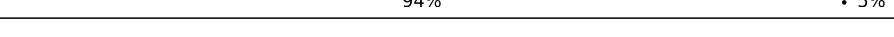
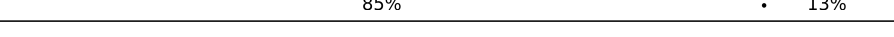

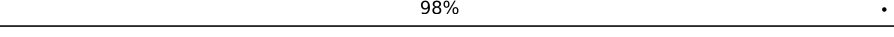
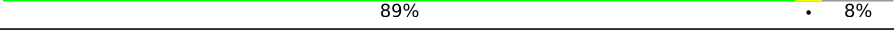


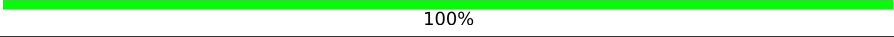
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Mol	Chain	Length	Quality of chain
10	C	273	 99% ..
11	D	209	 99%
12	E	201	 100%
13	F	179	 95% . .
14	G	177	 98% ..
15	H	149	 99% .
16	I	142	 99% .
17	J	142	 97% .
18	K	123	 99% .
19	L	144	 97% ..
20	M	136	 99% .
21	N	127	 94% 6%
22	O	117	 95% . .
23	P	115	 97% ..
24	Q	118	 97% ..
25	R	103	 95% 5%
26	S	110	 95% 5%
27	T	100	 91% . 7%
28	U	104	 96% ..
29	V	94	 100%
30	W	85	 87% . 12%
31	X	78	 96% ..
32	Y	63	 92% 8%
33	Z	59	 98% .
34	a	1542	 60% 38% .

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Mol	Chain	Length	Quality of chain
35	b	240	
36	c	233	
37	d	206	
38	e	167	
39	f	135	
40	g	179	
41	h	130	
42	i	130	
43	j	103	
44	k	129	
45	l	124	
46	m	118	
47	n	102	
48	o	89	
49	p	82	
50	q	84	
51	r	75	
52	s	92	
53	t	87	
54	u	71	
55	v	77	
56	w	76	
57	y	2	
58	z	33	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 147222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2902	Total	C	N	O	P	0	0
			62317	27806	11469	20140	2902		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 15 is a protein called 50S ribosomal protein L9.

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	102	Total	C	N	O	0	0
			779	492	146	141		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S17.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Dipeptide (FME-PHE).

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

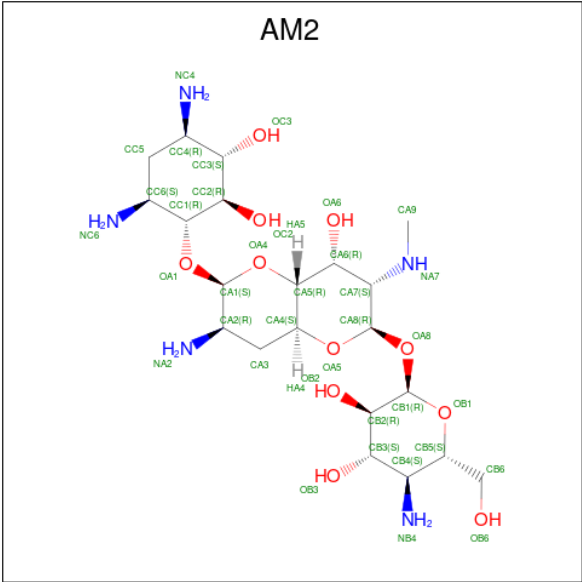
- Molecule 58 is a RNA chain called mRNA.

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

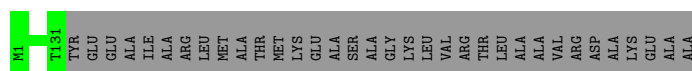
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	4	1	Total	Zn	0
			1	1	
59	6	1	Total	Zn	0
			1	1	

- Molecule 60 is APRAMYCIN (three-letter code: AM2) (formula: C₂₁H₄₁N₅O₁₁).



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



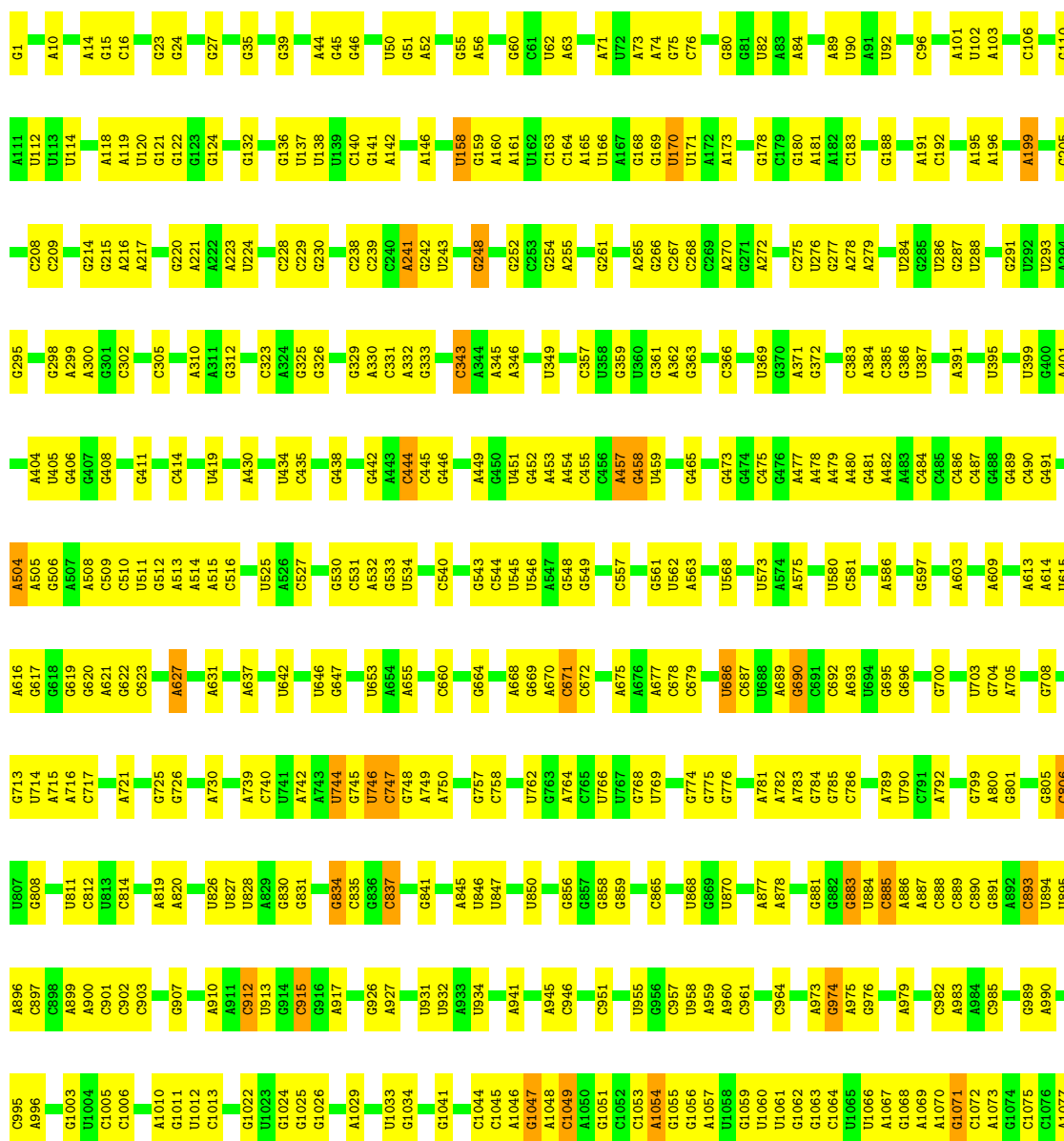
- Molecule 7: 50S ribosomal protein L31

Chain 6: 84% 10% 6%



- Molecule 8: 23S ribosomal RNA

Chain A: 57% 40% 3%



U2404	G2405	A2406	A2418	G2419	C2420	G2421	C2422	G2423	C2424	A2425	C2426	G2427	G2428	C2429	A2430	G2431	A2432	A2433	A2434	G2435	G2436	G2437	A2438	A2439	C2440	U2441	C2442	G2443	G2444	A2445	G2446	A2447	A2448	U2449	C2456	U2457	G2458	A2459	C2462	C2465	C2466	A2468	A2469	U2474	C2475	A2476	C2488	C2489	A2490	A2481	A2482	C2483	G2484	G2490		
C2300	U2305	C2306	G2307	G2308	A2309	C2310	G2318	A2319	C2320	A2321	A2322	G2323	G2324	C2325	A2326	A2327	A2333	U2334	A2335	A2336	G2337	U2343	U2344	G2345	A2346	C2347	U2348	G2349	C2350	A2358	G2361	G2367	G2373	C2374	G2379	C2380	G2382	G2383	U2384	C2385	A2388	A2392	G2396	U2402	C2403											
A2042	C2043	C2044	G2049	C2050	A2051	A2052	C2055	A2056	G2057	A2060	G2061	A2062	C2063	G2067	U2068	C2069	C2073	U2076	A2077	U2081	C2089	A2090	C2091	U2092	G2093	A2097	A2101	C2102	C2103	C2104	U2109	G2110	U2111	G2112	A2114	G2115	U2118	A2119	G2123	G2124	G2125	A2126	G2127	A2128	A2129	G2130	G2131	U2132	A2133	A2134	C2135	G2139	A2142	A2143	U2144	C2145
C2129	U2130	U2131	U2132	G2133	A2134	A2135	U2137	G2138	U2139	C2143	G2144	C2145	A2146	G2147	U2148	C2149	C2150	U2151	G2152	C2153	A2154	U2155	G2156	U2157	A2158	C2159	G2160	A2161	G2162	A2163	C2164	C2165	U2166	A2169	A2170	A2171	U2172	A2173	C2174	C2175	A2176	U2180	U2181	U2182	A2183	G2186	G2190	A2191	U2192	G2193	A2198	A2199				
C2200	U2203	G2204	C2208	G2209	A2210	U2211	A2212	U2213	C2214	C2215	C2222	U2223	A2224	C2225	A2226	G2228	G2239	U2245	C2248	U2249	G2250	G2251	G2259	U2262	U2265	U2266	A2267	A2268	G2269	U2272	A2273	A2274	G2279	G2280	A2281	G2282	C2283	A2284	C2285	A2287	A2288	A2297	U2298	C2300												
U1778	U1779	U1782	A1783	A1784	A1785	G1786	A1787	C1788	G1797	C1800	A1801	C1804	A1808	A1809	A1810	G1811	U1812	G1813	G1814	U1715	U1716	C1726	C1727	U1729	C1730	G1731	C1732	G1733	G1734	A1735	G1738	U1750	U1751	C1752	G1753	A1754	A1757	U1758	A1759	G1764	A1765	G1767	G1768	U1769	A1773	C1774	U1775	C1776	C1777	C1778						
G1869	G1873	C1874	A1875	A1876	G1884	U1885	A1886	C1889	A1890	A1891	C1892	G1905	G1906	G1907	C1908	C1909	G1910	U1911	C1914	3D	A1916	U1917	A1918	A1919	C1920	G1921	U1922	U1923	C1924	C1925	U1926	A1927	A1928	G1929	U1930	U1931	A1932	G1935	U1938	U1939	U1940	C1941	U1944	G1945	U1946	U1955	U1956	C1962								
U1963	G1964	C1965	A1966	C1967	A1968	A1969	U1970	G1972	A1977	U1979	G1980	A1981	U1982	C1985	C1990	U1991	G1992	U1993	C1997	C2001	G2002	A2003	U2007	C2008	A2009	G2012	A2013	A2014	A2015	U2016	A2019	A2020	C2021	U2022	C2023	G2027	U2028	G2029	A2030	A2031	A2032	A2033	G2034	C2035	C2036	G2040	U2041									
A2042	C2043	C2044	G2049	C2050	A2051	A2052	C2055	A2056	G2057	A2060	G2061	A2062	C2063	G2067	U2068	C2069	C2073	U2076	A2077	U2081	C2089	A2090	C2091	U2092	G2093	A2097	A2101	C2102	C2103	C2104	U2109	G2110	U2111	G2112	A2114	G2115	U2118	A2119	G2123	G2124	G2125	A2126	G2127	A2128	A2129	G2130	G2131	U2132	A2133	A2134	C2135	G2139	A2142	A2143	U2144	C2145
C2129	U2130	U2131	U2132	G2133	A2134	A2135	U2137	G2138	U2139	C2143	G2144	C2145	A2146	G2147	U2148	C2149	C2150	U2151	G2152	C2153	A2154	U2155	G2156	U2157	A2158	C2159	G2160	A2161	G2162	A2163	C2164	C2165	U2166	A2169	A2170	A2171	U2172	A2173	C2174	C2175	A2176	U2180	U2181	U2182	A2183	G2186	G2190	A2191	U2192	G2193	A2198	A2199				
C2200	U2203	G2204	C2208	G2209	A2210	U2211	A2212	U2213	C2214	C2215	C2222	U2223	A2224	C2225	A2226	G2228	G2239	U2245	C2248	U2249	G2250	G2251	G2259	U2262	U2265	U2266	A2267	A2268	G2269	U2272	A2273	A2274	G2279	G2280	A2281	G2282	C2283	A2284	C2285	A2287	A2288	A2297	U2298	C2300												
U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	U1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095	U1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	G1106	C1109	G1110	A1111	U1112	C1122	C1123	G1128	A1129	U1130	G1131	U1132	A1133	A1134	C1135	G1139	A1142	A1143	U1144	C1145	G1149									



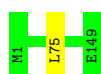
- Molecule 14: 50S ribosomal protein L6

Chain G:  98%



- Molecule 15: 50S ribosomal protein L9

Chain H:  99%



- Molecule 16: 50S ribosomal protein L11

Chain I:  99%



- Molecule 17: 50S ribosomal protein L13

Chain J:  97%



- Molecule 18: 50S ribosomal protein L14

Chain K:  99%



- Molecule 19: 50S ribosomal protein L15

Chain L:  97%



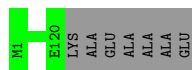
- Molecule 20: 50S ribosomal protein L16

Chain M:  99%



- Molecule 21: 50S ribosomal protein L17

Chain N: 94% 6%



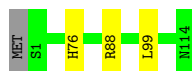
- Molecule 22: 50S ribosomal protein L18

Chain O: 95% ..



- Molecule 23: 50S ribosomal protein L19

Chain P: 97% ..



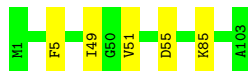
- Molecule 24: 50S ribosomal protein L20

Chain Q: 97% ..



- Molecule 25: 50S ribosomal protein L21

Chain R: 95% 5%



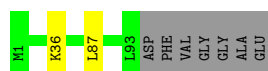
- Molecule 26: 50S ribosomal protein L22

Chain S: 95% 5%



- Molecule 27: 50S ribosomal protein L23

Chain T: 91% • 7%



- Molecule 28: 50S ribosomal protein L24

Chain U: 96%



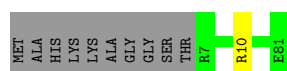
- Molecule 29: 50S ribosomal protein L25

Chain V: 100%

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L27

Chain W: 87%



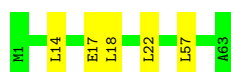
- Molecule 31: 50S ribosomal protein L28

Chain X: 96%



- Molecule 32: 50S ribosomal protein L29

Chain Y: 92%



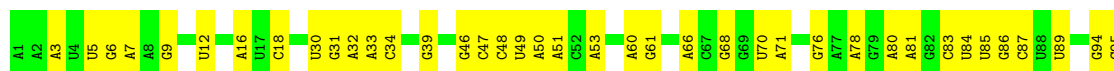
- Molecule 33: 50S ribosomal protein L30

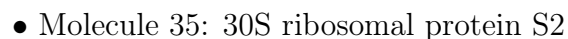
Chain Z: 98%




- Molecule 34: 16S ribosomal RNA

Chain a: 60%



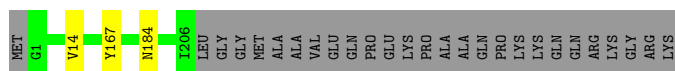


Chain b:  90% 9%



- Molecule 36: 30S ribosomal protein S3

Chain c:  87% 12%



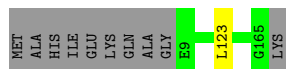
- Molecule 37: 30S ribosomal protein S4

Chain d:  97%



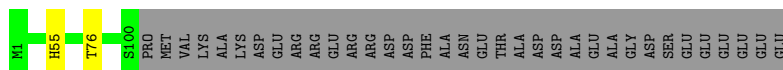
- Molecule 38: 30S ribosomal protein S5

Chain e:  93% 6%




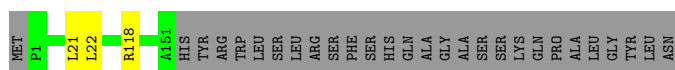
- Molecule 39: 30S ribosomal protein S6

Chain f:  73% 26%



- Molecule 40: 30S ribosomal protein S7

Chain g:  83% 16%



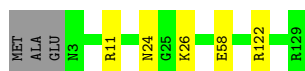
- Molecule 41: 30S ribosomal protein S8

Chain h:  98%



- Molecule 42: 30S ribosomal protein S9

Chain i:  94% ..




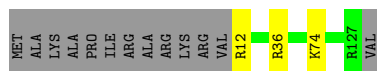
- Molecule 43: 30S ribosomal protein S10

Chain j:  94% • 5%



- Molecule 44: 30S ribosomal protein S11

Chain k:  88% • 10%



- Molecule 45: 30S ribosomal protein S12

Chain l:  98% ..



- Molecule 46: 30S ribosomal protein S13

Chain m:  95% • •



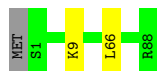
- Molecule 47: 30S ribosomal protein S14

Chain n:  95% • •



- Molecule 48: 30S ribosomal protein S15

Chain o:  97% • •



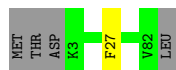
- Molecule 49: 30S ribosomal protein S16

Chain p:  100%


There are no outlier residues recorded for this chain.

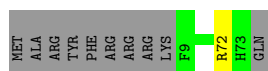
- Molecule 50: 30S ribosomal protein S17

Chain q:  94% 5%




- Molecule 51: 30S ribosomal protein S18

Chain r:  85% 13%



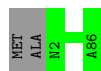
- Molecule 52: 30S ribosomal protein S19

Chain s:  83% 7% 11%




- Molecule 53: 30S ribosomal protein S20

Chain t:  98%



- Molecule 54: 30S ribosomal protein S21

Chain u:  89% 8%



- Molecule 55: P-site tRNA(fMet)

Chain v:  55% 38% 8%



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

Chain w:  50% 45% 5%



- Molecule 57: Dipeptide (FME-PHE)



There are no outlier residues recorded for this chain.

