Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:03 pm GMT

PDB ID	:	5OPT
EMDB ID	:	EMD-3844
Title	:	Structure of KSRP in context of Trypanosoma cruzi 40S
Authors	:	Brito Querido, J.; Mancera-Martinez, E.; Vicens, Q.; Bochler, A.; Chicher, J.; Simonetti, A.; Hashem, Y.
Deposited on	:	2017-08-10
Resolution	:	4.00 Å(reported)

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:

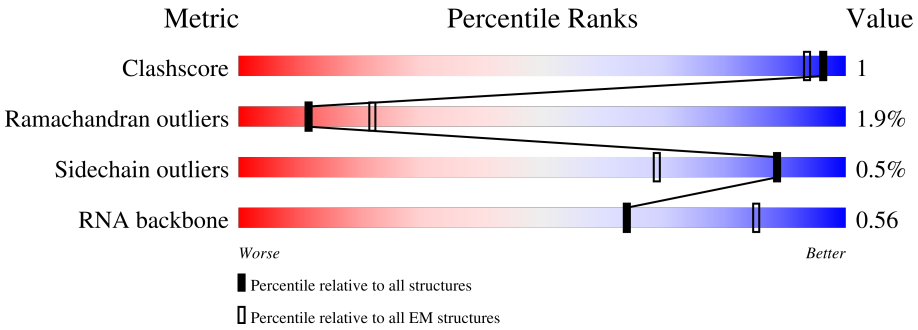
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	p	318	85% 95%
2	q	57	37% 63% 33%
3	r	149	50% 84% 9% 6%
4	t	152	55% 74% 22%
5	u	153	51% 74% 22%
6	L	273	26% 94% 5%
7	M	143	22% 99%

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Mol	Chain	Length	Quality of chain
8	O	190	58% 95% 5%
9	Q	211	22% 91% 5%
10	R	151	25% 92% 7%
11	S	86	37% 93% 5%
12	T	112	32% 93% 7%
13	U	112	43% 60% 39%
14	V	144	33% 92% 6%
15	W	261	21% 81% 17%
16	X	173	27% 84% 14%
17	Y	137	13% 90% 10%
18	Z	221	15% 77% 21%
19	b	190	17% 85% 14%
20	f	245	23% 82% 16%
21	d	263	24% 84% 15%
22	e	130	19% 98%
23	g	236	11% 35% 65%
24	a	110	40% 56% 7% 36%
25	i	141	79% 82% 14%
26	j	150	35% 38% 57%
27	P	250	27% 99%
28	k	196	32% 59% 40%
29	l	117	57% 85% 15%
30	m	214	67% 88% 5% 7%
31	n	161	41% 55% 42%
32	o	167	44% 79% 16%

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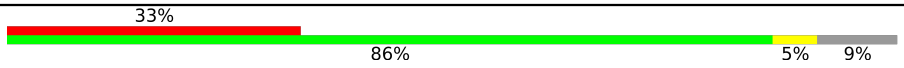
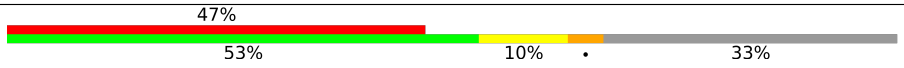
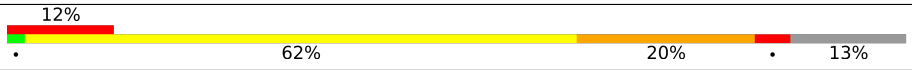
Mol	Chain	Length	Quality of chain
33	c	66	
34	h	257	
35	E	2319	

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 82219 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 Activated protein kinase C receptor, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	p	310	2405	1505	424	463	13	0	0

- Molecule 2 is a protein called Ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	q	38	311	191	64	52	4	0	0

- Molecule 3 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	r	140	1113	706	212	192	3	0	0

- Molecule 4 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	t	119	969	615	185	165	4	0	0

- Molecule 5 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	u	120	981	614	194	169	4	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	258	2038	1290	383	354	11	0	0

- Molecule 7 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	142	Total	C	N	O	S	0	0
			1116	706	220	188	2		

- Molecule 8 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	190	Total	C	N	O	S	0	0
			1493	932	286	269	6		

- Molecule 9 is a protein called Ribosomal protein S7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	200	Total	C	N	O	S	0	0
			1670	1063	324	277	6		

- Molecule 10 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	141	Total	C	N	O	S	0	0
			1143	724	221	190	8		

- Molecule 11 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	82	Total	C	N	O	S	0	0
			630	384	121	116	9		

- Molecule 12 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	104	Total	C	N	O	S	0	0
			829	510	177	132	10		

- Molecule 13 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	68	Total	C	N	O	S	0	0
			526	315	107	100	4		

- Molecule 14 is a protein called 40S ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	135	Total	C	N	O	S	0	0
			1011	620	195	187	9		

- Molecule 15 is a protein called 40S ribosomal protein S3a-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	217	Total	C	N	O	S	0	0
			1781	1124	337	313	7		

- Molecule 16 is a protein called 40S ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	148	Total	C	N	O	S	0	0
			1212	760	239	207	6		

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	123	Total	C	N	O	S	0	0
			989	628	194	165	2		

- Molecule 18 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	175	Total	C	N	O	S	0	0
			1404	885	283	233	3		

- Molecule 19 is a protein called 40S ribosomal protein S9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	164	Total	C	N	O	S	0	0
			1365	864	266	227	8		

- Molecule 20 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	f	207	Total	C	N	O	S	0	0
			1658	1060	299	288	11		

- Molecule 21 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	223	Total	C	N	O	S	0	0
			1726	1098	304	314	10		

- Molecule 22 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	129	Total	C	N	O	S	0	0
			1019	647	188	176	8		

- Molecule 23 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	83	Total	C	N	O	S	0	0
			635	395	116	122	2		

- Molecule 24 is a protein called Ribosomal protein S25, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	70	Total	C	N	O	S	0	0
			553	356	97	97	3		

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	i	121	Total	C	N	O	S	0	0
			958	594	174	185	5		

- Molecule 26 is a protein called Ubiquitin/ribosomal protein S27a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	j	64	Total	C	N	O	S	0	0
			518	324	98	90	6		

- Molecule 27 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	249	Total	C	N	O	S	0	0
			1983	1244	402	333	4		

- Molecule 28 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	118	Total	C	N	O	S	0	0
			972	610	187	170	5		

- Molecule 29 is a protein called Ribosomal protein S20, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	l	99	Total	C	N	O	S	0	0
			784	497	144	140	3		

- Molecule 30 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	m	200	Total	C	N	O	S	0	0
			1587	995	302	279	11		

- Molecule 31 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	n	93	Total	C	N	O	S	0	0
			780	508	136	132	4		

- Molecule 32 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	o	140	Total	C	N	O	S	0	0
			1116	702	221	185	8		

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	60	Total	C	N	O	S	0	0
			480	303	98	78	1		

- Molecule 34 is a protein called RNA-binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	173	Total	C	N	O	S	0	0
			1358	862	259	234	3		

- Molecule 35 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E	2022	Total	C	N	O	P	0	0
			43106	19268	7710	14111	2017		

There are 5 discrepancies between the modelled and reference sequences:

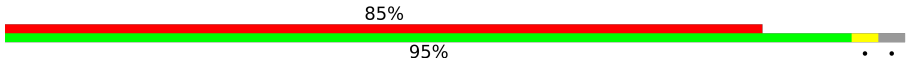
Chain	Residue	Modelled	Actual	Comment	Reference
E	143	C	A	conflict	GB 320364483
E	805	C	U	conflict	GB 320364483
E	2316	U	-	insertion	GB 320364483
E	2317	U	-	insertion	GB 320364483
E	2318	U	-	insertion	GB 320364483

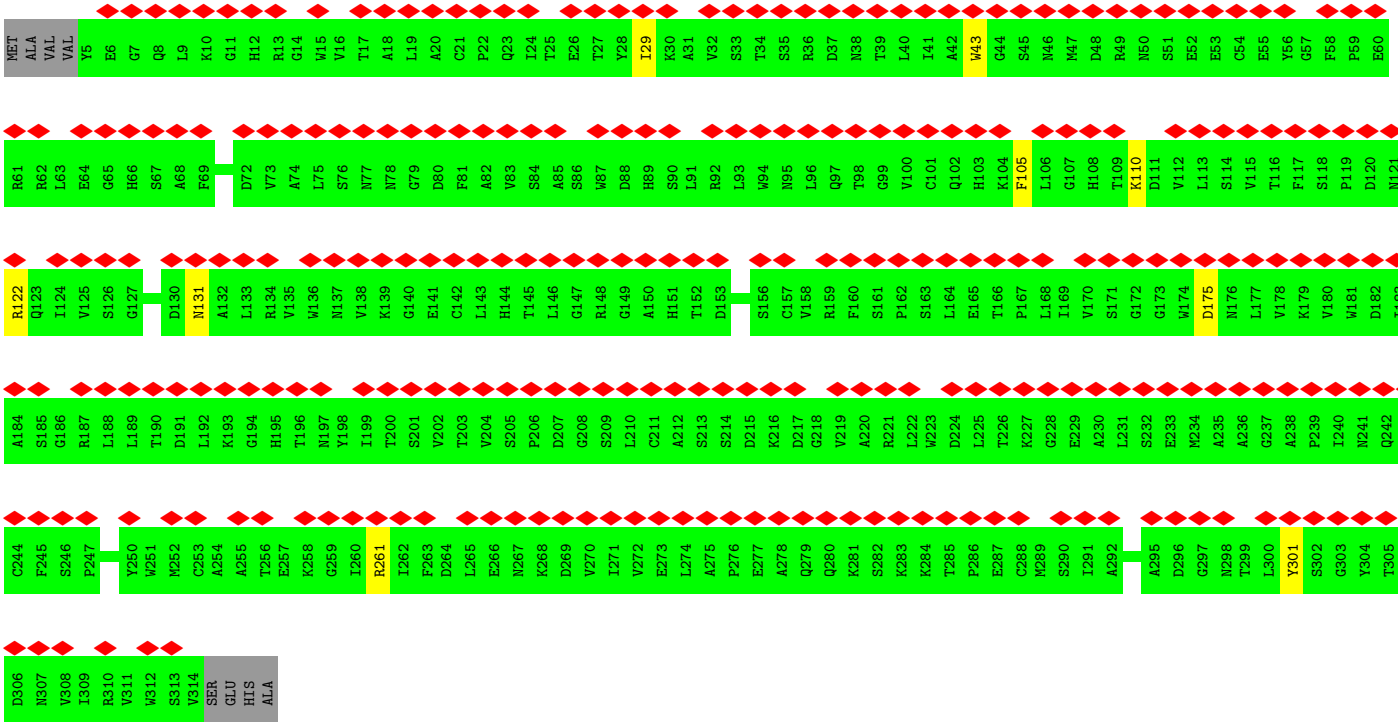
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Activated protein kinase C receptor, putative

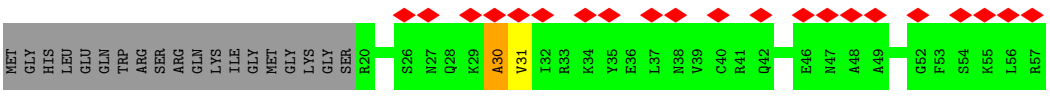
Chain p:





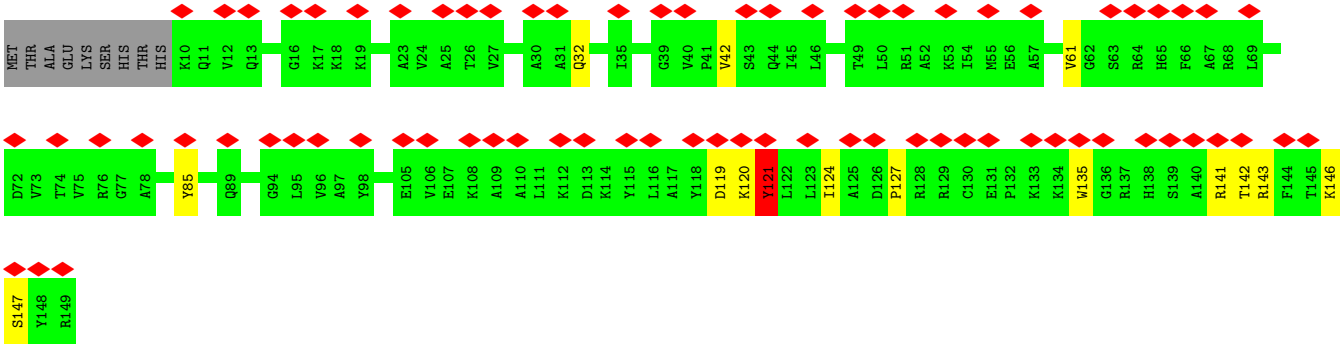
• Molecule 2: Ribosomal protein S29, putative

Chain q:



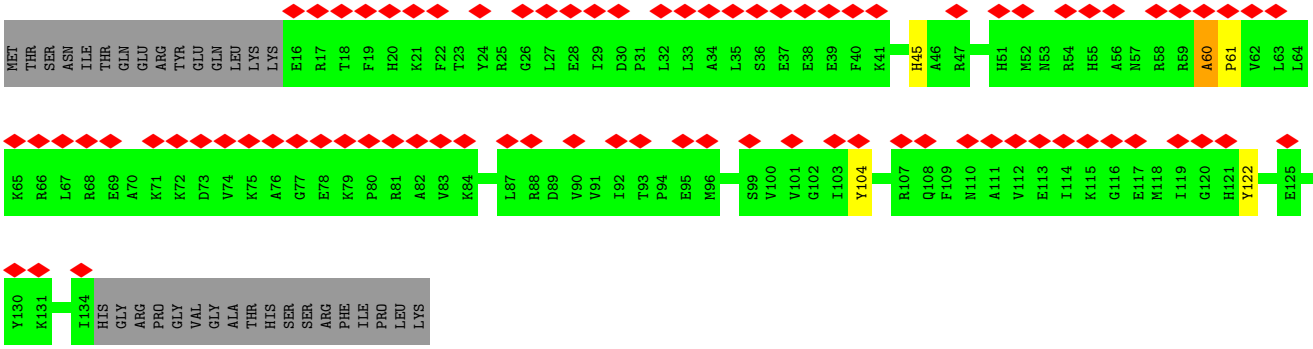
• Molecule 3: 40S ribosomal protein S16, putative

Chain r:



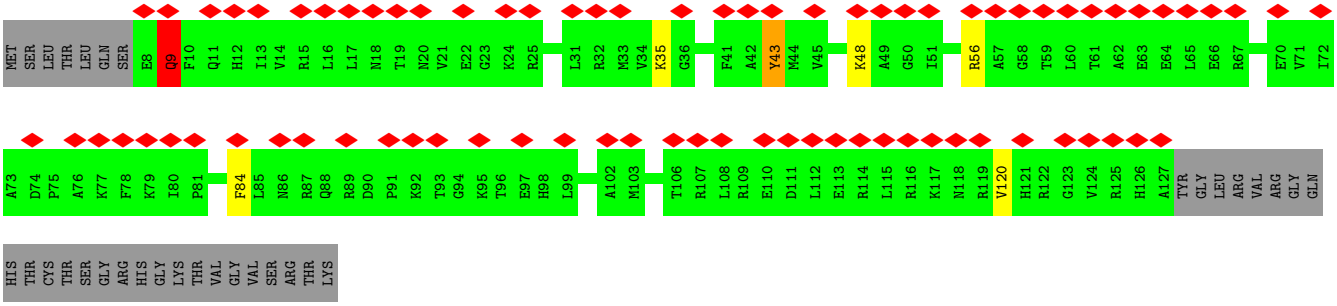
• Molecule 4: 40S ribosomal protein S15, putative

Chain t:



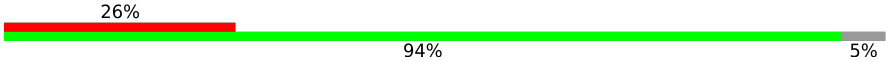
• Molecule 5: 40S ribosomal protein S18, putative

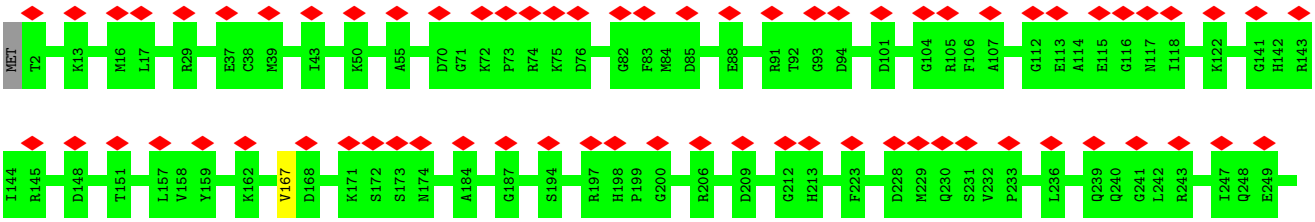
Chain u:

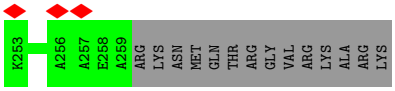


• Molecule 6: 40S ribosomal protein S4

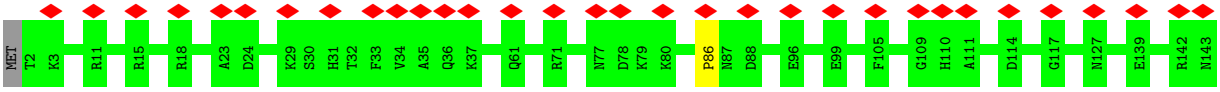
Chain L:



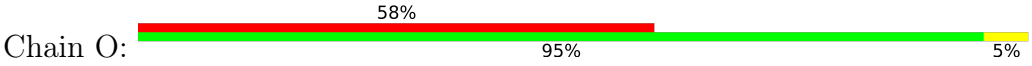


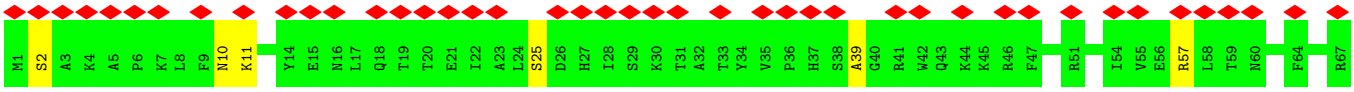


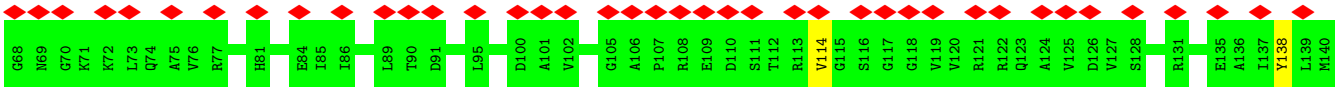
• Molecule 7: 40S ribosomal protein S23, putative

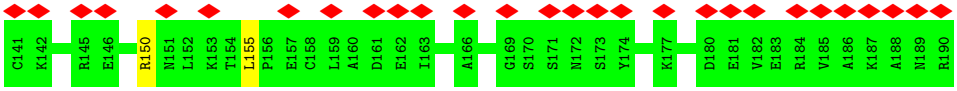


• Molecule 8: 40S ribosomal protein S5, putative

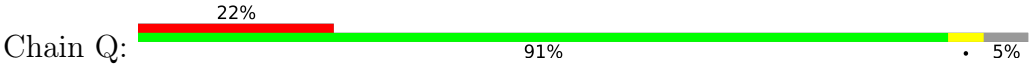


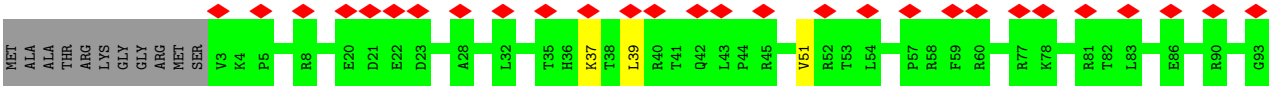


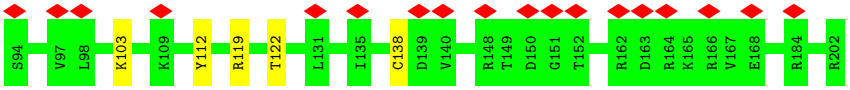




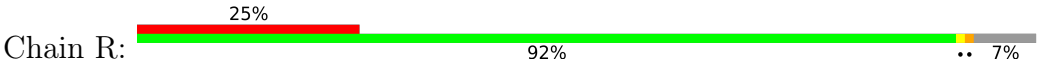
• Molecule 9: Ribosomal protein S7, putative

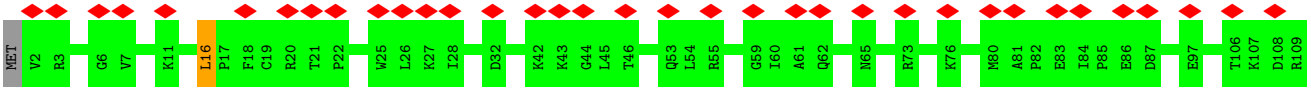


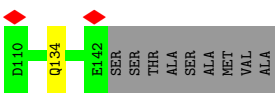




• Molecule 10: 40S ribosomal protein S13, putative

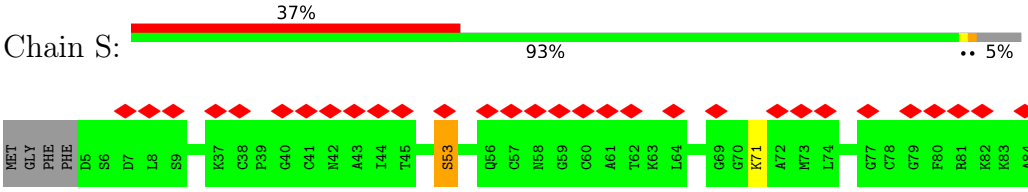






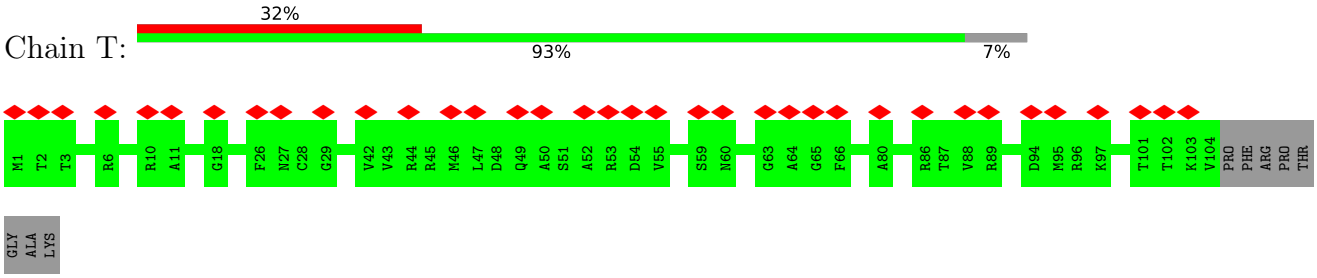
• Molecule 11: 40S ribosomal protein S27, putative

Chain S:



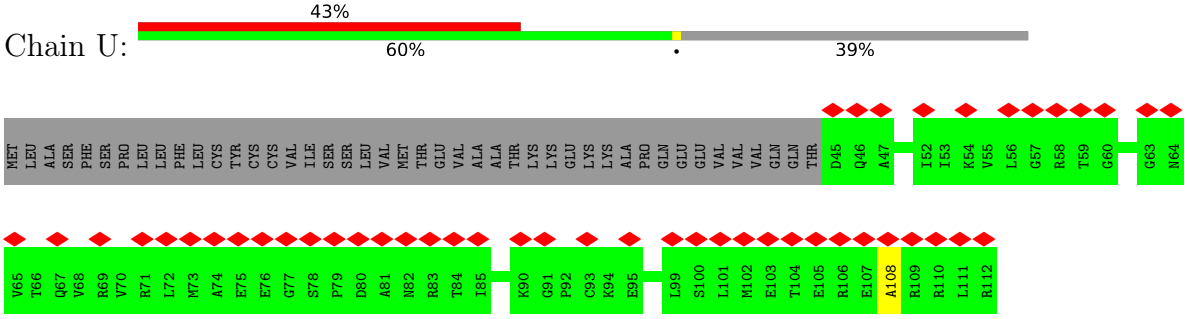
• Molecule 12: 40S ribosomal protein S26

Chain T:



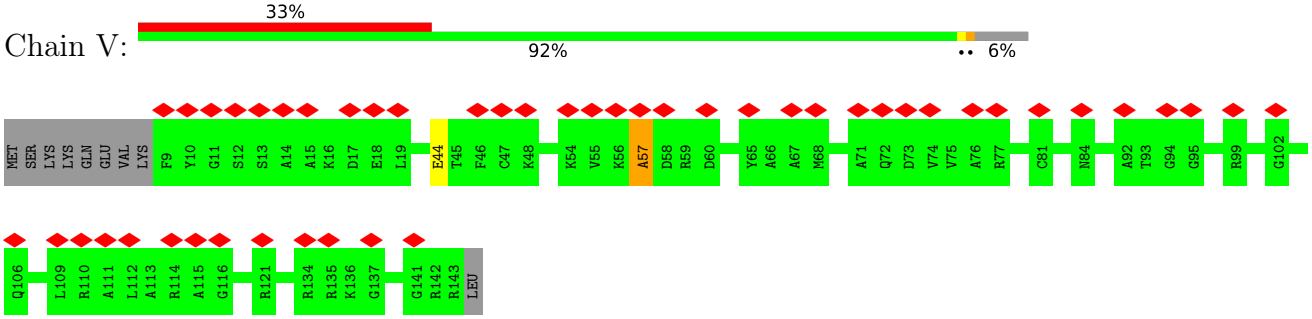
• Molecule 13: 40S ribosomal protein S33, putative

Chain U:



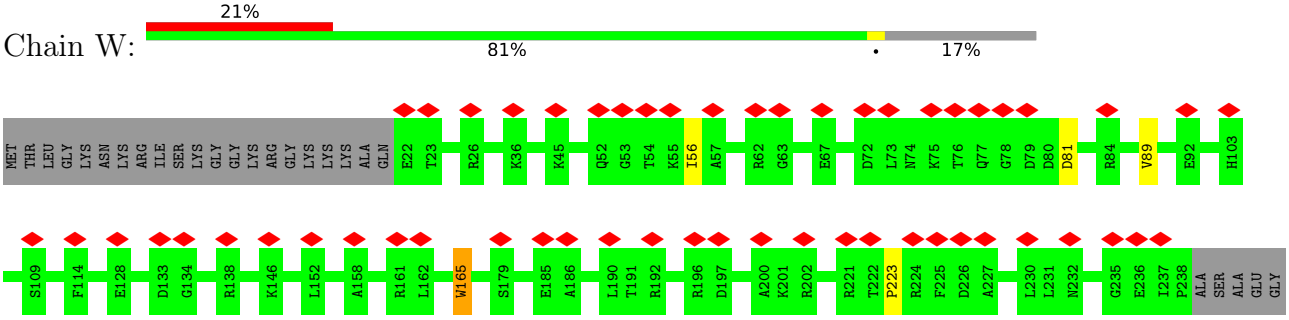
• Molecule 14: 40S ribosomal protein S14, putative

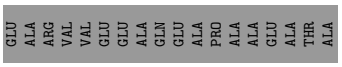
Chain V:



• Molecule 15: 40S ribosomal protein S3a-2

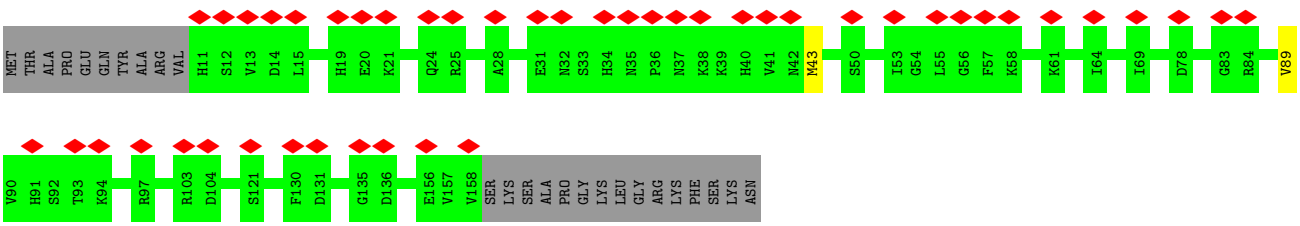
Chain W:





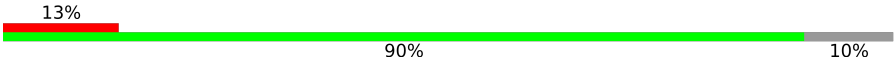
• Molecule 16: 40S ribosomal protein S11, putative

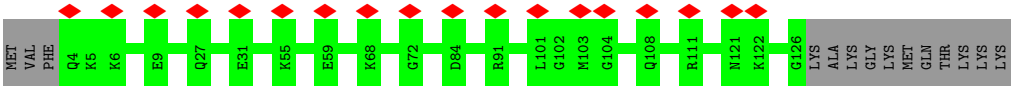
Chain X:



• Molecule 17: 40S ribosomal protein S24

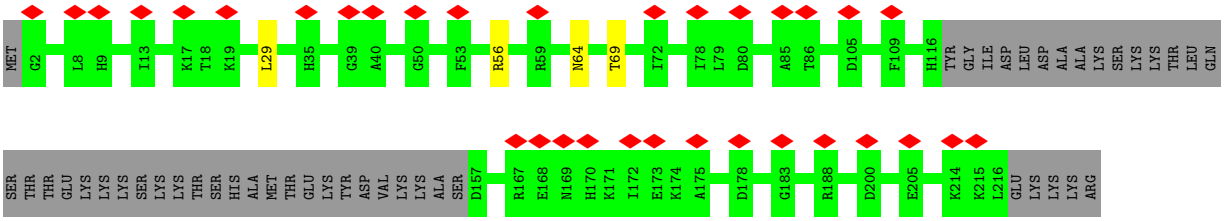
Chain Y:





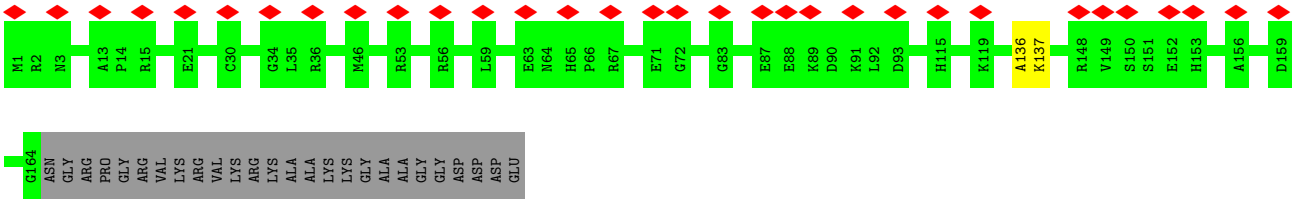
• Molecule 18: 40S ribosomal protein S8

Chain Z:



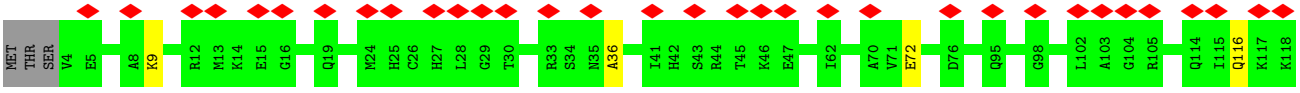
• Molecule 19: 40S ribosomal protein S9, putative

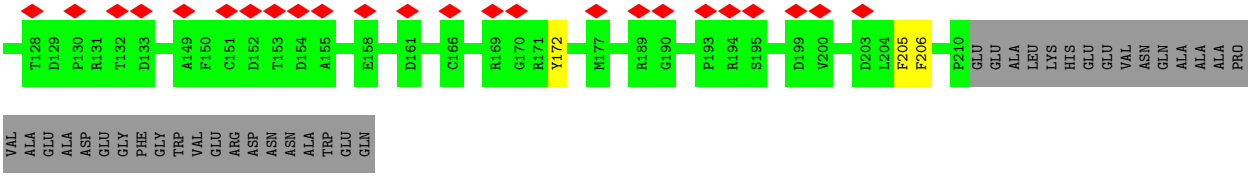
Chain b:



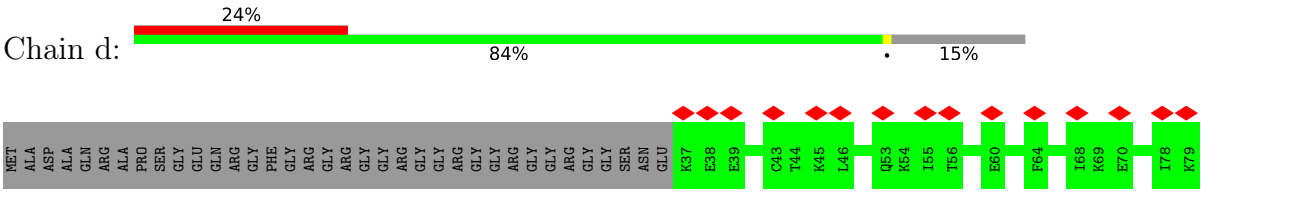
• Molecule 20: 40S ribosomal protein SA

Chain f:

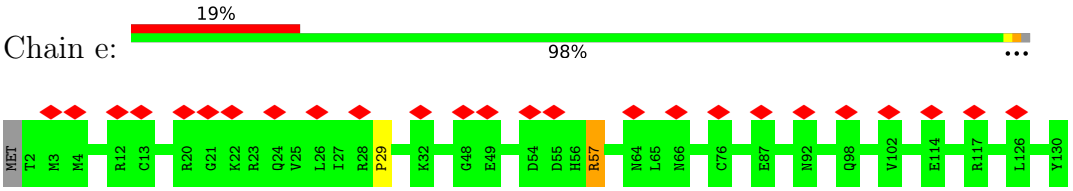




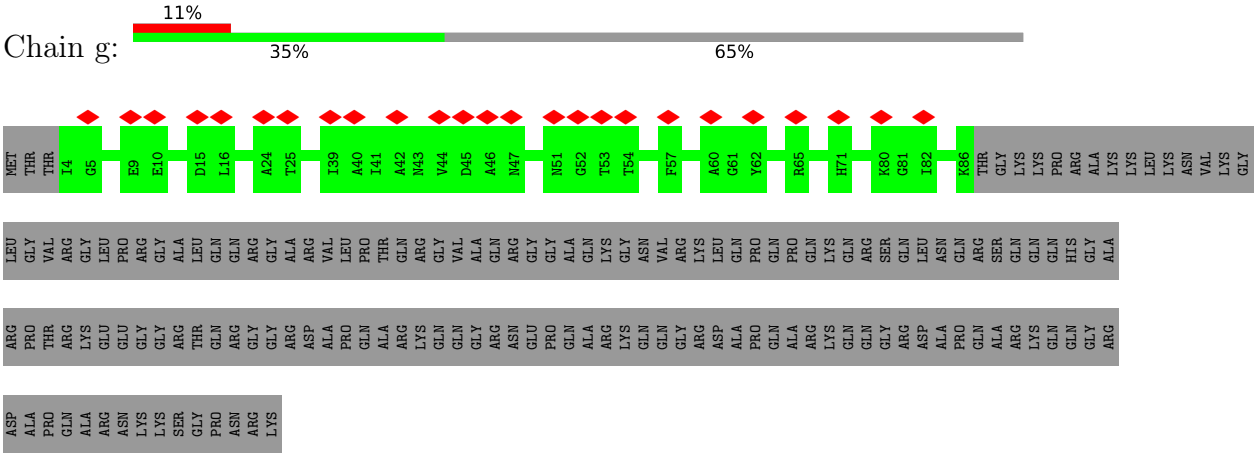
• Molecule 21: 40S ribosomal protein S2, putative



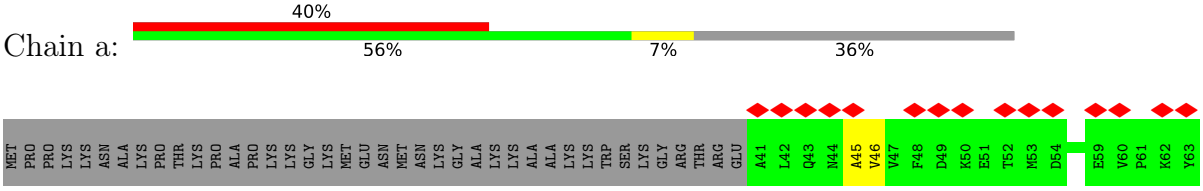
• Molecule 22: 40S ribosomal protein S15a, putative

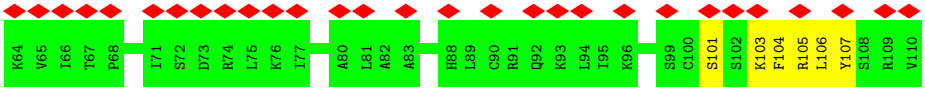


• Molecule 23: 40S ribosomal protein S21, putative



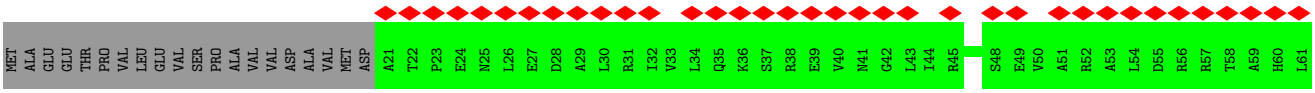
• Molecule 24: Ribosomal protein S25, putative

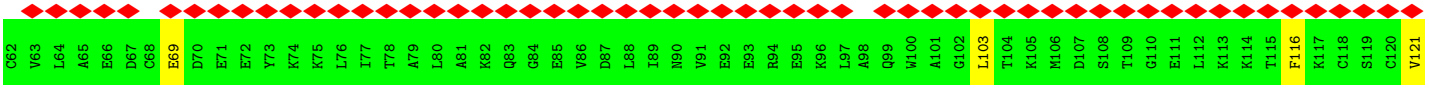


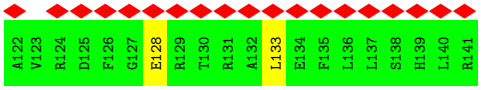


• Molecule 25: 40S ribosomal protein S12

Chain i:

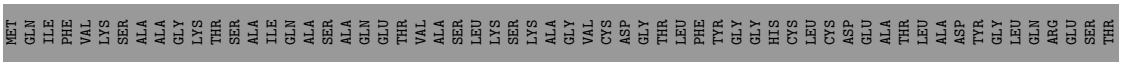


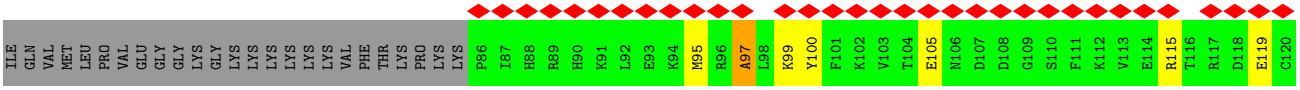


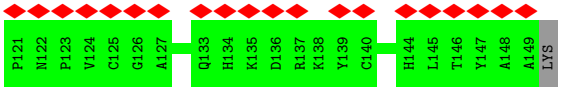


• Molecule 26: Ubiquitin/ribosomal protein S27a, putative

Chain j:

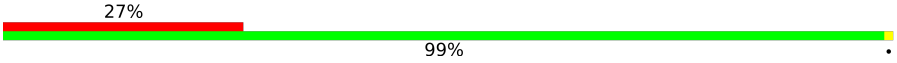


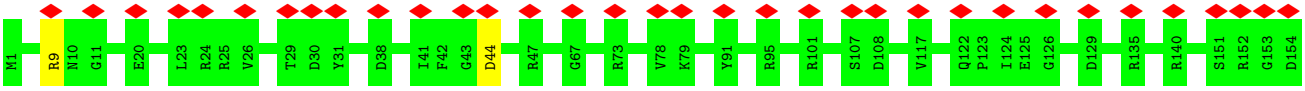


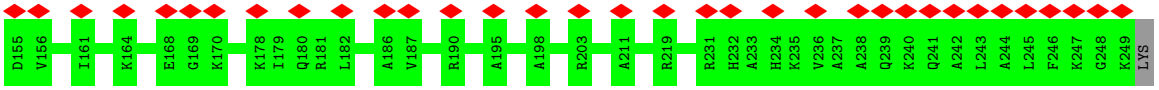


• Molecule 27: 40S ribosomal protein S6

Chain P:

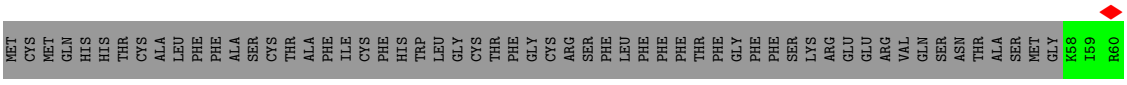


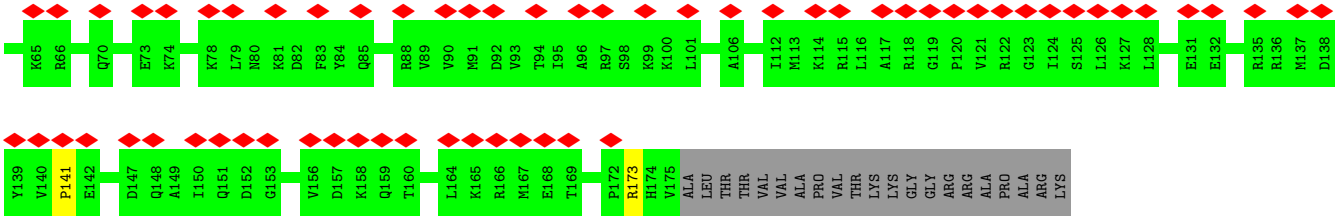




• Molecule 28: 40S ribosomal protein S17, putative

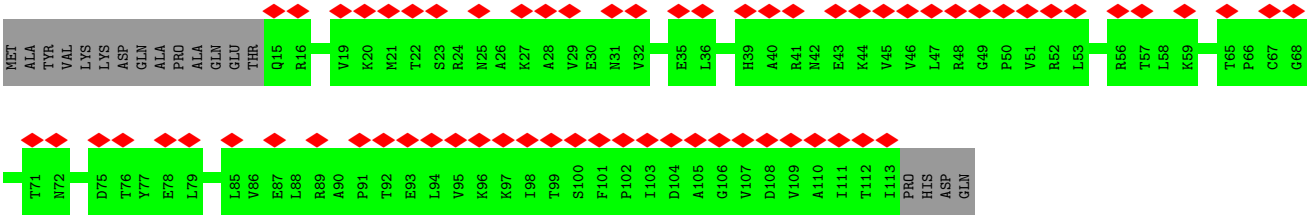
Chain k:





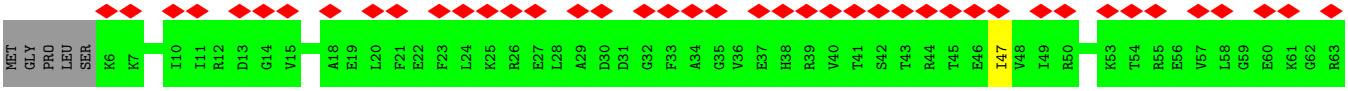
• Molecule 29: Ribosomal protein S20, putative

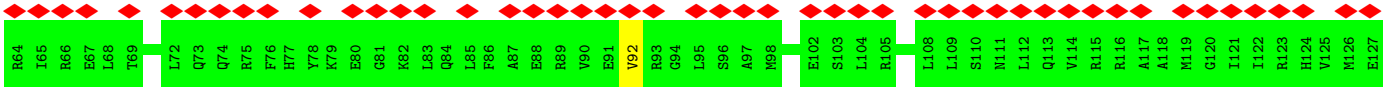
Chain l:

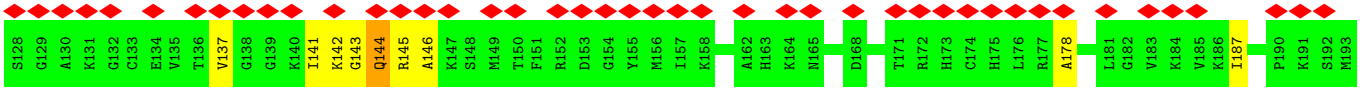


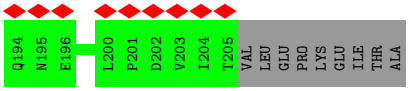
• Molecule 30: 40S ribosomal protein S3, putative

Chain m:



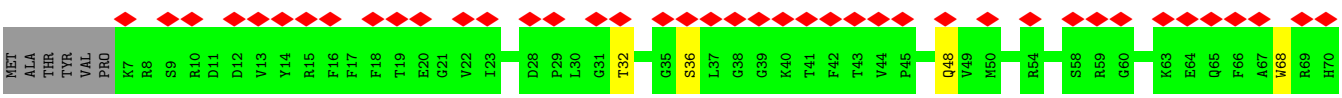


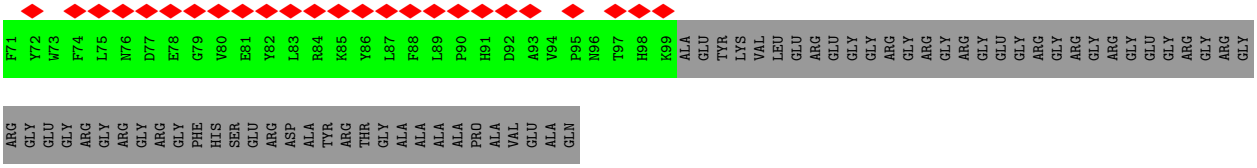




• Molecule 31: 40S ribosomal protein S10, putative

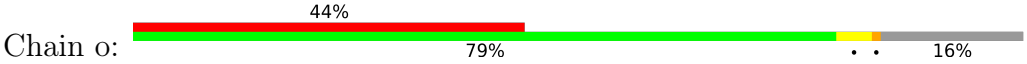
Chain n:

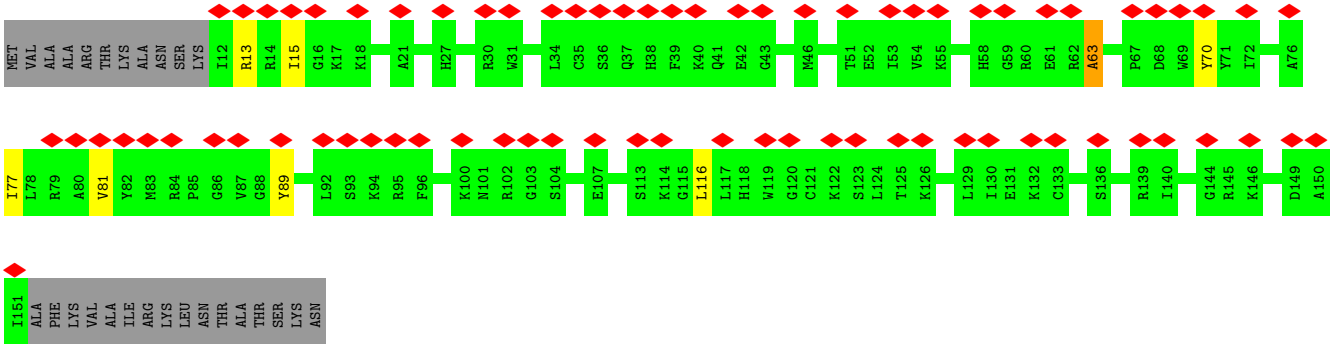




• Molecule 32: Ribosomal protein S19, putative

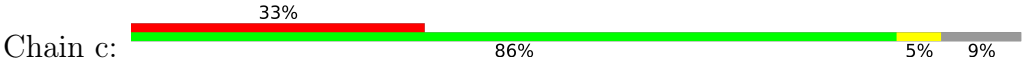
Chain o:

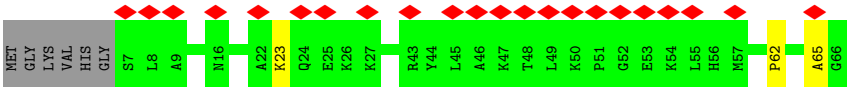




• Molecule 33: 40S ribosomal protein S30

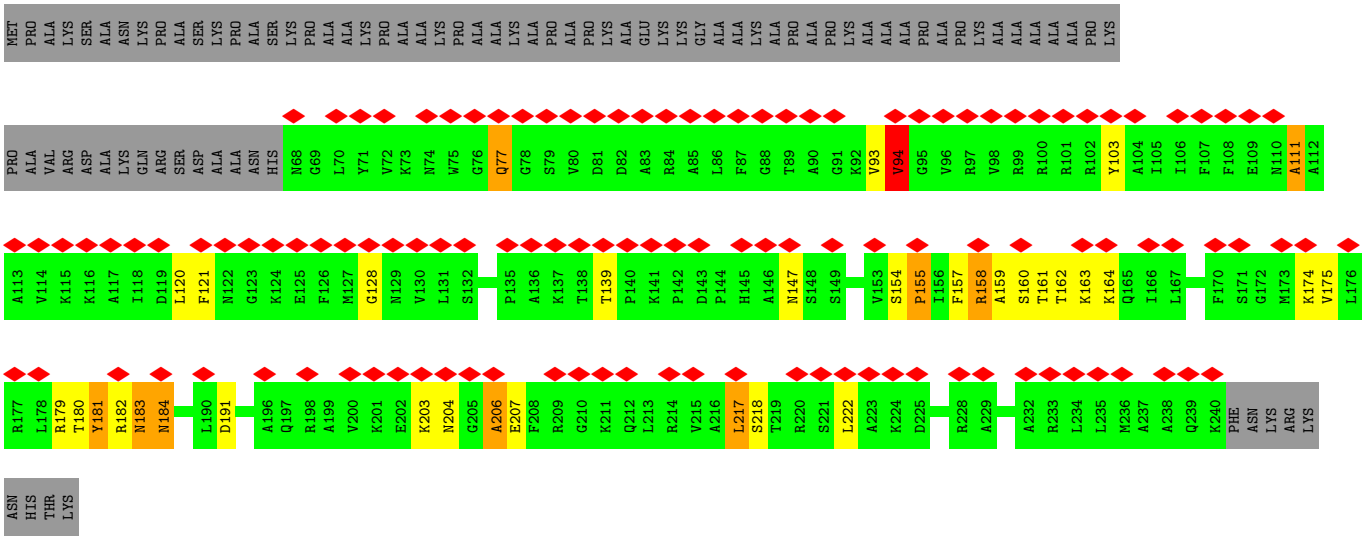
Chain c:





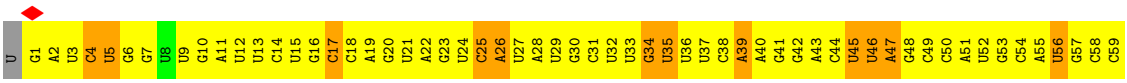
• Molecule 34: RNA-binding protein, putative

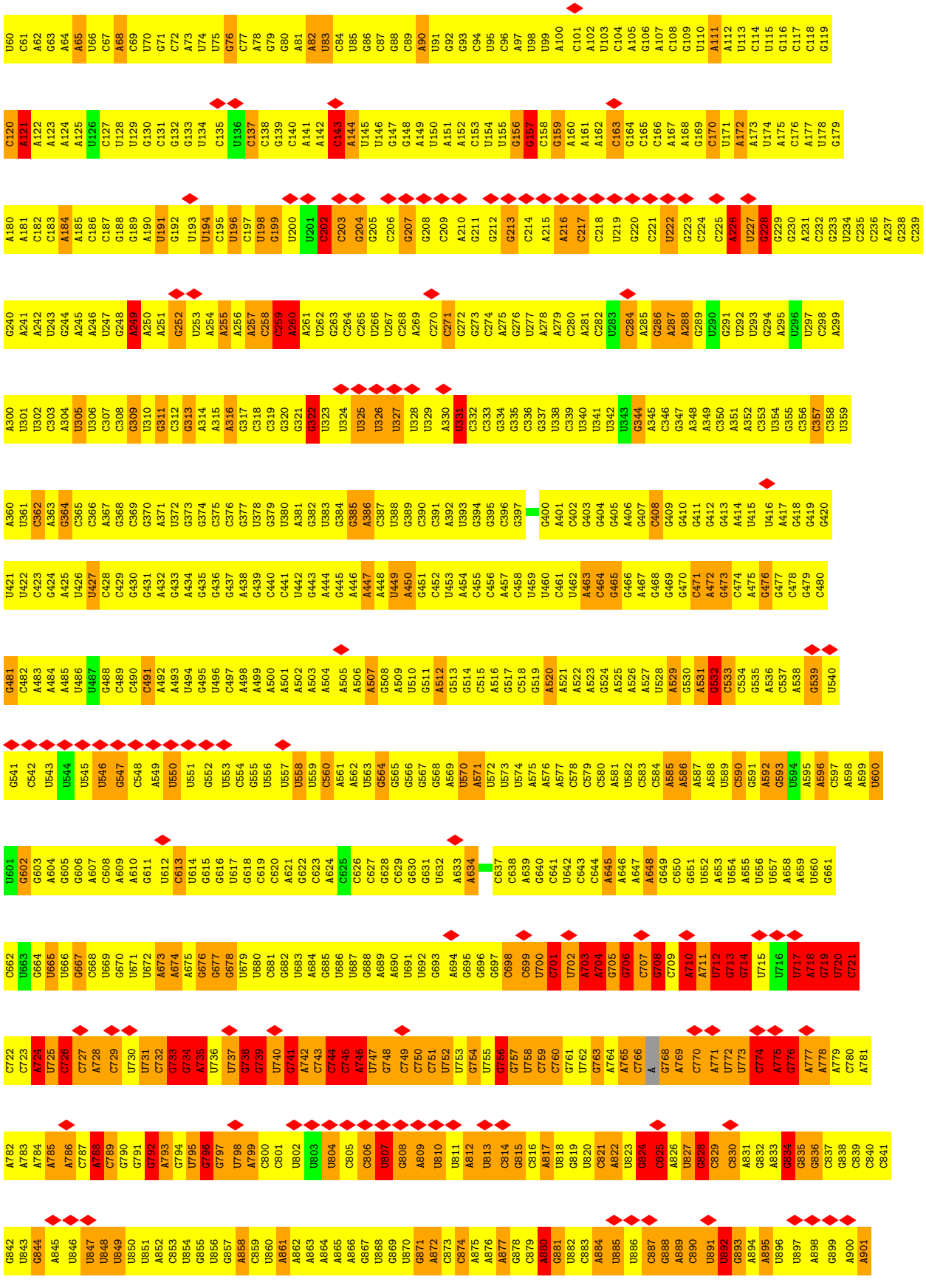
Chain h:



• Molecule 35: 18S rRNA

Chain E:

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C120 A121 A122 A123 A124 A125 U126 C127 U128 U129 G130 C131 G132 G133 U134 C135 U136 C137 C138 G139 C140 A141 A142 C143 A144 U145 U146 G147 G148 A149 U150 A151 A152 C153 U154 U155 G156 G157 C158 G159 A160 A161 A162 C163 G164 C165 C166 A167 A168 G169 C170 U171 A172 A173 U174 A175 C176 A177 U178 G179
A180 A181 C182 C183 A184 A185 C186 C187 G188 G189 A190 U191 G192 U193 U194 C195 U196 C197 U198 G199 U200 U201 G202 C203 A204 G205 C206 G207 G208 C209 A210 G211 G212 G213 C214 A215 A216 C217 C218 U219 G220 C221 U222 G223 C224 C225 A226 U227 G228 G229 G230 A231 C232 G233 U234 C235 C236 A237 G238 C239
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A300 U301 U302 C303 A304 U305 U306 C307 C308 G309 U310 G311 C312 G313 A314 A315 A316 G317 C318 C319 G320 G321 G322 U323 U324 U325 U326 U327 U328 U329 A330 U331 C332 C333 G334 G335 C336 G337 U338 C339 U340 U341 U342 U343 G344 A345 G346 A347 A348 A349 C350 A351 A352 C353 U354 G355 C356 C357 C358 U359
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C722 C723 A724 U725 C726 C727 A728 C729 U730 U731 C732 G733 G734 A735 U736 U737 G738 G739 U740 G741 A742 G743 C744 C745 A746 U747 G748 C749 C750 C751 U752 U753 G754 U755 G756 G757 U758 C759 C760 G761 U762 G763 A764 A765 C766 A G768 A769 C770 A771 U772 U773 C774 A775 G776 A777 A778 A779 C780 A781
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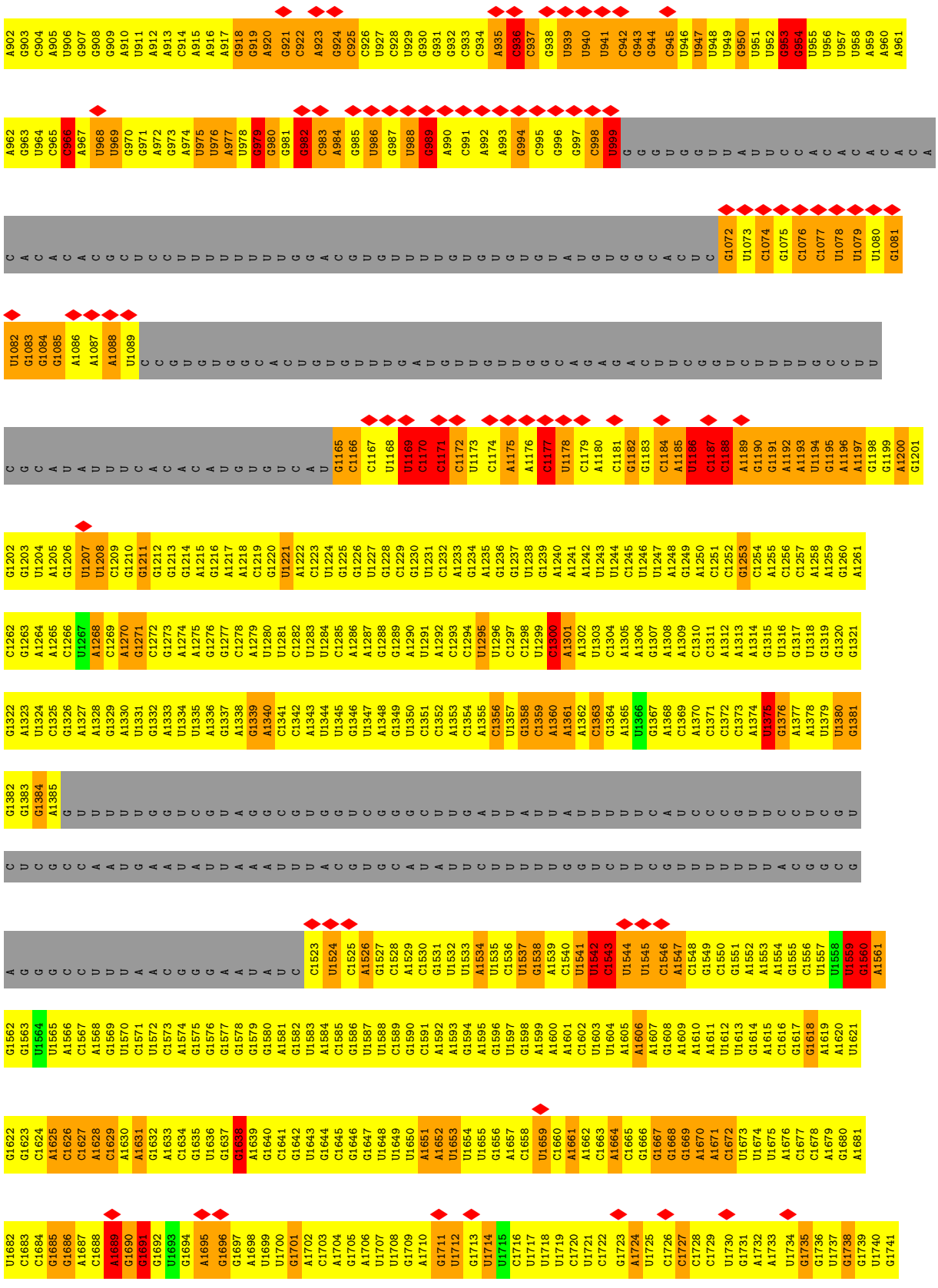