- Molecule 58: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 1MG, UR3, 4SU, MIA, AM2, 6MZ, OMG, FME, OMC, 5MC, OMU, 2MG, 4OC, PSU, MA6, ZN, 2MA, 5MU, G7M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.53	0/450	0.60	0/599
2	1	0.39	0/416	0.52	0/554
3	2	0.46	0/380	0.66	0/498
4	3	0.50	0/513	0.69	0/676
5	4	0.43	0/303	0.60	0/397
6	5	0.26	0/646	0.51	0/898
7	6	0.49	0/531	0.73	0/709
8	A	1.04	22/69266 (0.0%)	1.20	242/108055 (0.2%)
9	B	0.87	2/2873 (0.1%)	1.10	1/4478 (0.0%)
10	C	0.48	0/2121	0.62	0/2852
11	D	0.47	0/1586	0.62	0/2134
12	E	0.46	0/1571	0.60	0/2113
13	F	0.43	0/1434	0.59	0/1926
14	G	0.40	0/1343	0.57	0/1816
15	H	0.38	0/1122	0.61	0/1515
16	I	0.26	0/692	0.50	0/960
17	J	0.50	0/1152	0.55	0/1551
18	K	0.43	0/947	0.61	0/1268
19	L	0.48	0/1054	0.69	1/1403 (0.1%)
20	M	0.46	0/1093	0.57	0/1460
21	N	0.42	0/973	0.62	0/1301
22	O	0.43	0/902	0.61	0/1209
23	P	0.47	0/929	0.63	2/1242 (0.2%)
24	Q	0.50	0/960	0.60	1/1278 (0.1%)
25	R	0.47	0/829	0.64	0/1107
26	S	0.44	0/864	0.61	0/1156
27	T	0.42	0/744	0.62	0/994
28	U	0.46	0/787	0.61	0/1051
29	V	0.46	0/766	0.57	0/1025
30	W	0.45	0/582	0.63	0/769
31	X	0.44	0/635	0.66	1/848 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.41	0/510	0.64	0/677
33	Z	0.40	0/453	0.55	0/605
34	a	0.91	3/36725 (0.0%)	1.17	121/57285 (0.2%)
35	b	0.37	0/1735	0.57	0/2338
36	c	0.43	0/1651	0.56	1/2225 (0.0%)
37	d	0.39	0/1665	0.59	0/2227
38	e	0.42	0/1154	0.58	0/1554
39	f	0.38	0/835	0.56	0/1128
40	g	0.37	0/1195	0.54	0/1602
41	h	0.41	0/989	0.59	0/1326
42	i	0.42	0/1034	0.60	0/1375
43	j	0.37	0/796	0.62	0/1077
44	k	0.43	0/885	0.61	0/1195
45	l	0.44	0/969	0.60	0/1300
46	m	0.37	0/892	0.60	0/1193
47	n	0.45	0/811	0.69	0/1081
48	o	0.40	0/722	0.63	1/964 (0.1%)
49	p	0.40	0/659	0.58	0/884
50	q	0.41	0/657	0.59	0/881
51	r	0.42	0/544	0.60	0/731
52	s	0.46	0/675	0.69	0/908
53	t	0.38	0/671	0.51	0/888
54	u	0.40	0/512	0.56	0/683
55	v	0.83	1/1745 (0.1%)	1.17	7/2716 (0.3%)
56	w	0.69	0/1650	1.17	5/2569 (0.2%)
57	y	0.63	0/11	0.43	0/13
58	z	0.53	0/255	0.95	0/394
All	All	0.86	28/158864 (0.0%)	1.07	383/237661 (0.2%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	1	C	OP3-P	-10.75	1.48	1.61
9	B	1	U	OP3-P	-10.74	1.48	1.61
8	A	1	G	OP3-P	-10.73	1.48	1.61
8	A	1786	A	N9-C4	-7.76	1.33	1.37
8	A	195	A	N9-C4	-6.71	1.33	1.37
8	A	1378	A	N9-C4	-6.71	1.33	1.37
34	a	1196	A	O3'-P	6.17	1.68	1.61
8	A	2726	A	N9-C4	-6.07	1.34	1.37
34	a	1483	A	N9-C4	-5.81	1.34	1.37
8	A	1156	A	N9-C4	-5.73	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	679	C	N1-C6	-5.61	1.33	1.37
8	A	241	A	N9-C4	-5.58	1.34	1.37
8	A	1286	A	N9-C4	-5.49	1.34	1.37
8	A	1626	A	N9-C4	-5.40	1.34	1.37
34	a	288	A	N9-C4	-5.35	1.34	1.37
9	B	39	A	N9-C4	-5.33	1.34	1.37
8	A	270	A	N9-C4	-5.31	1.34	1.37
8	A	2616	C	N1-C6	-5.30	1.33	1.37
8	A	457	A	N9-C4	-5.25	1.34	1.37
8	A	627	A	N9-C4	-5.15	1.34	1.37
8	A	1029	A	N9-C4	-5.13	1.34	1.37
8	A	1378	A	C5-C6	-5.09	1.36	1.41
8	A	2014	A	N9-C4	-5.09	1.34	1.37
8	A	2456	C	N1-C6	-5.09	1.34	1.37
8	A	2432	A	N9-C4	-5.07	1.34	1.37
8	A	1662	U	C2-N3	-5.03	1.34	1.37
8	A	199	A	N9-C4	-5.03	1.34	1.37
8	A	454	A	N9-C4	-5.01	1.34	1.37

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1054	C	O5'-P-OP1	14.14	127.67	110.70
34	a	1196	A	C2'-C3'-O3'	9.93	131.35	109.50
34	a	1053	G	O3'-P-O5'	-9.74	85.50	104.00
34	a	1421	G	N9-C4-C5	9.61	109.24	105.40
34	a	1421	G	C8-N9-C1'	9.46	139.30	127.00
8	A	2731	G	C4-C5-N7	9.19	114.47	110.80
31	X	28	PHE	C-N-CA	-8.89	99.47	121.70
34	a	1421	G	N3-C4-N9	-8.74	120.76	126.00
34	a	1420	U	C2-N1-C1'	8.59	128.01	117.70
34	a	1466	C	N3-C2-O2	-8.57	115.90	121.90
34	a	811	C	C2-N1-C1'	8.53	128.18	118.80
55	v	17	C	N1-C1'-C2'	-8.52	102.63	112.00
8	A	951	C	C6-N1-C2	8.36	123.64	120.30
8	A	1902	C	N1-C2-O2	8.36	123.92	118.90
8	A	2129	C	C2-N1-C1'	8.25	127.88	118.80
8	A	1730	C	N1-C2-O2	8.24	123.84	118.90
8	A	1985	C	C6-N1-C2	8.20	123.58	120.30
8	A	1730	C	C2-N1-C1'	8.15	127.77	118.80
8	A	2731	G	C6-C5-N7	-8.06	125.57	130.40
55	v	42	G	O4'-C1'-N9	8.05	114.64	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2129	C	N1-C2-O2	7.87	123.62	118.90
8	A	799	G	N1-C2-N3	7.85	128.61	123.90
8	A	1533	C	N3-C2-O2	-7.78	116.46	121.90
8	A	1643	G	N1-C6-O6	-7.64	115.32	119.90
34	a	431	A	N1-C6-N6	-7.63	114.02	118.60
8	A	2683	C	N1-C2-O2	7.56	123.44	118.90
34	a	1421	G	C4-N9-C1'	-7.54	116.69	126.50
8	A	1418	G	N7-C8-N9	7.50	116.85	113.10
34	a	176	C	N3-C2-O2	-7.50	116.65	121.90
34	a	1053	G	OP1-P-O3'	-7.39	88.94	105.20
8	A	2506	U	C2-N1-C1'	7.39	126.57	117.70
8	A	1703	G	C8-N9-C4	7.38	109.35	106.40
34	a	1421	G	C6-C5-N7	7.35	134.81	130.40
8	A	686	U	O4'-C1'-N1	-7.33	102.33	108.20
8	A	2245	U	C5-C6-N1	-7.33	119.04	122.70
8	A	2731	G	N9-C4-C5	-7.26	102.50	105.40
34	a	176	C	N3-C4-N4	-7.23	112.94	118.00
8	A	1985	C	C5-C6-N1	-7.15	117.42	121.00
8	A	2159	G	N3-C4-N9	-7.11	121.73	126.00
8	A	2501	C	C2-N1-C1'	-7.08	111.01	118.80
34	a	106	C	N3-C2-O2	-7.06	116.96	121.90
34	a	1421	G	O4'-C1'-N9	7.05	113.84	108.20
8	A	964	C	C6-N1-C2	7.03	123.11	120.30
8	A	2052	A	N9-C4-C5	-7.02	102.99	105.80
8	A	183	C	N3-C2-O2	-7.01	116.99	121.90
8	A	2506	U	N1-C2-O2	7.01	127.70	122.80
8	A	799	G	C6-N1-C2	-6.99	120.91	125.10
8	A	214	G	N1-C2-N2	-6.92	109.97	116.20
34	a	1210	C	N3-C2-O2	-6.84	117.11	121.90
34	a	176	C	C2-N1-C1'	-6.81	111.31	118.80
8	A	2103	C	C2-N1-C1'	6.80	126.28	118.80
8	A	2731	G	C8-N9-C1'	-6.80	118.16	127.00
8	A	2731	G	N3-C4-N9	6.79	130.07	126.00
8	A	2731	G	C4-N9-C1'	6.78	135.31	126.50
34	a	866	C	N3-C2-O2	-6.78	117.15	121.90
8	A	1774	C	C2-N1-C1'	6.77	126.25	118.80
8	A	2159	G	N3-C4-C5	6.75	131.98	128.60
34	a	1158	C	N1-C2-O2	6.75	122.95	118.90
34	a	1420	U	C6-N1-C1'	-6.73	111.77	121.20
8	A	170	U	C2-N1-C1'	6.70	125.73	117.70
34	a	1043	G	N3-C4-N9	-6.69	121.98	126.00
8	A	1902	C	N3-C2-O2	-6.69	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1043	G	N9-C4-C5	6.69	108.08	105.40
8	A	1577	C	N3-C2-O2	-6.68	117.22	121.90
19	L	60	ARG	C-N-CA	-6.67	105.02	121.70
34	a	215	C	N1-C2-O2	6.66	122.90	118.90
8	A	2129	C	N3-C2-O2	-6.66	117.24	121.90
34	a	811	C	C6-N1-C1'	-6.65	112.82	120.80
34	a	751	U	C2-N1-C1'	6.62	125.64	117.70
8	A	2834	G	C8-N9-C4	6.60	109.04	106.40
8	A	2040	G	C8-N9-C4	6.59	109.03	106.40
8	A	1336	A	C8-N9-C4	6.58	108.43	105.80
8	A	2674	G	C8-N9-C4	6.56	109.02	106.40
56	w	19	G	N9-C4-C5	-6.52	102.79	105.40
8	A	238	C	C6-N1-C2	6.51	122.91	120.30
8	A	1779	U	C5-C6-N1	-6.48	119.46	122.70
34	a	811	C	N1-C2-O2	6.47	122.78	118.90
8	A	2103	C	N1-C2-O2	6.46	122.78	118.90
34	a	1053	G	OP2-P-O3'	-6.46	90.99	105.20
8	A	1398	C	N1-C2-O2	6.45	122.77	118.90
8	A	192	C	N3-C2-O2	-6.39	117.42	121.90
23	P	76	HIS	C-N-CA	-6.36	105.79	121.70
34	a	754	C	N1-C2-O2	6.36	122.72	118.90
8	A	964	C	C5-C6-N1	-6.34	117.83	121.00
8	A	1418	G	C5-N7-C8	-6.33	101.14	104.30
8	A	2248	C	N1-C2-O2	6.32	122.69	118.90
8	A	414	C	C6-N1-C2	6.32	122.83	120.30
34	a	577	G	C8-N9-C4	6.32	108.93	106.40
8	A	799	G	N1-C6-O6	-6.30	116.12	119.90
34	a	993	G	C6-C5-N7	-6.29	126.63	130.40
34	a	1421	G	N1-C6-O6	-6.28	116.13	119.90
8	A	192	C	N1-C2-O2	6.28	122.67	118.90
8	A	806	C	C6-N1-C2	6.27	122.81	120.30
8	A	2248	C	N3-C2-O2	-6.27	117.51	121.90
8	A	883	G	N3-C4-N9	-6.25	122.25	126.00
34	a	993	G	C4-N9-C1'	6.24	134.61	126.50
34	a	1356	G	N9-C4-C5	-6.23	102.91	105.40
8	A	1774	C	C6-N1-C1'	-6.22	113.33	120.80
8	A	2165	C	N1-C2-O2	6.22	122.63	118.90
34	a	176	C	C5-C6-N1	-6.21	117.89	121.00
8	A	2272	U	C5-C6-N1	-6.20	119.60	122.70
34	a	603	U	N3-C2-O2	-6.19	117.87	122.20
8	A	183	C	N1-C2-O2	6.19	122.61	118.90
8	A	627	A	C8-N9-C4	6.16	108.26	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2683	C	N3-C2-O2	-6.15	117.59	121.90
34	a	1307	U	C2-N1-C1'	6.15	125.08	117.70
36	c	14	VAL	C-N-CA	-6.14	106.35	121.70
8	A	806	C	C2-N3-C4	-6.14	116.83	119.90
8	A	1730	C	N3-C2-O2	-6.11	117.62	121.90
34	a	756	C	N3-C2-O2	-6.10	117.63	121.90
48	o	66	LEU	CA-CB-CG	-6.10	101.27	115.30
8	A	2159	G	C4-N9-C1'	-6.09	118.58	126.50
8	A	678	C	N3-C2-O2	-6.09	117.64	121.90
34	a	998	C	C6-N1-C1'	6.09	128.11	120.80
34	a	1043	G	C8-N9-C1'	6.09	134.91	127.00
8	A	2103	C	C6-N1-C2	-6.08	117.87	120.30
8	A	357	C	N3-C2-O2	-6.07	117.65	121.90
8	A	214	G	N1-C6-O6	-6.05	116.27	119.90
8	A	2731	G	C5-C6-O6	-6.04	124.97	128.60
34	a	754	C	N3-C2-O2	-6.04	117.68	121.90
8	A	2591	C	C6-N1-C2	-6.03	117.89	120.30
8	A	2588	G	C2-N3-C4	-6.03	108.89	111.90
34	a	1421	G	N3-C2-N2	-6.03	115.68	119.90
8	A	1730	C	C6-N1-C1'	-6.01	113.59	120.80
8	A	2129	C	C6-N1-C2	-6.01	117.90	120.30
8	A	893	C	C2-N3-C4	-6.01	116.89	119.90
34	a	1356	G	C6-C5-N7	-6.00	126.80	130.40
8	A	2023	C	N3-C4-C5	5.99	124.30	121.90
34	a	1421	G	C8-N9-C4	-5.99	104.00	106.40
8	A	2619	C	C6-N1-C2	5.99	122.69	120.30
8	A	696	G	C8-N9-C4	5.97	108.79	106.40
8	A	343	C	C2-N1-C1'	5.95	125.34	118.80
34	a	1466	C	N1-C2-O2	5.94	122.47	118.90
8	A	1324	G	O4'-C1'-N9	5.94	112.95	108.20
8	A	1054	A	N9-C4-C5	-5.93	103.43	105.80
8	A	1905	C	C5-C6-N1	-5.93	118.04	121.00
8	A	1234	U	N3-C2-O2	-5.92	118.05	122.20
8	A	742	A	C8-N9-C4	5.92	108.17	105.80
34	a	216	U	N1-C2-O2	5.90	126.93	122.80
56	w	19	G	C4-C5-N7	5.90	113.16	110.80
8	A	1900	A	O4'-C1'-N9	5.90	112.92	108.20
34	a	1158	C	N3-C2-O2	-5.89	117.77	121.90
8	A	268	C	C6-N1-C2	5.89	122.66	120.30
8	A	2815	C	C6-N1-C2	5.88	122.65	120.30
8	A	1662	U	N3-C4-O4	-5.88	115.28	119.40
8	A	2420	C	N1-C2-O2	5.88	122.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	177	G	C8-N9-C1'	-5.88	119.36	127.00
8	A	2543	G	C8-N9-C4	-5.88	104.05	106.40
34	a	998	C	C2-N1-C1'	-5.87	112.34	118.80
8	A	2215	C	C6-N1-C2	5.87	122.65	120.30
34	a	993	G	C8-N9-C1'	-5.86	119.39	127.00
8	A	700	G	C8-N9-C4	5.85	108.74	106.40
8	A	2300	C	C2-N1-C1'	5.83	125.22	118.80
8	A	2506	U	C6-N1-C1'	-5.82	113.05	121.20
34	a	751	U	C5-C6-N1	5.82	125.61	122.70
8	A	2127	G	O4'-C1'-N9	5.81	112.85	108.20
8	A	2551	C	N3-C4-N4	-5.81	113.94	118.00
8	A	1533	C	N1-C2-O2	5.79	122.37	118.90
24	Q	23	TYR	CB-CA-C	5.79	121.97	110.40
8	A	1049	C	C5-C6-N1	5.78	123.89	121.00
34	a	404	G	C8-N9-C1'	5.77	134.50	127.00
8	A	1845	G	C8-N9-C4	5.77	108.71	106.40
8	A	2483	C	C6-N1-C2	5.76	122.61	120.30
8	A	834	G	N1-C6-O6	-5.74	116.45	119.90
8	A	915	C	C2-N1-C1'	5.73	125.10	118.80
8	A	1930	G	N3-C4-C5	5.71	131.46	128.60
34	a	1140	C	N1-C2-O2	5.71	122.33	118.90
8	A	2501	C	C6-N1-C1'	5.70	127.64	120.80
8	A	1378	A	C2-N3-C4	-5.70	107.75	110.60
34	a	1103	C	C6-N1-C2	5.69	122.58	120.30
8	A	2731	G	C5-N7-C8	-5.68	101.46	104.30
8	A	806	C	N3-C4-C5	5.67	124.17	121.90
8	A	1398	C	N3-C2-O2	-5.67	117.93	121.90
8	A	806	C	C5-C6-N1	-5.67	118.17	121.00
34	a	1431	A	O4'-C1'-N9	5.67	112.73	108.20
8	A	885	C	OP2-P-O3'	5.67	117.67	105.20
34	a	177	G	C4-N9-C1'	5.67	133.87	126.50
34	a	1174	G	N9-C4-C5	-5.67	103.13	105.40
8	A	2707	U	C5-C6-N1	-5.66	119.87	122.70
8	A	893	C	C2-N1-C1'	-5.66	112.58	118.80
34	a	1059	C	N3-C4-N4	-5.66	114.04	118.00
8	A	2123	G	N3-C4-C5	5.65	131.43	128.60
8	A	1049	C	C6-N1-C2	-5.64	118.05	120.30
8	A	2337	G	N9-C4-C5	-5.63	103.15	105.40
34	a	993	G	N3-C4-N9	5.63	129.38	126.00
8	A	2052	A	C6-C5-N7	-5.62	128.37	132.30
34	a	1307	U	C6-N1-C1'	-5.62	113.34	121.20
34	a	1157	A	O4'-C1'-N9	-5.58	103.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2828	G	C8-N9-C4	5.57	108.63	106.40
8	A	1100	C	N1-C2-O2	5.57	122.24	118.90
8	A	1179	G	C4-N9-C1'	5.57	133.74	126.50
8	A	2159	G	C8-N9-C1'	5.57	134.24	127.00
8	A	2146	C	N1-C2-O2	5.56	122.24	118.90
34	a	1210	C	C6-N1-C2	-5.56	118.08	120.30
55	v	17	C	O4'-C1'-N1	5.56	112.65	108.20
8	A	837	C	N1-C2-O2	5.56	122.23	118.90
34	a	716	A	C8-N9-C4	5.55	108.02	105.80
34	a	1149	C	C5-C6-N1	5.55	123.77	121.00
8	A	2742	G	C8-N9-C4	5.54	108.62	106.40
8	A	2129	C	C6-N1-C1'	-5.53	114.17	120.80
34	a	305	G	N3-C4-N9	-5.52	122.69	126.00
8	A	214	G	N3-C2-N2	5.52	123.76	119.90
34	a	821	G	C8-N9-C4	5.51	108.61	106.40
8	A	814	C	C6-N1-C2	5.51	122.50	120.30
34	a	1103	C	C5-C6-N1	-5.51	118.25	121.00
55	v	19	G	O4'-C1'-N9	-5.50	103.80	108.20
8	A	2103	C	N3-C2-O2	-5.50	118.05	121.90
8	A	357	C	N1-C2-O2	5.50	122.20	118.90
34	a	105	G	C8-N9-C4	5.50	108.60	106.40
8	A	2052	A	C4-C5-N7	5.49	113.44	110.70
8	A	1252	G	C8-N9-C4	5.48	108.59	106.40
8	A	1071	G	C4-N9-C1'	5.48	133.62	126.50
8	A	678	C	N1-C2-O2	5.48	122.19	118.90
34	a	910	C	C6-N1-C2	5.48	122.49	120.30
8	A	1662	U	C5-C6-N1	-5.47	119.96	122.70
8	A	744	U	C2-N1-C1'	5.47	124.27	117.70
34	a	176	C	C5-C4-N4	5.47	124.03	120.20
56	w	9	A	O4'-C1'-N9	5.45	112.56	108.20
34	a	386	C	N3-C2-O2	-5.45	118.08	121.90
8	A	708	G	N3-C4-N9	-5.45	122.73	126.00
8	A	2892	G	C8-N9-C4	5.45	108.58	106.40
8	A	1491	G	N9-C4-C5	5.44	107.58	105.40
34	a	476	U	C2-N1-C1'	5.44	124.23	117.70
8	A	1649	G	N1-C6-O6	-5.43	116.64	119.90
8	A	775	G	N3-C4-C5	5.42	131.31	128.60
8	A	705	A	N1-C6-N6	5.41	121.85	118.60
8	A	238	C	C5-C6-N1	-5.40	118.30	121.00
34	a	1356	G	C4-C5-N7	5.40	112.96	110.80
34	a	1292	G	N9-C4-C5	-5.40	103.24	105.40
8	A	671	C	N3-C4-N4	-5.39	114.22	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2867	G	O4'-C1'-N9	5.39	112.51	108.20
34	a	1401	G	N1-C6-O6	-5.39	116.67	119.90
34	a	1421	G	C4-C5-N7	-5.39	108.64	110.80
34	a	1292	G	C4-C5-N7	5.39	112.95	110.80
8	A	695	G	C8-N9-C4	5.38	108.55	106.40
8	A	1824	G	C8-N9-C4	5.38	108.55	106.40
8	A	2103	C	C5-C6-N1	5.38	123.69	121.00
8	A	2676	C	C6-N1-C2	5.38	122.45	120.30
8	A	721	A	C8-N9-C4	5.38	107.95	105.80
8	A	2465	C	C6-N1-C2	5.37	122.45	120.30
8	A	1644	C	O4'-C1'-N1	5.37	112.49	108.20
8	A	1990	C	N3-C2-O2	-5.37	118.14	121.90
8	A	2040	G	N9-C4-C5	-5.36	103.25	105.40
34	a	655	A	C8-N9-C4	5.36	107.94	105.80
34	a	1491	G	C8-N9-C4	-5.36	104.26	106.40
8	A	2128	G	C4-N9-C1'	5.35	133.45	126.50
8	A	1662	U	C2-N3-C4	-5.35	123.79	127.00
8	A	721	A	N9-C4-C5	-5.34	103.66	105.80
9	B	7	G	C4-N9-C1'	-5.34	119.56	126.50
8	A	1946	U	C5-C6-N1	-5.34	120.03	122.70
8	A	901	C	N1-C2-O2	5.33	122.10	118.90
8	A	2793	C	N1-C2-O2	5.33	122.10	118.90
8	A	2551	C	C5-C6-N1	-5.32	118.34	121.00
34	a	528	C	C2-N1-C1'	-5.32	112.94	118.80
8	A	1905	C	C6-N1-C2	5.32	122.43	120.30
8	A	1292	G	C8-N9-C4	5.31	108.53	106.40
8	A	1902	C	N3-C4-C5	5.31	124.02	121.90
34	a	169	C	N1-C2-O2	5.31	122.09	118.90
8	A	1902	C	C6-N1-C1'	-5.30	114.44	120.80
8	A	2551	C	C6-N1-C2	5.30	122.42	120.30
8	A	1170	C	N1-C2-O2	5.30	122.08	118.90
8	A	799	G	N1-C2-N2	-5.30	111.43	116.20
8	A	671	C	C5-C6-N1	-5.30	118.35	121.00
8	A	458	G	N3-C4-C5	5.29	131.25	128.60
34	a	1142	G	C8-N9-C4	5.29	108.52	106.40
8	A	1156	A	C8-N9-C4	5.29	107.92	105.80
8	A	2367	G	C8-N9-C4	5.29	108.52	106.40
8	A	2520	C	N3-C4-C5	5.29	124.02	121.90
56	w	48	C	C6-N1-C2	5.29	122.42	120.30
34	a	750	C	N3-C2-O2	-5.28	118.20	121.90
8	A	1905	C	C2-N3-C4	-5.28	117.26	119.90
8	A	504	A	C2'-C3'-O3'	5.27	122.13	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	628	G	N9-C4-C5	-5.26	103.29	105.40
8	A	1370	C	C2-N3-C4	-5.26	117.27	119.90
8	A	89	A	C2-N3-C4	-5.26	107.97	110.60
8	A	2215	C	N3-C4-C5	5.25	124.00	121.90
34	a	1174	G	C4-C5-N7	5.25	112.90	110.80
8	A	2773	C	C6-N1-C2	5.25	122.40	120.30
34	a	808	C	O4'-C1'-N1	5.25	112.40	108.20
34	a	800	G	N3-C4-N9	-5.24	122.86	126.00
34	a	1356	G	N3-C4-N9	5.23	129.14	126.00
34	a	1415	G	C5-C6-O6	-5.23	125.46	128.60
8	A	690	G	C4-N9-C1'	-5.22	119.72	126.50
8	A	1093	G	N3-C4-N9	5.21	129.13	126.00
34	a	476	U	N1-C2-O2	5.21	126.44	122.80
34	a	1420	U	C5-C6-N1	5.20	125.30	122.70
55	v	7	G	O4'-C1'-N9	5.20	112.36	108.20
8	A	2186	G	N3-C4-C5	5.20	131.20	128.60
8	A	444	C	C2-N3-C4	-5.19	117.30	119.90
8	A	1251	C	C2-N1-C1'	5.19	124.51	118.80
8	A	1703	G	N7-C8-N9	-5.19	110.51	113.10
8	A	1814	G	N3-C4-N9	-5.18	122.89	126.00
8	A	1638	C	C5-C6-N1	-5.18	118.41	121.00
34	a	1162	C	C6-N1-C2	5.18	122.37	120.30
8	A	1779	U	C2-N3-C4	-5.18	123.89	127.00
8	A	1902	C	C2-N1-C1'	5.18	124.50	118.80
8	A	1145	C	C6-N1-C2	5.18	122.37	120.30
34	a	313	A	C5-C6-N1	5.17	120.29	117.70
34	a	323	U	C5-C6-N1	5.17	125.29	122.70
34	a	843	U	P-O3'-C3'	5.17	125.91	119.70
8	A	1675	C	N3-C2-O2	-5.17	118.28	121.90
8	A	1179	G	N3-C4-N9	5.17	129.10	126.00
34	a	476	U	C6-N1-C1'	-5.16	113.98	121.20
23	P	99	LEU	CA-CB-CG	-5.16	103.43	115.30
34	a	106	C	N1-C2-O2	5.16	122.00	118.90
34	a	824	G	N9-C4-C5	-5.16	103.34	105.40
8	A	974	G	C4-C5-N7	5.16	112.86	110.80
34	a	296	U	C5-C6-N1	-5.15	120.12	122.70
8	A	692	C	C6-N1-C2	5.15	122.36	120.30
8	A	1346	G	C6-C5-N7	-5.15	127.31	130.40
8	A	1425	G	N3-C4-N9	-5.15	122.91	126.00
8	A	2337	G	C8-N9-C4	5.15	108.46	106.40
34	a	404	G	C4-N9-C1'	-5.15	119.81	126.50
8	A	1466	U	C5-C4-O4	5.15	128.99	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1372	U	N3-C2-O2	-5.14	118.60	122.20
8	A	2186	G	C8-N9-C4	5.13	108.45	106.40
8	A	912	C	C2-N1-C1'	5.13	124.44	118.80
8	A	158	U	N3-C2-O2	-5.12	118.61	122.20
8	A	1425	G	C2-N3-C4	-5.12	109.34	111.90
8	A	1968	G	C8-N9-C4	5.12	108.45	106.40
34	a	1417	G	C8-N9-C4	5.12	108.45	106.40
8	A	2579	C	N1-C2-O2	5.12	121.97	118.90
8	A	1639	C	N1-C2-O2	5.12	121.97	118.90
34	a	324	G	N3-C4-C5	5.12	131.16	128.60
8	A	1346	G	N9-C4-C5	-5.11	103.36	105.40
34	a	508	U	C6-N1-C2	5.11	124.07	121.00
8	A	893	C	C6-N1-C1'	5.11	126.93	120.80
55	v	41	C	N1-C2-O2	5.10	121.96	118.90
8	A	2249	U	C4-C5-C6	5.10	122.76	119.70
8	A	293	U	C5-C6-N1	-5.09	120.15	122.70
8	A	1628	G	N1-C6-O6	-5.09	116.84	119.90
34	a	1300	G	P-O3'-C3'	5.09	125.81	119.70
8	A	1398	C	C2-N1-C1'	5.09	124.40	118.80
8	A	2718	G	C6-C5-N7	-5.09	127.35	130.40
8	A	2775	G	C8-N9-C4	5.09	108.44	106.40
34	a	1140	C	N3-C2-O2	-5.09	118.34	121.90
8	A	1244	A	C8-N9-C4	5.08	107.83	105.80
8	A	1894	C	N3-C2-O2	-5.08	118.34	121.90
34	a	679	C	C6-N1-C2	5.08	122.33	120.30
34	a	1103	C	C2-N1-C1'	-5.08	113.21	118.80
8	A	164	C	C2-N1-C1'	5.08	124.39	118.80
8	A	1600	C	C6-N1-C2	-5.08	118.27	120.30
34	a	176	C	C2-N3-C4	-5.07	117.36	119.90
8	A	979	A	C8-N9-C4	5.07	107.83	105.80
34	a	575	G	N3-C4-N9	-5.07	122.96	126.00
8	A	2578	G	N3-C4-C5	5.07	131.13	128.60
34	a	372	C	C2-N1-C1'	-5.07	113.22	118.80
8	A	1413	A	C5-C6-N6	-5.07	119.65	123.70
8	A	708	G	N3-C4-C5	5.06	131.13	128.60
8	A	1228	G	C8-N9-C4	5.06	108.42	106.40
8	A	1047	G	O4'-C1'-N9	5.06	112.25	108.20
8	A	1209	U	C6-N1-C2	5.06	124.03	121.00
8	A	2235	G	C8-N9-C4	5.06	108.42	106.40
56	w	19	G	C8-N9-C4	5.05	108.42	106.40
8	A	617	G	C8-N9-C4	5.05	108.42	106.40
34	a	5	U	C2-N1-C1'	5.05	123.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	343	C	C6-N1-C1'	-5.04	114.75	120.80
8	A	679	C	N1-C2-O2	5.04	121.93	118.90
8	A	951	C	C5-C6-N1	-5.04	118.48	121.00
34	a	1050	G	N3-C4-N9	-5.04	122.98	126.00
8	A	2418	A	C8-N9-C4	5.04	107.81	105.80
8	A	2632	A	C8-N9-C4	5.04	107.81	105.80
8	A	1778	U	C5-C6-N1	-5.03	120.18	122.70
8	A	90	U	N1-C2-N3	5.03	117.92	114.90
34	a	508	U	C5-C6-N1	-5.03	120.18	122.70
8	A	241	A	C8-N9-C4	5.03	107.81	105.80
34	a	215	C	N3-C2-O2	-5.03	118.38	121.90
8	A	883	G	C4-N9-C1'	-5.03	119.96	126.50
8	A	2834	G	N3-C4-C5	5.03	131.11	128.60
34	a	445	G	C4-N9-C1'	-5.03	119.97	126.50
34	a	586	C	C5-C6-N1	-5.02	118.49	121.00
8	A	1130	U	C5-C6-N1	-5.02	120.19	122.70
8	A	2666	C	N1-C2-O2	5.02	121.91	118.90
8	A	248	G	N3-C4-N9	5.02	129.01	126.00
8	A	1395	A	O4'-C1'-N9	5.02	112.21	108.20
8	A	170	U	C6-N1-C1'	-5.01	114.18	121.20
8	A	487	C	N3-C2-O2	-5.01	118.39	121.90
8	A	2222	C	N3-C2-O2	-5.01	118.39	121.90
8	A	2420	C	C6-N1-C1'	-5.01	114.79	120.80
34	a	1415	G	N3-C4-N9	5.01	129.00	126.00
34	a	1043	G	C4-N9-C1'	-5.01	119.99	126.50
34	a	68	G	N3-C4-C5	5.00	131.10	128.60
55	v	13	C	C6-N1-C2	5.00	122.30	120.30

There are no chirality outliers.

There are no planarity outliers.

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

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

5.3 Torsion angles [\(i\)](#)

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

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	42 (78%)	12 (22%)	0	100	100
2	1	48/55 (87%)	38 (79%)	10 (21%)	0	100	100
3	2	44/46 (96%)	27 (61%)	17 (39%)	0	100	100
4	3	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
5	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
6	5	129/165 (78%)	100 (78%)	29 (22%)	0	100	100
7	6	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
10	C	269/273 (98%)	213 (79%)	56 (21%)	0	100	100
11	D	207/209 (99%)	172 (83%)	34 (16%)	1 (0%)	25	65
12	E	199/201 (99%)	165 (83%)	34 (17%)	0	100	100
13	F	175/179 (98%)	153 (87%)	22 (13%)	0	100	100
14	G	174/177 (98%)	149 (86%)	25 (14%)	0	100	100
15	H	147/149 (99%)	117 (80%)	30 (20%)	0	100	100
16	I	139/142 (98%)	104 (75%)	35 (25%)	0	100	100
17	J	140/142 (99%)	109 (78%)	31 (22%)	0	100	100
18	K	120/123 (98%)	101 (84%)	19 (16%)	0	100	100
19	L	141/144 (98%)	108 (77%)	33 (23%)	0	100	100
20	M	134/136 (98%)	109 (81%)	24 (18%)	1 (1%)	19	57
21	N	118/127 (93%)	87 (74%)	31 (26%)	0	100	100
22	O	114/117 (97%)	101 (89%)	13 (11%)	0	100	100
23	P	112/115 (97%)	98 (88%)	14 (12%)	0	100	100
24	Q	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
25	R	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
26	S	108/110 (98%)	89 (82%)	19 (18%)	0	100	100
27	T	91/100 (91%)	74 (81%)	17 (19%)	0	100	100
28	U	100/104 (96%)	81 (81%)	19 (19%)	0	100	100
29	V	92/94 (98%)	79 (86%)	13 (14%)	0	100	100
30	W	73/85 (86%)	56 (77%)	17 (23%)	0	100	100
31	X	75/78 (96%)	63 (84%)	12 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	Y	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
33	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
35	b	216/240 (90%)	184 (85%)	32 (15%)	0	100	100
36	c	204/233 (88%)	181 (89%)	23 (11%)	0	100	100
37	d	203/206 (98%)	160 (79%)	42 (21%)	1 (0%)	25	65
38	e	155/167 (93%)	119 (77%)	36 (23%)	0	100	100
39	f	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
40	g	149/179 (83%)	130 (87%)	19 (13%)	0	100	100
41	h	127/130 (98%)	107 (84%)	20 (16%)	0	100	100
42	i	125/130 (96%)	98 (78%)	27 (22%)	0	100	100
43	j	96/103 (93%)	76 (79%)	19 (20%)	1 (1%)	13	49
44	k	114/129 (88%)	92 (81%)	22 (19%)	0	100	100
45	l	121/124 (98%)	96 (79%)	25 (21%)	0	100	100
46	m	112/118 (95%)	99 (88%)	13 (12%)	0	100	100
47	n	99/102 (97%)	87 (88%)	12 (12%)	0	100	100
48	o	86/89 (97%)	74 (86%)	12 (14%)	0	100	100
49	p	80/82 (98%)	61 (76%)	19 (24%)	0	100	100
50	q	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
51	r	63/75 (84%)	49 (78%)	14 (22%)	0	100	100
52	s	80/92 (87%)	70 (88%)	10 (12%)	0	100	100
53	t	83/87 (95%)	66 (80%)	17 (20%)	0	100	100
54	u	63/71 (89%)	50 (79%)	13 (21%)	0	100	100
All	All	5850/6220 (94%)	4809 (82%)	1037 (18%)	4 (0%)	50	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	j	60	ASP
37	d	144	ILE
11	D	138	LEU
20	M	59	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	45 (96%)	2 (4%)	25	46
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	37 (97%)	1 (3%)	41	59
4	3	51/52 (98%)	45 (88%)	6 (12%)	4	16
5	4	34/34 (100%)	32 (94%)	2 (6%)	16	38
7	6	59/62 (95%)	52 (88%)	7 (12%)	4	16
10	C	216/218 (99%)	214 (99%)	2 (1%)	75	83
11	D	164/164 (100%)	162 (99%)	2 (1%)	67	79
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	141 (95%)	7 (5%)	22	44
14	G	137/138 (99%)	134 (98%)	3 (2%)	47	65
15	H	114/114 (100%)	113 (99%)	1 (1%)	75	83
17	J	116/116 (100%)	112 (97%)	4 (3%)	32	51
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	100 (98%)	2 (2%)	50	68
20	M	109/109 (100%)	108 (99%)	1 (1%)	75	83
21	N	100/103 (97%)	100 (100%)	0	100	100
22	O	86/87 (99%)	81 (94%)	5 (6%)	17	38
23	P	99/100 (99%)	98 (99%)	1 (1%)	73	82
24	Q	89/90 (99%)	87 (98%)	2 (2%)	47	65
25	R	84/84 (100%)	79 (94%)	5 (6%)	16	37
26	S	93/93 (100%)	88 (95%)	5 (5%)	18	40
27	T	80/84 (95%)	78 (98%)	2 (2%)	42	61
28	U	83/85 (98%)	81 (98%)	2 (2%)	44	62
29	V	78/78 (100%)	78 (100%)	0	100	100
30	W	57/63 (90%)	56 (98%)	1 (2%)	54	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	X	67/68 (98%)	66 (98%)	1 (2%)	60	75
32	Y	55/55 (100%)	50 (91%)	5 (9%)	7	24
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	178 (99%)	2 (1%)	70	80
36	c	170/190 (90%)	168 (99%)	2 (1%)	67	79
37	d	172/173 (99%)	168 (98%)	4 (2%)	45	64
38	e	114/126 (90%)	113 (99%)	1 (1%)	75	83
39	f	87/116 (75%)	85 (98%)	2 (2%)	45	64
40	g	124/147 (84%)	121 (98%)	3 (2%)	44	62
41	h	104/105 (99%)	102 (98%)	2 (2%)	52	69
42	i	105/107 (98%)	100 (95%)	5 (5%)	21	43
43	j	86/90 (96%)	86 (100%)	0	100	100
44	k	89/99 (90%)	86 (97%)	3 (3%)	32	51
45	l	103/104 (99%)	102 (99%)	1 (1%)	73	82
46	m	92/96 (96%)	90 (98%)	2 (2%)	47	65
47	n	79/84 (94%)	75 (95%)	4 (5%)	20	41
48	o	76/77 (99%)	75 (99%)	1 (1%)	65	77
49	p	65/65 (100%)	65 (100%)	0	100	100
50	q	74/78 (95%)	73 (99%)	1 (1%)	62	75
51	r	56/65 (86%)	55 (98%)	1 (2%)	54	71
52	s	72/79 (91%)	66 (92%)	6 (8%)	9	27
53	t	65/66 (98%)	65 (100%)	0	100	100
54	u	46/61 (75%)	44 (96%)	2 (4%)	25	46
57	y	1/1 (100%)	1 (100%)	0	100	100
All	All	4627/4830 (96%)	4516 (98%)	111 (2%)	45	62