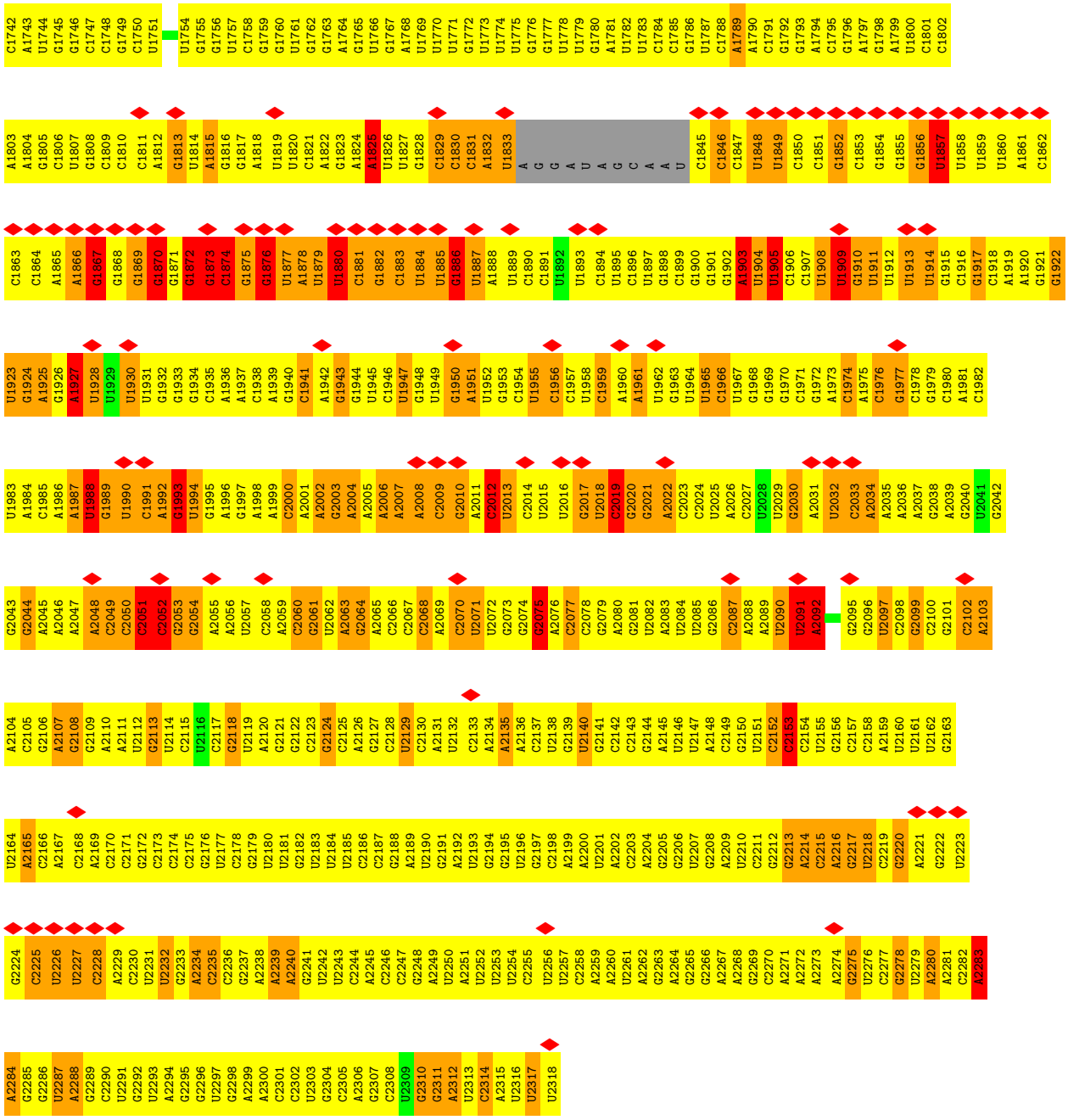
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A1803 A1804 G1805 C1806 U1807 G1808 C1809 C1810 C1811 A1812 G1813 U1814 A1815 G1816 G1817 A1818 U1819 U1820 C1821 A1822 G1823 A1824 A1825 U1826 U1827 G1828 C1829 C1830 C1831 A1832 U1833 A G G G A U A G C A A U C1845 C1846 C1847 U1848 U1849 C1850 C1851 G1852 C1853 G1854 G1855 G1856 U1857 U1858 U1859 U1860 A1861 C1862
C1863 C1864 A1865 A1866 G1867 G1868 G1869 G1870 G1871 G1872 G1873 C1874 G1875 G1876 U1877 A1878 U1879 U1880 C1881 G1882 C1883 U1884 U1885 G1886 U1887 A1888 U1889 C1890 C1891 U1892 U1893 C1894 U1895 C1896 U1897 G1898 C1899 G1900 G1901 G1902 A1903 U1904 U1905 C1906 C1907 U1908 U1909 G1910 U1911 U1912 U1913 U1914 G1915 C1916 G1917 C1918 A1919 A1920 G1921 G1922
U1923 G1924 A1925 G1926 A1927 U1928 U1929 U1930 U1931 G1932 G1933 G1934 C1935 A1936 A1937 C1938 A1939 G1940 C1941 A1942 G1943 G1944 U1945 G1946 U1947 G1948 U1949 G1950 A1951 U1952 G1953 C1954 U1955 C1956 C1957 U1958 C1959 A1960 A1961 U1962 G1963 U1964 U1965 C1966 U1967 G1968 G1969 G1970 C1971 G1972 A1973 C1974 A1975 C1976 G1977 C1978 G1979 C1980 A1981 C1982
U1983 A1984 C1985 A1986 A1987 U1988 G1989 U1990 C1991 A1992 G1993 U1994 G1995 A1996 G1997 A1998 A1999 C2000 A2001 A2002 G2003 A2004 A2005 A2006 A2007 A2008 C2009 G2010 A2011 C2012 U2013 C2014 U2015 U2016 G2017 U2018 C2019 G2020 G2021 A2022 C2023 C2024 U2025 A2026 C2027 U2028 U2029 G2030 A2031 U2032 C2033 A2034 A2035 A2036 A2037 G2038 A2039 G2040 U2041 G2042
G2043 G2044 A2045 A2046 A2047 A2048 C2049 C2050 C2051 C2052 G2053 G2054 A2055 A2056 U2057 C2058 A2059 C2060 G2061 U2062 A2063 G2064 A2065 C2066 C2067 C2068 A2069 C2070 U2071 U2072 G2073 G2074 G2075 A2076 C2077 C2078 G2079 A2080 G2081 U2082 A2083 U2084 U2085 G2086 C2087 A2088 A2089 U2090 U2091 A2092 G2095 G2096 U2097 G2098 G2099 C2100 C2101 C2102 A2103
A2104 C2105 G2106 A2107 G2108 G2109 A2110 A2111 U2112 G2113 U2114 C2115 U2116 C2117 G2118 U2119 A2120 G2121 G2122 C2123 G2124 C2125 A2126 G2127 C2128 U2129 C2130 A2131 U2132 C2133 A2134 A2135 A2136 C2137 U2138 G2139 U2140 G2141 C2142 C2143 G2144 A2145 U2146 U2147 A2148 C2149 G2150 U2151 C2152 C2153 C2154 U2155 G2156 C2157 C2158 A2159 U2160 U2161 U2162 G2163
U2164 A2165 C2166 A2167 C2168 A2169 C2170 C2171 G2172 C2173 C2174 C2175 G2176 U2177 C2178 G2179 U2180 U2181 G2182 U2183 U2184 U2185 C2186 C2187 G2188 A2189 U2190 G2191 A2192 U2193 G2194 G2195 U2196 G2197 C2198 A2199 A2200 U2201 A2202 C2203 A2204 G2205 G2206 U2207 G2208 A2209 U2210 C2211 G2212 G2213 A2214 C2215 A2216 G2217 U2218 C2219 G2220 A2221 G2222 U2223
G2224 C2225 U2226 U2227 C2228 A2229 C2230 U2231 U2232 G2233 A2234 C2235 C2236 G2237 A2238 A2239 A2240 G2241 U2242 U2243 C2244 A2245 C2246 C2247 G2248 A2249 U2250 A2251 U2252 U2253 U2254 C2255 U2256 U2257 C2258 A2259 A2260 U2261 A2262 G2263 A2264 G2265 G2266 A2267 A2268 G2269 C2270 A2271 A2272 A2273 A2274 G2275 U2276 C2277 G2278 U2279 A2280 A2281 C2282 A2283
A2284 G2285 G2286 U2287 A2288 G2289 C2290 U2291 G2292 U2293 A2294 G2295 G2296 U2297 G2298 A2299 A2300 C2301 C2302 U2303 G2304 C2305 A2306 G2307 C2308 U2309 G2310 G2311 A2312 U2313 C2314 A2315 U2316 U2317 U2318

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86000	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 ($e^-/Å^2$)	2.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.132	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0549	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	p	0.94	0/2461	1.01	3/3347 (0.1%)
2	q	1.09	0/314	1.04	1/416 (0.2%)
3	r	1.02	0/1131	1.11	5/1520 (0.3%)
4	t	1.02	0/988	1.05	3/1325 (0.2%)
5	u	1.05	0/996	1.10	5/1334 (0.4%)
6	L	0.99	0/2073	0.98	0/2787
7	M	0.97	0/1137	0.94	0/1520
8	O	0.99	0/1515	0.96	0/2034
9	Q	1.06	0/1703	1.01	0/2290
10	R	1.00	0/1164	0.96	0/1559
11	S	0.99	0/641	1.01	1/858 (0.1%)
12	T	1.13	0/845	1.00	0/1129
13	U	1.13	0/527	1.04	0/702
14	V	1.04	0/1026	1.02	1/1376 (0.1%)
15	W	1.03	0/1809	1.01	1/2437 (0.0%)
16	X	1.02	0/1238	0.96	0/1662
17	Y	1.01	0/1004	0.98	0/1335
18	Z	1.06	0/1424	1.01	0/1904
19	b	1.03	0/1394	0.95	0/1874
20	f	0.97	0/1693	1.01	5/2290 (0.2%)
21	d	0.94	0/1760	1.03	2/2376 (0.1%)
22	e	1.00	0/1037	1.03	0/1391
23	g	0.92	0/644	0.89	0/875
24	a	0.92	0/559	1.03	1/748 (0.1%)
25	i	0.98	0/966	0.97	2/1295 (0.2%)
26	j	0.98	0/530	1.10	3/707 (0.4%)
27	P	1.09	0/2008	0.98	0/2678
28	k	1.00	0/985	0.98	0/1313
29	l	0.99	0/794	1.06	0/1076
30	m	1.03	0/1606	1.02	4/2141 (0.2%)
31	n	0.98	0/804	0.99	0/1082
32	o	1.00	0/1140	1.09	2/1524 (0.1%)
33	c	0.98	0/488	0.97	0/644
34	h	1.06	0/1381	1.22	4/1857 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
35	E	1.63	86/48215 (0.2%)	2.51	5573/75140 (7.4%)
All	All	1.38	86/88000 (0.1%)	2.03	5616/128546 (4.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	p	0	3
3	r	0	7
4	t	0	2
5	u	0	4
8	O	0	3
9	Q	0	3
15	W	0	1
18	Z	0	1
22	e	0	1
24	a	0	2
26	j	0	1
27	P	0	2
28	k	0	1
30	m	0	2
32	o	0	2
33	c	0	2
34	h	0	22
35	E	4	121
All	All	4	180

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	724	A	N9-C4	-14.62	1.29	1.37
35	E	734	G	N9-C4	-13.56	1.27	1.38
35	E	711	A	N9-C4	-10.05	1.31	1.37
35	E	718	A	N9-C4	-9.61	1.32	1.37
35	E	738	G	N9-C4	-8.96	1.30	1.38
35	E	746	A	N9-C4	-8.02	1.33	1.37
35	E	733	G	N1-C2	8.02	1.44	1.37
35	E	724	A	N3-C4	-7.54	1.30	1.34
35	E	724	A	N7-C5	-7.52	1.34	1.39
35	E	1873	G	C6-N1	6.76	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	953	G	N1-C2	6.71	1.43	1.37
35	E	162	A	N7-C5	-6.59	1.35	1.39
35	E	746	A	N7-C5	-6.45	1.35	1.39
35	E	172	A	N7-C5	-6.44	1.35	1.39
35	E	2189	A	N7-C5	-6.42	1.35	1.39
35	E	1600	A	N7-C5	-6.35	1.35	1.39
35	E	1327	A	N7-C5	-6.30	1.35	1.39
35	E	1305	A	N7-C5	-6.29	1.35	1.39
35	E	1852	G	N1-C2	6.11	1.42	1.37
35	E	711	A	N7-C5	-6.09	1.35	1.39
35	E	2104	A	N7-C5	-6.07	1.35	1.39
35	E	1593	A	N7-C5	-6.06	1.35	1.39
35	E	1082	U	C2'-C1'	-6.01	1.46	1.53
35	E	1768	A	N7-C5	-6.00	1.35	1.39
35	E	1872	G	C2'-C1'	-5.95	1.46	1.53
35	E	256	A	N7-C5	-5.94	1.35	1.39
35	E	954	G	N1-C2	5.85	1.42	1.37
35	E	1083	G	C2'-C1'	-5.82	1.47	1.53
35	E	2264	A	N7-C5	-5.75	1.35	1.39
35	E	1554	A	N7-C5	-5.73	1.35	1.39
35	E	1348	A	N7-C5	-5.66	1.35	1.39
35	E	1328	A	N7-C5	-5.60	1.35	1.39
35	E	1872	G	C2-N3	5.58	1.37	1.32
35	E	97	A	N7-C5	-5.54	1.35	1.39
35	E	1384	G	N1-C2	5.50	1.42	1.37
35	E	1873	G	N1-C2	5.50	1.42	1.37
35	E	1185	A	N7-C5	-5.49	1.35	1.39
35	E	734	G	N1-C2	5.46	1.42	1.37
35	E	40	A	N7-C5	-5.46	1.35	1.39
35	E	952	U	C2-N3	5.46	1.41	1.37
35	E	1634	C	N3-C4	5.44	1.37	1.33
35	E	2120	A	N7-C5	-5.41	1.36	1.39
35	E	833	A	C2'-C1'	-5.40	1.47	1.53
35	E	895	A	N7-C5	-5.38	1.36	1.39
35	E	734	G	C6-N1	5.36	1.43	1.39
35	E	259	C	N3-C4	5.33	1.37	1.33
35	E	1876	G	N1-C2	5.31	1.42	1.37
35	E	1186	U	C2-N3	5.30	1.41	1.37
35	E	1601	A	N7-C5	-5.28	1.36	1.39
35	E	90	A	N7-C5	-5.27	1.36	1.39
35	E	953	G	N9-C4	-5.26	1.33	1.38
35	E	725	U	C2-N3	5.24	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	2113	G	N1-C2	5.23	1.42	1.37
35	E	1625	A	N7-C5	-5.21	1.36	1.39
35	E	2134	A	N7-C5	-5.21	1.36	1.39
35	E	1730	U	C2-N3	5.20	1.41	1.37
35	E	260	A	N7-C5	-5.20	1.36	1.39
35	E	175	A	N7-C5	-5.18	1.36	1.39
35	E	738	G	N1-C2	5.18	1.41	1.37
35	E	51	A	N7-C5	-5.17	1.36	1.39
35	E	2214	A	N7-C5	-5.17	1.36	1.39
35	E	1675	U	C2-N3	5.17	1.41	1.37
35	E	2204	A	N7-C5	-5.17	1.36	1.39
35	E	2145	A	N7-C5	-5.15	1.36	1.39
35	E	1599	A	N7-C5	-5.13	1.36	1.39
35	E	446	A	N7-C5	-5.12	1.36	1.39
35	E	777	A	N7-C5	-5.12	1.36	1.39
35	E	202	C	N3-C4	5.12	1.37	1.33
35	E	807	U	O3'-P	-5.11	1.55	1.61
35	E	1233	A	N7-C5	-5.11	1.36	1.39
35	E	1773	U	C2-N3	5.09	1.41	1.37
35	E	710	A	N7-C5	-5.08	1.36	1.39
35	E	774	C	O3'-P	-5.08	1.55	1.61
35	E	2152	C	N3-C4	5.08	1.37	1.33
35	E	979	G	C2-N3	5.07	1.36	1.32
35	E	1553	A	N7-C5	-5.06	1.36	1.39
35	E	757	G	C2-N3	5.06	1.36	1.32
35	E	834	G	C2-N3	5.06	1.36	1.32
35	E	909	G	C2-N3	5.06	1.36	1.32
35	E	592	A	N7-C5	-5.05	1.36	1.39
35	E	756	G	N1-C2	5.04	1.41	1.37
35	E	722	C	N1-C2	-5.04	1.35	1.40
35	E	1825	A	N7-C5	-5.03	1.36	1.39
35	E	1899	C	N3-C4	5.03	1.37	1.33
35	E	363	A	N7-C5	-5.03	1.36	1.39
35	E	718	A	N7-C5	-5.01	1.36	1.39