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	SER
1	0	38	LEU
3	2	41	ARG
4	3	15	LYS
4	3	29	ARG

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Mol	Chain	Res	Type
4	3	31	ILE
4	3	35	LYS
4	3	42	HIS
4	3	53	ASP
5	4	1	MET
5	4	12	ARG
7	6	37	CYS
7	6	47	LYS
7	6	49	ARG
7	6	50	ASP
7	6	53	THR
7	6	56	ARG
7	6	61	ASN
10	C	264	LYS
10	C	270	ARG
11	D	33	ARG
11	D	138	LEU
13	F	22	ASN
13	F	29	ARG
13	F	48	LEU
13	F	51	ASN
13	F	68	LYS
13	F	79	ARG
13	F	177	ARG
14	G	59	ASP
14	G	94	ARG
14	G	98	LYS
15	H	75	LEU
17	J	12	LYS
17	J	48	VAL
17	J	77	HIS
17	J	116	ARG
19	L	39	LYS
19	L	40	SER
20	M	6	ARG
22	O	30	ARG
22	O	31	THR
22	O	53	THR
22	O	67	ASN
22	O	103	VAL
23	P	88	ARG
24	Q	21	LYS

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Mol	Chain	Res	Type
24	Q	50	ARG
25	R	5	PHE
25	R	49	ILE
25	R	51	VAL
25	R	55	ASP
25	R	85	LYS
26	S	77	ASP
26	S	78	GLU
26	S	83	LYS
26	S	101	SER
26	S	104	THR
27	T	36	LYS
27	T	87	LEU
28	U	72	PHE
28	U	81	ARG
30	W	10	ARG
31	X	76	LYS
32	Y	14	LEU
32	Y	17	GLU
32	Y	18	LEU
32	Y	22	LEU
32	Y	57	LEU
35	b	73	ARG
35	b	131	LYS
36	c	167	TYR
36	c	184	ASN
37	d	44	LYS
37	d	57	LYS
37	d	75	TYR
37	d	150	LYS
38	e	123	LEU
39	f	55	HIS
39	f	76	THR
40	g	21	LEU
40	g	22	LEU
40	g	118	ARG
41	h	68	LYS
41	h	104	SER
42	i	11	ARG
42	i	24	ASN
42	i	26	LYS
42	i	58	GLU

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Mol	Chain	Res	Type
42	i	122	ARG
44	k	12	ARG
44	k	36	ARG
44	k	74	LYS
45	l	45	ASN
46	m	103	THR
46	m	104	ASN
47	n	5	MET
47	n	47	LYS
47	n	61	ARG
47	n	63	ARG
48	o	9	LYS
50	q	27	PHE
51	r	72	ARG
52	s	9	PHE
52	s	28	LYS
52	s	40	PHE
52	s	68	HIS
52	s	78	THR
52	s	80	ARG
54	u	15	LEU
54	u	37	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
3	2	6	GLN
3	2	13	ASN
3	2	26	ASN
3	2	29	GLN
5	4	13	ASN
7	6	61	ASN
7	6	65	ASN
10	C	85	ASN
10	C	127	ASN
10	C	133	ASN
10	C	142	ASN
10	C	162	GLN
10	C	196	ASN
10	C	238	ASN
10	C	259	ASN
11	D	32	ASN

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Mol	Chain	Res	Type
11	D	136	ASN
11	D	167	ASN
11	D	173	GLN
12	E	62	GLN
13	F	20	ASN
13	F	62	GLN
14	G	21	GLN
14	G	44	HIS
14	G	110	HIS
14	G	138	GLN
15	H	43	ASN
15	H	73	ASN
15	H	135	HIS
18	K	3	GLN
19	L	99	ASN
19	L	104	GLN
20	M	60	GLN
20	M	97	GLN
21	N	9	GLN
21	N	11	ASN
21	N	16	HIS
21	N	31	HIS
21	N	107	ASN
22	O	116	GLN
23	P	9	GLN
24	Q	36	GLN
24	Q	55	GLN
25	R	18	GLN
25	R	66	HIS
25	R	82	HIS
25	R	86	GLN
26	S	7	HIS
26	S	60	HIS
26	S	61	ASN
27	T	59	ASN
29	V	87	GLN
30	W	46	ASN
31	X	16	ASN
31	X	22	ASN
32	Y	31	GLN
32	Y	36	GLN
32	Y	45	GLN

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Mol	Chain	Res	Type
33	Z	19	HIS
35	b	17	HIS
35	b	119	GLN
37	d	58	GLN
37	d	115	GLN
38	e	72	ASN
38	e	77	ASN
39	f	3	HIS
39	f	68	GLN
40	g	121	ASN
40	g	147	ASN
41	h	37	ASN
41	h	66	GLN
41	h	75	GLN
43	j	58	ASN
44	k	28	ASN
44	k	39	ASN
44	k	80	ASN
45	l	28	GLN
47	n	62	ASN
47	n	66	GLN
48	o	37	HIS
48	o	41	HIS
48	o	45	HIS
49	p	9	HIS
51	r	51	GLN
51	r	53	GLN
52	s	42	ASN
52	s	55	GLN
52	s	56	HIS
52	s	82	HIS
53	t	47	GLN
53	t	51	ASN
53	t	60	GLN
53	t	77	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	575 (37%)	0
55	v	76/77 (98%)	30 (39%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	w	74/76 (97%)	32 (43%)	0
58	z	10/33 (30%)	6 (60%)	0
8	A	2897/2903 (99%)	1092 (37%)	86 (2%)
9	B	119/120 (99%)	46 (38%)	2 (1%)
All	All	4712/4751 (99%)	1781 (37%)	88 (1%)

All (1781) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	14	A
8	A	15	G
8	A	16	C
8	A	23	G
8	A	24	G
8	A	27	G
8	A	35	G
8	A	39	G
8	A	44	A
8	A	45	G
8	A	46	G
8	A	50	U
8	A	51	G
8	A	52	A
8	A	55	G
8	A	56	A
8	A	60	G
8	A	62	U
8	A	63	A
8	A	71	A
8	A	73	A
8	A	74	A
8	A	75	G
8	A	76	C
8	A	80	G
8	A	82	U
8	A	84	A
8	A	92	U
8	A	96	C
8	A	101	A
8	A	102	U
8	A	103	A

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Mol	Chain	Res	Type
8	A	106	C
8	A	110	G
8	A	112	U
8	A	114	U
8	A	118	A
8	A	119	A
8	A	120	U
8	A	121	G
8	A	122	G
8	A	124	G
8	A	132	G
8	A	136	G
8	A	137	U
8	A	138	U
8	A	140	C
8	A	141	G
8	A	142	A
8	A	146	A
8	A	158	U
8	A	159	G
8	A	160	A
8	A	161	A
8	A	163	C
8	A	165	A
8	A	166	U
8	A	168	G
8	A	169	G
8	A	170	U
8	A	171	U
8	A	173	A
8	A	178	G
8	A	180	G
8	A	181	A
8	A	188	G
8	A	191	A
8	A	196	A
8	A	199	A
8	A	205	G
8	A	208	C
8	A	209	C
8	A	215	G
8	A	216	A

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Mol	Chain	Res	Type
8	A	217	A
8	A	220	G
8	A	221	A
8	A	223	A
8	A	224	U
8	A	228	C
8	A	229	C
8	A	230	G
8	A	239	C
8	A	241	A
8	A	242	G
8	A	243	U
8	A	248	G
8	A	252	G
8	A	254	G
8	A	255	A
8	A	261	G
8	A	265	A
8	A	266	G
8	A	267	C
8	A	272	A
8	A	275	C
8	A	276	U
8	A	277	G
8	A	278	A
8	A	279	A
8	A	284	U
8	A	286	U
8	A	287	G
8	A	288	U
8	A	291	G
8	A	295	G
8	A	298	G
8	A	299	A
8	A	300	A
8	A	302	C
8	A	305	C
8	A	310	A
8	A	312	G
8	A	323	C
8	A	325	G
8	A	326	G

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Mol	Chain	Res	Type
8	A	329	G
8	A	330	A
8	A	331	C
8	A	332	A
8	A	333	G
8	A	343	C
8	A	345	A
8	A	346	A
8	A	349	U
8	A	359	G
8	A	361	G
8	A	362	A
8	A	363	G
8	A	366	C
8	A	369	U
8	A	371	A
8	A	372	G
8	A	383	C
8	A	384	A
8	A	385	C
8	A	386	G
8	A	387	U
8	A	391	A
8	A	395	U
8	A	399	U
8	A	401	A
8	A	404	A
8	A	405	U
8	A	406	G
8	A	408	G
8	A	411	G
8	A	419	U
8	A	430	A
8	A	434	U
8	A	435	C
8	A	438	G
8	A	442	G
8	A	445	C
8	A	446	G
8	A	449	A
8	A	451	U
8	A	452	G

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Mol	Chain	Res	Type
8	A	453	A
8	A	455	C
8	A	457	A
8	A	458	G
8	A	459	U
8	A	465	G
8	A	473	G
8	A	475	C
8	A	477	A
8	A	478	A
8	A	480	A
8	A	481	G
8	A	482	A
8	A	484	C
8	A	486	C
8	A	489	G
8	A	490	C
8	A	491	G
8	A	504	A
8	A	505	A
8	A	506	G
8	A	508	A
8	A	509	C
8	A	510	C
8	A	511	U
8	A	512	G
8	A	513	A
8	A	514	A
8	A	515	A
8	A	516	C
8	A	525	U
8	A	527	C
8	A	530	G
8	A	531	C
8	A	532	A
8	A	533	G
8	A	534	U
8	A	540	C
8	A	543	G
8	A	544	C
8	A	546	U
8	A	548	G

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Mol	Chain	Res	Type
8	A	549	G
8	A	557	C
8	A	561	G
8	A	562	U
8	A	563	A
8	A	568	U
8	A	573	U
8	A	575	A
8	A	581	C
8	A	586	A
8	A	597	G
8	A	603	A
8	A	609	A
8	A	613	A
8	A	614	A
8	A	615	U
8	A	616	A
8	A	620	G
8	A	621	A
8	A	622	G
8	A	623	C
8	A	627	A
8	A	631	A
8	A	637	A
8	A	642	U
8	A	646	U
8	A	647	G
8	A	653	U
8	A	655	A
8	A	660	C
8	A	664	G
8	A	668	A
8	A	669	G
8	A	670	A
8	A	672	C
8	A	675	A
8	A	677	A
8	A	686	U
8	A	687	C
8	A	689	A
8	A	690	G
8	A	693	A

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Mol	Chain	Res	Type
8	A	703	U
8	A	704	G
8	A	713	G
8	A	714	U
8	A	715	A
8	A	716	A
8	A	717	C
8	A	725	G
8	A	726	G
8	A	730	A
8	A	739	A
8	A	740	C
8	A	744	U
8	A	747	5MC
8	A	748	G
8	A	749	A
8	A	750	A
8	A	757	G
8	A	762	U
8	A	764	A
8	A	766	U
8	A	768	G
8	A	769	U
8	A	774	G
8	A	776	G
8	A	781	A
8	A	782	A
8	A	783	A
8	A	784	G
8	A	785	G
8	A	786	C
8	A	789	A
8	A	790	U
8	A	792	A
8	A	800	A
8	A	801	G
8	A	805	G
8	A	806	C
8	A	808	G
8	A	811	U
8	A	812	C
8	A	819	A

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Mol	Chain	Res	Type
8	A	820	A
8	A	826	U
8	A	827	U
8	A	828	U
8	A	831	G
8	A	834	G
8	A	835	C
8	A	837	C
8	A	841	G
8	A	845	A
8	A	846	U
8	A	847	U
8	A	850	U
8	A	856	G
8	A	858	G
8	A	859	G
8	A	865	C
8	A	868	U
8	A	870	U
8	A	877	A
8	A	878	A
8	A	881	G
8	A	883	G
8	A	884	U
8	A	885	C
8	A	886	A
8	A	887	A
8	A	888	C
8	A	889	C
8	A	890	C
8	A	891	G
8	A	893	C
8	A	894	U
8	A	895	U
8	A	896	A
8	A	897	C
8	A	899	A
8	A	900	A
8	A	902	C
8	A	903	C
8	A	907	G
8	A	910	A

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Mol	Chain	Res	Type
8	A	912	C
8	A	913	U
8	A	915	C
8	A	917	A
8	A	927	A
8	A	931	U
8	A	932	U
8	A	934	U
8	A	941	A
8	A	945	A
8	A	946	C
8	A	957	C
8	A	959	A
8	A	961	C
8	A	973	A
8	A	974	G
8	A	975	A
8	A	976	G
8	A	982	C
8	A	983	A
8	A	985	C
8	A	989	G
8	A	990	A
8	A	995	C
8	A	996	A
8	A	1003	G
8	A	1005	C
8	A	1006	C
8	A	1010	A
8	A	1011	G
8	A	1012	U
8	A	1013	C
8	A	1022	G
8	A	1025	G
8	A	1026	G
8	A	1033	U
8	A	1034	G
8	A	1041	G
8	A	1044	C
8	A	1045	C
8	A	1046	A
8	A	1047	G

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Mol	Chain	Res	Type
8	A	1048	A
8	A	1049	C
8	A	1051	G
8	A	1053	C
8	A	1054	A
8	A	1055	G
8	A	1056	G
8	A	1057	A
8	A	1059	G
8	A	1060	U
8	A	1061	U
8	A	1062	G
8	A	1063	G
8	A	1064	C
8	A	1066	U
8	A	1067	A
8	A	1068	G
8	A	1069	A
8	A	1070	A
8	A	1071	G
8	A	1072	C
8	A	1073	A
8	A	1075	C
8	A	1077	A
8	A	1078	U
8	A	1079	C
8	A	1080	A
8	A	1081	U
8	A	1083	U
8	A	1084	A
8	A	1085	A
8	A	1086	A
8	A	1087	G
8	A	1088	A
8	A	1089	A
8	A	1090	A
8	A	1091	G
8	A	1092	C
8	A	1093	G
8	A	1094	U
8	A	1096	A
8	A	1098	A

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Mol	Chain	Res	Type
8	A	1100	C
8	A	1101	U
8	A	1102	C
8	A	1103	A
8	A	1105	U
8	A	1106	G
8	A	1109	C
8	A	1111	A
8	A	1112	G
8	A	1114	C
8	A	1115	G
8	A	1116	G
8	A	1122	G
8	A	1123	C
8	A	1128	G
8	A	1129	A
8	A	1130	U
8	A	1131	G
8	A	1132	U
8	A	1133	A
8	A	1134	A
8	A	1135	C
8	A	1139	G
8	A	1142	A
8	A	1143	A
8	A	1144	A
8	A	1149	G
8	A	1152	C
8	A	1155	A
8	A	1157	G
8	A	1170	C
8	A	1171	G
8	A	1173	U
8	A	1174	U
8	A	1175	A
8	A	1176	U
8	A	1179	G
8	A	1180	U
8	A	1186	G
8	A	1187	G
8	A	1188	U
8	A	1193	G

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Mol	Chain	Res	Type
8	A	1204	A
8	A	1205	A
8	A	1209	U
8	A	1210	G
8	A	1211	C
8	A	1212	G
8	A	1214	A
8	A	1218	G
8	A	1225	G
8	A	1226	A
8	A	1227	G
8	A	1235	G
8	A	1236	G
8	A	1238	G
8	A	1241	A
8	A	1245	G
8	A	1248	G
8	A	1249	U
8	A	1251	C
8	A	1252	G
8	A	1253	A
8	A	1255	U
8	A	1256	G
8	A	1264	A
8	A	1268	A
8	A	1269	A
8	A	1271	G
8	A	1272	A
8	A	1273	U
8	A	1284	A
8	A	1285	A
8	A	1289	C
8	A	1293	C
8	A	1300	G
8	A	1301	A
8	A	1302	A
8	A	1303	G
8	A	1306	C
8	A	1311	G
8	A	1312	U
8	A	1313	U
8	A	1314	C

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Mol	Chain	Res	Type
8	A	1315	C
8	A	1322	A
8	A	1325	U
8	A	1328	A
8	A	1332	G
8	A	1340	U
8	A	1342	A
8	A	1344	U
8	A	1345	C
8	A	1346	G
8	A	1352	U
8	A	1365	A
8	A	1368	G
8	A	1369	G
8	A	1370	C
8	A	1376	C
8	A	1378	A
8	A	1379	U
8	A	1380	G
8	A	1383	A
8	A	1384	A
8	A	1385	A
8	A	1386	C
8	A	1393	A
8	A	1395	A
8	A	1396	U
8	A	1397	U
8	A	1398	C
8	A	1410	G
8	A	1411	U
8	A	1415	U
8	A	1416	G
8	A	1418	G
8	A	1419	A
8	A	1420	A
8	A	1421	G
8	A	1428	C
8	A	1429	G
8	A	1432	G
8	A	1433	A
8	A	1435	G
8	A	1448	G

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Mol	Chain	Res	Type
8	A	1451	C
8	A	1452	G
8	A	1453	A
8	A	1454	C
8	A	1455	G
8	A	1458	U
8	A	1459	G
8	A	1460	U
8	A	1461	C
8	A	1467	U
8	A	1472	C
8	A	1473	G
8	A	1474	U
8	A	1482	G
8	A	1484	U
8	A	1488	C
8	A	1490	A
8	A	1491	G
8	A	1493	C
8	A	1494	A
8	A	1495	A
8	A	1496	A
8	A	1497	U
8	A	1502	A
8	A	1503	A
8	A	1504	A
8	A	1506	U
8	A	1509	A
8	A	1512	C
8	A	1515	A
8	A	1521	G
8	A	1524	G
8	A	1528	A
8	A	1532	A
8	A	1534	U
8	A	1535	A
8	A	1536	C
8	A	1537	G
8	A	1544	A
8	A	1547	C
8	A	1551	A
8	A	1553	A

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Mol	Chain	Res	Type
8	A	1554	U
8	A	1557	C
8	A	1558	C
8	A	1562	U
8	A	1563	U
8	A	1566	A
8	A	1569	A
8	A	1570	A
8	A	1578	U
8	A	1584	U
8	A	1585	C
8	A	1591	A
8	A	1594	U
8	A	1596	A
8	A	1598	A
8	A	1600	C
8	A	1607	C
8	A	1608	A
8	A	1609	A
8	A	1610	A
8	A	1616	A
8	A	1617	C
8	A	1619	G
8	A	1622	G
8	A	1623	G
8	A	1626	A
8	A	1627	G
8	A	1628	G
8	A	1631	G
8	A	1635	A
8	A	1643	G
8	A	1644	C
8	A	1645	G
8	A	1646	C
8	A	1647	U
8	A	1648	U
8	A	1649	G
8	A	1651	G
8	A	1654	A
8	A	1657	U
8	A	1658	C
8	A	1664	A

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Mol	Chain	Res	Type
8	A	1668	A
8	A	1669	A
8	A	1674	G
8	A	1691	C
8	A	1693	U
8	A	1695	G
8	A	1698	A
8	A	1699	G
8	A	1700	A
8	A	1702	G
8	A	1705	A
8	A	1715	G
8	A	1716	U
8	A	1726	C
8	A	1727	C
8	A	1729	U
8	A	1730	C
8	A	1731	G
8	A	1732	C
8	A	1733	G
8	A	1735	A
8	A	1738	G
8	A	1750	G
8	A	1752	C
8	A	1754	A
8	A	1757	A
8	A	1758	U
8	A	1759	A
8	A	1764	C
8	A	1767	G
8	A	1769	U
8	A	1773	A
8	A	1774	C
8	A	1775	U
8	A	1782	U
8	A	1784	A
8	A	1787	A
8	A	1788	C
8	A	1797	G
8	A	1800	C
8	A	1801	A
8	A	1804	C

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Mol	Chain	Res	Type
8	A	1808	A
8	A	1809	A
8	A	1810	A
8	A	1812	U
8	A	1813	G
8	A	1816	C
8	A	1817	G
8	A	1820	U
8	A	1821	A
8	A	1828	G
8	A	1829	A
8	A	1830	C
8	A	1833	C
8	A	1835	2MG
8	A	1848	A
8	A	1852	U
8	A	1857	G
8	A	1859	U
8	A	1860	G
8	A	1862	G
8	A	1865	U
8	A	1866	A
8	A	1868	C
8	A	1869	G
8	A	1873	G
8	A	1874	C
8	A	1876	A
8	A	1884	G
8	A	1895	C
8	A	1900	A
8	A	1901	A
8	A	1902	C
8	A	1906	G
8	A	1908	C
8	A	1910	G
8	A	1917	PSU
8	A	1918	A
8	A	1919	A
8	A	1921	G
8	A	1922	G
8	A	1923	U
8	A	1925	C

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Mol	Chain	Res	Type
8	A	1926	U
8	A	1928	A
8	A	1930	G
8	A	1932	A
8	A	1935	G
8	A	1938	A
8	A	1939	5MU
8	A	1940	U
8	A	1941	C
8	A	1944	U
8	A	1946	U
8	A	1955	U
8	A	1956	U
8	A	1962	5MC
8	A	1963	U
8	A	1964	G
8	A	1965	C
8	A	1967	C
8	A	1970	A
8	A	1972	G
8	A	1977	A
8	A	1979	U
8	A	1982	U
8	A	1991	U
8	A	1992	G
8	A	1993	U
8	A	1997	C
8	A	2001	C
8	A	2002	G
8	A	2003	A
8	A	2007	U
8	A	2009	A
8	A	2012	G
8	A	2013	A
8	A	2015	A
8	A	2016	U
8	A	2019	A
8	A	2021	C
8	A	2022	U
8	A	2023	C
8	A	2027	G
8	A	2028	U

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Mol	Chain	Res	Type
8	A	2029	G
8	A	2031	A
8	A	2032	G
8	A	2033	A
8	A	2034	U
8	A	2036	C
8	A	2042	A
8	A	2043	C
8	A	2044	C
8	A	2049	G
8	A	2051	A
8	A	2052	A
8	A	2055	C
8	A	2056	G
8	A	2057	G
8	A	2060	A
8	A	2061	G
8	A	2062	A
8	A	2063	C
8	A	2067	G
8	A	2068	U
8	A	2069	G7M
8	A	2073	C
8	A	2076	U
8	A	2077	A
8	A	2081	U
8	A	2089	C
8	A	2091	C
8	A	2092	U
8	A	2093	G
8	A	2097	A
8	A	2101	A
8	A	2102	G
8	A	2103	C
8	A	2104	C
8	A	2109	U
8	A	2110	G
8	A	2111	U
8	A	2112	G
8	A	2114	A
8	A	2115	G
8	A	2116	G

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Mol	Chain	Res	Type
8	A	2118	U
8	A	2119	A
8	A	2124	G
8	A	2125	G
8	A	2126	A
8	A	2127	G
8	A	2128	G
8	A	2129	C
8	A	2130	U
8	A	2131	U
8	A	2132	U
8	A	2133	G
8	A	2134	A
8	A	2135	A
8	A	2136	G
8	A	2138	G
8	A	2139	U
8	A	2143	C
8	A	2144	G
8	A	2145	C
8	A	2146	C
8	A	2147	A
8	A	2148	G
8	A	2150	C
8	A	2151	U
8	A	2152	G
8	A	2153	C
8	A	2155	U
8	A	2156	G
8	A	2157	G
8	A	2158	A
8	A	2159	G
8	A	2160	C
8	A	2161	C
8	A	2162	G
8	A	2163	A
8	A	2164	C
8	A	2166	U
8	A	2169	A
8	A	2170	A
8	A	2171	A
8	A	2172	U

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Mol	Chain	Res	Type
8	A	2173	A
8	A	2175	C
8	A	2176	A
8	A	2180	U
8	A	2181	U
8	A	2183	A
8	A	2186	G
8	A	2190	G
8	A	2193	G
8	A	2198	A
8	A	2199	A
8	A	2200	C
8	A	2203	U
8	A	2204	G
8	A	2208	C
8	A	2210	U
8	A	2211	A
8	A	2212	A
8	A	2214	C
8	A	2225	A
8	A	2226	C
8	A	2232	C
8	A	2238	G
8	A	2239	G
8	A	2248	C
8	A	2251	OMG
8	A	2259	U
8	A	2262	U
8	A	2265	U
8	A	2266	A
8	A	2267	A
8	A	2269	G
8	A	2273	A
8	A	2274	A
8	A	2279	G
8	A	2281	A
8	A	2283	C
8	A	2285	C
8	A	2286	G
8	A	2287	A
8	A	2288	A
8	A	2297	A

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Mol	Chain	Res	Type
8	A	2300	C
8	A	2305	U
8	A	2307	G
8	A	2308	G
8	A	2309	A
8	A	2310	C
8	A	2318	G
8	A	2320	U
8	A	2321	U
8	A	2322	A
8	A	2325	G
8	A	2327	A
8	A	2333	A
8	A	2334	U
8	A	2335	A
8	A	2336	A
8	A	2337	G
8	A	2343	U
8	A	2344	U
8	A	2345	G
8	A	2347	C
8	A	2349	G
8	A	2350	C
8	A	2358	A
8	A	2361	G
8	A	2373	G
8	A	2374	C
8	A	2379	G
8	A	2380	C
8	A	2382	G
8	A	2383	G
8	A	2384	U
8	A	2385	C
8	A	2388	A
8	A	2392	A
8	A	2396	G
8	A	2402	U
8	A	2403	C
8	A	2406	A
8	A	2422	C
8	A	2423	U
8	A	2424	C

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Mol	Chain	Res	Type
8	A	2425	A
8	A	2426	A
8	A	2427	C
8	A	2428	G
8	A	2429	G
8	A	2430	A
8	A	2432	A
8	A	2433	A
8	A	2434	A
8	A	2435	A
8	A	2437	G
8	A	2439	A
8	A	2441	U
8	A	2442	C
8	A	2445	2MG
8	A	2447	G
8	A	2448	A
8	A	2449	U
8	A	2456	C
8	A	2458	G
8	A	2459	A
8	A	2462	C
8	A	2467	C
8	A	2469	A
8	A	2474	U
8	A	2475	C
8	A	2476	A
8	A	2480	C
8	A	2482	A
8	A	2484	G
8	A	2490	G
8	A	2491	U
8	A	2494	G
8	A	2496	C
8	A	2498	OMC
8	A	2499	C
8	A	2500	U
8	A	2502	G
8	A	2505	G
8	A	2513	A
8	A	2518	A
8	A	2520	C

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Mol	Chain	Res	Type
8	A	2524	G
8	A	2528	U
8	A	2529	G
8	A	2532	G
8	A	2534	A
8	A	2535	G
8	A	2536	G
8	A	2543	G
8	A	2547	A
8	A	2553	G
8	A	2554	U
8	A	2555	U
8	A	2560	A
8	A	2564	A
8	A	2566	A
8	A	2567	G
8	A	2572	A
8	A	2573	C
8	A	2574	G
8	A	2576	G
8	A	2577	A
8	A	2578	G
8	A	2579	C
8	A	2581	G
8	A	2582	G
8	A	2583	G
8	A	2584	U
8	A	2585	U
8	A	2595	G
8	A	2599	G
8	A	2600	A
8	A	2602	A
8	A	2603	G
8	A	2606	C
8	A	2609	U
8	A	2610	C
8	A	2613	U
8	A	2618	G
8	A	2623	G
8	A	2627	G
8	A	2629	U
8	A	2633	G

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Mol	Chain	Res	Type
8	A	2634	A
8	A	2635	A
8	A	2636	C
8	A	2644	G
8	A	2646	C
8	A	2648	G
8	A	2650	U
8	A	2651	C
8	A	2654	A
8	A	2656	U
8	A	2660	A
8	A	2661	G
8	A	2663	G
8	A	2671	G
8	A	2682	A
8	A	2683	C
8	A	2684	U
8	A	2688	G
8	A	2690	U
8	A	2694	G
8	A	2699	C
8	A	2702	G
8	A	2707	U
8	A	2710	C
8	A	2711	A
8	A	2712	C
8	A	2714	G
8	A	2718	G
8	A	2719	G
8	A	2720	U
8	A	2721	A
8	A	2729	G
8	A	2732	G
8	A	2733	A
8	A	2739	U
8	A	2744	G
8	A	2748	A
8	A	2750	A
8	A	2751	G
8	A	2752	C
8	A	2755	C
8	A	2757	A

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Mol	Chain	Res	Type
8	A	2758	A
8	A	2761	A
8	A	2764	A
8	A	2765	A
8	A	2767	C
8	A	2778	A
8	A	2779	U
8	A	2780	G
8	A	2782	G
8	A	2787	C
8	A	2790	U
8	A	2791	G
8	A	2793	C
8	A	2796	U
8	A	2797	U
8	A	2798	U
8	A	2799	A
8	A	2800	A
8	A	2801	G
8	A	2803	G
8	A	2804	U
8	A	2809	A
8	A	2812	G
8	A	2813	A
8	A	2820	A
8	A	2821	A
8	A	2823	A
8	A	2824	C
8	A	2825	G
8	A	2831	G
8	A	2833	U
8	A	2834	G
8	A	2835	A
8	A	2849	U
8	A	2850	A
8	A	2861	U
8	A	2867	G
8	A	2868	A
8	A	2869	G
8	A	2872	A
8	A	2879	A
8	A	2883	A

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Mol	Chain	Res	Type
8	A	2884	U
8	A	2886	A
8	A	2889	C
8	A	2891	U
8	A	2892	G
8	A	2893	A
8	A	2895	G
8	A	2900	A
8	A	2901	C
9	B	3	C
9	B	7	G
9	B	9	G
9	B	10	G
9	B	13	G
9	B	14	U
9	B	16	G
9	B	17	C
9	B	18	G
9	B	19	C
9	B	22	U
9	B	25	U
9	B	30	C
9	B	32	U
9	B	34	A
9	B	35	C
9	B	37	C
9	B	40	U
9	B	41	G
9	B	42	C
9	B	44	G
9	B	46	A
9	B	47	C
9	B	51	G
9	B	53	A
9	B	56	G
9	B	57	A
9	B	58	A
9	B	62	C
9	B	65	U
9	B	66	A
9	B	67	G
9	B	73	A

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Mol	Chain	Res	Type
9	B	80	U
9	B	84	G
9	B	88	C
9	B	89	U
9	B	90	C
9	B	91	C
9	B	101	A
9	B	102	G
9	B	108	A
9	B	109	A
9	B	116	G
9	B	119	A
9	B	120	U
34	a	3	A
34	a	6	G
34	a	7	A
34	a	9	G
34	a	12	U
34	a	16	A
34	a	18	C
34	a	30	U
34	a	31	G
34	a	32	A
34	a	33	A
34	a	34	C
34	a	39	G
34	a	46	G
34	a	47	C
34	a	48	C
34	a	49	U
34	a	50	A
34	a	51	A
34	a	53	A
34	a	60	A
34	a	61	G
34	a	66	A
34	a	70	U
34	a	71	A
34	a	76	G
34	a	78	A
34	a	80	A
34	a	81	A

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Mol	Chain	Res	Type
34	a	83	C
34	a	84	U
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	94	G
34	a	95	C
34	a	96	U
34	a	99	C
34	a	107	G
34	a	108	G
34	a	109	A
34	a	110	C
34	a	117	G
34	a	121	U
34	a	122	G
34	a	130	A
34	a	131	A
34	a	144	G
34	a	145	G
34	a	149	A
34	a	153	C
34	a	159	G
34	a	160	A
34	a	161	A
34	a	163	C
34	a	165	G
34	a	166	U
34	a	169	C
34	a	171	A
34	a	173	U
34	a	174	A
34	a	175	C
34	a	179	A
34	a	180	U
34	a	182	A
34	a	183	C
34	a	184	G
34	a	185	U
34	a	196	A
34	a	197	A

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Mol	Chain	Res	Type
34	a	198	G
34	a	200	G
34	a	205	A
34	a	208	U
34	a	210	C
34	a	211	G
34	a	214	C
34	a	216	U
34	a	217	C
34	a	220	G
34	a	223	A
34	a	226	G
34	a	228	A
34	a	230	G
34	a	240	G
34	a	245	U
34	a	246	A
34	a	247	G
34	a	251	G
34	a	253	A
34	a	262	A
34	a	263	A
34	a	266	G
34	a	267	C
34	a	270	A
34	a	271	C
34	a	274	A
34	a	275	G
34	a	280	C
34	a	281	G
34	a	289	G
34	a	293	G
34	a	294	U
34	a	298	A
34	a	301	G
34	a	306	A
34	a	317	U
34	a	321	A
34	a	322	C
34	a	323	U
34	a	324	G
34	a	326	G

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Mol	Chain	Res	Type
34	a	328	C
34	a	329	A
34	a	330	C
34	a	338	A
34	a	344	A
34	a	345	C
34	a	351	G
34	a	352	C
34	a	353	A
34	a	354	G
34	a	356	A
34	a	361	G
34	a	363	A
34	a	364	A
34	a	365	U
34	a	366	A
34	a	367	U
34	a	371	A
34	a	372	C
34	a	374	A
34	a	375	U
34	a	376	G
34	a	377	G
34	a	382	A
34	a	387	U
34	a	388	G
34	a	390	U
34	a	397	A
34	a	398	U
34	a	404	G
34	a	406	G
34	a	407	U
34	a	411	A
34	a	413	G
34	a	414	A
34	a	421	U
34	a	423	G
34	a	429	U
34	a	431	A
34	a	439	U
34	a	443	C
34	a	446	G

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Mol	Chain	Res	Type
34	a	448	A
34	a	449	G
34	a	456	A
34	a	458	U
34	a	461	A
34	a	462	G
34	a	464	U
34	a	465	A
34	a	466	A
34	a	468	A
34	a	469	C
34	a	470	C
34	a	473	U
34	a	479	U
34	a	480	U
34	a	483	C
34	a	484	G
34	a	485	U
34	a	486	U
34	a	493	A
34	a	495	A
34	a	496	A
34	a	505	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	516	PSU
34	a	517	G
34	a	518	C
34	a	519	C
34	a	521	G
34	a	525	C
34	a	530	G
34	a	531	U
34	a	532	A
34	a	533	A
34	a	534	U
34	a	535	A
34	a	536	C
34	a	537	G
34	a	541	G
34	a	547	A

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Mol	Chain	Res	Type
34	a	548	G
34	a	554	A
34	a	560	A
34	a	561	U
34	a	562	U
34	a	563	A
34	a	564	C
34	a	567	G
34	a	570	G
34	a	572	A
34	a	574	A
34	a	576	C
34	a	577	G
34	a	582	C
34	a	583	A
34	a	589	U
34	a	592	G
34	a	595	A
34	a	596	A
34	a	597	G
34	a	599	C
34	a	607	A
34	a	614	C
34	a	615	G
34	a	618	C
34	a	626	G
34	a	629	A
34	a	631	C
34	a	633	G
34	a	645	G
34	a	650	G
34	a	656	G
34	a	659	U
34	a	665	A
34	a	666	G
34	a	680	C
34	a	681	A
34	a	687	A
34	a	692	U
34	a	698	G
34	a	701	U
34	a	703	G