All (5616) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	774	C	P-O3'-C3'	37.91	165.19	119.70
35	E	1187	C	P-O3'-C3'	33.90	160.37	119.70
35	E	976	U	O5'-P-OP2	-24.56	81.23	110.70
35	E	976	U	O5'-P-OP1	-24.39	81.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	703	A	P-O3'-C3'	23.77	148.22	119.70
35	E	531	A	P-O3'-C3'	22.35	146.52	119.70
35	E	1904	U	P-O3'-C3'	21.62	145.65	119.70
35	E	807	U	P-O3'-C3'	20.81	144.67	119.70
35	E	769	A	P-O3'-C3'	20.03	143.74	119.70
35	E	998	C	P-O3'-C3'	18.73	142.18	119.70
35	E	1546	C	P-O3'-C3'	18.58	141.99	119.70
35	E	1191	G	P-O3'-C3'	18.57	141.98	119.70
35	E	2048	A	P-O3'-C3'	18.40	141.78	119.70
35	E	2049	C	P-O3'-C3'	17.14	140.26	119.70
35	E	939	U	P-O3'-C3'	16.81	139.87	119.70
35	E	756	G	P-O3'-C3'	16.39	139.37	119.70
35	E	808	G	P-O3'-C3'	16.26	139.21	119.70
35	E	227	U	P-O3'-C3'	16.06	138.97	119.70
35	E	701	C	P-O3'-C3'	15.68	138.51	119.70
35	E	711	A	N1-C6-N6	15.56	127.94	118.60
35	E	918	G	P-O3'-C3'	15.32	138.08	119.70
35	E	810	U	P-O3'-C3'	15.11	137.83	119.70
35	E	724	A	N1-C6-N6	15.06	127.64	118.60
35	E	275	A	N1-C6-N6	14.90	127.54	118.60
35	E	279	A	N1-C6-N6	14.80	127.48	118.60
35	E	697	G	P-O3'-C3'	14.59	137.21	119.70
35	E	1088	A	N1-C6-N6	14.56	127.34	118.60
35	E	795	U	P-O3'-C3'	14.56	137.17	119.70
35	E	975	U	O3'-P-O5'	14.46	131.48	104.00
35	E	890	C	P-O3'-C3'	14.46	137.05	119.70
35	E	175	A	N1-C6-N6	14.43	127.26	118.60
35	E	765	A	P-O3'-C3'	14.34	136.91	119.70
35	E	727	C	P-O3'-C3'	14.27	136.82	119.70
35	E	1639	A	N1-C6-N6	14.23	127.14	118.60
35	E	705	G	P-O3'-C3'	14.04	136.54	119.70
35	E	1607	A	N1-C6-N6	13.97	126.98	118.60
35	E	962	A	N1-C6-N6	13.96	126.97	118.60
35	E	1534	A	N1-C6-N6	13.92	126.95	118.60
35	E	260	A	N1-C6-N6	13.88	126.93	118.60
35	E	1200	A	N1-C6-N6	13.84	126.90	118.60
35	E	942	C	P-O3'-C3'	13.78	136.24	119.70
35	E	2136	A	N1-C6-N6	13.76	126.85	118.60
35	E	536	A	N1-C6-N6	13.74	126.84	118.60
35	E	738	G	N1-C6-O6	13.65	128.09	119.90
35	E	777	A	P-O3'-C3'	13.64	136.07	119.70
35	E	813	U	P-O3'-C3'	13.63	136.05	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	210	A	N1-C6-N6	13.57	126.74	118.60
35	E	734	G	N1-C6-O6	13.57	128.04	119.90
35	E	984	A	N1-C6-N6	13.55	126.73	118.60
35	E	1554	A	N1-C6-N6	13.54	126.73	118.60
35	E	1903	A	P-O3'-C3'	13.47	135.86	119.70
35	E	2306	A	N1-C6-N6	13.42	126.65	118.60
35	E	2281	A	N1-C6-N6	13.39	126.64	118.60
35	E	746	A	N1-C6-N6	13.35	126.61	118.60
35	E	1593	A	N1-C6-N6	13.35	126.61	118.60
35	E	561	A	N1-C6-N6	13.25	126.55	118.60
35	E	1287	A	N1-C6-N6	13.25	126.55	118.60
35	E	483	A	N1-C6-N6	13.25	126.55	118.60
35	E	261	A	N1-C6-N6	13.24	126.54	118.60
35	E	1998	A	N1-C6-N6	13.23	126.54	118.60
35	E	920	A	N1-C6-N6	13.21	126.52	118.60
35	E	2280	A	N1-C6-N6	13.20	126.52	118.60
35	E	2092	A	N1-C6-N6	13.20	126.52	118.60
35	E	646	A	N1-C6-N6	13.15	126.49	118.60
35	E	2217	G	P-O3'-C3'	13.14	135.47	119.70
35	E	2229	A	N1-C6-N6	13.13	126.48	118.60
35	E	1374	A	N1-C6-N6	13.12	126.47	118.60
35	E	1193	A	N1-C6-N6	13.09	126.46	118.60
35	E	2245	A	N1-C6-N6	13.09	126.45	118.60
35	E	1981	A	N1-C6-N6	13.05	126.43	118.60
35	E	434	A	N1-C6-N6	13.05	126.43	118.60
35	E	2268	A	N1-C6-N6	13.04	126.43	118.60
35	E	889	A	N1-C6-N6	13.04	126.42	118.60
35	E	1652	A	N1-C6-N6	13.04	126.42	118.60
35	E	910	A	N1-C6-N6	13.03	126.42	118.60
35	E	1986	A	N1-C6-N6	13.02	126.41	118.60
35	E	1790	A	N1-C6-N6	13.00	126.40	118.60
35	E	1218	A	N1-C6-N6	13.00	126.40	118.60
35	E	892	U	P-O3'-C3'	12.98	135.27	119.70
35	E	1866	A	N1-C6-N6	12.96	126.38	118.60
35	E	1799	A	N1-C6-N6	12.95	126.37	118.60
35	E	2022	A	N1-C6-N6	12.94	126.37	118.60
35	E	1925	A	N1-C6-N6	12.94	126.36	118.60
35	E	1268	A	N1-C6-N6	12.93	126.36	118.60
35	E	1301	A	N1-C6-N6	12.92	126.35	118.60
35	E	1804	A	N1-C6-N6	12.92	126.35	118.60
35	E	864	A	N1-C6-N6	12.91	126.35	118.60
35	E	492	A	N1-C6-N6	12.89	126.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2080	A	N1-C6-N6	12.89	126.33	118.60
35	E	2251	A	N1-C6-N6	12.88	126.33	118.60
35	E	923	A	N1-C6-N6	12.88	126.33	118.60
35	E	1240	A	N1-C6-N6	12.87	126.32	118.60
35	E	538	A	N1-C6-N6	12.86	126.32	118.60
35	E	1595	A	N1-C6-N6	12.86	126.32	118.60
35	E	2264	A	N1-C6-N6	12.86	126.31	118.60
35	E	2059	A	N1-C6-N6	12.85	126.31	118.60
35	E	278	A	N1-C6-N6	12.82	126.30	118.60
35	E	457	A	N1-C6-N6	12.79	126.28	118.60
35	E	1973	A	N1-C6-N6	12.79	126.28	118.60
35	E	526	A	N1-C6-N6	12.78	126.27	118.60
35	E	645	A	N1-C6-N6	12.78	126.27	118.60
35	E	1615	A	N1-C6-N6	12.77	126.26	118.60
35	E	1360	A	N1-C6-N6	12.76	126.26	118.60
35	E	160	A	N1-C6-N6	12.76	126.25	118.60
35	E	2004	A	N1-C6-N6	12.75	126.25	118.60
35	E	976	U	OP1-P-OP2	12.74	138.71	119.60
35	E	2002	A	N1-C6-N6	12.74	126.25	118.60
35	E	1290	A	N1-C6-N6	12.74	126.24	118.60
35	E	1815	A	N1-C6-N6	12.73	126.24	118.60
35	E	702	U	P-O3'-C3'	12.72	134.97	119.70
35	E	22	A	N1-C6-N6	12.72	126.23	118.60
35	E	1702	A	N1-C6-N6	12.72	126.23	118.60
35	E	549	A	N1-C6-N6	12.71	126.22	118.60
35	E	1261	A	N1-C6-N6	12.71	126.22	118.60
35	E	1082	U	P-O3'-C3'	12.70	134.94	119.70
35	E	2221	A	N1-C6-N6	12.70	126.22	118.60
35	E	450	A	N1-C6-N6	12.69	126.21	118.60
35	E	1336	A	N1-C6-N6	12.69	126.21	118.60
35	E	2209	A	N1-C6-N6	12.69	126.21	118.60
35	E	414	A	N1-C6-N6	12.68	126.21	118.60
35	E	1628	A	N1-C6-N6	12.67	126.20	118.60
35	E	1196	A	N1-C6-N6	12.64	126.19	118.60
35	E	1302	A	N1-C6-N6	12.64	126.19	118.60
35	E	604	A	N1-C6-N6	12.64	126.18	118.60
35	E	658	A	N1-C6-N6	12.62	126.17	118.60
35	E	202	C	P-O3'-C3'	12.62	134.84	119.70
35	E	226	A	N1-C6-N6	12.61	126.17	118.60
35	E	1309	A	N1-C6-N6	12.61	126.17	118.60
35	E	73	A	N1-C6-N6	12.60	126.16	118.60
35	E	1235	A	N1-C6-N6	12.60	126.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	105	A	N1-C6-N6	12.60	126.16	118.60
35	E	1818	A	N1-C6-N6	12.58	126.14	118.60
35	E	2234	A	N1-C6-N6	12.56	126.14	118.60
35	E	144	A	N1-C6-N6	12.56	126.13	118.60
35	E	1355	A	N1-C6-N6	12.55	126.13	118.60
35	E	1222	A	N1-C6-N6	12.55	126.13	118.60
35	E	281	A	N1-C6-N6	12.54	126.12	118.60
35	E	121	A	N1-C6-N6	12.53	126.12	118.60
35	E	1275	A	N1-C6-N6	12.53	126.12	118.60
35	E	1679	A	N1-C6-N6	12.53	126.12	118.60
35	E	62	A	N1-C6-N6	12.53	126.12	118.60
35	E	111	A	N1-C6-N6	12.52	126.11	118.60
35	E	1188	C	P-O5'-C5'	12.52	140.94	120.90
35	E	2047	A	N1-C6-N6	12.51	126.11	118.60
35	E	1241	A	N1-C6-N6	12.51	126.11	118.60
35	E	2234	A	P-O3'-C3'	12.50	134.70	119.70
35	E	814	C	P-O3'-C3'	12.50	134.70	119.70
35	E	1185	A	N1-C6-N6	12.49	126.10	118.60
35	E	78	A	N1-C6-N6	12.49	126.09	118.60
35	E	1951	A	N1-C6-N6	12.49	126.09	118.60
35	E	1308	A	N1-C6-N6	12.48	126.09	118.60
35	E	1657	A	N1-C6-N6	12.48	126.09	118.60
35	E	1732	A	N1-C6-N6	12.48	126.09	118.60
35	E	1681	A	N1-C6-N6	12.47	126.08	118.60
35	E	381	A	N1-C6-N6	12.47	126.08	118.60
35	E	2200	A	N1-C6-N6	12.47	126.08	118.60
35	E	392	A	N1-C6-N6	12.47	126.08	118.60
35	E	472	A	N1-C6-N6	12.46	126.08	118.60
35	E	2288	A	N1-C6-N6	12.45	126.07	118.60
35	E	1286	A	N1-C6-N6	12.45	126.07	118.60
35	E	2001	A	N1-C6-N6	12.45	126.07	118.60
35	E	251	A	N1-C6-N6	12.44	126.06	118.60
35	E	1314	A	N1-C6-N6	12.44	126.06	118.60
35	E	935	A	P-O3'-C3'	12.44	134.62	119.70
35	E	505	A	N1-C6-N6	12.43	126.06	118.60
35	E	1279	A	N1-C6-N6	12.43	126.06	118.60
35	E	799	A	N1-C6-N6	12.42	126.05	118.60
35	E	1609	A	N1-C6-N6	12.42	126.05	118.60
35	E	1574	A	N1-C6-N6	12.42	126.05	118.60
35	E	1553	A	N1-C6-N6	12.41	126.05	118.60
35	E	2145	A	N1-C6-N6	12.40	126.04	118.60
35	E	2202	A	N1-C6-N6	12.40	126.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	852	A	N1-C6-N6	12.40	126.04	118.60
35	E	581	A	N1-C6-N6	12.40	126.04	118.60
35	E	475	A	N1-C6-N6	12.39	126.04	118.60
35	E	588	A	N1-C6-N6	12.39	126.04	118.60
35	E	1086	A	N1-C6-N6	12.38	126.03	118.60
35	E	1706	A	N1-C6-N6	12.37	126.02	118.60
35	E	123	A	N1-C6-N6	12.36	126.02	118.60
35	E	349	A	N1-C6-N6	12.36	126.02	118.60
35	E	2088	A	N1-C6-N6	12.36	126.01	118.60
35	E	1192	A	P-O3'-C3'	12.35	134.52	119.70
35	E	1710	A	N1-C6-N6	12.35	126.01	118.60
35	E	1936	A	N1-C6-N6	12.35	126.01	118.60
35	E	831	A	N1-C6-N6	12.34	126.00	118.60
35	E	639	A	N1-C6-N6	12.34	126.00	118.60
35	E	509	A	N1-C6-N6	12.34	126.00	118.60
35	E	215	A	N1-C6-N6	12.33	126.00	118.60
35	E	406	A	N1-C6-N6	12.33	126.00	118.60
35	E	1330	A	N1-C6-N6	12.33	126.00	118.60
35	E	785	A	N1-C6-N6	12.33	126.00	118.60
35	E	704	A	N1-C6-N6	12.32	125.99	118.60
35	E	190	A	N1-C6-N6	12.31	125.98	118.60
35	E	287	A	N1-C6-N6	12.30	125.98	118.60
35	E	872	A	N1-C6-N6	12.30	125.98	118.60
35	E	1794	A	N1-C6-N6	12.29	125.98	118.60
35	E	788	A	N1-C6-N6	12.29	125.97	118.60
35	E	1704	A	N1-C6-N6	12.29	125.97	118.60
35	E	1768	A	N1-C6-N6	12.28	125.97	118.60
35	E	1781	A	N1-C6-N6	12.28	125.97	118.60
35	E	241	A	N1-C6-N6	12.27	125.96	118.60
35	E	647	A	N1-C6-N6	12.27	125.96	118.60
35	E	599	A	N1-C6-N6	12.27	125.96	118.60
35	E	764	A	N1-C6-N6	12.26	125.95	118.60
35	E	522	A	N1-C6-N6	12.26	125.95	118.60
35	E	1797	A	N1-C6-N6	12.25	125.95	118.60
35	E	2046	A	N1-C6-N6	12.25	125.95	118.60
35	E	2262	A	N1-C6-N6	12.25	125.95	118.60
35	E	257	A	N1-C6-N6	12.25	125.95	118.60
35	E	569	A	N1-C6-N6	12.25	125.95	118.60
35	E	653	A	N1-C6-N6	12.25	125.95	118.60
35	E	432	A	N1-C6-N6	12.24	125.95	118.60
35	E	703	A	N1-C6-N6	12.24	125.95	118.60
35	E	1259	A	N1-C6-N6	12.24	125.95	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2111	A	N1-C6-N6	12.24	125.95	118.60
35	E	1265	A	N1-C6-N6	12.23	125.94	118.60
35	E	314	A	N1-C6-N6	12.22	125.94	118.60
35	E	1217	A	N1-C6-N6	12.22	125.93	118.60
35	E	438	A	N1-C6-N6	12.22	125.93	118.60
35	E	1192	A	N1-C6-N6	12.22	125.93	118.60
35	E	304	A	N1-C6-N6	12.22	125.93	118.60
35	E	1561	A	N1-C6-N6	12.21	125.93	118.60
35	E	256	A	N1-C6-N6	12.21	125.93	118.60
35	E	1292	A	N1-C6-N6	12.21	125.93	118.60
35	E	778	A	N1-C6-N6	12.21	125.92	118.60
35	E	348	A	N1-C6-N6	12.20	125.92	118.60
35	E	655	A	N1-C6-N6	12.20	125.92	118.60
35	E	1832	A	N1-C6-N6	12.20	125.92	118.60
35	E	2048	A	N1-C6-N6	12.20	125.92	118.60
35	E	1822	A	N1-C6-N6	12.20	125.92	118.60
35	E	576	A	N1-C6-N6	12.19	125.91	118.60
35	E	10	G	N1-C6-O6	12.19	127.21	119.90
35	E	1661	A	N1-C6-N6	12.19	125.91	118.60
35	E	161	A	N1-C6-N6	12.18	125.91	118.60
35	E	454	A	N1-C6-N6	12.18	125.91	118.60
35	E	1205	A	N1-C6-N6	12.18	125.91	118.60
35	E	742	A	N1-C6-N6	12.18	125.91	118.60
35	E	1215	A	N1-C6-N6	12.18	125.91	118.60
35	E	11	A	N1-C6-N6	12.17	125.90	118.60
35	E	710	A	N1-C6-N6	12.17	125.90	118.60
35	E	1913	U	P-O3'-C3'	12.17	134.30	119.70
35	E	1676	A	N1-C6-N6	12.16	125.90	118.60
35	E	894	A	N1-C6-N6	12.16	125.89	118.60
35	E	2167	A	N1-C6-N6	12.16	125.89	118.60
35	E	1258	A	N1-C6-N6	12.15	125.89	118.60
35	E	1176	A	N1-C6-N6	12.15	125.89	118.60
35	E	1619	A	N1-C6-N6	12.15	125.89	118.60
35	E	417	A	N1-C6-N6	12.14	125.89	118.60
35	E	2031	A	N1-C6-N6	12.14	125.89	118.60
35	E	1764	A	N1-C6-N6	12.14	125.88	118.60
35	E	168	A	N1-C6-N6	12.12	125.88	118.60
35	E	845	A	N1-C6-N6	12.12	125.88	118.60
35	E	728	A	N1-C6-N6	12.12	125.87	118.60
35	E	884	A	N1-C6-N6	12.12	125.87	118.60
35	E	371	A	N1-C6-N6	12.12	125.87	118.60
35	E	1385	A	N1-C6-N6	12.11	125.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1592	A	N1-C6-N6	12.11	125.87	118.60
35	E	28	A	N1-C6-N6	12.11	125.87	118.60
35	E	2036	A	N1-C6-N6	12.11	125.87	118.60
35	E	2083	A	N1-C6-N6	12.11	125.86	118.60
35	E	142	A	N1-C6-N6	12.11	125.86	118.60
35	E	592	A	N1-C6-N6	12.10	125.86	118.60
35	E	826	A	N1-C6-N6	12.10	125.86	118.60
35	E	1362	A	N1-C6-N6	12.10	125.86	118.60
35	E	1611	A	N1-C6-N6	12.10	125.86	118.60
35	E	2299	A	N1-C6-N6	12.10	125.86	118.60
35	E	65	A	N1-C6-N6	12.10	125.86	118.60
35	E	1825	A	N1-C6-N6	12.10	125.86	118.60
35	E	1526	A	N1-C6-N6	12.09	125.86	118.60
35	E	783	A	N1-C6-N6	12.09	125.85	118.60
35	E	1865	A	N1-C6-N6	12.09	125.85	118.60
35	E	586	A	N1-C6-N6	12.09	125.85	118.60
35	E	659	A	N1-C6-N6	12.08	125.85	118.60
35	E	1270	A	N1-C6-N6	12.08	125.85	118.60
35	E	875	A	N1-C6-N6	12.08	125.85	118.60
35	E	245	A	N1-C6-N6	12.07	125.84	118.60
35	E	916	A	N1-C6-N6	12.07	125.84	118.60
35	E	2294	A	N1-C6-N6	12.07	125.84	118.60
35	E	577	A	N1-C6-N6	12.07	125.84	118.60
35	E	503	A	N1-C6-N6	12.06	125.84	118.60
35	E	2089	A	N1-C6-N6	12.06	125.83	118.60
35	E	809	A	N1-C6-N6	12.05	125.83	118.60
35	E	2076	A	N1-C6-N6	12.05	125.83	118.60
35	E	26	A	N1-C6-N6	12.05	125.83	118.60
35	E	935	A	N1-C6-N6	12.04	125.83	118.60
35	E	974	A	N1-C6-N6	12.04	125.83	118.60
35	E	124	A	N1-C6-N6	12.04	125.82	118.60
35	E	507	A	N1-C6-N6	12.04	125.82	118.60
35	E	977	A	N1-C6-N6	12.04	125.82	118.60
35	E	2026	A	N1-C6-N6	12.04	125.82	118.60
35	E	863	A	N1-C6-N6	12.04	125.82	118.60
35	E	1175	A	N1-C6-N6	12.04	125.82	118.60
35	E	2283	A	N1-C6-N6	12.03	125.82	118.60
35	E	990	A	N1-C6-N6	12.03	125.82	118.60
35	E	506	A	N1-C6-N6	12.02	125.81	118.60
35	E	2189	A	N1-C6-N6	12.02	125.81	118.60
35	E	610	A	N1-C6-N6	12.02	125.81	118.60
35	E	246	A	N1-C6-N6	12.02	125.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	295	A	N1-C6-N6	12.02	125.81	118.60
35	E	891	U	P-O3'-C3'	12.02	134.12	119.70
35	E	386	A	N1-C6-N6	12.01	125.81	118.60
35	E	833	A	N1-C6-N6	12.01	125.81	118.60
35	E	2216	A	N1-C6-N6	12.01	125.81	118.60
35	E	2	A	N1-C6-N6	12.01	125.81	118.60
35	E	595	A	N1-C6-N6	12.01	125.80	118.60
35	E	675	A	N1-C6-N6	12.01	125.80	118.60
35	E	2126	A	N1-C6-N6	12.01	125.80	118.60
35	E	905	A	N1-C6-N6	12.00	125.80	118.60
35	E	1255	A	N1-C6-N6	12.00	125.80	118.60
35	E	2272	A	N1-C6-N6	12.00	125.80	118.60
35	E	504	A	N1-C6-N6	12.00	125.80	118.60
35	E	499	A	N1-C6-N6	11.99	125.80	118.60
35	E	2267	A	N1-C6-N6	11.99	125.80	118.60
35	E	587	A	N1-C6-N6	11.99	125.79	118.60
35	E	698	C	P-O3'-C3'	11.99	134.08	119.70
35	E	444	A	N1-C6-N6	11.98	125.79	118.60
35	E	915	A	N1-C6-N6	11.98	125.79	118.60
35	E	1984	A	N1-C6-N6	11.98	125.79	118.60
35	E	1180	A	N1-C6-N6	11.98	125.79	118.60
35	E	2011	A	N1-C6-N6	11.98	125.79	118.60
35	E	2135	A	N1-C6-N6	11.98	125.79	118.60
35	E	1903	A	N1-C6-N6	11.97	125.78	118.60
35	E	858	A	N1-C6-N6	11.97	125.78	118.60
35	E	300	A	N1-C6-N6	11.97	125.78	118.60
35	E	1368	A	N1-C6-N6	11.97	125.78	118.60
35	E	1633	A	N1-C6-N6	11.97	125.78	118.60
35	E	1529	A	N1-C6-N6	11.96	125.78	118.60
35	E	1902	G	P-O3'-C3'	11.96	134.06	119.70
35	E	2260	A	N1-C6-N6	11.96	125.78	118.60
35	E	2037	A	N1-C6-N6	11.96	125.78	118.60
35	E	979	G	N1-C6-O6	11.96	127.08	119.90
35	E	1353	A	N1-C6-N6	11.96	125.77	118.60
35	E	765	A	N1-C6-N6	11.95	125.77	118.60
35	E	1960	A	N1-C6-N6	11.95	125.77	118.60
35	E	1327	A	N1-C6-N6	11.95	125.77	118.60
35	E	141	A	N1-C6-N6	11.95	125.77	118.60
35	E	516	A	N1-C6-N6	11.95	125.77	118.60
35	E	1087	A	N1-C6-N6	11.94	125.77	118.60
35	E	68	A	N1-C6-N6	11.94	125.77	118.60
35	E	531	A	N1-C6-N6	11.94	125.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	781	A	N1-C6-N6	11.94	125.76	118.60
35	E	598	A	N1-C6-N6	11.94	125.76	118.60
35	E	1539	A	N1-C6-N6	11.94	125.76	118.60
35	E	1568	A	N1-C6-N6	11.93	125.76	118.60
35	E	40	A	N1-C6-N6	11.93	125.76	118.60
35	E	242	A	N1-C6-N6	11.93	125.76	118.60
35	E	498	A	N1-C6-N6	11.93	125.76	118.60
35	E	467	A	N1-C6-N6	11.92	125.75	118.60
35	E	2259	A	N1-C6-N6	11.92	125.75	118.60
35	E	596	A	N1-C6-N6	11.92	125.75	118.60
35	E	2065	A	N1-C6-N6	11.92	125.75	118.60
35	E	107	A	N1-C6-N6	11.92	125.75	118.60
35	E	782	A	N1-C6-N6	11.92	125.75	118.60
35	E	793	A	N1-C6-N6	11.91	125.75	118.60
35	E	960	A	N1-C6-N6	11.91	125.75	118.60
35	E	912	A	N1-C6-N6	11.91	125.75	118.60
35	E	562	A	N1-C6-N6	11.91	125.74	118.60
35	E	1370	A	N1-C6-N6	11.90	125.74	118.60
35	E	1333	A	N1-C6-N6	11.90	125.74	118.60
35	E	525	A	N1-C6-N6	11.90	125.74	118.60
35	E	2005	A	N1-C6-N6	11.90	125.74	118.60
35	E	1343	A	N1-C6-N6	11.89	125.74	118.60
35	E	529	A	N1-C6-N6	11.89	125.73	118.60
35	E	2199	A	N1-C6-N6	11.89	125.73	118.60
35	E	81	A	N1-C6-N6	11.89	125.73	118.60
35	E	1264	A	N1-C6-N6	11.89	125.73	118.60
35	E	1189	A	N1-C6-N6	11.89	125.73	118.60
35	E	1888	A	N1-C6-N6	11.89	125.73	118.60
35	E	1996	A	N1-C6-N6	11.88	125.73	118.60
35	E	47	A	N1-C6-N6	11.88	125.73	118.60
35	E	352	A	N1-C6-N6	11.88	125.73	118.60
35	E	634	A	N1-C6-N6	11.88	125.73	118.60
35	E	1743	A	N1-C6-N6	11.88	125.73	118.60
35	E	1631	A	N1-C6-N6	11.87	125.72	118.60
35	E	1733	A	N1-C6-N6	11.87	125.72	118.60
35	E	2238	A	N1-C6-N6	11.87	125.72	118.60
35	E	792	G	N1-C6-O6	11.87	127.02	119.90
35	E	1662	A	N1-C6-N6	11.87	125.72	118.60
35	E	1920	A	N1-C6-N6	11.87	125.72	118.60
35	E	1999	A	N1-C6-N6	11.87	125.72	118.60
35	E	64	A	N1-C6-N6	11.86	125.72	118.60
35	E	501	A	N1-C6-N6	11.87	125.72	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	607	A	N1-C6-N6	11.87	125.72	118.60
35	E	769	A	N1-C6-N6	11.86	125.72	118.60
35	E	571	A	N1-C6-N6	11.86	125.72	118.60
35	E	2192	A	N1-C6-N6	11.86	125.72	118.60
35	E	82	A	N1-C6-N6	11.86	125.72	118.60
35	E	184	A	N1-C6-N6	11.86	125.71	118.60
35	E	181	A	N1-C6-N6	11.86	125.71	118.60
35	E	775	A	N1-C6-N6	11.86	125.71	118.60
35	E	898	A	N1-C6-N6	11.86	125.71	118.60
35	E	97	A	N1-C6-N6	11.85	125.71	118.60
35	E	2103	A	N1-C6-N6	11.85	125.71	118.60
35	E	1610	A	N1-C6-N6	11.85	125.71	118.60
35	E	527	A	N1-C6-N6	11.84	125.71	118.60
35	E	425	A	N1-C6-N6	11.83	125.70	118.60
35	E	861	A	N1-C6-N6	11.83	125.70	118.60
35	E	180	A	N1-C6-N6	11.83	125.70	118.60
35	E	624	A	N1-C6-N6	11.83	125.70	118.60
35	E	690	A	N1-C6-N6	11.83	125.70	118.60
35	E	1651	A	N1-C6-N6	11.83	125.70	118.60
35	E	1689	A	N1-C6-N6	11.83	125.70	118.60
35	E	2273	A	N1-C6-N6	11.83	125.70	118.60
35	E	992	A	N1-C6-N6	11.83	125.70	118.60
35	E	1987	A	N1-C6-N6	11.83	125.69	118.60
35	E	19	A	N1-C6-N6	11.82	125.69	118.60
35	E	648	A	N1-C6-N6	11.82	125.69	118.60
35	E	1975	A	N1-C6-N6	11.82	125.69	118.60
35	E	917	A	N1-C6-N6	11.82	125.69	118.60
35	E	177	A	N1-C6-N6	11.82	125.69	118.60
35	E	1312	A	N1-C6-N6	11.81	125.69	118.60
35	E	959	A	N1-C6-N6	11.81	125.69	118.60
35	E	447	A	N1-C6-N6	11.80	125.68	118.60
35	E	585	A	N1-C6-N6	11.80	125.68	118.60
35	E	249	A	N1-C6-N6	11.80	125.68	118.60
35	E	2035	A	N1-C6-N6	11.80	125.68	118.60
35	E	112	A	N1-C6-N6	11.80	125.68	118.60
35	E	902	A	N1-C6-N6	11.80	125.68	118.60
35	E	1878	A	N1-C6-N6	11.80	125.68	118.60
35	E	865	A	N1-C6-N6	11.79	125.67	118.60
35	E	1248	A	N1-C6-N6	11.79	125.67	118.60
35	E	1313	A	N1-C6-N6	11.79	125.67	118.60
35	E	250	A	N1-C6-N6	11.79	125.67	118.60
35	E	502	A	N1-C6-N6	11.79	125.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	500	A	N1-C6-N6	11.78	125.67	118.60
35	E	167	A	N1-C6-N6	11.78	125.67	118.60
35	E	1724	A	N1-C6-N6	11.78	125.67	118.60
35	E	1992	A	N1-C6-N6	11.78	125.67	118.60
35	E	2008	A	N1-C6-N6	11.78	125.67	118.60
35	E	493	A	N1-C6-N6	11.78	125.67	118.60
35	E	2055	A	N1-C6-N6	11.77	125.66	118.60
35	E	254	A	N1-C6-N6	11.77	125.66	118.60
35	E	694	A	N1-C6-N6	11.77	125.66	118.60
35	E	2274	A	N1-C6-N6	11.77	125.66	118.60
35	E	1919	A	N1-C6-N6	11.77	125.66	118.60
35	E	735	A	N1-C6-N6	11.76	125.66	118.60
35	E	673	A	N1-C6-N6	11.76	125.66	118.60
35	E	718	A	N1-C6-N6	11.76	125.66	118.60
35	E	231	A	N1-C6-N6	11.76	125.65	118.60
35	E	2069	A	N1-C6-N6	11.76	125.65	118.60
35	E	1323	A	N1-C6-N6	11.75	125.65	118.60
35	E	330	A	N1-C6-N6	11.75	125.65	118.60
35	E	523	A	N1-C6-N6	11.74	125.65	118.60
35	E	779	A	N1-C6-N6	11.74	125.65	118.60
35	E	913	A	N1-C6-N6	11.74	125.65	118.60
35	E	961	A	N1-C6-N6	11.74	125.64	118.60
35	E	51	A	N1-C6-N6	11.74	125.64	118.60
35	E	269	A	N1-C6-N6	11.74	125.64	118.60
35	E	345	A	N1-C6-N6	11.73	125.64	118.60
35	E	829	C	P-O3'-C3'	11.73	133.78	119.70
35	E	185	A	N1-C6-N6	11.73	125.64	118.60
35	E	1197	A	N1-C6-N6	11.73	125.64	118.60
35	E	43	A	N1-C6-N6	11.72	125.63	118.60
35	E	786	A	N1-C6-N6	11.72	125.63	118.60
35	E	812	A	N1-C6-N6	11.72	125.63	118.60
35	E	2039	A	N1-C6-N6	11.72	125.63	118.60
35	E	1942	A	N1-C6-N6	11.72	125.63	118.60
35	E	149	A	N1-C6-N6	11.72	125.63	118.60
35	E	771	A	N1-C6-N6	11.71	125.63	118.60
35	E	932	G	N1-C6-O6	11.71	126.93	119.90
35	E	972	A	N1-C6-N6	11.71	125.63	118.60
35	E	1620	A	N1-C6-N6	11.71	125.63	118.60
35	E	2315	A	N1-C6-N6	11.71	125.62	118.60
35	E	55	A	N1-C6-N6	11.70	125.62	118.60
35	E	2134	A	N1-C6-N6	11.70	125.62	118.60
35	E	2169	A	N1-C6-N6	11.70	125.62	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	866	A	N1-C6-N6	11.70	125.62	118.60
35	E	2104	A	N1-C6-N6	11.70	125.62	118.60
35	E	1803	A	N1-C6-N6	11.69	125.61	118.60
35	E	1961	A	N1-C6-N6	11.69	125.61	118.60
35	E	122	A	N1-C6-N6	11.68	125.61	118.60
35	E	1601	A	N1-C6-N6	11.68	125.61	118.60
35	E	729	C	P-O3'-C3'	11.68	133.71	119.70
35	E	1698	A	N1-C6-N6	11.68	125.61	118.60
35	E	2284	A	N1-C6-N6	11.68	125.61	118.60
35	E	520	A	N1-C6-N6	11.67	125.60	118.60
35	E	689	A	N1-C6-N6	11.67	125.60	118.60
35	E	784	A	N1-C6-N6	11.66	125.60	118.60
35	E	102	A	N1-C6-N6	11.66	125.59	118.60
35	E	1937	A	N1-C6-N6	11.65	125.59	118.60
35	E	1348	A	N1-C6-N6	11.65	125.59	118.60
35	E	901	A	N1-C6-N6	11.64	125.59	118.60
35	E	2113	G	N1-C6-O6	11.64	126.89	119.90
35	E	125	A	N1-C6-N6	11.64	125.58	118.60
35	E	1695	A	N1-C6-N6	11.64	125.58	118.60
35	E	817	A	N1-C6-N6	11.63	125.58	118.60
35	E	1378	A	N1-C6-N6	11.63	125.58	118.60
35	E	993	A	N1-C6-N6	11.63	125.58	118.60
35	E	1599	A	N1-C6-N6	11.63	125.58	118.60
35	E	1939	A	N1-C6-N6	11.62	125.58	118.60
35	E	1566	A	N1-C6-N6	11.62	125.57	118.60
35	E	39	A	N1-C6-N6	11.61	125.57	118.60
35	E	900	A	N1-C6-N6	11.61	125.56	118.60
35	E	2271	A	N1-C6-N6	11.61	125.56	118.60
35	E	2300	A	N1-C6-N6	11.60	125.56	118.60
35	E	2312	A	N1-C6-N6	11.59	125.55	118.60
35	E	1812	A	N1-C6-N6	11.58	125.55	118.60
35	E	885	U	P-O3'-C3'	11.56	133.57	119.70
35	E	1552	A	N1-C6-N6	11.55	125.53	118.60
35	E	1671	A	N1-C6-N6	11.55	125.53	118.60
35	E	2159	A	N1-C6-N6	11.55	125.53	118.60
35	E	216	A	N1-C6-N6	11.54	125.52	118.60
35	E	1076	C	P-O3'-C3'	11.54	133.54	119.70
35	E	1340	A	N1-C6-N6	11.53	125.52	118.60
35	E	2227	U	P-O3'-C3'	11.53	133.53	119.70
35	E	532	G	P-O3'-C3'	11.52	133.52	119.70
35	E	674	A	N1-C6-N6	11.51	125.51	118.60
35	E	351	A	N1-C6-N6	11.50	125.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	367	A	N1-C6-N6	11.50	125.50	118.60
35	E	162	A	N1-C6-N6	11.49	125.50	118.60
35	E	1630	A	N1-C6-N6	11.49	125.50	118.60
35	E	1328	A	N1-C6-N6	11.48	125.49	118.60
35	E	1081	G	P-O3'-C3'	11.48	133.48	119.70
35	E	148	G	N1-C6-O6	11.48	126.79	119.90
35	E	463	A	N1-C6-N6	11.48	125.49	118.60
35	E	2239	A	N1-C6-N6	11.48	125.49	118.60
35	E	446	A	N1-C6-N6	11.47	125.48	118.60
35	E	90	A	N1-C6-N6	11.46	125.48	118.60
35	E	360	A	N1-C6-N6	11.46	125.47	118.60
35	E	2063	A	N1-C6-N6	11.44	125.47	118.60
35	E	2056	A	N1-C6-N6	11.44	125.47	118.60
35	E	719	G	P-O3'-C3'	11.44	133.42	119.70
35	E	967	A	N1-C6-N6	11.43	125.46	118.60
35	E	1868	G	N1-C6-O6	11.43	126.76	119.90
35	E	968	U	P-O3'-C3'	11.42	133.40	119.70
35	E	1085	G	N1-C6-O6	11.42	126.75	119.90
35	E	1377	A	N1-C6-N6	11.42	125.45	118.60
35	E	2034	A	N1-C6-N6	11.41	125.45	118.60
35	E	288	A	N1-C6-N6	11.41	125.44	118.60
35	E	835	G	N1-C6-O6	11.40	126.74	119.90
35	E	1365	A	N1-C6-N6	11.39	125.43	118.60
35	E	950	G	N1-C6-O6	11.38	126.73	119.90
35	E	944	G	N1-C6-O6	11.38	126.72	119.90
35	E	621	A	N1-C6-N6	11.36	125.42	118.60
35	E	2038	G	N1-C6-O6	11.36	126.72	119.90
35	E	980	G	N1-C6-O6	11.32	126.69	119.90
35	E	485	A	N1-C6-N6	11.32	125.39	118.60
35	E	706	G	P-O5'-C5'	11.32	139.00	120.90
35	E	2007	A	N1-C6-N6	11.31	125.39	118.60
35	E	2213	G	P-O3'-C3'	11.31	133.27	119.70
35	E	777	A	N1-C6-N6	11.30	125.38	118.60
35	E	1305	A	N1-C6-N6	11.30	125.38	118.60
35	E	877	A	N1-C6-N6	11.29	125.38	118.60
35	E	316	A	N1-C6-N6	11.29	125.37	118.60
35	E	2107	A	N1-C6-N6	11.27	125.36	118.60
35	E	2204	A	N1-C6-N6	11.26	125.36	118.60
35	E	709	C	P-O3'-C3'	11.25	133.20	119.70
35	E	2148	A	N1-C6-N6	11.25	125.35	118.60
35	E	2110	A	N1-C6-N6	11.21	125.33	118.60
35	E	1338	A	N1-C6-N6	11.20	125.32	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1746	G	N1-C6-O6	11.20	126.62	119.90
35	E	940	U	P-O3'-C3'	11.20	133.14	119.70
35	E	1242	A	N1-C6-N6	11.19	125.31	118.60
35	E	1250	A	N1-C6-N6	11.18	125.31	118.60
35	E	237	A	N1-C6-N6	11.17	125.30	118.60
35	E	172	A	N1-C6-N6	11.17	125.30	118.60
35	E	1789	A	N1-C6-N6	11.16	125.30	118.60
35	E	1664	A	N1-C6-N6	11.16	125.30	118.60
35	E	575	A	N1-C6-N6	11.13	125.28	118.60
35	E	684	A	N1-C6-N6	11.13	125.28	118.60
35	E	1584	A	N1-C6-N6	11.12	125.27	118.60
35	E	484	A	N1-C6-N6	11.12	125.27	118.60
35	E	609	A	N1-C6-N6	11.12	125.27	118.60
35	E	953	G	N1-C6-O6	11.12	126.57	119.90
35	E	1808	G	N1-C6-O6	11.09	126.55	119.90
35	E	633	A	N1-C6-N6	11.06	125.24	118.60
35	E	979	G	C5-C6-O6	-11.05	121.97	128.60
35	E	2113	G	C5-C6-O6	-11.05	121.97	128.60
35	E	535	G	N1-C6-O6	10.98	126.49	119.90
35	E	2224	G	N1-C6-O6	10.98	126.49	119.90
35	E	63	G	N1-C6-O6	10.98	126.49	119.90
35	E	285	A	N1-C6-N6	10.97	125.18	118.60
35	E	1670	A	N1-C6-N6	10.89	125.14	118.60
35	E	2240	A	N1-C6-N6	10.89	125.13	118.60
35	E	862	A	N1-C6-N6	10.88	125.12	118.60
35	E	975	U	OP2-P-O3'	-10.86	81.31	105.20
35	E	788	A	P-O3'-C3'	10.83	132.70	119.70
35	E	335	G	N1-C6-O6	10.83	126.40	119.90
35	E	23	G	N1-C6-O6	10.80	126.38	119.90
35	E	822	A	N1-C6-N6	10.79	125.08	118.60
35	E	71	G	N1-C6-O6	10.79	126.37	119.90
35	E	931	G	N1-C6-O6	10.77	126.36	119.90
35	E	2131	A	N1-C6-N6	10.76	125.06	118.60
35	E	169	G	N1-C6-O6	10.75	126.35	119.90
35	E	1953	G	N1-C6-O6	10.75	126.35	119.90
35	E	1854	G	N1-C6-O6	10.74	126.35	119.90
35	E	1361	A	N1-C6-N6	10.74	125.05	118.60
35	E	2006	A	N1-C6-N6	10.74	125.05	118.60
35	E	276	G	N1-C6-O6	10.73	126.34	119.90
35	E	2051	C	P-O3'-C3'	10.73	132.58	119.70
35	E	263	G	N1-C6-O6	10.73	126.34	119.90
35	E	1384	G	N1-C6-O6	10.73	126.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	530	G	N1-C6-O6	10.72	126.33	119.90
35	E	567	G	N1-C6-O6	10.72	126.33	119.90
35	E	255	A	N1-C6-N6	10.71	125.03	118.60
35	E	1605	A	N1-C6-N6	10.71	125.03	118.60
35	E	1749	G	N1-C6-O6	10.69	126.31	119.90
35	E	1886	G	P-O3'-C3'	10.68	132.51	119.70
35	E	1606	A	N1-C6-N6	10.63	124.98	118.60
35	E	521	A	N1-C6-N6	10.62	124.97	118.60
35	E	100	A	N1-C6-N6	10.62	124.97	118.60
35	E	10	G	C5-C6-O6	-10.61	122.24	128.60
35	E	724	A	C5-C6-N1	-10.61	112.40	117.70
35	E	1644	G	N1-C6-O6	10.60	126.26	119.90
35	E	1625	A	N1-C6-N6	10.60	124.96	118.60
35	E	394	G	N1-C6-O6	10.59	126.26	119.90
35	E	291	G	N1-C6-O6	10.59	126.25	119.90
35	E	315	A	N1-C6-N6	10.57	124.94	118.60
35	E	2122	G	N1-C6-O6	10.55	126.23	119.90
35	E	1186	U	P-O3'-C3'	10.55	132.36	119.70
35	E	2165	A	N1-C6-N6	10.54	124.92	118.60
35	E	1898	G	N1-C6-O6	10.53	126.22	119.90
35	E	1306	A	N1-C6-N6	10.53	124.92	118.60
35	E	1547	A	N1-C6-N6	10.52	124.91	118.60
35	E	1873	G	N1-C6-O6	10.50	126.20	119.90
35	E	133	G	N1-C6-O6	10.47	126.19	119.90
35	E	1861	A	N1-C6-N6	10.47	124.88	118.60
35	E	983	C	O4'-C1'-N1	10.46	116.57	108.20
35	E	488	G	N1-C6-O6	10.45	126.17	119.90
35	E	1598	G	N1-C6-O6	10.45	126.17	119.90
35	E	53	G	N1-C6-O6	10.45	126.17	119.90
35	E	712	U	P-O3'-C3'	10.45	132.24	119.70
35	E	79	G	N1-C6-O6	10.44	126.16	119.90
35	E	2017	G	P-O3'-C3'	10.44	132.22	119.70
35	E	1824	A	N1-C6-N6	10.43	124.86	118.60
35	E	1555	G	N1-C6-O6	10.43	126.16	119.90
35	E	1277	G	N1-C6-O6	10.41	126.15	119.90
35	E	2296	G	N1-C6-O6	10.41	126.14	119.90
35	E	524	G	N1-C6-O6	10.40	126.14	119.90
35	E	2289	G	N1-C6-O6	10.39	126.13	119.90
35	E	895	A	N1-C6-N6	10.38	124.83	118.60
35	E	2120	A	N1-C6-N6	10.37	124.82	118.60
35	E	1871	G	N1-C6-O6	10.36	126.12	119.90
35	E	420	G	N1-C6-O6	10.36	126.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	555	G	N1-C6-O6	10.35	126.11	119.90
35	E	766	C	O4'-C1'-N1	10.34	116.47	108.20
35	E	106	G	N1-C6-O6	10.34	126.10	119.90
35	E	2043	G	N1-C6-O6	10.34	126.10	119.90
35	E	299	A	N1-C6-N6	10.33	124.80	118.60
35	E	1210	G	N1-C6-O6	10.33	126.10	119.90
35	E	855	G	N1-C6-O6	10.32	126.09	119.90
35	E	2249	A	N1-C6-N6	10.32	124.79	118.60
35	E	1233	A	N1-C6-N6	10.31	124.79	118.60
35	E	857	G	N1-C6-O6	10.29	126.08	119.90
35	E	2045	A	N1-C6-N6	10.29	124.78	118.60
35	E	661	G	N1-C6-O6	10.29	126.07	119.90
35	E	2214	A	N1-C6-N6	10.29	124.77	118.60
35	E	1808	G	C5-C6-O6	-10.28	122.43	128.60
35	E	2195	G	N1-C6-O6	10.27	126.06	119.90
35	E	188	G	N1-C6-O6	10.27	126.06	119.90
35	E	2237	G	N1-C6-O6	10.27	126.06	119.90
35	E	1869	G	N1-C6-O6	10.26	126.05	119.90
35	E	702	U	O4'-C1'-N1	10.25	116.40	108.20
35	E	907	G	N1-C6-O6	10.25	126.05	119.90
35	E	711	A	C5-C6-N1	-10.25	112.58	117.70
35	E	1943	G	N1-C6-O6	10.25	126.05	119.90
35	E	1182	G	N1-C6-O6	10.23	126.04	119.90
35	E	975	U	OP1-P-O3'	-10.22	82.72	105.20
35	E	1731	G	N1-C6-O6	10.22	126.03	119.90
35	E	1900	G	N1-C6-O6	10.21	126.02	119.90
35	E	970	G	N1-C6-O6	10.20	126.02	119.90
35	E	943	G	N1-C6-O6	10.19	126.02	119.90
35	E	706	G	N1-C6-O6	10.19	126.01	119.90
35	E	552	G	N1-C6-O6	10.18	126.01	119.90
35	E	541	G	N1-C6-O6	10.18	126.01	119.90
35	E	86	G	N1-C6-O6	10.17	126.00	119.90
35	E	1237	G	N1-C6-O6	10.17	126.00	119.90
35	E	1545	U	P-O3'-C3'	10.17	131.90	119.70
35	E	1367	G	N1-C6-O6	10.15	125.99	119.90
35	E	220	G	N1-C6-O6	10.15	125.99	119.90
35	E	1763	G	N1-C6-O6	10.15	125.99	119.90
35	E	223	G	N1-C6-O6	10.14	125.98	119.90
35	E	1855	G	N1-C6-O6	10.14	125.98	119.90
35	E	2139	G	N1-C6-O6	10.13	125.98	119.90
35	E	2233	G	N1-C6-O6	10.13	125.98	119.90
35	E	1927	A	N1-C6-N6	10.12	124.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	508	G	N1-C6-O6	10.12	125.97	119.90
35	E	347	G	N1-C6-O6	10.11	125.96	119.90
35	E	2121	G	N1-C6-O6	10.10	125.96	119.90
35	E	836	G	N1-C6-O6	10.10	125.96	119.90
35	E	403	G	N1-C6-O6	10.09	125.95	119.90
35	E	734	G	C5-C6-O6	-10.08	122.55	128.60
35	E	211	G	N1-C6-O6	10.08	125.95	119.90
35	E	6	G	N1-C6-O6	10.07	125.94	119.90
35	E	1817	G	N1-C6-O6	10.07	125.94	119.90
35	E	1577	G	N1-C6-O6	10.06	125.94	119.90
35	E	2152	C	P-O3'-C3'	10.05	131.76	119.70
35	E	943	G	C5-C6-O6	-10.04	122.58	128.60
35	E	713	G	P-O3'-C3'	10.04	131.75	119.70
35	E	204	G	N1-C6-O6	10.04	125.92	119.90
35	E	1735	G	N1-C6-O6	10.03	125.92	119.90
35	E	363	A	N1-C6-N6	10.03	124.62	118.60
35	E	517	G	N1-C6-O6	10.03	125.92	119.90
35	E	888	G	N1-C6-O6	10.02	125.91	119.90
35	E	410	G	N1-C6-O6	10.02	125.91	119.90
35	E	1274	A	N1-C6-N6	10.01	124.61	118.60
35	E	954	G	N1-C6-O6	10.00	125.90	119.90
35	E	564	G	N1-C6-O6	10.00	125.90	119.90
35	E	42	G	N1-C6-O6	9.99	125.90	119.90
35	E	651	G	N1-C6-O6	9.98	125.89	119.90
35	E	470	G	N1-C6-O6	9.97	125.88	119.90
35	E	431	G	N1-C6-O6	9.97	125.88	119.90
35	E	1549	G	N1-C6-O6	9.97	125.88	119.90
35	E	1776	G	N1-C6-O6	9.96	125.88	119.90
35	E	230	G	N1-C6-O6	9.96	125.87	119.90
35	E	7	G	N1-C6-O6	9.95	125.87	119.90
35	E	717	U	P-O3'-C3'	9.95	131.64	119.70
35	E	996	G	N1-C6-O6	9.95	125.87	119.90
35	E	2217	G	N1-C6-O6	9.94	125.86	119.90
35	E	944	G	C5-C6-O6	-9.93	122.64	128.60
35	E	1687	A	N1-C6-N6	9.93	124.56	118.60
35	E	532	G	N1-C6-O6	9.93	125.86	119.90
35	E	2265	G	N1-C6-O6	9.93	125.86	119.90
35	E	2304	G	N1-C6-O6	9.93	125.86	119.90
35	E	1852	G	N1-C6-O6	9.92	125.85	119.90
35	E	1870	G	N1-C6-O6	9.92	125.85	119.90
35	E	785	A	P-O3'-C3'	9.92	131.60	119.70
35	E	1608	G	N1-C6-O6	9.92	125.85	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	57	G	N1-C6-O6	9.91	125.85	119.90
35	E	132	G	N1-C6-O6	9.90	125.84	119.90
35	E	1213	G	N1-C6-O6	9.90	125.84	119.90
35	E	2220	G	N1-C6-O6	9.89	125.84	119.90
35	E	205	G	N1-C6-O6	9.89	125.83	119.90
35	E	1880	U	O4'-C1'-N1	9.88	116.10	108.20
35	E	982	G	N1-C6-O6	9.87	125.82	119.90
35	E	2197	G	N1-C6-O6	9.87	125.82	119.90
35	E	473	G	N1-C6-O6	9.87	125.82	119.90
35	E	2176	G	N1-C6-O6	9.87	125.82	119.90
35	E	208	G	N1-C6-O6	9.87	125.82	119.90
35	E	835	G	C5-C6-O6	-9.87	122.68	128.60
35	E	409	G	N1-C6-O6	9.86	125.82	119.90
35	E	756	G	N1-C6-O6	9.86	125.81	119.90
35	E	2275	G	N1-C6-O6	9.86	125.82	119.90
35	E	1220	G	N1-C6-O6	9.86	125.81	119.90
35	E	1307	G	N1-C6-O6	9.86	125.81	119.90
35	E	311	G	N1-C6-O6	9.85	125.81	119.90
35	E	772	U	P-O3'-C3'	9.85	131.51	119.70
35	E	30	G	N1-C6-O6	9.84	125.81	119.90
35	E	34	G	N1-C6-O6	9.84	125.80	119.90
35	E	1381	G	N1-C6-O6	9.83	125.80	119.90
35	E	466	G	N1-C6-O6	9.83	125.80	119.90
35	E	189	G	N1-C6-O6	9.82	125.80	119.90
35	E	233	G	N1-C6-O6	9.82	125.79	119.90
35	E	963	G	N1-C6-O6	9.82	125.79	119.90
35	E	971	G	N1-C6-O6	9.82	125.79	119.90
35	E	1886	G	N1-C6-O6	9.82	125.79	119.90
35	E	109	G	N1-C6-O6	9.81	125.78	119.90
35	E	606	G	N1-C6-O6	9.81	125.78	119.90
35	E	1635	G	N1-C6-O6	9.80	125.78	119.90
35	E	1206	G	N1-C6-O6	9.79	125.78	119.90
35	E	1997	G	N1-C6-O6	9.79	125.78	119.90
35	E	413	G	N1-C6-O6	9.79	125.78	119.90
35	E	229	G	N1-C6-O6	9.79	125.77	119.90
35	E	430	G	N1-C6-O6	9.79	125.77	119.90
35	E	2127	G	N1-C6-O6	9.79	125.77	119.90
35	E	1666	G	N1-C6-O6	9.79	125.77	119.90
35	E	156	G	N1-C6-O6	9.78	125.77	119.90
35	E	1382	G	N1-C6-O6	9.78	125.77	119.90
35	E	2163	G	N1-C6-O6	9.78	125.77	119.90
35	E	514	G	N1-C6-O6	9.76	125.76	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	611	G	N1-C6-O6	9.76	125.76	119.90
35	E	1876	G	C5-C6-O6	-9.75	122.75	128.60
35	E	334	G	N1-C6-O6	9.74	125.75	119.90
35	E	395	G	N1-C6-O6	9.74	125.75	119.90
35	E	1777	G	N1-C6-O6	9.74	125.75	119.90
35	E	93	G	N1-C6-O6	9.74	125.74	119.90
35	E	1339	G	N1-C6-O6	9.74	125.74	119.90
35	E	842	G	N1-C6-O6	9.73	125.74	119.90
35	E	2278	G	N1-C6-O6	9.73	125.74	119.90
35	E	1979	G	N1-C6-O6	9.73	125.74	119.90
35	E	1594	G	N1-C6-O6	9.73	125.74	119.90
35	E	2266	G	N1-C6-O6	9.73	125.74	119.90
35	E	192	G	N1-C6-O6	9.72	125.73	119.90
35	E	451	G	N1-C6-O6	9.71	125.72	119.90
35	E	495	G	N1-C6-O6	9.69	125.72	119.90
35	E	173	A	N1-C6-N6	9.69	124.41	118.60
35	E	2222	G	N1-C6-O6	9.69	125.71	119.90
35	E	1230	G	N1-C6-O6	9.68	125.71	119.90
35	E	320	G	N1-C6-O6	9.67	125.70	119.90
35	E	2194	G	N1-C6-O6	9.67	125.70	119.90
35	E	2073	G	N1-C6-O6	9.66	125.70	119.90
35	E	2206	G	N1-C6-O6	9.65	125.69	119.90
35	E	207	G	N1-C6-O6	9.65	125.69	119.90
35	E	401	A	N1-C6-N6	9.65	124.39	118.60
35	E	1579	G	N1-C6-O6	9.64	125.69	119.90
35	E	791	G	N1-C6-O6	9.64	125.69	119.90
35	E	272	G	N1-C6-O6	9.64	125.68	119.90
35	E	1289	G	N1-C6-O6	9.64	125.68	119.90
35	E	566	G	N1-C6-O6	9.63	125.68	119.90
35	E	1329	G	N1-C6-O6	9.63	125.68	119.90
35	E	48	G	N1-C6-O6	9.63	125.68	119.90
35	E	1867	G	N1-C6-O6	9.63	125.68	119.90
35	E	2205	G	N1-C6-O6	9.63	125.68	119.90
35	E	513	G	N1-C6-O6	9.62	125.67	119.90
35	E	1793	G	N1-C6-O6	9.62	125.67	119.90
35	E	389	G	N1-C6-O6	9.62	125.67	119.90
35	E	987	G	N1-C6-O6	9.62	125.67	119.90
35	E	1085	G	C5-C6-O6	-9.61	122.83	128.60
35	E	775	A	P-O5'-C5'	9.61	136.28	120.90
35	E	1563	G	N1-C6-O6	9.61	125.67	119.90
35	E	2003	G	N1-C6-O6	9.61	125.67	119.90
35	E	1786	G	N1-C6-O6	9.61	125.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2295	G	N1-C6-O6	9.60	125.66	119.90
35	E	151	A	N1-C6-N6	9.60	124.36	118.60
35	E	678	G	N1-C6-O6	9.60	125.66	119.90
35	E	317	G	N1-C6-O6	9.60	125.66	119.90
35	E	1697	G	N1-C6-O6	9.60	125.66	119.90
35	E	477	G	N1-C6-O6	9.59	125.65	119.90
35	E	1216	G	N1-C6-O6	9.59	125.65	119.90
35	E	615	G	N1-C6-O6	9.57	125.64	119.90
35	E	1746	G	C5-C6-O6	-9.57	122.86	128.60
35	E	1762	G	N1-C6-O6	9.57	125.64	119.90
35	E	405	G	N1-C6-O6	9.56	125.64	119.90
35	E	1165	G	N1-C6-O6	9.55	125.63	119.90
35	E	2150	G	N1-C6-O6	9.54	125.63	119.90
35	E	199	G	N1-C6-O6	9.54	125.62	119.90
35	E	2292	G	N1-C6-O6	9.53	125.62	119.90
35	E	412	G	N1-C6-O6	9.53	125.62	119.90
35	E	633	A	P-O3'-C3'	9.53	131.13	119.70
35	E	404	G	N1-C6-O6	9.52	125.61	119.90
35	E	1349	G	N1-C6-O6	9.52	125.61	119.90
35	E	1600	A	N1-C6-N6	9.52	124.31	118.60
35	E	1749	G	C5-C6-O6	-9.52	122.89	128.60
35	E	1578	G	N1-C6-O6	9.51	125.61	119.90
35	E	616	G	N1-C6-O6	9.51	125.61	119.90
35	E	2156	G	N1-C6-O6	9.51	125.61	119.90
35	E	130	G	N1-C6-O6	9.51	125.60	119.90
35	E	157	G	N1-C6-O6	9.50	125.60	119.90
35	E	2147	U	O4'-C1'-N1	9.50	115.80	108.20
35	E	148	G	C5-C6-O6	-9.49	122.90	128.60
35	E	1922	G	N1-C6-O6	9.49	125.59	119.90
35	E	640	G	N1-C6-O6	9.49	125.59	119.90
35	E	670	G	N1-C6-O6	9.49	125.59	119.90
35	E	1332	G	N1-C6-O6	9.48	125.59	119.90
35	E	1263	G	N1-C6-O6	9.48	125.59	119.90
35	E	2208	G	N1-C6-O6	9.47	125.58	119.90
35	E	738	G	C5-C6-O6	-9.47	122.92	128.60
35	E	1326	G	N1-C6-O6	9.46	125.58	119.90
35	E	2141	G	N1-C6-O6	9.46	125.58	119.90
35	E	919	G	P-O3'-C3'	9.46	131.05	119.70
35	E	2044	G	N1-C6-O6	9.46	125.58	119.90
35	E	1319	G	N1-C6-O6	9.46	125.57	119.90
35	E	1562	G	N1-C6-O6	9.46	125.58	119.90
35	E	1705	G	N1-C6-O6	9.46	125.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1970	G	N1-C6-O6	9.46	125.57	119.90
35	E	708	G	N1-C6-O6	9.45	125.57	119.90
35	E	370	G	N1-C6-O6	9.45	125.57	119.90
35	E	878	G	N1-C6-O6	9.45	125.57	119.90
35	E	812	A	P-O3'-C3'	9.45	131.03	119.70
35	E	71	G	C5-C6-O6	-9.44	122.94	128.60
35	E	364	G	N1-C6-O6	9.44	125.56	119.90