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Mol	Chain	Res	Type
34	a	704	A
34	a	708	C
34	a	711	G
34	a	714	G
34	a	718	A
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	729	A
34	a	732	C
34	a	733	G
34	a	734	G
34	a	735	C
34	a	746	A
34	a	748	G
34	a	751	U
34	a	753	A
34	a	755	G
34	a	756	C
34	a	759	A
34	a	765	G
34	a	773	G
34	a	774	G
34	a	777	A
34	a	781	A
34	a	782	A
34	a	787	A
34	a	788	U
34	a	790	A
34	a	792	A
34	a	793	U
34	a	794	A
34	a	796	C
34	a	805	C
34	a	808	C
34	a	810	C
34	a	811	C
34	a	812	G
34	a	814	A
34	a	815	A
34	a	816	A

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Mol	Chain	Res	Type
34	a	817	C
34	a	820	U
34	a	821	G
34	a	822	U
34	a	828	U
34	a	832	G
34	a	838	G
34	a	841	C
34	a	843	U
34	a	844	G
34	a	846	G
34	a	848	C
34	a	849	G
34	a	851	G
34	a	854	U
34	a	858	G
34	a	862	C
34	a	864	A
34	a	867	G
34	a	872	A
34	a	874	G
34	a	876	C
34	a	884	U
34	a	885	G
34	a	889	A
34	a	890	G
34	a	891	U
34	a	898	G
34	a	902	G
34	a	910	C
34	a	916	U
34	a	919	A
34	a	920	U
34	a	926	G
34	a	927	G
34	a	934	C
34	a	935	A
34	a	938	A
34	a	939	G
34	a	945	G
34	a	946	A
34	a	957	U

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Mol	Chain	Res	Type
34	a	960	U
34	a	964	A
34	a	966	2MG
34	a	967	5MC
34	a	968	A
34	a	969	A
34	a	971	G
34	a	973	G
34	a	975	A
34	a	976	G
34	a	977	A
34	a	980	C
34	a	982	U
34	a	984	C
34	a	986	U
34	a	992	U
34	a	993	G
34	a	994	A
34	a	996	A
34	a	997	U
34	a	998	C
34	a	1003	G
34	a	1004	A
34	a	1005	A
34	a	1006	G
34	a	1009	U
34	a	1010	U
34	a	1014	A
34	a	1020	G
34	a	1021	A
34	a	1022	A
34	a	1023	U
34	a	1024	G
34	a	1025	U
34	a	1026	G
34	a	1027	C
34	a	1028	C
34	a	1029	U
34	a	1030	U
34	a	1031	C
34	a	1032	G
34	a	1035	A

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Mol	Chain	Res	Type
34	a	1042	A
34	a	1043	G
34	a	1044	A
34	a	1045	C
34	a	1050	G
34	a	1053	G
34	a	1054	C
34	a	1055	A
34	a	1056	U
34	a	1060	U
34	a	1064	G
34	a	1065	U
34	a	1066	C
34	a	1071	C
34	a	1079	G
34	a	1081	A
34	a	1085	U
34	a	1088	G
34	a	1092	A
34	a	1094	G
34	a	1095	U
34	a	1101	A
34	a	1103	C
34	a	1108	G
34	a	1109	C
34	a	1111	A
34	a	1113	C
34	a	1120	C
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1127	G
34	a	1129	C
34	a	1130	A
34	a	1131	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1139	G
34	a	1140	C
34	a	1143	G
34	a	1145	A

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Mol	Chain	Res	Type
34	a	1147	C
34	a	1150	A
34	a	1151	A
34	a	1152	A
34	a	1157	A
34	a	1158	C
34	a	1159	U
34	a	1160	G
34	a	1161	C
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1179	A
34	a	1184	G
34	a	1190	G
34	a	1191	A
34	a	1193	G
34	a	1194	U
34	a	1196	A
34	a	1197	A
34	a	1198	G
34	a	1200	C
34	a	1206	G
34	a	1210	C
34	a	1212	U
34	a	1213	A
34	a	1214	C
34	a	1219	A
34	a	1222	G
34	a	1224	U
34	a	1225	A
34	a	1226	C
34	a	1237	C
34	a	1238	A
34	a	1239	A
34	a	1240	U
34	a	1241	G
34	a	1248	A
34	a	1250	A
34	a	1252	A
34	a	1253	G
34	a	1254	A

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Mol	Chain	Res	Type
34	a	1256	A
34	a	1257	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1262	C
34	a	1267	C
34	a	1270	G
34	a	1274	A
34	a	1275	A
34	a	1278	G
34	a	1279	G
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1294	G
34	a	1295	U
34	a	1297	G
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1303	C
34	a	1304	G
34	a	1305	G
34	a	1307	U
34	a	1317	C
34	a	1320	C
34	a	1325	C
34	a	1328	C
34	a	1330	U
34	a	1331	G
34	a	1332	A
34	a	1338	G
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1347	G
34	a	1348	U
34	a	1350	A

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Mol	Chain	Res	Type
34	a	1351	U
34	a	1358	U
34	a	1361	G
34	a	1363	A
34	a	1364	U
34	a	1370	G
34	a	1372	U
34	a	1374	A
34	a	1375	A
34	a	1378	C
34	a	1379	G
34	a	1381	U
34	a	1383	C
34	a	1386	G
34	a	1387	G
34	a	1388	C
34	a	1394	A
34	a	1395	C
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1403	C
34	a	1408	A
34	a	1413	A
34	a	1416	G
34	a	1417	G
34	a	1418	A
34	a	1419	G
34	a	1420	U
34	a	1421	G
34	a	1423	G
34	a	1426	G
34	a	1427	C
34	a	1429	A
34	a	1430	A
34	a	1432	G
34	a	1433	A
34	a	1436	U
34	a	1437	A
34	a	1440	U
34	a	1441	A
34	a	1442	G

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Mol	Chain	Res	Type
34	a	1446	A
34	a	1448	C
34	a	1451	U
34	a	1452	C
34	a	1457	G
34	a	1459	G
34	a	1467	C
34	a	1472	U
34	a	1474	U
34	a	1475	G
34	a	1476	A
34	a	1483	A
34	a	1484	C
34	a	1485	U
34	a	1486	G
34	a	1489	G
34	a	1491	G
34	a	1492	A
34	a	1494	G
34	a	1497	G
34	a	1498	UR3
34	a	1499	A
34	a	1500	A
34	a	1503	A
34	a	1504	G
34	a	1506	U
34	a	1507	A
34	a	1508	A
34	a	1515	G
34	a	1517	G
34	a	1520	C
34	a	1524	C
34	a	1526	G
34	a	1527	U
34	a	1529	G
34	a	1530	G
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1538	C
34	a	1539	C
34	a	1540	U

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Mol	Chain	Res	Type
55	v	2	G
55	v	7	G
55	v	14	A
55	v	16	C
55	v	17	C
55	v	17(A)	U
55	v	18	G
55	v	19	G
55	v	20	H2U
55	v	21	A
55	v	24	U
55	v	33	U
55	v	34	C
55	v	35	A
55	v	38	A
55	v	42	G
55	v	43	A
55	v	44	A
55	v	47	U
55	v	48	C
55	v	52	G
55	v	55	PSU
55	v	56	C
55	v	59	A
55	v	63	G
55	v	69	C
55	v	72	A
55	v	73	A
55	v	75	C
55	v	76	A
56	w	8	4SU
56	w	13	C
56	w	16	U
56	w	17	C
56	w	18	G
56	w	19	G
56	w	20	U
56	w	21	A
56	w	22	G
56	w	31	A
56	w	33	U
56	w	40	C

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Mol	Chain	Res	Type
56	w	45	U
56	w	46	G7M
56	w	47	U
56	w	49	C
56	w	50	U
56	w	52	G
56	w	53	G
56	w	54	5MU
56	w	57	G
56	w	58	A
56	w	59	U
56	w	60	U
56	w	61	C
56	w	64	A
56	w	67	C
56	w	68	C
56	w	73	A
56	w	74	C
56	w	75	C
56	w	76	A
58	z	-1	C
58	z	0	U
58	z	2	U
58	z	4	U
58	z	5	U
58	z	8	U

All (88) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	73	A
8	A	141	G
8	A	242	G
8	A	361	G
8	A	444	C
8	A	457	A
8	A	458	G
8	A	479	A
8	A	481	G
8	A	504	A
8	A	510	C
8	A	545	U

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Mol	Chain	Res	Type
8	A	562	U
8	A	580	U
8	A	619	G
8	A	671	C
8	A	686	U
8	A	715	A
8	A	746	PSU
8	A	758	C
8	A	784	G
8	A	819	A
8	A	827	U
8	A	830	G
8	A	846	U
8	A	883	G
8	A	884	U
8	A	885	C
8	A	894	U
8	A	926	G
8	A	958	U
8	A	960	A
8	A	982	C
8	A	1024	G
8	A	1062	G
8	A	1082	U
8	A	1090	A
8	A	1093	G
8	A	1143	A
8	A	1183	U
8	A	1224	U
8	A	1300	G
8	A	1331	G
8	A	1385	A
8	A	1432	G
8	A	1552	A
8	A	1607	C
8	A	1643	G
8	A	1663	G
8	A	1715	G
8	A	1808	A
8	A	1816	C
8	A	1847	G
8	A	1875	G

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Mol	Chain	Res	Type
8	A	1899	A
8	A	1907	G
8	A	1920	C
8	A	1921	G
8	A	1981	A
8	A	2015	A
8	A	2031	A
8	A	2149	U
8	A	2150	C
8	A	2158	A
8	A	2159	G
8	A	2192	U
8	A	2287	A
8	A	2319	G
8	A	2324	U
8	A	2343	U
8	A	2344	U
8	A	2405	G
8	A	2426	A
8	A	2445	2MG
8	A	2468	A
8	A	2474	U
8	A	2481	G
8	A	2572	A
8	A	2655	G
8	A	2706	A
8	A	2728	U
8	A	2732	G
8	A	2756	U
8	A	2796	U
8	A	2808	G
8	A	2848	G
9	B	66	A
9	B	89	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	4SU	v	8	55	18,21,22	3.56	7 (38%)	26,30,33	2.08	6 (23%)
8	PSU	A	2604	8	18,21,22	1.06	2 (11%)	22,30,33	2.03	5 (22%)
56	4SU	w	8	56	18,21,22	3.57	8 (44%)	26,30,33	2.31	4 (15%)
8	6MZ	A	1618	8	18,25,26	4.09	8 (44%)	16,36,39	2.40	6 (37%)
8	PSU	A	2504	8	18,21,22	1.10	3 (16%)	22,30,33	2.17	5 (22%)
55	H2U	v	20	55	18,21,22	2.95	5 (27%)	21,30,33	2.17	5 (23%)
56	5MU	w	54	56	19,22,23	1.45	6 (31%)	28,32,35	2.26	7 (25%)
8	PSU	A	2605	8	18,21,22	1.00	1 (5%)	22,30,33	2.05	4 (18%)
56	PSU	w	32	56	18,21,22	1.06	1 (5%)	22,30,33	1.65	5 (22%)
34	2MG	a	1516	34	18,26,27	2.46	7 (38%)	16,38,41	1.32	3 (18%)
8	2MG	A	1835	8	18,26,27	2.51	7 (38%)	16,38,41	1.49	3 (18%)
8	OMC	A	2498	8	19,22,23	0.95	1 (5%)	26,31,34	1.49	2 (7%)
34	G7M	a	527	34	20,26,27	2.29	7 (35%)	17,39,42	1.37	2 (11%)
8	2MA	A	2503	8	19,25,26	2.99	7 (36%)	21,37,40	1.84	4 (19%)
55	PSU	v	55	55	18,21,22	1.11	1 (5%)	22,30,33	1.80	4 (18%)
34	2MG	a	966	34	18,26,27	2.57	7 (38%)	16,38,41	1.49	3 (18%)
56	PSU	w	55	56	18,21,22	1.43	3 (16%)	22,30,33	1.89	7 (31%)
57	FME	y	101	57	8,9,10	0.90	0	7,9,11	1.14	0
8	OMG	A	2251	8,56	18,26,27	2.53	8 (44%)	19,38,41	1.60	4 (21%)
56	PSU	w	39	56	18,21,22	1.10	1 (5%)	22,30,33	1.74	3 (13%)
8	5MU	A	1939	8	19,22,23	4.76	7 (36%)	28,32,35	3.71	13 (46%)
8	PSU	A	955	8	18,21,22	1.05	1 (5%)	22,30,33	1.88	5 (22%)
56	G7M	w	46	56	20,26,27	2.31	7 (35%)	17,39,42	1.26	1 (5%)
34	MA6	a	1519	34	18,26,27	1.05	1 (5%)	19,38,41	2.66	2 (10%)
34	PSU	a	516	34	18,21,22	1.07	1 (5%)	22,30,33	1.62	3 (13%)
8	2MG	A	2445	8	18,26,27	2.45	7 (38%)	16,38,41	1.59	4 (25%)
34	UR3	a	1498	34	19,22,23	2.48	6 (31%)	26,32,35	1.27	1 (3%)
34	MA6	a	1518	34	18,26,27	1.11	1 (5%)	19,38,41	1.90	2 (10%)
56	MIA	w	37	56	24,31,32	2.44	4 (16%)	26,44,47	3.10	9 (34%)
8	PSU	A	2457	8	18,21,22	1.05	2 (11%)	22,30,33	1.99	5 (22%)
34	5MC	a	967	34	18,22,23	3.66	7 (38%)	26,32,35	1.18	3 (11%)
8	1MG	A	745	8	18,26,27	2.57	4 (22%)	19,39,42	1.42	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PSU	A	1911	8	18,21,22	1.07	2 (11%)	22,30,33	2.15	6 (27%)
8	5MC	A	1962	8	18,22,23	3.49	7 (38%)	26,32,35	1.34	4 (15%)
8	PSU	A	1917	8	18,21,22	0.97	1 (5%)	22,30,33	1.88	4 (18%)
34	5MC	a	1407	34	18,22,23	3.44	7 (38%)	26,32,35	1.18	3 (11%)
34	2MG	a	1207	34	18,26,27	2.40	7 (38%)	16,38,41	1.44	3 (18%)
34	4OC	a	1402	34	20,23,24	2.94	8 (40%)	26,32,35	1.24	5 (19%)
8	G7M	A	2069	8	20,26,27	2.25	8 (40%)	17,39,42	1.26	1 (5%)
8	OMU	A	2552	8	19,22,23	2.90	7 (36%)	26,31,34	1.95	6 (23%)
55	5MU	v	54	55	19,22,23	4.80	7 (36%)	28,32,35	3.54	11 (39%)
8	PSU	A	746	8	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
8	PSU	A	2580	8	18,21,22	1.32	2 (11%)	22,30,33	2.23	7 (31%)
8	5MC	A	747	8	18,22,23	3.51	7 (38%)	26,32,35	1.50	2 (7%)
8	6MZ	A	2030	8	18,25,26	4.06	8 (44%)	16,36,39	2.60	4 (25%)

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
55	4SU	v	8	55	-	0/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
56	4SU	w	8	56	-	2/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	5/5/27/28	0/3/3/3
8	PSU	A	2504	8	-	0/7/25/26	0/2/2/2
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
56	5MU	w	54	56	-	3/7/25/26	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	OMC	A	2498	8	-	3/9/27/28	0/2/2/2
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
8	2MA	A	2503	8	-	3/3/25/26	0/3/3/3
55	PSU	v	55	55	-	3/7/25/26	0/2/2/2
34	2MG	a	966	34	-	1/5/27/28	0/3/3/3
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	FME	y	101	57	-	6/7/9/11	-
8	OMG	A	2251	8,56	-	3/5/27/28	0/3/3/3
56	PSU	w	39	56	-	5/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	1/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
56	G7M	w	46	56	-	3/3/25/26	0/3/3/3
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
34	PSU	a	516	34	-	1/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	4/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	3/7/29/30	0/3/3/3
56	MIA	w	37	56	-	3/11/33/34	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
34	5MC	a	967	34	-	1/7/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
8	PSU	A	1911	8	-	1/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	4/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	4OC	a	1402	34	-	3/9/29/30	0/2/2/2
8	G7M	A	2069	8	-	2/3/25/26	0/3/3/3
8	OMU	A	2552	8	-	6/9/27/28	0/2/2/2
55	5MU	v	54	55	-	2/7/25/26	0/2/2/2
8	PSU	A	746	8	-	1/7/25/26	0/2/2/2
8	PSU	A	2580	8	-	2/7/25/26	0/2/2/2
8	5MC	A	747	8	-	2/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	54	5MU	C2-N1	11.24	1.56	1.38
8	A	1939	5MU	C2-N1	11.04	1.56	1.38
55	v	54	5MU	C6-N1	10.29	1.55	1.38
8	A	1939	5MU	C6-N1	10.01	1.55	1.38
55	v	54	5MU	C4-C5	9.91	1.61	1.44
8	A	747	5MC	C6-C5	9.14	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1939	5MU	C4-C5	9.05	1.59	1.44
55	v	20	H2U	C2-N1	9.01	1.48	1.35
34	a	967	5MC	C6-C5	9.00	1.49	1.34
8	A	2030	6MZ	C3'-C4'	-8.88	1.30	1.53
8	A	1618	6MZ	C3'-C4'	-8.75	1.30	1.53
34	a	1407	5MC	C6-C5	8.68	1.48	1.34
8	A	1939	5MU	C4-N3	-8.63	1.22	1.38
8	A	1962	5MC	C6-C5	8.50	1.48	1.34
55	v	8	4SU	C4-N3	8.29	1.46	1.37
8	A	2030	6MZ	O4'-C4'	8.07	1.63	1.45
56	w	8	4SU	C4-N3	7.84	1.46	1.37
55	v	54	5MU	C4-N3	-7.73	1.24	1.38
8	A	1618	6MZ	O4'-C1'	-7.62	1.30	1.41
8	A	1618	6MZ	O4'-C4'	7.61	1.62	1.45
8	A	1618	6MZ	C6-N6	7.56	1.47	1.35
8	A	2503	2MA	C4-N3	7.51	1.47	1.35
8	A	2030	6MZ	O4'-C1'	-7.49	1.30	1.41
8	A	2030	6MZ	C6-N6	7.37	1.47	1.35
56	w	8	4SU	C2-N1	7.28	1.50	1.38
8	A	745	1MG	C2-N2	7.28	1.47	1.34
55	v	8	4SU	C2-N1	7.26	1.50	1.38
56	w	37	MIA	C13-C14	7.03	1.52	1.32
34	a	967	5MC	C4-N3	6.89	1.45	1.34
34	a	1402	4OC	C4-N3	6.82	1.44	1.32
8	A	1962	5MC	C4-N3	6.70	1.45	1.34
56	w	37	MIA	C2-S10	6.64	1.81	1.75
8	A	2552	OMU	C2-N3	6.61	1.49	1.38
8	A	747	5MC	C4-N3	6.47	1.45	1.34
8	A	2552	OMU	C2-N1	6.34	1.48	1.38
8	A	1962	5MC	C2-N3	6.27	1.49	1.36
34	a	967	5MC	C2-N3	6.19	1.48	1.36
34	a	1516	2MG	C2-N2	6.17	1.47	1.33
34	a	966	2MG	C2-N2	6.14	1.47	1.33
8	A	1835	2MG	C2-N2	6.12	1.47	1.33
55	v	20	H2U	C2-N3	6.12	1.48	1.38
8	A	2445	2MG	C2-N2	6.06	1.46	1.33
34	a	1498	UR3	C6-C5	5.98	1.49	1.35
34	a	1207	2MG	C2-N2	5.93	1.46	1.33
34	a	1407	5MC	C4-N3	5.81	1.44	1.34
8	A	1939	5MU	C6-C5	5.70	1.44	1.34
34	a	527	G7M	C2-N3	5.69	1.47	1.33
56	w	8	4SU	C4-S4	-5.69	1.57	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	8	4SU	C6-C5	5.68	1.48	1.35
8	A	2503	2MA	C2-N3	5.65	1.44	1.34
34	a	1498	UR3	C2-N1	5.65	1.46	1.38
8	A	2503	2MA	C2-N1	5.64	1.44	1.34
55	v	8	4SU	C2-N3	5.64	1.48	1.38
55	v	8	4SU	C6-C5	5.63	1.48	1.35
34	a	1407	5MC	C2-N3	5.63	1.47	1.36
8	A	747	5MC	C2-N3	5.55	1.47	1.36
34	a	1402	4OC	C6-C5	5.51	1.47	1.35
56	w	8	4SU	C2-N3	5.50	1.47	1.38
55	v	54	5MU	C6-C5	5.47	1.43	1.34
34	a	1402	4OC	C2-N3	5.42	1.47	1.36
56	w	46	G7M	C2-N3	5.41	1.46	1.33
56	w	37	MIA	C6-N6	5.41	1.44	1.34
8	A	2251	OMG	C2-N3	5.39	1.46	1.33
8	A	2552	OMU	C6-C5	5.37	1.47	1.35
8	A	2069	G7M	C2-N3	5.09	1.45	1.33
8	A	745	1MG	C2-N3	5.05	1.43	1.34
8	A	1835	2MG	C4-N3	5.04	1.49	1.37
8	A	2503	2MA	C6-N1	5.02	1.42	1.33
55	v	8	4SU	C4-S4	-4.96	1.59	1.68
34	a	1516	2MG	C4-N3	4.86	1.49	1.37
34	a	966	2MG	C4-N3	4.85	1.49	1.37
8	A	745	1MG	C4-N3	4.76	1.48	1.37
8	A	1962	5MC	C4-N4	4.73	1.46	1.34
8	A	2251	OMG	C2-N2	4.70	1.45	1.34
8	A	747	5MC	C4-N4	4.69	1.46	1.34
34	a	967	5MC	C4-N4	4.67	1.46	1.34
8	A	2251	OMG	C4-N3	4.66	1.48	1.37
55	v	20	H2U	C4-N3	4.66	1.45	1.37
34	a	1407	5MC	C4-N4	4.64	1.46	1.34
8	A	2445	2MG	C4-N3	4.62	1.48	1.37
34	a	527	G7M	C4-N3	4.53	1.48	1.37
34	a	1402	4OC	C4-N4	4.41	1.45	1.35
34	a	967	5MC	C6-N1	4.41	1.45	1.38
34	a	1207	2MG	C4-N3	4.38	1.48	1.37
34	a	967	5MC	C2-N1	4.33	1.49	1.40
34	a	1498	UR3	C2-N3	4.30	1.47	1.39
8	A	2069	G7M	C4-N3	4.28	1.47	1.37
56	w	46	G7M	C4-N3	4.27	1.47	1.37
34	a	1407	5MC	C2-N1	4.16	1.49	1.40
34	a	966	2MG	C2-N1	4.14	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	46	G7M	C2-N2	4.13	1.44	1.34
8	A	1618	6MZ	O3'-C3'	4.06	1.52	1.43
8	A	2069	G7M	C2-N2	4.00	1.43	1.34
34	a	1207	2MG	C2-N1	4.00	1.43	1.36
34	a	1407	5MC	C6-N1	3.98	1.44	1.38
34	a	527	G7M	C2-N2	3.96	1.43	1.34
34	a	1402	4OC	C2-N1	3.82	1.48	1.40
8	A	747	5MC	C6-N1	3.79	1.44	1.38
8	A	2552	OMU	C4-N3	3.76	1.45	1.38
8	A	1962	5MC	C2-N1	3.69	1.48	1.40
34	a	1516	2MG	C2-N1	3.66	1.42	1.36
55	v	55	PSU	C6-C5	3.65	1.39	1.35
8	A	2445	2MG	C2-N1	3.65	1.42	1.36
8	A	747	5MC	C2-N1	3.62	1.47	1.40
8	A	1962	5MC	C6-N1	3.56	1.44	1.38
56	w	39	PSU	C6-C5	3.55	1.39	1.35
34	a	1402	4OC	C5-C4	3.55	1.48	1.40
34	a	1407	5MC	O2-C2	-3.52	1.17	1.23
8	A	2552	OMU	O4-C4	-3.51	1.17	1.24
8	A	747	5MC	O2-C2	-3.50	1.17	1.23
8	A	2445	2MG	O6-C6	-3.48	1.16	1.23
8	A	1835	2MG	C2-N1	3.42	1.42	1.36
56	w	46	G7M	C6-N1	3.38	1.42	1.37
56	w	55	PSU	C2'-C1'	-3.37	1.49	1.53
8	A	2445	2MG	C5-C4	-3.36	1.34	1.43
34	a	1402	4OC	O2-C2	-3.33	1.17	1.23
8	A	1962	5MC	O2-C2	-3.33	1.17	1.23
34	a	966	2MG	C5-C4	-3.29	1.34	1.43
8	A	746	PSU	C6-C5	3.28	1.39	1.35
34	a	1516	2MG	O6-C6	-3.26	1.16	1.23
8	A	1835	2MG	C5-C4	-3.21	1.34	1.43
8	A	2251	OMG	C6-N1	3.21	1.42	1.37
34	a	1516	2MG	C5-C4	-3.19	1.34	1.43
34	a	966	2MG	O6-C6	-3.18	1.16	1.23
8	A	1835	2MG	O6-C6	-3.18	1.16	1.23
34	a	1207	2MG	O6-C6	-3.17	1.16	1.23
56	w	32	PSU	C6-C5	3.16	1.39	1.35
34	a	967	5MC	O2-C2	-3.16	1.17	1.23
56	w	46	G7M	C5-C6	3.16	1.53	1.45
8	A	2580	PSU	O4'-C1'	-3.11	1.39	1.43
8	A	2030	6MZ	O3'-C3'	3.09	1.50	1.43
8	A	2069	G7M	C5-C6	3.09	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1207	2MG	C5-C4	-3.07	1.35	1.43
34	a	966	2MG	C6-N1	3.07	1.42	1.37
8	A	745	1MG	C5-C4	-3.06	1.35	1.43
34	a	527	G7M	C5-C6	3.06	1.53	1.45
8	A	1939	5MU	O4-C4	-3.05	1.17	1.23
8	A	2030	6MZ	O2'-C2'	-3.04	1.35	1.43
34	a	1518	MA6	C5-C4	-3.00	1.33	1.40
8	A	1618	6MZ	O2'-C2'	-2.99	1.35	1.43
56	w	54	5MU	C4-N3	-2.98	1.33	1.38
8	A	1618	6MZ	C5-C4	-2.97	1.33	1.40
56	w	55	PSU	C2-N1	-2.97	1.32	1.36
56	w	8	4SU	C5-C4	2.97	1.46	1.42
34	a	527	G7M	O6-C6	-2.96	1.17	1.23
56	w	37	MIA	C5-C4	-2.94	1.33	1.40
8	A	1939	5MU	O2-C2	-2.94	1.17	1.23
8	A	2030	6MZ	C5-C4	-2.92	1.33	1.40
34	a	516	PSU	C6-C5	2.91	1.38	1.35
34	a	1498	UR3	O2-C2	-2.89	1.17	1.22
8	A	2069	G7M	C6-N1	2.83	1.42	1.37
8	A	1618	6MZ	C2-N3	2.82	1.36	1.32
34	a	1519	MA6	C5-C4	-2.81	1.33	1.40
8	A	2251	OMG	C5-C4	-2.81	1.35	1.43
8	A	2605	PSU	C6-C5	2.80	1.38	1.35
8	A	2069	G7M	O6-C6	-2.76	1.17	1.23
8	A	2030	6MZ	C2-N3	2.76	1.36	1.32
8	A	2552	OMU	O2-C2	-2.75	1.18	1.23
34	a	966	2MG	C5-C6	2.73	1.53	1.47
8	A	1835	2MG	C5-C6	2.70	1.52	1.47
8	A	2251	OMG	C5-C6	2.69	1.52	1.47
55	v	8	4SU	C5-C4	2.68	1.46	1.42
8	A	2251	OMG	O6-C6	-2.65	1.17	1.23
55	v	54	5MU	O4-C4	-2.64	1.18	1.23
8	A	1835	2MG	C6-N1	2.61	1.41	1.37
8	A	1911	PSU	C6-C5	2.60	1.38	1.35
56	w	46	G7M	C2-N1	2.57	1.44	1.37
56	w	46	G7M	O6-C6	-2.57	1.18	1.23
55	v	54	5MU	O2-C2	-2.57	1.18	1.23
34	a	1498	UR3	C6-N1	2.56	1.44	1.38
8	A	2604	PSU	C6-C5	2.56	1.38	1.35
8	A	2251	OMG	C2-N1	2.55	1.44	1.37
34	a	1207	2MG	C6-N1	2.54	1.41	1.37
34	a	1516	2MG	C6-N1	2.52	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	527	G7M	C6-N1	2.50	1.41	1.37
8	A	2503	2MA	C5-C4	-2.50	1.34	1.40
56	w	54	5MU	C6-C5	2.49	1.38	1.34
55	v	8	4SU	O2-C2	-2.48	1.18	1.23
34	a	1402	4OC	C6-N1	2.46	1.43	1.38
8	A	2504	PSU	C6-C5	2.45	1.38	1.35
8	A	955	PSU	C6-C5	2.44	1.38	1.35
8	A	2552	OMU	C6-N1	2.43	1.43	1.38
8	A	2457	PSU	C6-C5	2.42	1.38	1.35
8	A	2503	2MA	C6-N6	-2.42	1.25	1.34
55	v	20	H2U	O4-C4	-2.40	1.18	1.23
8	A	1917	PSU	C6-C5	2.39	1.38	1.35
55	v	20	H2U	O2-C2	-2.37	1.18	1.23
34	a	1207	2MG	C5-C6	2.36	1.52	1.47
8	A	2069	G7M	C5-C4	-2.34	1.34	1.39
56	w	54	5MU	C6-N1	-2.34	1.34	1.38
56	w	8	4SU	O2-C2	-2.33	1.18	1.23
34	a	1498	UR3	O4-C4	-2.32	1.18	1.23
8	A	2503	2MA	C6-C5	2.27	1.51	1.43
8	A	1911	PSU	C4-C5	-2.23	1.37	1.44
8	A	2580	PSU	C4-C5	-2.23	1.37	1.44
56	w	54	5MU	C2-N1	2.22	1.42	1.38
8	A	2445	2MG	C6-N1	2.22	1.41	1.37
8	A	2604	PSU	O4'-C1'	-2.20	1.40	1.43
56	w	55	PSU	C2-N3	-2.20	1.33	1.37
56	w	54	5MU	C2-N3	-2.20	1.34	1.38
8	A	2504	PSU	C4-C5	-2.17	1.38	1.44
56	w	54	5MU	C4-C5	2.12	1.48	1.44
8	A	2445	2MG	C5-C6	2.11	1.51	1.47
34	a	527	G7M	C2-N1	2.11	1.42	1.37
8	A	2069	G7M	C2-N1	2.08	1.42	1.37
8	A	2504	PSU	O4'-C1'	-2.08	1.41	1.43
8	A	2457	PSU	O4'-C1'	-2.05	1.41	1.43
34	a	1516	2MG	C5-C6	2.02	1.51	1.47
56	w	8	4SU	C6-N1	2.01	1.42	1.38
8	A	2498	OMC	C5-C4	-2.01	1.38	1.42