35	E	568	G	N1-C6-O6	9.44	125.56	119.90
35	E	1260	G	N1-C6-O6	9.44	125.56	119.90
35	E	344	G	N1-C6-O6	9.43	125.56	119.90
35	E	76	G	N1-C6-O6	9.43	125.56	119.90
35	E	628	G	N1-C6-O6	9.42	125.55	119.90
35	E	869	G	N1-C6-O6	9.42	125.55	119.90
35	E	535	G	C5-C6-O6	-9.41	122.95	128.60
35	E	1944	G	N1-C6-O6	9.41	125.55	119.90
35	E	322	G	N1-C6-O6	9.41	125.55	119.90
35	E	664	G	N1-C6-O6	9.40	125.54	119.90
35	E	980	G	C5-C6-O6	-9.40	122.96	128.60
35	E	1856	G	N1-C6-O6	9.40	125.54	119.90
35	E	792	G	P-O3'-C3'	9.39	130.97	119.70
35	E	355	G	N1-C6-O6	9.39	125.53	119.90
35	E	733	G	N1-C6-O6	9.38	125.53	119.90
35	E	238	G	N1-C6-O6	9.38	125.53	119.90
35	E	880	A	N1-C6-N6	9.38	124.23	118.60
35	E	2241	G	N1-C6-O6	9.38	125.53	119.90
35	E	1910	G	N1-C6-O6	9.37	125.52	119.90
35	E	139	G	N1-C6-O6	9.37	125.52	119.90
35	E	705	G	N1-C6-O6	9.36	125.51	119.90
35	E	2118	G	N1-C6-O6	9.36	125.51	119.90
35	E	908	G	N1-C6-O6	9.35	125.51	119.90
35	E	1315	G	N1-C6-O6	9.34	125.51	119.90
35	E	1203	G	N1-C6-O6	9.34	125.50	119.90
35	E	605	G	N1-C6-O6	9.34	125.50	119.90
35	E	481	G	N1-C6-O6	9.33	125.50	119.90
35	E	276	G	C5-C6-O6	-9.33	123.00	128.60
35	E	1656	G	N1-C6-O6	9.33	125.50	119.90
35	E	240	G	N1-C6-O6	9.32	125.50	119.90
35	E	622	G	N1-C6-O6	9.32	125.49	119.90
35	E	994	G	N1-C6-O6	9.32	125.49	119.90
35	E	1950	G	N1-C6-O6	9.32	125.49	119.90
35	E	1968	G	N1-C6-O6	9.32	125.49	119.90
35	E	41	G	N1-C6-O6	9.31	125.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	794	G	N1-C6-O6	9.31	125.49	119.90
35	E	1569	G	N1-C6-O6	9.31	125.49	119.90
35	E	435	G	N1-C6-O6	9.31	125.48	119.90
35	E	1756	G	N1-C6-O6	9.30	125.48	119.90
35	E	1868	G	C5-C6-O6	-9.30	123.02	128.60
35	E	244	G	N1-C6-O6	9.30	125.48	119.90
35	E	1932	G	N1-C6-O6	9.29	125.48	119.90
35	E	2310	G	N1-C6-O6	9.29	125.47	119.90
35	E	1816	G	N1-C6-O6	9.28	125.47	119.90
35	E	147	G	N1-C6-O6	9.27	125.46	119.90
35	E	1876	G	N1-C6-O6	9.27	125.46	119.90
35	E	1320	G	N1-C6-O6	9.27	125.46	119.90
35	E	2172	G	N1-C6-O6	9.27	125.46	119.90
35	E	712	U	O4'-C1'-N1	9.27	115.61	108.20
35	E	1759	G	N1-C6-O6	9.26	125.45	119.90
35	E	133	G	C5-C6-O6	-9.26	123.05	128.60
35	E	291	G	C5-C6-O6	-9.25	123.05	128.60
35	E	439	G	N1-C6-O6	9.25	125.45	119.90
35	E	448	A	N1-C6-N6	9.23	124.14	118.60
35	E	1214	G	N1-C6-O6	9.23	125.44	119.90
35	E	1854	G	C5-C6-O6	-9.23	123.06	128.60
35	E	847	U	P-O3'-C3'	9.22	130.77	119.70
35	E	313	G	N1-C6-O6	9.20	125.42	119.90
35	E	1972	G	N1-C6-O6	9.20	125.42	119.90
35	E	106	G	C5-C6-O6	-9.20	123.08	128.60
35	E	1075	G	N1-C6-O6	9.20	125.42	119.90
35	E	1623	G	N1-C6-O6	9.20	125.42	119.90
35	E	2182	G	N1-C6-O6	9.19	125.41	119.90
35	E	179	G	N1-C6-O6	9.19	125.41	119.90
35	E	547	G	N1-C6-O6	9.18	125.41	119.90
35	E	2086	G	N1-C6-O6	9.17	125.40	119.90
35	E	2269	G	N1-C6-O6	9.17	125.40	119.90
35	E	2038	G	C5-C6-O6	-9.17	123.10	128.60
35	E	1083	G	N1-C6-O6	9.16	125.40	119.90
35	E	1898	G	C5-C6-O6	-9.15	123.11	128.60
35	E	1776	G	C5-C6-O6	-9.13	123.12	128.60
35	E	790	G	N1-C6-O6	9.13	125.38	119.90
35	E	377	G	N1-C6-O6	9.12	125.37	119.90
35	E	757	G	N1-C6-O6	9.12	125.37	119.90
35	E	1212	G	N1-C6-O6	9.12	125.37	119.90
35	E	469	G	N1-C6-O6	9.11	125.37	119.90
35	E	468	G	N1-C6-O6	9.11	125.36	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	699	C	O4'-C1'-N1	9.11	115.48	108.20
35	E	1228	G	N1-C6-O6	9.11	125.36	119.90
35	E	1940	G	N1-C6-O6	9.10	125.36	119.90
35	E	1694	G	N1-C6-O6	9.10	125.36	119.90
35	E	1555	G	C5-C6-O6	-9.10	123.14	128.60
35	E	567	G	C5-C6-O6	-9.09	123.14	128.60
35	E	1692	G	N1-C6-O6	9.09	125.35	119.90
35	E	1337	G	N1-C6-O6	9.08	125.35	119.90
35	E	2064	G	N1-C6-O6	9.08	125.35	119.90
35	E	1538	G	N1-C6-O6	9.08	125.35	119.90
35	E	2285	G	N1-C6-O6	9.08	125.35	119.90
35	E	748	G	N1-C6-O6	9.08	125.35	119.90
35	E	263	G	C5-C6-O6	-9.07	123.16	128.60
35	E	321	G	N1-C6-O6	9.07	125.34	119.90
35	E	433	G	N1-C6-O6	9.07	125.34	119.90
35	E	79	G	C5-C6-O6	-9.07	123.16	128.60
35	E	1234	G	N1-C6-O6	9.06	125.34	119.90
35	E	228	G	N1-C6-O6	9.06	125.34	119.90
35	E	1796	G	N1-C6-O6	9.06	125.34	119.90
35	E	1798	G	N1-C6-O6	9.06	125.34	119.90
35	E	931	G	C5-C6-O6	-9.05	123.17	128.60
35	E	119	G	N1-C6-O6	9.05	125.33	119.90
35	E	1953	G	C5-C6-O6	-9.05	123.17	128.60
35	E	1317	G	N1-C6-O6	9.05	125.33	119.90
35	E	1969	G	N1-C6-O6	9.05	125.33	119.90
35	E	1288	G	N1-C6-O6	9.05	125.33	119.90
35	E	530	G	C5-C6-O6	-9.04	123.18	128.60
35	E	792	G	C5-C6-O6	-9.04	123.18	128.60
35	E	824	G	N1-C6-O6	9.04	125.32	119.90
35	E	918	G	N1-C6-O6	9.04	125.32	119.90
35	E	1736	G	N1-C6-O6	9.04	125.32	119.90
35	E	436	G	N1-C6-O6	9.03	125.32	119.90
35	E	555	G	C5-C6-O6	-9.03	123.18	128.60
35	E	2224	G	C5-C6-O6	-9.03	123.18	128.60
35	E	539	G	N1-C6-O6	9.03	125.32	119.90
35	E	1921	G	N1-C6-O6	9.03	125.32	119.90
35	E	63	G	C5-C6-O6	-9.02	123.19	128.60
35	E	188	G	C5-C6-O6	-9.02	123.19	128.60
35	E	1277	G	C5-C6-O6	-9.02	123.19	128.60
35	E	273	G	N1-C6-O6	9.02	125.31	119.90
35	E	2050	C	P-O3'-C3'	9.02	130.52	119.70
35	E	1614	G	N1-C6-O6	9.01	125.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1253	G	N1-C6-O6	9.01	125.31	119.90
35	E	1575	G	N1-C6-O6	9.01	125.31	119.90
35	E	733	G	C5-C6-O6	-9.01	123.20	128.60
35	E	2144	G	N1-C6-O6	9.00	125.30	119.90
35	E	1739	G	N1-C6-O6	9.00	125.30	119.90
35	E	86	G	C5-C6-O6	-9.00	123.20	128.60
35	E	1644	G	C5-C6-O6	-9.00	123.20	128.60
35	E	1817	G	C5-C6-O6	-9.00	123.20	128.60
35	E	443	G	N1-C6-O6	8.99	125.30	119.90
35	E	2020	G	N1-C6-O6	8.99	125.30	119.90
35	E	1933	G	N1-C6-O6	8.99	125.29	119.90
35	E	1914	U	O4'-C1'-N1	8.99	115.39	108.20
35	E	2124	G	N1-C6-O6	8.99	125.29	119.90
35	E	289	G	N1-C6-O6	8.98	125.29	119.90
35	E	23	G	C5-C6-O6	-8.98	123.21	128.60
35	E	465	G	N1-C6-O6	8.97	125.28	119.90
35	E	2061	G	N1-C6-O6	8.97	125.28	119.90
35	E	1873	G	C5-C6-O6	-8.97	123.22	128.60
35	E	1701	G	N1-C6-O6	8.96	125.28	119.90
35	E	2012	C	P-O5'-C5'	8.96	135.23	120.90
35	E	1617	G	N1-C6-O6	8.95	125.27	119.90
35	E	921	G	N1-C6-O6	8.95	125.27	119.90
35	E	1225	G	N1-C6-O6	8.94	125.27	119.90
35	E	1995	G	N1-C6-O6	8.94	125.27	119.90
35	E	479	G	N1-C6-O6	8.94	125.26	119.90
35	E	888	G	C5-C6-O6	-8.94	123.24	128.60
35	E	164	G	N1-C6-O6	8.93	125.26	119.90
35	E	249	A	O4'-C1'-N9	8.93	115.35	108.20
35	E	512	A	N1-C6-N6	8.93	123.96	118.60
35	E	682	G	N1-C6-O6	8.93	125.26	119.90
35	E	1367	G	C5-C6-O6	-8.93	123.24	128.60
35	E	2023	C	O4'-C1'-N1	8.93	115.35	108.20
35	E	2108	G	N1-C6-O6	8.93	125.26	119.90
35	E	814	C	C2-N1-C1'	8.93	128.62	118.80
35	E	833	A	P-O3'-C3'	8.93	130.41	119.70
35	E	1713	G	N1-C6-O6	8.93	125.26	119.90
35	E	1640	G	N1-C6-O6	8.92	125.25	119.90
35	E	1823	G	N1-C6-O6	8.92	125.25	119.90
35	E	400	G	N1-C6-O6	8.91	125.25	119.90
35	E	838	G	N1-C6-O6	8.91	125.25	119.90
35	E	1691	G	N1-C6-O6	8.91	125.25	119.90
35	E	893	G	N1-C6-O6	8.91	125.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2212	G	N1-C6-O6	8.91	125.25	119.90
35	E	1190	G	N1-C6-O6	8.90	125.24	119.90
35	E	335	G	C5-C6-O6	-8.90	123.26	128.60
35	E	385	G	N1-C6-O6	8.90	125.24	119.90
35	E	1199	G	N1-C6-O6	8.90	125.24	119.90
35	E	685	G	N1-C6-O6	8.90	125.24	119.90
35	E	761	G	N1-C6-O6	8.90	125.24	119.90
35	E	796	G	N1-C6-O6	8.90	125.24	119.90
35	E	1081	G	N1-C6-O6	8.90	125.24	119.90
35	E	1560	G	N1-C6-O6	8.90	125.24	119.90
35	E	213	G	N1-C6-O6	8.89	125.24	119.90
35	E	985	G	N1-C6-O6	8.89	125.24	119.90
35	E	1249	G	N1-C6-O6	8.89	125.24	119.90
35	E	1875	G	N1-C6-O6	8.89	125.23	119.90
35	E	1901	G	N1-C6-O6	8.89	125.23	119.90
35	E	2123	C	O4'-C1'-N1	8.89	115.31	108.20
35	E	745	C	O4'-C1'-N1	8.88	115.31	108.20
35	E	1993	G	N1-C6-O6	8.89	125.23	119.90
35	E	1183	G	N1-C6-O6	8.88	125.23	119.90
35	E	693	G	N1-C6-O6	8.88	125.23	119.90
35	E	511	G	N1-C6-O6	8.88	125.22	119.90
35	E	1792	G	N1-C6-O6	8.87	125.22	119.90
35	E	2049	C	O4'-C1'-N1	8.87	115.30	108.20
35	E	2079	G	N1-C6-O6	8.87	125.22	119.90
35	E	248	G	N1-C6-O6	8.87	125.22	119.90
35	E	602	G	N1-C6-O6	8.87	125.22	119.90
35	E	2151	U	O4'-C1'-N1	8.86	115.29	108.20
35	E	661	G	C5-C6-O6	-8.86	123.28	128.60
35	E	53	G	C5-C6-O6	-8.86	123.28	128.60
35	E	419	G	N1-C6-O6	8.86	125.22	119.90
35	E	1765	G	N1-C6-O6	8.86	125.22	119.90
35	E	2043	G	C5-C6-O6	-8.86	123.28	128.60
35	E	1618	G	N1-C6-O6	8.85	125.21	119.90
35	E	1198	G	N1-C6-O6	8.84	125.20	119.90
35	E	2286	G	N1-C6-O6	8.84	125.20	119.90
35	E	1072	G	N1-C6-O6	8.84	125.20	119.90
35	E	1917	G	N1-C6-O6	8.84	125.20	119.90
35	E	424	G	N1-C6-O6	8.83	125.20	119.90
35	E	476	G	N1-C6-O6	8.83	125.20	119.90
35	E	1364	G	N1-C6-O6	8.83	125.20	119.90
35	E	1376	G	N1-C6-O6	8.83	125.20	119.90
35	E	2179	G	N1-C6-O6	8.83	125.20	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1738	G	N1-C6-O6	8.83	125.20	119.90
35	E	1226	G	N1-C6-O6	8.82	125.19	119.90
35	E	2109	G	N1-C6-O6	8.82	125.19	119.90
35	E	1276	G	N1-C6-O6	8.82	125.19	119.90
35	E	2074	G	N1-C6-O6	8.82	125.19	119.90
35	E	815	G	N1-C6-O6	8.82	125.19	119.90
35	E	1813	G	N1-C6-O6	8.82	125.19	119.90
35	E	989	G	N1-C6-O6	8.81	125.19	119.90
35	E	2030	G	N1-C6-O6	8.81	125.19	119.90
35	E	631	G	N1-C6-O6	8.80	125.18	119.90
35	E	411	G	N1-C6-O6	8.80	125.18	119.90
35	E	1236	G	N1-C6-O6	8.80	125.18	119.90
35	E	1322	G	N1-C6-O6	8.80	125.18	119.90
35	E	1551	G	N1-C6-O6	8.80	125.18	119.90
35	E	1924	G	N1-C6-O6	8.80	125.18	119.90
35	E	137	C	O4'-C1'-N1	8.79	115.24	108.20
35	E	212	G	N1-C6-O6	8.80	125.18	119.90
35	E	2040	G	N1-C6-O6	8.79	125.18	119.90
35	E	46	U	O4'-C1'-N1	8.79	115.23	108.20
35	E	938	G	N1-C6-O6	8.79	125.17	119.90
35	E	2011	A	P-O3'-C3'	8.79	130.25	119.70
35	E	1632	G	N1-C6-O6	8.79	125.17	119.90
35	E	649	G	N1-C6-O6	8.78	125.17	119.90
35	E	2101	G	N1-C6-O6	8.78	125.17	119.90
35	E	379	G	N1-C6-O6	8.78	125.17	119.90
35	E	1963	G	N1-C6-O6	8.78	125.17	119.90
35	E	407	G	N1-C6-O6	8.78	125.17	119.90
35	E	1590	G	N1-C6-O6	8.77	125.17	119.90
35	E	309	G	N1-C6-O6	8.77	125.16	119.90
35	E	930	G	N1-C6-O6	8.77	125.16	119.90
35	E	1596	G	N1-C6-O6	8.77	125.16	119.90
35	E	1084	G	N1-C6-O6	8.77	125.16	119.90
35	E	1165	G	C5-C6-O6	-8.77	123.34	128.60
35	E	1890	C	O4'-C1'-N1	8.76	115.21	108.20
35	E	20	G	N1-C6-O6	8.76	125.16	119.90
35	E	754	G	N1-C6-O6	8.76	125.16	119.90
35	E	909	G	N1-C6-O6	8.76	125.16	119.90
35	E	1915	G	N1-C6-O6	8.76	125.15	119.90
35	E	903	G	N1-C6-O6	8.75	125.15	119.90
35	E	1383	G	N1-C6-O6	8.75	125.15	119.90
35	E	919	G	N1-C6-O6	8.75	125.15	119.90
35	E	30	G	C5-C6-O6	-8.74	123.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	828	G	N1-C6-O6	8.74	125.15	119.90
35	E	1696	G	N1-C6-O6	8.74	125.14	119.90
35	E	688	G	N1-C6-O6	8.74	125.14	119.90
35	E	1622	G	N1-C6-O6	8.74	125.14	119.90
35	E	2106	G	N1-C6-O6	8.74	125.14	119.90
35	E	591	G	N1-C6-O6	8.73	125.14	119.90
35	E	618	G	N1-C6-O6	8.73	125.14	119.90
35	E	2081	G	N1-C6-O6	8.73	125.14	119.90
35	E	667	G	N1-C6-O6	8.73	125.14	119.90
35	E	1906	C	O4'-C1'-N1	8.72	115.18	108.20
35	E	92	G	N1-C6-O6	8.72	125.13	119.90
35	E	2152	C	O4'-C1'-N1	8.72	115.17	108.20
35	E	1637	G	N1-C6-O6	8.72	125.13	119.90
35	E	1358	G	N1-C6-O6	8.71	125.13	119.90
35	E	1926	G	N1-C6-O6	8.71	125.13	119.90
35	E	1772	G	N1-C6-O6	8.71	125.13	119.90
35	E	2213	G	N1-C6-O6	8.71	125.13	119.90
35	E	80	G	N1-C6-O6	8.71	125.12	119.90
35	E	1549	G	C5-C6-O6	-8.71	123.38	128.60
35	E	1902	G	N1-C6-O6	8.71	125.13	119.90
35	E	981	G	N1-C6-O6	8.70	125.12	119.90
35	E	466	G	C5-C6-O6	-8.70	123.38	128.60
35	E	532	G	C5-C6-O6	-8.70	123.38	128.60
35	E	2296	G	C5-C6-O6	-8.70	123.38	128.60
35	E	1531	G	N1-C6-O6	8.69	125.12	119.90
35	E	1853	C	O4'-C1'-N1	8.69	115.16	108.20
35	E	2096	G	N1-C6-O6	8.69	125.11	119.90
35	E	876	A	N1-C6-N6	8.69	123.81	118.60
35	E	1384	G	C5-C6-O6	-8.68	123.39	128.60
35	E	412	G	C5-C6-O6	-8.68	123.39	128.60
35	E	1535	U	O4'-C1'-N1	8.68	115.14	108.20
35	E	973	G	N1-C6-O6	8.67	125.10	119.90
35	E	1201	G	N1-C6-O6	8.67	125.10	119.90
35	E	397	G	N1-C6-O6	8.67	125.10	119.90
35	E	1182	G	C5-C6-O6	-8.66	123.40	128.60
35	E	881	G	N1-C6-O6	8.65	125.09	119.90
35	E	924	G	N1-C6-O6	8.65	125.09	119.90
35	E	1580	G	N1-C6-O6	8.65	125.09	119.90
35	E	2237	G	C5-C6-O6	-8.65	123.41	128.60
35	E	286	G	N1-C6-O6	8.65	125.09	119.90
35	E	797	G	N1-C6-O6	8.65	125.09	119.90
35	E	1187	C	O4'-C1'-N1	8.65	115.12	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	16	G	N1-C6-O6	8.65	125.09	119.90
35	E	1210	G	C5-C6-O6	-8.65	123.41	128.60
35	E	1943	G	C5-C6-O6	-8.65	123.41	128.60
35	E	2010	G	N1-C6-O6	8.65	125.09	119.90
35	E	1321	G	N1-C6-O6	8.65	125.09	119.90
35	E	867	G	N1-C6-O6	8.64	125.08	119.90
35	E	819	G	N1-C6-O6	8.64	125.08	119.90
35	E	899	G	N1-C6-O6	8.63	125.08	119.90
35	E	132	G	C5-C6-O6	-8.63	123.42	128.60
35	E	440	C	O4'-C1'-N1	8.63	115.10	108.20
35	E	6	G	C5-C6-O6	-8.63	123.42	128.60
35	E	418	G	N1-C6-O6	8.63	125.08	119.90
35	E	2233	G	C5-C6-O6	-8.63	123.42	128.60
35	E	1977	G	N1-C6-O6	8.63	125.08	119.90
35	E	1767	G	N1-C6-O6	8.62	125.07	119.90
35	E	763	G	N1-C6-O6	8.62	125.07	119.90
35	E	1723	G	N1-C6-O6	8.61	125.07	119.90
35	E	2217	G	C5-C6-O6	-8.61	123.43	128.60
35	E	2248	G	N1-C6-O6	8.61	125.06	119.90
35	E	223	G	C5-C6-O6	-8.61	123.44	128.60
35	E	337	G	N1-C6-O6	8.60	125.06	119.90
35	E	519	G	N1-C6-O6	8.60	125.06	119.90
35	E	1755	G	N1-C6-O6	8.60	125.06	119.90
35	E	1646	G	N1-C6-O6	8.59	125.06	119.90
35	E	768	G	N1-C6-O6	8.59	125.05	119.90
35	E	677	G	N1-C6-O6	8.59	125.05	119.90
35	E	696	G	N1-C6-O6	8.59	125.05	119.90
35	E	1668	G	N1-C6-O6	8.59	125.05	119.90
35	E	1731	G	C5-C6-O6	-8.59	123.45	128.60
35	E	108	C	O4'-C1'-N1	8.58	115.06	108.20
35	E	159	G	N1-C6-O6	8.58	125.05	119.90
35	E	676	G	N1-C6-O6	8.58	125.05	119.90
35	E	697	G	N1-C6-O6	8.58	125.05	119.90
35	E	368	G	N1-C6-O6	8.57	125.05	119.90
35	E	252	G	N1-C6-O6	8.57	125.04	119.90
35	E	1586	G	N1-C6-O6	8.57	125.04	119.90
35	E	69	C	O4'-C1'-N1	8.56	115.05	108.20
35	E	739	G	N1-C6-O6	8.56	125.04	119.90
35	E	1709	G	N1-C6-O6	8.56	125.04	119.90
35	E	116	G	N1-C6-O6	8.56	125.03	119.90
35	E	970	G	C5-C6-O6	-8.56	123.47	128.60
35	E	169	G	C5-C6-O6	-8.55	123.47	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2188	G	N1-C6-O6	8.56	125.03	119.90
35	E	1780	G	N1-C6-O6	8.55	125.03	119.90
35	E	1882	G	N1-C6-O6	8.55	125.03	119.90
35	E	2021	G	N1-C6-O6	8.55	125.03	119.90
35	E	695	G	N1-C6-O6	8.54	125.03	119.90
35	E	871	G	N1-C6-O6	8.55	125.03	119.90
35	E	2298	G	N1-C6-O6	8.54	125.03	119.90
35	E	1256	C	O4'-C1'-N1	8.54	115.03	108.20
35	E	808	G	N1-C6-O6	8.54	125.02	119.90
35	E	2053	G	N1-C6-O6	8.54	125.02	119.90
35	E	603	G	N1-C6-O6	8.53	125.02	119.90
35	E	816	C	O4'-C1'-N1	8.53	115.03	108.20
35	E	1934	G	N1-C6-O6	8.53	125.02	119.90
35	E	714	G	N1-C6-O6	8.52	125.01	119.90
35	E	311	G	C5-C6-O6	-8.52	123.49	128.60
35	E	724	A	C2-N3-C4	-8.52	106.34	110.60
35	E	1548	C	C2-N1-C1'	8.52	128.17	118.80
35	E	2191	G	N1-C6-O6	8.51	125.01	119.90
35	E	997	G	N1-C6-O6	8.51	125.01	119.90
35	E	2112	U	O4'-C1'-N1	8.51	115.01	108.20
35	E	431	G	C5-C6-O6	-8.50	123.50	128.60
35	E	923	A	P-O3'-C3'	8.50	129.90	119.70
35	E	2054	G	N1-C6-O6	8.50	125.00	119.90
35	E	2042	G	N1-C6-O6	8.50	125.00	119.90
35	E	1805	G	N1-C6-O6	8.49	125.00	119.90
35	E	1869	G	C5-C6-O6	-8.49	123.51	128.60
35	E	1989	G	N1-C6-O6	8.49	124.99	119.90
35	E	2032	U	O4'-C1'-N1	8.49	114.99	108.20
35	E	88	G	N1-C6-O6	8.49	124.99	119.90
35	E	1891	C	O4'-C1'-N1	8.49	114.99	108.20
35	E	2075	G	N1-C6-O6	8.49	124.99	119.90
35	E	541	G	C5-C6-O6	-8.48	123.51	128.60
35	E	1582	G	N1-C6-O6	8.48	124.99	119.90
35	E	220	G	C5-C6-O6	-8.47	123.52	128.60
35	E	564	G	C5-C6-O6	-8.47	123.52	128.60
35	E	2311	G	N1-C6-O6	8.47	124.98	119.90
35	E	1075	G	O4'-C1'-N9	8.46	114.97	108.20
35	E	2095	G	N1-C6-O6	8.46	124.98	119.90
35	E	275	A	C5-C6-N6	-8.46	116.93	123.70
35	E	1527	G	N1-C6-O6	8.46	124.98	119.90
35	E	698	C	O4'-C1'-N1	8.46	114.97	108.20
35	E	1239	G	N1-C6-O6	8.45	124.97	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2017	G	N1-C6-O6	8.45	124.97	119.90
35	E	857	G	C5-C6-O6	-8.45	123.53	128.60
35	E	1647	G	N1-C6-O6	8.45	124.97	119.90
35	E	1202	G	N1-C6-O6	8.45	124.97	119.90
35	E	2289	G	C5-C6-O6	-8.45	123.53	128.60
35	E	2263	G	N1-C6-O6	8.45	124.97	119.90
35	E	834	G	N1-C6-O6	8.44	124.96	119.90
35	E	713	G	N1-C6-O6	8.43	124.96	119.90
35	E	950	G	C5-C6-O6	-8.42	123.55	128.60
35	E	445	G	N1-C6-O6	8.42	124.95	119.90
35	E	1346	G	N1-C6-O6	8.41	124.95	119.90
35	E	1910	G	C5-C6-O6	-8.41	123.55	128.60
35	E	1257	C	O4'-C1'-N1	8.41	114.93	108.20
35	E	211	G	C5-C6-O6	-8.41	123.56	128.60
35	E	2122	G	C5-C6-O6	-8.41	123.56	128.60
35	E	1642	G	N1-C6-O6	8.41	124.94	119.90
35	E	2023	C	C2-N1-C1'	8.41	128.05	118.80
35	E	1598	G	C5-C6-O6	-8.39	123.56	128.60
35	E	2139	G	C5-C6-O6	-8.39	123.56	128.60
35	E	963	G	C5-C6-O6	-8.39	123.57	128.60
35	E	832	G	N1-C6-O6	8.39	124.93	119.90
35	E	749	C	P-O3'-C3'	8.39	129.76	119.70
35	E	753	U	O4'-C1'-N1	8.38	114.91	108.20
35	E	719	G	N1-C6-O6	8.38	124.93	119.90
35	E	1548	C	O4'-C1'-N1	8.38	114.91	108.20
35	E	48	G	C5-C6-O6	-8.38	123.57	128.60
35	E	189	G	C5-C6-O6	-8.38	123.57	128.60
35	E	230	G	C5-C6-O6	-8.37	123.58	128.60
35	E	1076	C	O4'-C1'-N1	8.38	114.90	108.20
35	E	996	G	C5-C6-O6	-8.37	123.58	128.60
35	E	1220	G	C5-C6-O6	-8.37	123.58	128.60
35	E	1	G	N1-C6-O6	8.37	124.92	119.90
35	E	394	G	C5-C6-O6	-8.37	123.58	128.60
35	E	741	G	N1-C6-O6	8.36	124.92	119.90
35	E	844	G	N1-C6-O6	8.35	124.91	119.90
35	E	31	C	O4'-C1'-N1	8.35	114.88	108.20
35	E	922	C	P-O3'-C3'	8.35	129.72	119.70
35	E	1195	G	N1-C6-O6	8.35	124.91	119.90
35	E	1262	C	O4'-C1'-N1	8.34	114.87	108.20
35	E	593	G	N1-C6-O6	8.34	124.90	119.90
35	E	57	G	C5-C6-O6	-8.34	123.60	128.60
35	E	1864	C	O4'-C1'-N1	8.33	114.87	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	262	U	O4'-C1'-N1	8.33	114.86	108.20
35	E	932	G	C5-C6-O6	-8.33	123.60	128.60
35	E	1188	C	O4'-C1'-N1	8.32	114.86	108.20
35	E	395	G	C5-C6-O6	-8.31	123.61	128.60
35	E	334	G	C5-C6-O6	-8.31	123.61	128.60
35	E	437	G	N1-C6-O6	8.31	124.89	119.90
35	E	524	G	C5-C6-O6	-8.31	123.61	128.60
35	E	1850	C	O4'-C1'-N1	8.31	114.85	108.20
35	E	272	G	C5-C6-O6	-8.30	123.62	128.60
35	E	1581	A	N1-C6-N6	8.30	123.58	118.60
35	E	2222	G	C5-C6-O6	-8.30	123.62	128.60
35	E	641	C	O4'-C1'-N1	8.30	114.84	108.20
35	E	2275	G	C5-C6-O6	-8.30	123.62	128.60
35	E	7	G	C5-C6-O6	-8.30	123.62	128.60
35	E	2307	G	N1-C6-O6	8.30	124.88	119.90
35	E	514	G	C5-C6-O6	-8.29	123.63	128.60
35	E	1680	G	N1-C6-O6	8.29	124.87	119.90
35	E	630	G	N1-C6-O6	8.29	124.87	119.90