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1939	5MU	C5-C4-N3	11.77	125.36	115.31
55	v	54	5MU	C5-C4-N3	11.06	124.75	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1939	5MU	C5-C6-N1	-10.15	112.89	123.34
34	a	1519	MA6	N1-C6-N6	-9.77	106.78	117.06
55	v	54	5MU	C5-C6-N1	-9.01	114.07	123.34
56	w	37	MIA	C12-C13-C14	-8.92	109.78	127.14
56	w	37	MIA	C11-S10-C2	8.85	108.87	102.27
56	w	8	4SU	C4-N3-C2	-7.79	119.77	127.34
55	v	20	H2U	C4-N3-C2	-7.71	119.39	125.79
8	A	2030	6MZ	C9-N6-C6	-7.18	116.69	122.87
56	w	8	4SU	C5-C4-N3	6.43	120.65	114.69
55	v	8	4SU	C4-N3-C2	-6.25	121.27	127.34
8	A	747	5MC	C5-C6-N1	-5.90	117.27	123.34
8	A	2605	PSU	C4-N3-C2	-5.84	117.92	126.34
8	A	2604	PSU	C4-N3-C2	-5.78	118.01	126.34
8	A	2504	PSU	C4-N3-C2	-5.72	118.10	126.34
8	A	2457	PSU	C4-N3-C2	-5.68	118.16	126.34
8	A	1939	5MU	N3-C2-N1	5.61	122.34	114.89
34	a	1518	MA6	N1-C6-N6	-5.55	111.21	117.06
8	A	2030	6MZ	N3-C2-N1	-5.51	120.06	128.68
8	A	1618	6MZ	N3-C2-N1	-5.45	120.17	128.68
8	A	1939	5MU	O4-C4-C5	-5.44	118.60	124.90
34	a	1519	MA6	N3-C2-N1	-5.44	120.18	128.68
56	w	54	5MU	C4-N3-C2	-5.42	120.34	127.35
34	a	1518	MA6	N3-C2-N1	-5.37	120.29	128.68
8	A	1939	5MU	C4-N3-C2	-5.35	120.43	127.35
56	w	54	5MU	N3-C2-N1	5.29	121.91	114.89
8	A	2552	OMU	C4-N3-C2	-5.28	119.62	126.58
8	A	1911	PSU	C4-N3-C2	-5.18	118.87	126.34
55	v	54	5MU	C5M-C5-C6	-5.17	115.95	122.85
8	A	2580	PSU	N1-C2-N3	5.15	120.97	115.13
8	A	1911	PSU	N1-C2-N3	5.10	120.91	115.13
8	A	1917	PSU	C4-N3-C2	-5.09	119.01	126.34
8	A	2580	PSU	C4-N3-C2	-5.08	119.01	126.34
8	A	2504	PSU	N1-C2-N3	5.07	120.88	115.13
8	A	2605	PSU	N1-C2-N3	5.06	120.86	115.13
8	A	1618	6MZ	C9-N6-C6	-5.05	118.53	122.87
8	A	2498	OMC	C2'-C1'-N1	-4.99	104.54	114.22
55	v	54	5MU	C5M-C5-C4	4.95	124.21	118.77
56	w	37	MIA	C15-C14-C13	-4.95	108.35	122.65
55	v	54	5MU	N3-C2-N1	4.95	121.45	114.89
8	A	2503	2MA	C1'-N9-C4	-4.90	118.04	126.64
55	v	55	PSU	N1-C2-N3	4.88	120.66	115.13
8	A	1917	PSU	N1-C2-N3	4.83	120.61	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	8	4SU	C5-C4-S4	-4.83	118.24	124.47
56	w	37	MIA	C16-C14-C13	-4.77	108.86	122.65
8	A	2457	PSU	N1-C2-N3	4.75	120.51	115.13
56	w	39	PSU	N1-C2-N3	4.75	120.51	115.13
8	A	955	PSU	N1-C2-N3	4.72	120.48	115.13
8	A	746	PSU	C4-N3-C2	-4.70	119.57	126.34
55	v	54	5MU	C4-N3-C2	-4.70	121.27	127.35
8	A	2604	PSU	N1-C2-N3	4.69	120.44	115.13
34	a	1498	UR3	C4-N3-C2	-4.63	120.20	124.56
56	w	32	PSU	C4-N3-C2	-4.58	119.73	126.34
55	v	54	5MU	O4-C4-C5	-4.57	119.61	124.90
56	w	54	5MU	C5-C4-N3	4.56	119.20	115.31
34	a	516	PSU	C4-N3-C2	-4.49	119.87	126.34
8	A	746	PSU	N1-C2-N3	4.48	120.21	115.13
55	v	8	4SU	C5-C4-N3	4.43	118.80	114.69
8	A	2580	PSU	C6-C5-C4	4.39	121.27	118.20
34	a	527	G7M	C2-N1-C6	-4.34	117.12	125.10
55	v	55	PSU	C4-N3-C2	-4.32	120.12	126.34
56	w	39	PSU	C4-N3-C2	-4.31	120.12	126.34
56	w	55	PSU	N1-C2-N3	4.27	119.97	115.13
8	A	745	1MG	C5-C6-N1	4.26	120.31	113.90
8	A	2503	2MA	C2-N3-C4	4.23	118.96	115.52
8	A	1911	PSU	C6-C5-C4	4.21	121.14	118.20
56	w	8	4SU	C5-C4-S4	-4.09	119.19	124.47
8	A	1962	5MC	C5-C6-N1	-4.00	119.22	123.34
8	A	2504	PSU	C6-C5-C4	3.95	120.96	118.20
8	A	1835	2MG	C5-C6-N1	3.86	120.77	113.95
34	a	966	2MG	C5-C6-N1	3.86	120.76	113.95
56	w	54	5MU	C5-C6-N1	-3.82	119.41	123.34
8	A	955	PSU	C4-N3-C2	-3.80	120.86	126.34
56	w	32	PSU	N1-C2-N3	3.78	119.41	115.13
8	A	2251	OMG	C5-C6-N1	3.76	120.59	113.95
56	w	46	G7M	C2-N1-C6	-3.75	118.18	125.10
34	a	516	PSU	N1-C2-N3	3.73	119.35	115.13
8	A	2552	OMU	C5-C4-N3	3.69	120.36	114.84
56	w	54	5MU	O4-C4-C5	-3.69	120.63	124.90
8	A	2552	OMU	N3-C2-N1	3.69	119.78	114.89
8	A	955	PSU	C6-C5-C4	3.68	120.77	118.20
34	a	967	5MC	C5-C6-N1	-3.63	119.60	123.34
8	A	2030	6MZ	C1'-N9-C4	-3.60	120.31	126.64
8	A	2445	2MG	C5-C6-N1	3.59	120.28	113.95
8	A	1618	6MZ	C1'-N9-C4	-3.51	120.47	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	55	PSU	C4-N3-C2	-3.50	121.29	126.34
34	a	1516	2MG	C5-C6-N1	3.47	120.08	113.95
8	A	2552	OMU	O4-C4-C5	-3.47	119.06	125.16
8	A	2251	OMG	C2-N1-C6	-3.43	118.78	125.10
56	w	55	PSU	O2-C2-N1	-3.40	119.04	122.79
56	w	54	5MU	C3'-C2'-C1'	3.37	107.84	101.43
8	A	2552	OMU	C1'-N1-C2	3.37	123.66	117.57
8	A	1939	5MU	C5M-C5-C6	-3.36	118.36	122.85
56	w	37	MIA	C2-N3-C4	3.33	119.92	115.32
55	v	20	H2U	N3-C2-N1	3.29	120.13	116.65
56	w	37	MIA	N3-C2-N1	-3.27	120.97	126.98
8	A	2069	G7M	C2-N1-C6	-3.24	119.13	125.10
56	w	8	4SU	N3-C2-N1	3.19	119.12	114.89
55	v	20	H2U	C5-C4-N3	3.15	120.19	116.65
34	a	1207	2MG	C5-C6-N1	3.15	119.51	113.95
8	A	2503	2MA	N3-C2-N1	-3.14	119.99	125.73
34	a	1407	5MC	C5-C6-N1	-3.12	120.12	123.34
8	A	1962	5MC	CM5-C5-C6	-3.04	118.79	122.85
55	v	55	PSU	C6-N1-C2	-3.02	119.59	122.68
8	A	1911	PSU	O2-C2-N1	-2.93	119.57	122.79
8	A	955	PSU	O2-C2-N1	-2.92	119.57	122.79
56	w	55	PSU	O4-C4-C5	-2.92	116.40	124.05
8	A	1939	5MU	C6-C5-C4	2.91	120.47	118.03
55	v	8	4SU	N3-C2-N1	2.89	118.73	114.89
8	A	955	PSU	C6-N1-C2	-2.88	119.74	122.68
8	A	2251	OMG	O6-C6-C5	-2.83	118.84	124.37
8	A	2503	2MA	CM2-C2-N1	2.81	121.53	117.15
34	a	1207	2MG	CM2-N2-C2	-2.81	117.67	123.86
8	A	1939	5MU	C6-N1-C2	-2.80	118.46	121.30
55	v	8	4SU	S4-C4-N3	2.79	122.96	120.21
8	A	2580	PSU	C5-C6-N1	-2.78	117.93	122.11
8	A	2030	6MZ	O4'-C1'-C2'	-2.78	102.86	106.93
8	A	1835	2MG	C8-N7-C5	2.78	108.28	102.99
56	w	39	PSU	C6-N1-C2	-2.74	119.88	122.68
56	w	55	PSU	C6-C5-C4	-2.74	116.28	118.20
8	A	1917	PSU	C6-N1-C2	-2.72	119.91	122.68
55	v	20	H2U	O2-C2-N1	-2.70	119.71	123.11
8	A	1618	6MZ	C2'-C3'-C4'	2.69	107.88	102.64
8	A	747	5MC	CM5-C5-C6	-2.69	119.25	122.85
34	a	966	2MG	C8-N7-C5	2.68	108.10	102.99
55	v	54	5MU	C6-N1-C2	-2.66	118.60	121.30
8	A	2251	OMG	C8-N7-C5	2.65	108.04	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	967	5MC	CM5-C5-C6	-2.64	119.32	122.85
8	A	746	PSU	O2-C2-N1	-2.64	119.89	122.79
55	v	54	5MU	O2-C2-N1	-2.64	119.28	122.79
8	A	745	1MG	C8-N7-C5	2.62	107.98	102.99
8	A	2498	OMC	O2-C2-N3	-2.62	118.07	122.33
56	w	37	MIA	C1'-N9-C4	2.61	131.23	126.64
34	a	1407	5MC	O2-C2-N3	-2.59	118.13	122.33
34	a	1516	2MG	O6-C6-C5	-2.55	119.39	124.37
55	v	8	4SU	C1'-N1-C2	2.55	122.18	117.57
8	A	2552	OMU	O2-C2-N1	-2.54	119.42	122.79
8	A	2604	PSU	C5-C6-N1	-2.52	118.33	122.11
8	A	2445	2MG	C8-N7-C5	2.51	107.78	102.99
8	A	1917	PSU	O2-C2-N1	-2.50	120.04	122.79
34	a	1402	4OC	C6-C5-C4	2.49	120.01	116.96
8	A	1618	6MZ	O3'-C3'-C2'	2.47	119.80	111.82
8	A	2504	PSU	C5-C6-N1	-2.46	118.42	122.11
8	A	745	1MG	O6-C6-C5	-2.45	119.85	124.19
8	A	1962	5MC	C1'-N1-C6	-2.45	117.05	121.12
34	a	1407	5MC	CM5-C5-C6	-2.42	119.61	122.85
34	a	1402	4OC	O2-C2-N3	-2.40	118.42	122.33
8	A	2580	PSU	O2-C2-N3	-2.40	117.29	121.82
34	a	1402	4OC	C1'-N1-C6	-2.40	115.61	120.84
34	a	1207	2MG	C8-N7-C5	2.39	107.54	102.99
56	w	54	5MU	O2-C2-N1	-2.38	119.62	122.79
8	A	2504	PSU	O2-C2-N1	-2.37	120.18	122.79
55	v	20	H2U	C5-C6-N1	2.37	119.43	111.61
55	v	54	5MU	O4-C4-N3	-2.37	115.57	120.12
34	a	966	2MG	O6-C6-C5	-2.36	119.77	124.37
8	A	2457	PSU	C5-C6-N1	-2.33	118.61	122.11
55	v	55	PSU	O2-C2-N1	-2.33	120.22	122.79
8	A	2580	PSU	O4'-C1'-C2'	2.33	108.43	105.14
8	A	2445	2MG	O6-C6-C5	-2.33	119.82	124.37
34	a	1516	2MG	C8-N7-C5	2.32	107.42	102.99
56	w	32	PSU	O2-C2-N1	-2.31	120.25	122.79
8	A	2445	2MG	C3'-C2'-C1'	2.29	104.43	100.98
56	w	37	MIA	C16-C14-C15	-2.28	109.56	114.60
34	a	1402	4OC	C1'-N1-C2	2.27	123.48	118.42
34	a	527	G7M	O6-C6-N1	-2.26	117.98	120.65
56	w	55	PSU	O4-C4-N3	2.26	124.45	120.12
8	A	2605	PSU	C5-C4-N3	2.26	121.68	116.58
8	A	1835	2MG	O6-C6-C5	-2.25	119.97	124.37
8	A	2604	PSU	C5-C4-N3	2.25	121.67	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	55	PSU	O3'-C3'-C4'	2.21	117.44	111.05
8	A	2604	PSU	O4'-C1'-C2'	2.20	108.25	105.14
56	w	37	MIA	S10-C2-N1	2.19	123.58	116.01
8	A	1939	5MU	C1'-N1-C2	2.18	121.52	117.57
8	A	1939	5MU	C5M-C5-C4	2.18	121.17	118.77
8	A	2457	PSU	C5-C4-N3	2.18	121.51	116.58
8	A	1911	PSU	C6-N1-C2	-2.17	120.46	122.68
8	A	1939	5MU	O4-C4-N3	-2.17	115.96	120.12
8	A	2605	PSU	C5-C6-N1	-2.17	118.86	122.11
8	A	1618	6MZ	C3'-C2'-C1'	2.16	104.23	100.98
34	a	516	PSU	O4'-C1'-C2'	2.15	108.17	105.14
8	A	2580	PSU	C3'-C2'-C1'	2.14	104.13	101.64
8	A	746	PSU	C6-N1-C2	-2.14	120.50	122.68
55	v	54	5MU	C6-C5-C4	2.13	119.81	118.03
8	A	1939	5MU	O2-C2-N3	-2.12	117.54	121.50
8	A	2457	PSU	C6-C5-C4	2.10	119.66	118.20
34	a	967	5MC	C1'-N1-C6	-2.09	117.64	121.12
8	A	1962	5MC	C5-C4-N3	-2.08	119.43	121.67
34	a	1402	4OC	C5-C4-N4	-2.05	118.43	122.61
56	w	32	PSU	O4'-C1'-C2'	2.03	108.00	105.14
8	A	1939	5MU	O2-C2-N1	-2.02	120.11	122.79
8	A	1911	PSU	C5-C6-N1	-2.01	119.10	122.11
56	w	32	PSU	C5-C4-N3	2.00	121.11	116.58

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	20	H2U	O4'-C1'-N1-C6
55	v	20	H2U	C2'-C1'-N1-C2
55	v	20	H2U	C2'-C1'-N1-C6
8	A	747	5MC	C3'-C4'-C5'-O5'
8	A	1618	6MZ	C5-C6-N6-C9
8	A	1618	6MZ	N1-C6-N6-C9
8	A	2251	OMG	O4'-C4'-C5'-O5'
8	A	2251	OMG	C3'-C4'-C5'-O5'
8	A	2498	OMC	C1'-C2'-O2'-CM2
8	A	2503	2MA	O4'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C1'-N1-C2
8	A	2552	OMU	O4'-C1'-N1-C6
8	A	2552	OMU	C1'-C2'-O2'-CM2
8	A	2580	PSU	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
34	a	1402	4OC	C1'-C2'-O2'-CM2
34	a	1498	UR3	O4'-C4'-C5'-O5'
34	a	1518	MA6	C5-C6-N6-C10
34	a	1518	MA6	N1-C6-N6-C10
34	a	1519	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	C2'-C1'-C5-C6
56	w	39	PSU	O4'-C1'-C5-C6
56	w	46	G7M	C3'-C4'-C5'-O5'
56	w	54	5MU	O4'-C4'-C5'-O5'
57	y	101	FME	O1-CN-N-CA
57	y	101	FME	N-CA-CB-CG
57	y	101	FME	O-C-CA-CB
34	a	1519	MA6	C4'-C5'-O5'-P
8	A	1618	6MZ	O4'-C4'-C5'-O5'
8	A	1618	6MZ	C3'-C4'-C5'-O5'
8	A	1962	5MC	O4'-C4'-C5'-O5'
8	A	2069	G7M	O4'-C4'-C5'-O5'
8	A	2445	2MG	O4'-C4'-C5'-O5'
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2498	OMC	O4'-C4'-C5'-O5'
34	a	1498	UR3	C3'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C2
8	A	747	5MC	O4'-C4'-C5'-O5'
8	A	1835	2MG	C3'-C4'-C5'-O5'
8	A	1962	5MC	C3'-C4'-C5'-O5'
8	A	2069	G7M	C3'-C4'-C5'-O5'
8	A	2503	2MA	C3'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
56	w	54	5MU	C3'-C4'-C5'-O5'
34	a	1519	MA6	N1-C6-N6-C9
34	a	1498	UR3	O4'-C1'-N1-C6
57	y	101	FME	CB-CG-SD-CE
55	v	55	PSU	C3'-C4'-C5'-O5'
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	2498	OMC	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	w	39	PSU	C3'-C4'-C5'-O5'
55	v	54	5MU	O4'-C4'-C5'-O5'
55	v	55	PSU	O4'-C4'-C5'-O5'
56	w	46	G7M	O4'-C4'-C5'-O5'
55	v	54	5MU	C3'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C4'-C5'-O5'
8	A	2251	OMG	C4'-C5'-O5'-P
56	w	39	PSU	O4'-C4'-C5'-O5'
34	a	966	2MG	C4'-C5'-O5'-P
55	v	55	PSU	C4'-C5'-O5'-P
8	A	2552	OMU	C4'-C5'-O5'-P
34	a	527	G7M	C4'-C5'-O5'-P
8	A	1962	5MC	C4'-C5'-O5'-P
34	a	1518	MA6	C5-C6-N6-C9
56	w	46	G7M	C4'-C5'-O5'-P
56	w	54	5MU	C4'-C5'-O5'-P
8	A	2030	6MZ	C3'-C4'-C5'-O5'
57	y	101	FME	C-CA-CB-CG
8	A	1618	6MZ	C4'-C5'-O5'-P
8	A	2030	6MZ	C4'-C5'-O5'-P
8	A	2503	2MA	C4'-C5'-O5'-P
55	v	20	H2U	C4'-C5'-O5'-P
8	A	1939	5MU	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
56	w	8	4SU	C4'-C5'-O5'-P
8	A	2552	OMU	C3'-C4'-C5'-O5'
8	A	746	PSU	O4'-C1'-C5-C6
8	A	2580	PSU	O4'-C1'-C5-C6
56	w	8	4SU	O4'-C4'-C5'-O5'
56	w	55	PSU	O4'-C4'-C5'-O5'
55	v	20	H2U	O4'-C1'-N1-C2
56	w	37	MIA	N1-C2-S10-C11
34	a	516	PSU	C3'-C4'-C5'-O5'
8	A	1962	5MC	C2'-C1'-N1-C6
57	y	101	FME	CB-CA-N-CN
8	A	1911	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
60	AM2	a	2001	-	40,40,40	1.66	10 (25%)	53,60,60	1.71	11 (20%)

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
60	AM2	a	2001	-	-	8/12/84/84	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	a	2001	AM2	OA4-CA1	4.04	1.52	1.41
60	a	2001	AM2	CB3-CB4	-3.69	1.48	1.53
60	a	2001	AM2	OA5-CA8	3.20	1.50	1.41
60	a	2001	AM2	OA5-CA4	3.08	1.51	1.44
60	a	2001	AM2	OB1-CB1	2.89	1.49	1.41
60	a	2001	AM2	OA8-CA8	-2.63	1.34	1.41
60	a	2001	AM2	OA8-CB1	-2.58	1.34	1.41
60	a	2001	AM2	OA4-CA5	2.57	1.48	1.44
60	a	2001	AM2	OA1-CA1	-2.50	1.34	1.41
60	a	2001	AM2	CA7-NA7	-2.27	1.43	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	a	2001	AM2	CA1-OA1-CC1	-5.36	104.71	117.96
60	a	2001	AM2	CA8-CA7-NA7	-3.99	103.86	111.00
60	a	2001	AM2	CB1-OA8-CA8	-3.84	107.56	114.42
60	a	2001	AM2	CA9-NA7-CA7	-3.31	109.57	114.38
60	a	2001	AM2	OA1-CA1-CA2	3.21	113.61	108.23
60	a	2001	AM2	CA8-OA5-CA4	-2.69	108.41	113.69
60	a	2001	AM2	CB1-OB1-CB5	-2.46	108.87	113.69
60	a	2001	AM2	OA5-CA4-CA3	2.41	113.38	108.39
60	a	2001	AM2	OA8-CB1-OB1	-2.38	104.03	110.67
60	a	2001	AM2	OA8-CA8-CA7	-2.11	104.60	108.24
60	a	2001	AM2	CA6-CA5-CA4	2.01	115.53	110.93

There are no chirality outliers.

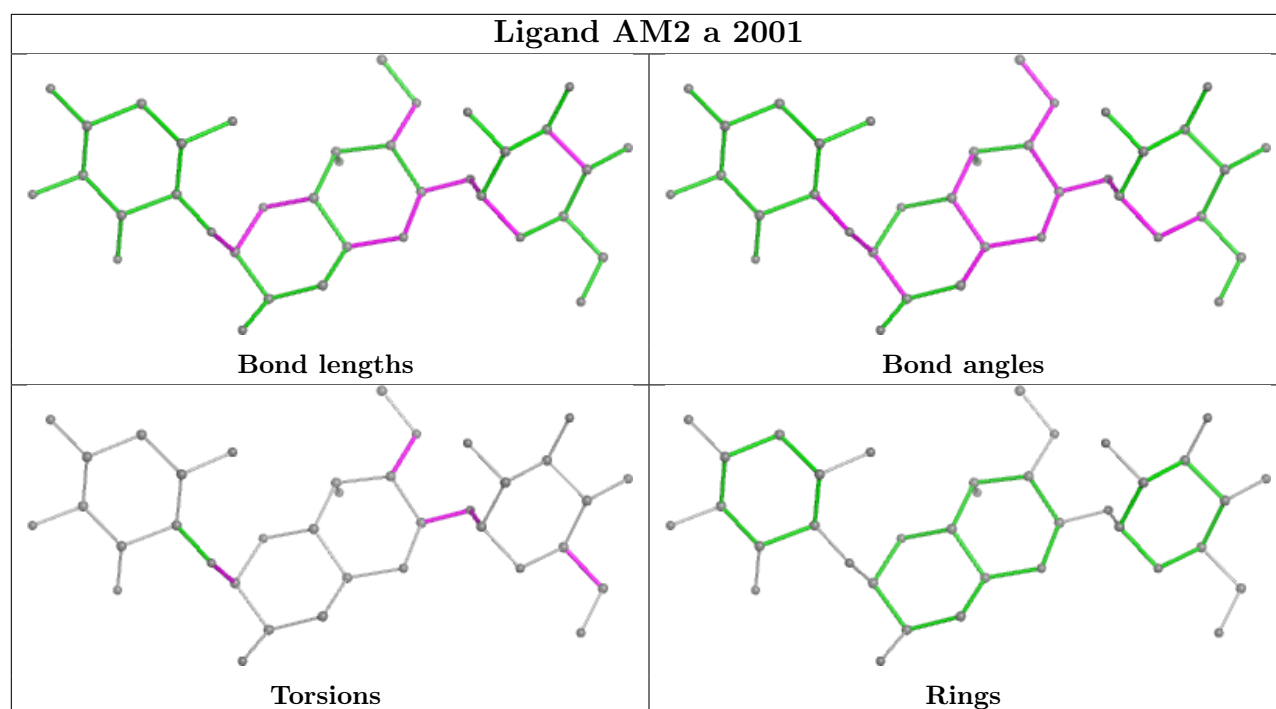
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	a	2001	AM2	CA7-CA8-OA8-CB1
60	a	2001	AM2	OA5-CA8-OA8-CB1
60	a	2001	AM2	OB1-CB5-CB6-OB6
60	a	2001	AM2	CB4-CB5-CB6-OB6
60	a	2001	AM2	OB1-CB1-OA8-CA8
60	a	2001	AM2	CB2-CB1-OA8-CA8
60	a	2001	AM2	CA6-CA7-NA7-CA9
60	a	2001	AM2	OA4-CA1-OA1-CC1

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.