35	E	2121	G	C5-C6-O6	-8.29	123.63	128.60
35	E	320	G	C5-C6-O6	-8.28	123.64	128.60
35	E	2176	G	C5-C6-O6	-8.27	123.64	128.60
35	E	640	G	C5-C6-O6	-8.27	123.64	128.60
35	E	430	G	C5-C6-O6	-8.27	123.64	128.60
35	E	771	A	P-O3'-C3'	8.27	129.62	119.70
35	E	1074	C	O4'-C1'-N1	8.27	114.81	108.20
35	E	1985	C	O4'-C1'-N1	8.26	114.81	108.20
35	E	157	G	C5-C6-O6	-8.25	123.65	128.60
35	E	165	C	O4'-C1'-N1	8.25	114.80	108.20
35	E	1741	G	N1-C6-O6	8.25	124.85	119.90
35	E	2206	G	C5-C6-O6	-8.25	123.65	128.60
35	E	1685	G	N1-C6-O6	8.25	124.85	119.90
35	E	1935	C	O4'-C1'-N1	8.25	114.80	108.20
35	E	552	G	C5-C6-O6	-8.24	123.66	128.60
35	E	2174	C	O4'-C1'-N1	8.24	114.79	108.20
35	E	373	G	N1-C6-O6	8.24	124.84	119.90
35	E	238	G	C5-C6-O6	-8.23	123.66	128.60
35	E	294	G	N1-C6-O6	8.23	124.84	119.90
35	E	420	G	C5-C6-O6	-8.23	123.66	128.60
35	E	488	G	C5-C6-O6	-8.23	123.66	128.60
35	E	776	G	N1-C6-O6	8.23	124.84	119.90
35	E	1982	C	O4'-C1'-N1	8.23	114.78	108.20
35	E	1594	G	C5-C6-O6	-8.22	123.67	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	428	C	O4'-C1'-N1	8.22	114.78	108.20
35	E	478	C	O4'-C1'-N1	8.22	114.78	108.20
35	E	1307	G	C5-C6-O6	-8.22	123.67	128.60
35	E	2235	C	O4'-C1'-N1	8.21	114.77	108.20
35	E	606	G	C5-C6-O6	-8.21	123.68	128.60
35	E	2265	G	C5-C6-O6	-8.21	123.68	128.60
35	E	2290	C	O4'-C1'-N1	8.20	114.76	108.20
35	E	1870	G	C5-C6-O6	-8.20	123.68	128.60
35	E	887	C	O4'-C1'-N1	8.20	114.76	108.20
35	E	2302	C	O4'-C1'-N1	8.20	114.76	108.20
35	E	700	U	O4'-C1'-N1	8.19	114.76	108.20
35	E	1735	G	C5-C6-O6	-8.19	123.69	128.60
35	E	1339	G	C5-C6-O6	-8.19	123.69	128.60
35	E	1906	C	C2-N1-C1'	8.19	127.81	118.80
35	E	2278	G	C5-C6-O6	-8.19	123.69	128.60
35	E	34	G	C5-C6-O6	-8.19	123.69	128.60
35	E	389	G	C5-C6-O6	-8.19	123.69	128.60
35	E	2246	C	O4'-C1'-N1	8.19	114.75	108.20
35	E	1750	C	O4'-C1'-N1	8.18	114.75	108.20
35	E	1711	G	N1-C6-O6	8.18	124.81	119.90
35	E	385	G	C5-C6-O6	-8.18	123.69	128.60
35	E	746	A	C6-C5-N7	-8.17	126.58	132.30
35	E	2198	C	O4'-C1'-N1	8.17	114.74	108.20
35	E	2197	G	C5-C6-O6	-8.17	123.70	128.60
35	E	2220	G	C5-C6-O6	-8.17	123.70	128.60
35	E	1203	G	C5-C6-O6	-8.16	123.70	128.60
35	E	1540	C	O4'-C1'-N1	8.16	114.73	108.20
35	E	718	A	C5-C6-N1	-8.16	113.62	117.70
35	E	192	G	C5-C6-O6	-8.15	123.71	128.60
35	E	204	G	C5-C6-O6	-8.15	123.71	128.60
35	E	1875	G	P-O3'-C3'	8.15	129.49	119.70
35	E	205	G	C5-C6-O6	-8.14	123.71	128.60
35	E	404	G	C5-C6-O6	-8.14	123.72	128.60
35	E	1793	G	C5-C6-O6	-8.14	123.72	128.60
35	E	2266	G	C5-C6-O6	-8.13	123.72	128.60
35	E	1219	C	O4'-C1'-N1	8.13	114.70	108.20
35	E	1907	C	O4'-C1'-N1	8.13	114.70	108.20
35	E	113	U	O4'-C1'-N1	8.12	114.70	108.20
35	E	1579	G	C5-C6-O6	-8.12	123.73	128.60
35	E	1082	U	O4'-C1'-N1	8.12	114.70	108.20
35	E	1230	G	C5-C6-O6	-8.12	123.73	128.60
35	E	1938	C	O4'-C1'-N1	8.12	114.70	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1979	G	C5-C6-O6	-8.12	123.73	128.60
35	E	319	C	O4'-C1'-N1	8.12	114.69	108.20
35	E	837	C	O4'-C1'-N1	8.11	114.69	108.20
35	E	1983	U	O4'-C1'-N1	8.11	114.69	108.20
35	E	2067	C	O4'-C1'-N1	8.11	114.69	108.20
35	E	135	C	O4'-C1'-N1	8.10	114.68	108.20
35	E	834	G	P-O3'-C3'	8.10	129.42	119.70
35	E	2194	G	C5-C6-O6	-8.10	123.74	128.60
35	E	391	C	O4'-C1'-N1	8.10	114.68	108.20
35	E	84	C	O4'-C1'-N1	8.10	114.68	108.20
35	E	318	C	O4'-C1'-N1	8.10	114.68	108.20
35	E	186	C	O4'-C1'-N1	8.09	114.67	108.20
35	E	405	G	C5-C6-O6	-8.09	123.74	128.60
35	E	232	C	O4'-C1'-N1	8.09	114.67	108.20
35	E	559	U	P-O3'-C3'	8.09	129.41	119.70
35	E	942	C	C2-N1-C1'	8.09	127.70	118.80
35	E	982	G	P-O3'-C3'	8.09	129.41	119.70
35	E	331	U	O4'-C1'-N1	8.09	114.67	108.20
35	E	508	G	C5-C6-O6	-8.09	123.75	128.60
35	E	423	C	O4'-C1'-N1	8.08	114.66	108.20
35	E	1237	G	C5-C6-O6	-8.08	123.75	128.60
35	E	1900	G	C5-C6-O6	-8.08	123.75	128.60
35	E	1211	G	N1-C6-O6	8.08	124.75	119.90
35	E	548	C	O4'-C1'-N1	8.07	114.66	108.20
35	E	104	C	O4'-C1'-N1	8.07	114.66	108.20
35	E	156	G	C5-C6-O6	-8.07	123.76	128.60
35	E	807	U	O4'-C1'-N1	8.07	114.66	108.20
35	E	374	G	N1-C6-O6	8.06	124.74	119.90
35	E	1273	G	N1-C6-O6	8.05	124.73	119.90
35	E	722	C	O4'-C1'-N1	8.05	114.64	108.20
35	E	720	U	O4'-C1'-N1	8.05	114.64	108.20
35	E	1577	G	C5-C6-O6	-8.05	123.77	128.60
35	E	2114	U	C2-N1-C1'	8.05	127.36	117.70
35	E	517	G	C5-C6-O6	-8.04	123.77	128.60
35	E	2295	G	C5-C6-O6	-8.04	123.78	128.60
35	E	971	G	C5-C6-O6	-8.03	123.78	128.60
35	E	1957	C	O4'-C1'-N1	8.03	114.62	108.20
35	E	668	C	O4'-C1'-N1	8.02	114.62	108.20
35	E	470	G	C5-C6-O6	-8.02	123.79	128.60
35	E	579	C	O4'-C1'-N1	8.02	114.61	108.20
35	E	409	G	C5-C6-O6	-8.01	123.79	128.60
35	E	1236	G	O4'-C1'-N9	8.01	114.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1325	C	O4'-C1'-N1	8.01	114.61	108.20
35	E	2157	C	O4'-C1'-N1	8.01	114.61	108.20
35	E	1777	G	C5-C6-O6	-8.01	123.80	128.60
35	E	2125	C	O4'-C1'-N1	8.01	114.61	108.20
35	E	2208	G	C5-C6-O6	-8.01	123.80	128.60
35	E	1851	C	O4'-C1'-N1	8.01	114.60	108.20
35	E	208	G	C5-C6-O6	-8.00	123.80	128.60
35	E	376	C	O4'-C1'-N1	8.00	114.60	108.20
35	E	217	C	O4'-C1'-N1	8.00	114.60	108.20
35	E	2236	C	O4'-C1'-N1	7.99	114.59	108.20
35	E	332	C	O4'-C1'-N1	7.99	114.59	108.20
35	E	907	G	C5-C6-O6	-7.99	123.81	128.60
35	E	240	G	C5-C6-O6	-7.98	123.81	128.60
35	E	2158	C	O4'-C1'-N1	7.97	114.58	108.20
35	E	1263	G	C5-C6-O6	-7.96	123.82	128.60
35	E	1289	G	C5-C6-O6	-7.96	123.82	128.60
35	E	1828	G	N1-C6-O6	7.96	124.68	119.90
35	E	1911	U	O4'-C1'-N1	7.96	114.57	108.20
35	E	477	G	C5-C6-O6	-7.96	123.82	128.60
35	E	746	A	C5-C6-N1	-7.96	113.72	117.70
35	E	162	A	C4-C5-C6	7.96	120.98	117.00
35	E	2244	C	O4'-C1'-N1	7.96	114.56	108.20
35	E	1809	C	O4'-C1'-N1	7.95	114.56	108.20
35	E	619	C	O4'-C1'-N1	7.95	114.56	108.20
35	E	563	U	O4'-C1'-N1	7.94	114.55	108.20
35	E	1216	G	C5-C6-O6	-7.94	123.83	128.60
35	E	2149	C	O4'-C1'-N1	7.94	114.55	108.20
35	E	370	G	C5-C6-O6	-7.94	123.84	128.60
35	E	364	G	C5-C6-O6	-7.93	123.84	128.60
35	E	473	G	C5-C6-O6	-7.93	123.84	128.60
35	E	2205	G	C5-C6-O6	-7.93	123.84	128.60
35	E	1282	C	O4'-C1'-N1	7.93	114.54	108.20
35	E	167	A	O4'-C1'-N9	7.92	114.54	108.20
35	E	410	G	C5-C6-O6	-7.92	123.85	128.60
35	E	1373	C	O4'-C1'-N1	7.92	114.54	108.20
35	E	723	C	O4'-C1'-N1	7.92	114.54	108.20
35	E	42	G	C5-C6-O6	-7.92	123.85	128.60
35	E	678	G	C5-C6-O6	-7.92	123.85	128.60
35	E	387	C	O4'-C1'-N1	7.91	114.53	108.20
35	E	199	G	C5-C6-O6	-7.91	123.85	128.60
35	E	1638	G	N1-C6-O6	7.91	124.65	119.90
35	E	1846	C	O4'-C1'-N1	7.91	114.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	921	G	P-O3'-C3'	7.91	129.19	119.70
35	E	756	G	C5-C6-O6	-7.90	123.86	128.60
35	E	1872	G	N1-C6-O6	7.90	124.64	119.90
35	E	1727	C	O4'-C1'-N1	7.90	114.52	108.20
35	E	1786	G	C5-C6-O6	-7.90	123.86	128.60
35	E	542	C	O4'-C1'-N1	7.89	114.52	108.20
35	E	347	G	C5-C6-O6	-7.89	123.86	128.60
35	E	2184	U	O4'-C1'-N1	7.89	114.51	108.20
35	E	322	G	C5-C6-O6	-7.89	123.86	128.60
35	E	855	G	C5-C6-O6	-7.89	123.87	128.60
35	E	2060	C	O4'-C1'-N1	7.89	114.51	108.20
35	E	131	C	O4'-C1'-N1	7.88	114.51	108.20
35	E	566	G	C5-C6-O6	-7.88	123.87	128.60
35	E	1775	U	O4'-C1'-N1	7.88	114.50	108.20
35	E	403	G	C5-C6-O6	-7.88	123.87	128.60
35	E	489	C	O4'-C1'-N1	7.88	114.50	108.20
35	E	1634	C	N3-C4-N4	7.88	123.51	118.00
35	E	260	A	C5-C6-N1	-7.87	113.77	117.70
35	E	2241	G	C5-C6-O6	-7.87	123.88	128.60
35	E	988	U	O4'-C1'-N1	7.87	114.49	108.20
35	E	2141	G	C5-C6-O6	-7.87	123.88	128.60
35	E	384	G	N1-C6-O6	7.86	124.62	119.90
35	E	382	G	N1-C6-O6	7.86	124.61	119.90
35	E	355	G	C5-C6-O6	-7.86	123.89	128.60
35	E	757	G	C5-C6-O6	-7.86	123.89	128.60
35	E	1082	U	P-O5'-C5'	7.86	133.47	120.90
35	E	568	G	C5-C6-O6	-7.85	123.89	128.60
35	E	2270	C	O4'-C1'-N1	7.85	114.48	108.20
32	o	70	TYR	CB-CG-CD1	-7.85	116.29	121.00
35	E	623	C	O4'-C1'-N1	7.85	114.48	108.20
35	E	217	C	C5'-C4'-C3'	7.85	128.56	116.00
35	E	236	C	O4'-C1'-N1	7.85	114.48	108.20
35	E	1251	C	O4'-C1'-N1	7.85	114.48	108.20
35	E	1980	C	O4'-C1'-N1	7.84	114.48	108.20
35	E	233	G	C5-C6-O6	-7.84	123.89	128.60
35	E	1683	C	O4'-C1'-N1	7.84	114.47	108.20
35	E	1272	C	O4'-C1'-N1	7.83	114.47	108.20
35	E	1645	C	O4'-C1'-N1	7.83	114.47	108.20
35	E	2211	C	O4'-C1'-N1	7.83	114.47	108.20
35	E	77	C	O4'-C1'-N1	7.83	114.46	108.20
35	E	203	C	O4'-C1'-N1	7.83	114.46	108.20
35	E	2137	C	O4'-C1'-N1	7.83	114.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2225	C	O4'-C1'-N1	7.83	114.46	108.20
35	E	207	G	C5-C6-O6	-7.83	123.91	128.60
35	E	1335	U	O4'-C1'-N1	7.83	114.46	108.20
35	E	1899	C	O4'-C1'-N1	7.83	114.46	108.20
35	E	1971	C	O4'-C1'-N1	7.82	114.46	108.20
35	E	158	C	O4'-C1'-N1	7.82	114.46	108.20
35	E	1332	G	C5-C6-O6	-7.81	123.91	128.60
35	E	1569	G	C5-C6-O6	-7.81	123.91	128.60
35	E	2044	G	C5-C6-O6	-7.81	123.91	128.60
35	E	615	G	C5-C6-O6	-7.81	123.91	128.60
35	E	38	C	O4'-C1'-N1	7.81	114.44	108.20
35	E	321	G	C5-C6-O6	-7.81	123.92	128.60
35	E	110	U	O4'-C1'-N1	7.80	114.44	108.20
35	E	1181	C	O4'-C1'-N1	7.80	114.44	108.20
35	E	1880	U	C4'-C3'-C2'	-7.80	94.80	102.60
35	E	1855	G	C5-C6-O6	-7.80	123.92	128.60
35	E	358	C	O4'-C1'-N1	7.80	114.44	108.20
35	E	221	C	O4'-C1'-N1	7.79	114.44	108.20
35	E	282	C	O4'-C1'-N1	7.79	114.43	108.20
35	E	955	U	O4'-C1'-N1	7.79	114.43	108.20
35	E	72	C	O4'-C1'-N1	7.79	114.43	108.20
35	E	560	C	O4'-C1'-N1	7.79	114.43	108.20
35	E	885	U	O4'-C1'-N1	7.79	114.43	108.20
35	E	725	U	O4'-C1'-N1	7.78	114.42	108.20
35	E	2313	U	O4'-C1'-N1	7.78	114.42	108.20
35	E	1291	U	O4'-C1'-N1	7.78	114.42	108.20
35	E	2066	C	O4'-C1'-N1	7.78	114.42	108.20
35	E	2189	A	C4-C5-C6	7.78	120.89	117.00
35	E	2304	G	C5-C6-O6	-7.77	123.94	128.60
35	E	235	C	O4'-C1'-N1	7.77	114.42	108.20
35	E	953	G	C5-C6-O6	-7.77	123.94	128.60
35	E	1320	G	C5-C6-O6	-7.77	123.94	128.60
35	E	482	C	O4'-C1'-N1	7.76	114.41	108.20
35	E	1763	G	C5-C6-O6	-7.76	123.94	128.60
35	E	495	G	C5-C6-O6	-7.76	123.95	128.60
35	E	840	C	O4'-C1'-N1	7.76	114.41	108.20
35	E	152	A	N1-C6-N6	7.75	123.25	118.60
35	E	578	C	O4'-C1'-N1	7.75	114.40	108.20
35	E	1889	U	O4'-C1'-N1	7.75	114.40	108.20
35	E	1191	G	N1-C6-O6	7.75	124.55	119.90
35	E	103	U	O4'-C1'-N1	7.75	114.40	108.20
35	E	651	G	C5-C6-O6	-7.75	123.95	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	828	G	P-O3'-C3'	7.75	129.00	119.70
35	E	2156	G	C5-C6-O6	-7.75	123.95	128.60
35	E	2255	C	O4'-C1'-N1	7.75	114.40	108.20
35	E	546	U	O4'-C1'-N1	7.74	114.39	108.20
35	E	1166	C	O4'-C1'-N1	7.74	114.39	108.20
35	E	1832	A	P-O3'-C3'	7.74	128.99	119.70
35	E	2247	C	O4'-C1'-N1	7.74	114.39	108.20
35	E	147	G	C5-C6-O6	-7.74	123.96	128.60
35	E	452	C	O4'-C1'-N1	7.74	114.39	108.20
35	E	683	U	O4'-C1'-N1	7.74	114.39	108.20
35	E	825	C	O4'-C1'-N1	7.74	114.39	108.20
35	E	1852	G	C5-C6-O6	-7.73	123.96	128.60
35	E	344	G	C5-C6-O6	-7.73	123.96	128.60
34	h	181	TYR	CB-CG-CD2	-7.73	116.36	121.00
35	E	2258	C	O4'-C1'-N1	7.73	114.38	108.20
35	E	139	G	C5-C6-O6	-7.72	123.97	128.60
35	E	1563	G	C5-C6-O6	-7.72	123.97	128.60
35	E	2052	C	O4'-C1'-N1	7.72	114.38	108.20
35	E	120	C	O4'-C1'-N1	7.72	114.38	108.20
35	E	1686	G	N1-C6-O6	7.72	124.53	119.90
35	E	2277	C	O4'-C1'-N1	7.72	114.37	108.20
35	E	2102	C	O4'-C1'-N1	7.71	114.37	108.20
35	E	650	C	O4'-C1'-N1	7.71	114.37	108.20
35	E	547	G	C5-C6-O6	-7.71	123.97	128.60
35	E	1905	U	O4'-C1'-N1	7.71	114.37	108.20
35	E	744	C	O4'-C1'-N1	7.71	114.36	108.20
35	E	1886	G	C5-C6-O6	-7.71	123.98	128.60
35	E	365	C	O4'-C1'-N1	7.71	114.36	108.20
35	E	87	C	O4'-C1'-N1	7.70	114.36	108.20
35	E	176	C	O4'-C1'-N1	7.70	114.36	108.20
35	E	153	C	O4'-C1'-N1	7.70	114.36	108.20
35	E	218	C	O4'-C1'-N1	7.70	114.36	108.20
35	E	333	C	O4'-C1'-N1	7.69	114.35	108.20
35	E	2078	C	O4'-C1'-N1	7.69	114.35	108.20
35	E	2310	G	C5-C6-O6	-7.69	123.99	128.60
35	E	513	G	C5-C6-O6	-7.69	123.99	128.60
35	E	681	C	O4'-C1'-N1	7.69	114.35	108.20
35	E	413	G	C5-C6-O6	-7.68	123.99	128.60
35	E	853	C	O4'-C1'-N1	7.68	114.35	108.20
35	E	1315	G	C5-C6-O6	-7.68	123.99	128.60
35	E	997	G	O4'-C1'-N9	7.68	114.34	108.20
35	E	1974	C	O4'-C1'-N1	7.68	114.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	197	C	O4'-C1'-N1	7.68	114.34	108.20
35	E	1863	C	O4'-C1'-N1	7.68	114.34	108.20
35	E	49	C	O4'-C1'-N1	7.68	114.34	108.20
35	E	1073	U	O4'-C1'-N1	7.67	114.34	108.20
35	E	1956	C	O4'-C1'-N1	7.67	114.34	108.20
35	E	1327	A	C4-C5-C6	7.67	120.84	117.00
35	E	1616	C	O4'-C1'-N1	7.67	114.34	108.20
35	E	41	G	C5-C6-O6	-7.67	124.00	128.60
35	E	59	C	O4'-C1'-N1	7.67	114.33	108.20
35	E	2292	G	C5-C6-O6	-7.67	124.00	128.60
35	E	1871	G	C5-C6-O6	-7.67	124.00	128.60
35	E	76	G	C5-C6-O6	-7.66	124.00	128.60
35	E	580	C	O4'-C1'-N1	7.66	114.33	108.20
35	E	1228	G	C5-C6-O6	-7.66	124.00	128.60
35	E	1271	G	N1-C6-O6	7.66	124.49	119.90
35	E	2173	C	O4'-C1'-N1	7.65	114.32	108.20
35	E	1369	C	O4'-C1'-N1	7.65	114.32	108.20
35	E	1862	C	O4'-C1'-N1	7.65	114.32	108.20
35	E	2000	C	O4'-C1'-N1	7.64	114.31	108.20
35	E	925	C	O4'-C1'-N1	7.64	114.31	108.20
35	E	605	G	C5-C6-O6	-7.64	124.02	128.60
35	E	1916	C	O4'-C1'-N1	7.64	114.31	108.20
35	E	2127	G	C5-C6-O6	-7.64	124.02	128.60
35	E	2195	G	C5-C6-O6	-7.64	124.02	128.60
35	E	1319	G	C5-C6-O6	-7.64	124.02	128.60
35	E	1897	U	O4'-C1'-N1	7.64	114.31	108.20
35	E	2228	C	O4'-C1'-N1	7.64	114.31	108.20
35	E	94	C	O4'-C1'-N1	7.63	114.31	108.20
35	E	279	A	C5-C6-N6	-7.63	117.59	123.70
35	E	1354	C	O4'-C1'-N1	7.63	114.31	108.20
35	E	244	G	C5-C6-O6	-7.63	124.02	128.60
35	E	357	C	O4'-C1'-N1	7.63	114.30	108.20
35	E	986	U	O4'-C1'-N1	7.63	114.30	108.20
35	E	1748	C	O4'-C1'-N1	7.62	114.30	108.20
35	E	611	G	C5-C6-O6	-7.62	124.03	128.60
35	E	12	U	O4'-C1'-N1	7.62	114.30	108.20
35	E	390	C	O4'-C1'-N1	7.62	114.30	108.20
35	E	292	U	O4'-C1'-N1	7.62	114.30	108.20
35	E	408	C	O4'-C1'-N1	7.62	114.30	108.20
35	E	481	G	C5-C6-O6	-7.62	124.03	128.60
35	E	1288	G	C5-C6-O6	-7.62	124.03	128.60
35	E	1948	G	N1-C6-O6	7.62	124.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2172	G	C5-C6-O6	-7.62	124.03	128.60
35	E	441	C	O4'-C1'-N1	7.62	114.29	108.20
35	E	303	C	O4'-C1'-N1	7.61	114.29	108.20
35	E	228	G	C5-C6-O6	-7.61	124.04	128.60
35	E	1712	U	O4'-C1'-N1	7.61	114.28	108.20
35	E	317	G	C5-C6-O6	-7.60	124.04	128.60
35	E	995	C	O4'-C1'-N1	7.60	114.28	108.20
35	E	1324	U	O4'-C1'-N1	7.60	114.28	108.20
35	E	1976	C	O4'-C1'-N1	7.60	114.28	108.20
35	E	1940	G	C5-C6-O6	-7.60	124.04	128.60
35	E	933	C	O4'-C1'-N1	7.60	114.28	108.20
35	E	1349	G	C5-C6-O6	-7.60	124.04	128.60
35	E	18	C	O4'-C1'-N1	7.60	114.28	108.20
35	E	1543	C	N3-C4-N4	7.60	123.32	118.00
35	E	2013	U	O4'-C1'-N1	7.59	114.28	108.20
35	E	213	G	N3-C2-N2	7.59	125.21	119.90
35	E	1918	C	O4'-C1'-N1	7.59	114.27	108.20
35	E	89	C	O4'-C1'-N1	7.59	114.27	108.20
35	E	490	C	O4'-C1'-N1	7.59	114.27	108.20
35	E	1634	C	O4'-C1'-N1	7.59	114.27	108.20
35	E	1666	G	C5-C6-O6	-7.59	124.05	128.60
35	E	313	G	C5-C6-O6	-7.58	124.05	128.60
35	E	1705	G	C5-C6-O6	-7.58	124.05	128.60
35	E	1703	C	O4'-C1'-N1	7.58	114.27	108.20
35	E	455	C	O4'-C1'-N1	7.58	114.26	108.20
35	E	869	G	C5-C6-O6	-7.58	124.06	128.60
35	E	1562	G	C5-C6-O6	-7.58	124.06	128.60
35	E	1310	C	O4'-C1'-N1	7.57	114.26	108.20
35	E	1944	G	C5-C6-O6	-7.57	124.06	128.60
35	E	2187	C	O4'-C1'-N1	7.57	114.26	108.20
35	E	537	C	O4'-C1'-N1	7.57	114.26	108.20
35	E	2140	U	O4'-C1'-N1	7.57	114.26	108.20
35	E	182	C	O4'-C1'-N1	7.57	114.25	108.20
35	E	1756	G	C5-C6-O6	-7.56	124.06	128.60
35	E	1188	C	N3-C4-N4	7.55	123.29	118.00
35	E	1530	C	O4'-C1'-N1	7.55	114.24	108.20
35	E	2190	U	O4'-C1'-N1	7.55	114.24	108.20
35	E	1254	C	O4'-C1'-N1	7.55	114.24	108.20
35	E	1648	U	O4'-C1'-N1	7.55	114.24	108.20
35	E	166	C	O4'-C1'-N1	7.55	114.24	108.20
35	E	206	C	O4'-C1'-N1	7.55	114.24	108.20
35	E	664	G	C5-C6-O6	-7.55	124.07	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	841	C	O4'-C1'-N1	7.55	114.24	108.20
35	E	1283	U	O4'-C1'-N1	7.55	114.24	108.20
35	E	2108	G	C5-C6-O6	-7.55	124.07	128.60
35	E	2058	C	O4'-C1'-N1	7.54	114.24	108.20
35	E	274	C	O4'-C1'-N1	7.54	114.23	108.20
35	E	2285	G	C5-C6-O6	-7.54	124.07	128.60
35	E	836	G	C5-C6-O6	-7.54	124.08	128.60
35	E	1974	C	C2-N1-C1'	7.54	127.10	118.80
35	E	842	G	C5-C6-O6	-7.54	124.08	128.60
35	E	117	C	O4'-C1'-N1	7.54	114.23	108.20
35	E	1880	U	P-O3'-C3'	7.54	128.74	119.70
35	E	130	G	C5-C6-O6	-7.53	124.08	128.60
35	E	415	U	O4'-C1'-N1	7.53	114.22	108.20
35	E	1623	G	C5-C6-O6	-7.53	124.08	128.60
35	E	239	C	O4'-C1'-N1	7.53	114.22	108.20
35	E	1747	C	O4'-C1'-N1	7.53	114.22	108.20
35	E	1223	C	O4'-C1'-N1	7.52	114.22	108.20
35	E	1269	C	O4'-C1'-N1	7.52	114.22	108.20
35	E	1571	C	O4'-C1'-N1	7.52	114.22	108.20
35	E	2154	C	O4'-C1'-N1	7.52	114.22	108.20
35	E	759	C	C6-N1-C2	-7.51	117.30	120.30
35	E	1908	U	O4'-C1'-N1	7.51	114.21	108.20
35	E	1950	G	C5-C6-O6	-7.51	124.09	128.60
34	h	181	TYR	CB-CG-CD1	7.51	125.51	121.00
35	E	662	C	O4'-C1'-N1	7.51	114.21	108.20
35	E	1639	A	C5-C6-N6	-7.51	117.69	123.70
35	E	54	C	O4'-C1'-N1	7.51	114.21	108.20
35	E	109	G	C5-C6-O6	-7.51	124.09	128.60
35	E	751	C	O4'-C1'-N1	7.51	114.21	108.20
35	E	1867	G	O4'-C1'-N9	7.51	114.21	108.20
35	E	5	U	O4'-C1'-N1	7.50	114.20	108.20
35	E	1739	G	C5-C6-O6	-7.50	124.10	128.60
35	E	58	C	O4'-C1'-N1	7.50	114.20	108.20
35	E	439	G	C5-C6-O6	-7.50	124.10	128.60
35	E	1758	C	O4'-C1'-N1	7.50	114.20	108.20
35	E	1213	G	C5-C6-O6	-7.50	124.10	128.60
35	E	956	U	O4'-C1'-N1	7.50	114.20	108.20
35	E	656	U	O4'-C1'-N1	7.50	114.20	108.20
35	E	2100	C	O4'-C1'-N1	7.50	114.20	108.20
35	E	435	G	C5-C6-O6	-7.49	124.10	128.60
35	E	458	C	O4'-C1'-N1	7.49	114.19	108.20
35	E	265	C	O4'-C1'-N1	7.49	114.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1932	G	C5-C6-O6	-7.49	124.11	128.60
35	E	2133	C	O4'-C1'-N1	7.49	114.19	108.20
35	E	670	G	C5-C6-O6	-7.49	124.11	128.60
35	E	1593	A	C4-C5-C6	7.49	120.74	117.00
35	E	1697	G	C5-C6-O6	-7.49	124.11	128.60
35	E	396	C	O4'-C1'-N1	7.48	114.19	108.20
35	E	2182	G	C5-C6-O6	-7.48	124.11	128.60
35	E	818	U	O4'-C1'-N1	7.48	114.18	108.20
35	E	787	C	O4'-C1'-N1	7.48	114.18	108.20
35	E	2150	G	C5-C6-O6	-7.47	124.11	128.60
35	E	259	C	N3-C4-C5	-7.47	118.91	121.90
35	E	451	G	C5-C6-O6	-7.47	124.12	128.60
35	E	1557	U	O4'-C1'-N1	7.47	114.18	108.20
35	E	1867	G	C5-C6-O6	-7.47	124.12	128.60
32	o	70	TYR	CB-CG-CD2	7.47	125.48	121.00
35	E	1602	C	O4'-C1'-N1	7.47	114.17	108.20
35	E	1744	U	O4'-C1'-N1	7.46	114.17	108.20
35	E	628	G	C5-C6-O6	-7.46	124.12	128.60
35	E	2087	C	O4'-C1'-N1	7.46	114.17	108.20
35	E	928	C	O4'-C1'-N1	7.46	114.17	108.20
35	E	175	A	C5-C6-N6	-7.46	117.73	123.70
35	E	1188	C	P-O3'-C3'	7.46	128.65	119.70
35	E	1922	G	C5-C6-O6	-7.46	124.13	128.60
35	E	1329	G	C5-C6-O6	-7.46	124.13	128.60
35	E	627	C	O4'-C1'-N1	7.45	114.16	108.20
35	E	2131	A	O4'-C1'-N9	7.45	114.16	108.20
35	E	2242	U	O4'-C1'-N1	7.45	114.16	108.20
35	E	1179	C	O4'-C1'-N1	7.45	114.16	108.20
35	E	66	U	O4'-C1'-N1	7.45	114.16	108.20
35	E	890	C	O4'-C1'-N1	7.44	114.15	108.20
35	E	1656	G	C5-C6-O6	-7.44	124.14	128.60
35	E	1372	C	O4'-C1'-N1	7.44	114.15	108.20
35	E	1382	G	C5-C6-O6	-7.43	124.14	128.60
35	E	118	C	O4'-C1'-N1	7.43	114.15	108.20
35	E	209	C	O4'-C1'-N1	7.43	114.14	108.20
35	E	212	G	C5-C6-O6	-7.43	124.14	128.60
35	E	375	C	O4'-C1'-N1	7.43	114.14	108.20
35	E	706	G	C5-C6-O6	-7.43	124.14	128.60
35	E	726	C	P-O3'-C3'	7.43	128.61	119.70
35	E	722	C	N3-C4-C5	-7.42	118.93	121.90
35	E	802	U	O4'-C1'-N1	7.42	114.14	108.20
35	E	1655	U	O4'-C1'-N1	7.42	114.14	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2183	U	O4'-C1'-N1	7.42	114.14	108.20
35	E	93	G	C5-C6-O6	-7.42	124.15	128.60
35	E	749	C	O4'-C1'-N1	7.42	114.13	108.20
35	E	1317	G	C5-C6-O6	-7.42	124.15	128.60
35	E	1823	G	C5-C6-O6	-7.42	124.15	128.60
35	E	969	U	O4'-C1'-N1	7.41	114.13	108.20
35	E	149	A	O4'-C1'-N9	7.41	114.13	108.20
35	E	622	G	C5-C6-O6	-7.41	124.15	128.60
35	E	1978	C	O4'-C1'-N1	7.41	114.13	108.20
35	E	679	U	O4'-C1'-N1	7.41	114.13	108.20
35	E	366	C	O4'-C1'-N1	7.40	114.12	108.20
35	E	710	A	O4'-C1'-N9	7.40	114.12	108.20
35	E	515	C	O4'-C1'-N1	7.40	114.12	108.20
35	E	1081	G	O4'-C1'-N9	7.40	114.12	108.20
35	E	1371	C	O4'-C1'-N1	7.40	114.12	108.20
35	E	1893	U	O4'-C1'-N1	7.40	114.12	108.20
35	E	2142	C	O4'-C1'-N1	7.40	114.12	108.20
35	E	1663	C	O4'-C1'-N1	7.39	114.11	108.20
35	E	2178	C	O4'-C1'-N1	7.39	114.12	108.20
35	E	2163	G	C5-C6-O6	-7.39	124.16	128.60
35	E	1305	A	C4-C5-C6	7.39	120.69	117.00
35	E	797	G	P-O3'-C3'	7.39	128.57	119.70
35	E	312	C	O4'-C1'-N1	7.38	114.10	108.20
35	E	402	C	O4'-C1'-N1	7.38	114.10	108.20
35	E	433	G	C5-C6-O6	-7.38	124.17	128.60
35	E	1260	G	C5-C6-O6	-7.38	124.17	128.60
35	E	1687	A	O4'-C1'-N9	7.38	114.10	108.20
35	E	1736	G	C5-C6-O6	-7.38	124.17	128.60
35	E	2256	U	O4'-C1'-N1	7.37	114.10	108.20
35	E	469	G	C5-C6-O6	-7.37	124.18	128.60
35	E	1352	C	O4'-C1'-N1	7.37	114.10	108.20
35	E	378	U	O4'-C1'-N1	7.37	114.09	108.20
35	E	1785	C	O4'-C1'-N1	7.37	114.09	108.20
35	E	2020	G	O4'-C1'-N9	7.37	114.10	108.20
35	E	15	U	O4'-C1'-N1	7.37	114.09	108.20
35	E	1088	A	C5-C6-N6	-7.37	117.81	123.70
35	E	1300	C	C6-N1-C1'	-7.36	111.96	120.80
35	E	1884	U	C2-N1-C1'	7.36	126.53	117.70
35	E	271	C	O4'-C1'-N1	7.36	114.09	108.20
35	E	1608	G	C5-C6-O6	-7.36	124.18	128.60
35	E	109	G	O4'-C1'-N9	7.36	114.09	108.20
35	E	616	G	C5-C6-O6	-7.36	124.19	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2254	U	O4'-C1'-N1	7.36	114.09	108.20
35	E	2186	C	O4'-C1'-N1	7.36	114.08	108.20
35	E	626	C	O4'-C1'-N1	7.35	114.08	108.20
35	E	1690	G	N1-C6-O6	7.35	124.31	119.90
35	E	758	U	O4'-C1'-N1	7.35	114.08	108.20
35	E	949	U	O4'-C1'-N1	7.35	114.08	108.20
35	E	256	A	C4-C5-C6	7.35	120.67	117.00
35	E	710	A	C4-C5-C6	7.35	120.67	117.00
35	E	1208	U	O4'-C1'-N1	7.35	114.08	108.20
35	E	1234	G	C5-C6-O6	-7.35	124.19	128.60
35	E	873	C	C2-N1-C1'	7.35	126.88	118.80
35	E	1084	G	O4'-C1'-N9	7.35	114.08	108.20
35	E	572	U	O4'-C1'-N1	7.34	114.08	108.20
35	E	2064	G	C5-C6-O6	-7.34	124.19	128.60
35	E	2203	C	O4'-C1'-N1	7.34	114.08	108.20
35	E	2230	C	O4'-C1'-N1	7.34	114.08	108.20
35	E	1997	G	C5-C6-O6	-7.34	124.19	128.60
35	E	2215	C	O4'-C1'-N1	7.34	114.07	108.20
35	E	1573	C	O4'-C1'-N1	7.34	114.07	108.20
35	E	709	C	O4'-C1'-N1	7.33	114.06	108.20
35	E	1762	G	C5-C6-O6	-7.33	124.20	128.60
35	E	669	U	O4'-C1'-N1	7.33	114.06	108.20
35	E	436	G	C5-C6-O6	-7.33	124.20	128.60
35	E	533	C	O4'-C1'-N1	7.33	114.06	108.20
35	E	892	U	O4'-C1'-N1	7.33	114.06	108.20
35	E	1895	U	O4'-C1'-N1	7.33	114.06	108.20
35	E	2061	G	C5-C6-O6	-7.33	124.20	128.60
35	E	339	C	O4'-C1'-N1	7.32	114.06	108.20
35	E	1356	C	O4'-C1'-N1	7.32	114.06	108.20
35	E	146	U	O4'-C1'-N1	7.32	114.06	108.20
35	E	353	C	N3-C4-N4	7.32	123.12	118.00
35	E	796	G	C5-C6-O6	-7.32	124.21	128.60
35	E	2196	U	O4'-C1'-N1	7.32	114.06	108.20
35	E	1845	C	O4'-C1'-N1	7.32	114.05	108.20
35	E	2261	U	O4'-C1'-N1	7.32	114.05	108.20
35	E	350	C	O4'-C1'-N1	7.32	114.05	108.20
35	E	1578	G	C5-C6-O6	-7.32	124.21	128.60
35	E	1816	G	C5-C6-O6	-7.32	124.21	128.60
35	E	1917	G	C5-C6-O6	-7.32	124.21	128.60
35	E	1856	G	C5-C6-O6	-7.31	124.21	128.60
35	E	2104	A	C4-C5-C6	7.31	120.66	117.00
35	E	2216	A	O4'-C1'-N9	7.31	114.05	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2019	C	N3-C4-N4	7.31	123.11	118.00
35	E	536	A	C5-C6-N6	-7.30	117.86	123.70
35	E	2023	C	C6-N1-C1'	-7.30	112.04	120.80
35	E	2118	G	C5-C6-O6	-7.30	124.22	128.60
35	E	2210	U	O4'-C1'-N1	7.30	114.04	108.20
35	E	1226	G	C5-C6-O6	-7.30	124.22	128.60
35	E	904	C	O4'-C1'-N1	7.30	114.04	108.20
35	E	1903	A	P-O5'-C5'	7.30	132.58	120.90
35	E	518	C	O4'-C1'-N1	7.29	114.04	108.20
35	E	1872	G	O4'-C1'-N9	7.29	114.03	108.20
35	E	1169	U	O4'-C1'-N1	7.29	114.03	108.20
35	E	1523	C	O4'-C1'-N1	7.29	114.03	108.20
35	E	748	G	C5-C6-O6	-7.28	124.23	128.60
35	E	1344	U	O4'-C1'-N1	7.28	114.02	108.20
35	E	680	U	O4'-C1'-N1	7.28	114.02	108.20
35	E	1677	C	O4'-C1'-N1	7.28	114.02	108.20
35	E	1209	C	O4'-C1'-N1	7.28	114.02	108.20
35	E	1694	G	C5-C6-O6	-7.27	124.24	128.60
35	E	814	C	C6-N1-C1'	-7.27	112.08	120.80
35	E	1206	G	C5-C6-O6	-7.27	124.24	128.60
35	E	1341	C	O4'-C1'-N1	7.26	114.01	108.20
35	E	2257	U	O4'-C1'-N1	7.26	114.01	108.20
35	E	1723	G	C5-C6-O6	-7.26	124.24	128.60
35	E	1654	U	O4'-C1'-N1	7.26	114.01	108.20
35	E	878	G	C5-C6-O6	-7.26	124.25	128.60
35	E	2082	U	O4'-C1'-N1	7.26	114.01	108.20
35	E	1303	U	O4'-C1'-N1	7.25	114.00	108.20
35	E	421	U	O4'-C1'-N1	7.25	114.00	108.20
35	E	456	C	O4'-C1'-N1	7.25	114.00	108.20
35	E	1665	C	O4'-C1'-N1	7.25	114.00	108.20
35	E	2062	U	O4'-C1'-N1	7.25	114.00	108.20
35	E	2175	C	O4'-C1'-N1	7.25	114.00	108.20
35	E	479	G	C5-C6-O6	-7.25	124.25	128.60
35	E	1719	U	O4'-C1'-N1	7.25	114.00	108.20
35	E	2075	G	C5-C6-O6	-7.25	124.25	128.60
35	E	270	C	O4'-C1'-N1	7.24	113.99	108.20
35	E	590	C	O4'-C1'-N1	7.24	113.99	108.20
35	E	1575	G	C5-C6-O6	-7.24	124.26	128.60
35	E	1607	A	C5-C6-N6	-7.24	117.91	123.70
35	E	480	C	O4'-C1'-N1	7.23	113.98	108.20
35	E	554	C	N3-C4-N4	7.23	123.06	118.00
35	E	755	U	O4'-C1'-N1	7.23	113.99	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	13	U	O4'-C1'-N1	7.23	113.98	108.20
35	E	850	U	O4'-C1'-N1	7.23	113.98	108.20
35	E	1083	G	C5-C6-O6	-7.23	124.26	128.60
35	E	2138	U	O4'-C1'-N1	7.23	113.98	108.20
35	E	1339	G	O4'-C1'-N9	7.22	113.98	108.20
35	E	1554	A	C4-C5-C6	7.22	120.61	117.00
35	E	1635	G	C5-C6-O6	-7.22	124.27	128.60
35	E	1768	A	C4-C5-C6	7.22	120.61	117.00
35	E	1278	C	O4'-C1'-N1	7.22	113.98	108.20
35	E	1629	C	O4'-C1'-N1	7.22	113.97	108.20
35	E	649	G	C5-C6-O6	-7.21	124.27	128.60
35	E	734	G	N1-C2-N3	-7.21	119.57	123.90
35	E	1668	G	C5-C6-O6	-7.21	124.27	128.60
35	E	422	U	O4'-C1'-N1	7.21	113.97	108.20
35	E	654	U	O4'-C1'-N1	7.21	113.97	108.20
35	E	1381	G	C5-C6-O6	-7.21	124.28	128.60
35	E	2143	C	O4'-C1'-N1	7.21	113.97	108.20
35	E	346	C	O4'-C1'-N1	7.21	113.96	108.20
35	E	620	C	O4'-C1'-N1	7.21	113.96	108.20
35	E	926	C	O4'-C1'-N1	7.20	113.96	108.20
35	E	1970	G	O4'-C1'-N9	7.20	113.96	108.20
35	E	2193	U	O4'-C1'-N1	7.20	113.96	108.20
35	E	1170	C	O4'-C1'-N1	7.20	113.96	108.20
35	E	1193	A	C5-C6-N6	-7.20	117.94	123.70
35	E	1229	C	O4'-C1'-N1	7.20	113.96	108.20
35	E	377	G	C5-C6-O6	-7.20	124.28	128.60
35	E	1926	G	C5-C6-O6	-7.20	124.28	128.60
35	E	1284	U	O4'-C1'-N1	7.20	113.96	108.20
35	E	1072	G	C5-C6-O6	-7.20	124.28	128.60
35	E	1295	U	O4'-C1'-N1	7.19	113.95	108.20
35	E	1721	U	O4'-C1'-N1	7.19	113.95	108.20
35	E	202	C	N3-C4-N4	7.19	123.03	118.00
35	E	1225	G	C5-C6-O6	-7.19	124.28	128.60
35	E	1692	G	C5-C6-O6	-7.19	124.28	128.60
35	E	310	U	O4'-C1'-N1	7.19	113.95	108.20
35	E	1970	G	C5-C6-O6	-7.19	124.29	128.60
35	E	584	C	N3-C4-N4	7.19	123.03	118.00
35	E	97	A	C4-C5-C6	7.19	120.59	117.00
35	E	2306	A	C5-C6-N6	-7.19	117.95	123.70
35	E	67	C	O4'-C1'-N1	7.18	113.95	108.20
35	E	921	G	C5-C6-O6	-7.18	124.29	128.60
35	E	229	G	C5-C6-O6	-7.18	124.29	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1899	C	N3-C4-N4	7.18	123.03	118.00
35	E	429	C	O4'-C1'-N1	7.18	113.94	108.20
35	E	1968	G	C5-C6-O6	-7.18	124.29	128.60
35	E	874	C	O4'-C1'-N1	7.18	113.94	108.20
35	E	994	G	C5-C6-O6	-7.18	124.29	128.60
35	E	1293	C	O4'-C1'-N1	7.17	113.94	108.20
35	E	497	C	O4'-C1'-N1	7.17	113.94	108.20
35	E	1729	C	O4'-C1'-N1	7.17	113.94	108.20
35	E	1811	C	O4'-C1'-N1	7.17	113.93	108.20
35	E	224	C	O4'-C1'-N1	7.17	113.93	108.20
35	E	1678	C	O4'-C1'-N1	7.17	113.93	108.20
35	E	1243	U	O4'-C1'-N1	7.16	113.93	108.20
35	E	1796	G	C5-C6-O6	-7.16	124.31	128.60
35	E	2253	U	O4'-C1'-N1	7.16	113.92	108.20
35	E	633	A	O4'-C1'-N9	7.15	113.92	108.20
35	E	1894	C	O4'-C1'-N1	7.15	113.92	108.20
35	E	884	A	O4'-C1'-N9	7.15	113.92	108.20
35	E	1546	C	O4'-C1'-N1	7.15	113.92	108.20
35	E	138	C	O4'-C1'-N1	7.15	113.92	108.20
35	E	794	G	C5-C6-O6	-7.15	124.31	128.60
35	E	830	C	O4'-C1'-N1	7.15	113.92	108.20
35	E	1847	C	O4'-C1'-N1	7.15	113.92	108.20
35	E	1879	U	O4'-C1'-N1	7.14	113.91	108.20
35	E	1311	C	O4'-C1'-N1	7.14	113.91	108.20
35	E	1990	U	O4'-C1'-N1	7.14	113.91	108.20
35	E	2084	U	O4'-C1'-N1	7.14	113.91	108.20
35	E	2264	A	C4-C5-C6	7.13	120.57	117.00
35	E	1791	C	O4'-C1'-N1	7.13	113.90	108.20
35	E	815	G	O4'-C1'-N9	7.13	113.90	108.20
35	E	2029	U	O4'-C1'-N1	7.13	113.90	108.20
35	E	539	G	C5-C6-O6	-7.13	124.32	128.60
35	E	1830	C	O4'-C1'-N1	7.12	113.90	108.20
35	E	1266	C	O4'-C1'-N1	7.12	113.89	108.20
35	E	790	G	C5-C6-O6	-7.12	124.33	128.60
35	E	2061	G	C4-N9-C1'	7.12	135.75	126.50
35	E	1585	C	O4'-C1'-N1	7.12	113.89	108.20
35	E	2308	C	O4'-C1'-N1	7.12	113.89	108.20
35	E	1185	A	C5-C6-N1	-7.11	114.14	117.70
35	E	388	U	O4'-C1'-N1	7.11	113.89	108.20
35	E	2057	U	O4'-C1'-N1	7.11	113.89	108.20
35	E	801	C	O4'-C1'-N1	7.10	113.88	108.20
35	E	686	U	O4'-C1'-N1	7.10	113.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	134	U	O4'-C1'-N1	7.10	113.88	108.20
35	E	962	A	C5-C6-N6	-7.10	118.02	123.70
35	E	1548	C	C6-N1-C1'	-7.10	112.28	120.80
35	E	827	U	O4'-C1'-N1	7.10	113.88	108.20
35	E	2105	C	O4'-C1'-N1	7.10	113.88	108.20
35	E	2181	U	O4'-C1'-N1	7.10	113.88	108.20
35	E	187	C	O4'-C1'-N1	7.10	113.88	108.20
35	E	1224	U	O4'-C1'-N1	7.09	113.87	108.20
35	E	1245	C	O4'-C1'-N1	7.09	113.87	108.20
35	E	671	U	O4'-C1'-N1	7.09	113.87	108.20
35	E	1348	A	C4-C5-C6	7.09	120.54	117.00
35	E	2146	U	O4'-C1'-N1	7.09	113.87	108.20
35	E	908	G	C5-C6-O6	-7.08	124.35	128.60
35	E	1347	U	O4'-C1'-N1	7.08	113.87	108.20
35	E	1667	G	N1-C6-O6	7.08	124.15	119.90
35	E	900	A	O4'-C1'-N9	7.08	113.86	108.20
35	E	1685	G	C5-C6-O6	-7.08	124.35	128.60
35	E	1714	U	O4'-C1'-N1	7.08	113.86	108.20
35	E	1947	U	O4'-C1'-N1	7.08	113.86	108.20
35	E	1377	A	O4'-C1'-N9	7.07	113.86	108.20
35	E	1326	G	C5-C6-O6	-7.07	124.36	128.60
35	E	1376	G	O4'-C1'-N9	7.07	113.86	108.20
35	E	17	C	O4'-C1'-N1	7.07	113.86	108.20
35	E	2301	C	O4'-C1'-N1	7.07	113.86	108.20
35	E	1183	G	C5-C6-O6	-7.07	124.36	128.60
35	E	1185	A	O4'-C1'-N9	7.07	113.85	108.20
35	E	1331	U	O4'-C1'-N1	7.07	113.85	108.20
35	E	1379	U	O4'-C1'-N1	7.07	113.85	108.20
35	E	1622	G	C5-C6-O6	-7.07	124.36	128.60
35	E	85	U	O4'-C1'-N1	7.07	113.85	108.20
35	E	1694	G	O4'-C1'-N9	7.07	113.85	108.20
35	E	368	G	O4'-C1'-N9	7.06	113.85	108.20
35	E	1909	U	O4'-C1'-N1	7.06	113.85	108.20
35	E	225	C	O4'-C1'-N1	7.06	113.85	108.20
35	E	534	C	O4'-C1'-N1	7.06	113.85	108.20
35	E	1075	G	C5-C6-O6	-7.06	124.37	128.60
35	E	2318	U	O4'-C1'-N1	7.05	113.84	108.20
35	E	465	G	C5-C6-O6	-7.05	124.37	128.60
35	E	2201	U	O4'-C1'-N1	7.05	113.84	108.20
35	E	573	U	O4'-C1'-N1	7.05	113.84	108.20
35	E	32	U	O4'-C1'-N1	7.05	113.84	108.20
35	E	1716	C	O4'-C1'-N1	7.05	113.84	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1901	G	C5-C6-O6	-7.05	124.37	128.60
35	E	2161	U	O4'-C1'-N1	7.05	113.84	108.20
35	E	2219	C	O4'-C1'-N1	7.05	113.84	108.20
35	E	92	G	C5-C6-O6	-7.04	124.37	128.60
35	E	1640	G	C5-C6-O6	-7.04	124.37	128.60
35	E	384	G	C5-C6-O6	-7.04	124.38	128.60
35	E	407	G	C5-C6-O6	-7.04	124.38	128.60
35	E	1337	G	C5-C6-O6	-7.04	124.38	128.60
35	E	27	U	O4'-C1'-N1	7.04	113.83	108.20
35	E	1871	G	O4'-C1'-N9	7.04	113.83	108.20
35	E	115	U	O4'-C1'-N1	7.04	113.83	108.20
35	E	1285	C	O4'-C1'-N1	7.04	113.83	108.20
35	E	534	C	N3-C4-N4	7.04	122.92	118.00
35	E	1538	G	C5-C6-O6	-7.04	124.38	128.60
35	E	2012	C	O4'-C1'-N1	7.04	113.83	108.20
35	E	745	C	N3-C4-N4	7.03	122.92	118.00
35	E	779	A	C4-C5-C6	7.03	120.52	117.00
35	E	1624	C	O4'-C1'-N1	7.03	113.82	108.20
35	E	178	U	O4'-C1'-N1	7.03	113.82	108.20
35	E	1252	C	O4'-C1'-N1	7.03	113.82	108.20
35	E	155	U	O4'-C1'-N1	7.03	113.82	108.20
35	E	719	G	O4'-C1'-N9	7.03	113.82	108.20
35	E	883	C	N3-C4-N4	7.03	122.92	118.00
35	E	1184	C	O4'-C1'-N1	7.03	113.82	108.20
35	E	1600	A	C4-C5-C6	7.02	120.51	117.00
35	E	1536	C	O4'-C1'-N1	7.02	113.82	108.20
35	E	1618	G	C5-C6-O6	-7.02	124.39	128.60
35	E	441	C	N3-C4-N4	7.02	122.92	118.00
35	E	1798	G	C5-C6-O6	-7.02	124.39	128.60
35	E	50	C	O4'-C1'-N1	7.02	113.81	108.20
35	E	964	U	O4'-C1'-N1	7.02	113.81	108.20
35	E	1081	G	C5-C6-O6	-7.02	124.39	128.60
35	E	280	C	O4'-C1'-N1	7.02	113.81	108.20
35	E	724	A	N1-C2-N3	7.02	132.81	129.30
35	E	1556	C	O4'-C1'-N1	7.02	113.81	108.20
35	E	643	C	O4'-C1'-N1	7.01	113.81	108.20
35	E	266	U	O4'-C1'-N1	7.01	113.81	108.20
35	E	772	U	O4'-C1'-C2'	-7.01	98.79	105.80
35	E	1760	G	N1-C6-O6	7.01	124.11	119.90
35	E	298	C	N3-C4-N4	7.01	122.91	118.00
35	E	1342	C	O4'-C1'-N1	7.01	113.81	108.20
35	E	286	G	C5-C6-O6	-7.01	124.39	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	708	G	O4'-C1'-N9	7.01	113.81	108.20
35	E	1171	C	O4'-C1'-N1	7.01	113.81	108.20
35	E	2160	U	O4'-C1'-N1	7.01	113.81	108.20
35	E	1820	U	O4'-C1'-N1	7.00	113.80	108.20
35	E	918	G	C5-C6-O6	-7.00	124.40	128.60
35	E	1364	G	C5-C6-O6	-7.00	124.40	128.60
35	E	2034	A	O4'-C1'-N9	7.00	113.80	108.20
35	E	612	U	O4'-C1'-N1	7.00	113.80	108.20
35	E	971	G	O4'-C1'-N9	7.00	113.80	108.20
35	E	1928	U	O4'-C1'-N1	7.00	113.80	108.20
35	E	14	C	O4'-C1'-N1	6.99	113.79	108.20
35	E	289	G	C5-C6-O6	-6.99	124.40	128.60
35	E	642	U	O4'-C1'-N1	6.99	113.79	108.20
35	E	897	U	O4'-C1'-N1	6.99	113.79	108.20
35	E	1921	G	C5-C6-O6	-6.99	124.41	128.60
35	E	1550	C	O4'-C1'-N1	6.99	113.79	108.20
35	E	234	U	O4'-C1'-N1	6.99	113.79	108.20
35	E	1949	U	O4'-C1'-N1	6.98	113.79	108.20
35	E	2086	G	C5-C6-O6	-6.98	124.41	128.60
35	E	459	U	O4'-C1'-N1	6.98	113.78	108.20
35	E	471	C	O4'-C1'-N1	6.98	113.78	108.20
35	E	638	C	O4'-C1'-N1	6.98	113.78	108.20
35	E	667	G	C5-C6-O6	-6.98	124.41	128.60
35	E	914	C	O4'-C1'-N1	6.98	113.78	108.20
35	E	1636	U	O4'-C1'-N1	6.98	113.78	108.20
35	E	652	U	O4'-C1'-N1	6.98	113.78	108.20
35	E	705	G	C5-C6-O6	-6.98	124.41	128.60
35	E	1872	G	C5-C6-O6	-6.98	124.41	128.60
35	E	1961	A	C4-C5-C6	6.98	120.49	117.00
35	E	613	C	O4'-C1'-N1	6.97	113.78	108.20
35	E	264	C	O4'-C1'-N1	6.97	113.78	108.20
35	E	554	C	O4'-C1'-N1	6.97	113.78	108.20
35	E	1718	U	O4'-C1'-N1	6.97	113.78	108.20
35	E	1589	C	O4'-C1'-N1	6.97	113.77	108.20
35	E	637	C	O4'-C1'-N1	6.96	113.77	108.20
35	E	859	C	O4'-C1'-N1	6.96	113.77	108.20
35	E	1198	G	C5-C6-O6	-6.96	124.42	128.60
35	E	2019	C	O4'-C1'-N1	6.96	113.77	108.20
35	E	731	U	O4'-C1'-N1	6.96	113.77	108.20
26	j	100	TYR	CB-CG-CD1	6.96	125.17	121.00
35	E	1806	C	O4'-C1'-N1	6.96	113.76	108.20
35	E	546	U	C2-N1-C1'	6.95	126.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1576	G	N1-C6-O6	6.95	124.07	119.90
35	E	1198	G	P-O3'-C3'	6.95	128.04	119.70
35	E	617	U	O4'-C1'-N1	6.95	113.76	108.20
35	E	1351	C	O4'-C1'-N1	6.95	113.76	108.20
35	E	1903	A	O4'-C1'-N9	6.95	113.76	108.20
35	E	210	A	C5-C6-N6	-6.95	118.14	123.70
35	E	1755	G	C5-C6-O6	-6.95	124.43	128.60
35	E	150	U	O4'-C1'-N1	6.94	113.75	108.20
35	E	2228	C	N3-C4-N4	6.94	122.86	118.00
35	E	657	U	O4'-C1'-N1	6.94	113.75	108.20
35	E	726	C	O4'-C1'-N1	6.94	113.75	108.20
35	E	910	A	C5-C6-N6	-6.94	118.15	123.70
35	E	1931	U	O4'-C1'-N1	6.94	113.75	108.20
35	E	2162	U	O4'-C1'-N1	6.94	113.75	108.20
35	E	528	U	O4'-C1'-N1	6.93	113.75	108.20
35	E	824	G	C5-C6-O6	-6.93	124.44	128.60
35	E	987	G	O4'-C1'-N9	6.93	113.75	108.20
35	E	353	C	O4'-C1'-N1	6.93	113.75	108.20
35	E	2021	G	C5-C6-O6	-6.93	124.44	128.60
35	E	2128	C	O4'-C1'-N1	6.93	113.75	108.20
35	E	305	U	O4'-C1'-N1	6.93	113.75	108.20
35	E	1544	U	O4'-C1'-N1	6.93	113.75	108.20
35	E	346	C	N3-C4-N4	6.93	122.85	118.00
35	E	789	C	O4'-C1'-N1	6.93	113.74	108.20
35	E	1322	G	C5-C6-O6	-6.93	124.44	128.60
35	E	752	U	O4'-C1'-N1	6.93	113.74	108.20
35	E	2252	U	O4'-C1'-N1	6.93	113.74	108.20
35	E	91	U	O4'-C1'-N1	6.92	113.74	108.20
35	E	719	G	C5-C6-O6	-6.92	124.45	128.60
35	E	938	G	C5-C6-O6	-6.92	124.45	128.60
35	E	1614	G	C5-C6-O6	-6.92	124.45	128.60
35	E	323	U	O4'-C1'-N1	6.92	113.74	108.20
35	E	618	G	C5-C6-O6	-6.92	124.45	128.60
35	E	1772	G	C5-C6-O6	-6.92	124.45	128.60
35	E	1896	C	O4'-C1'-N1	6.92	113.74	108.20
35	E	416	U	O4'-C1'-N1	6.92	113.74	108.20
35	E	424	G	C5-C6-O6	-6.92	124.45	128.60
35	E	970	G	O4'-C1'-N9	6.92	113.73	108.20
35	E	2250	U	O4'-C1'-N1	6.92	113.73	108.20
35	E	2282	C	O4'-C1'-N1	6.91	113.73	108.20
35	E	565	G	N1-C6-O6	6.91	124.05	119.90
35	E	37	U	O4'-C1'-N1	6.91	113.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	336	C	O4'-C1'-N1	6.91	113.72	108.20
35	E	492	A	C5-C6-N6	-6.91	118.18	123.70
35	E	833	A	O4'-C1'-N9	6.91	113.72	108.20
35	E	1810	C	O4'-C1'-N1	6.91	113.72	108.20
35	E	2074	G	C5-C6-O6	-6.91	124.46	128.60
35	E	550	U	O4'-C1'-N1	6.90	113.72	108.20
35	E	614	U	O4'-C1'-N1	6.90	113.72	108.20
35	E	750	C	O4'-C1'-N1	6.90	113.72	108.20
35	E	780	C	O4'-C1'-N1	6.90	113.72	108.20
35	E	77	C	N3-C4-N4	6.90	122.83	118.00
35	E	179	G	C5-C6-O6	-6.90	124.46	128.60
35	E	2180	U	O4'-C1'-N1	6.89	113.72	108.20
35	E	2053	G	C5-C6-O6	-6.89	124.47	128.60
35	E	1713	G	C5-C6-O6	-6.89	124.47	128.60
35	E	114	C	O4'-C1'-N1	6.89	113.71	108.20
35	E	164	G	C5-C6-O6	-6.89	124.47	128.60
35	E	2207	U	O4'-C1'-N1	6.89	113.71	108.20
26	j	100	TYR	CB-CG-CD2	-6.88	116.87	121.00
35	E	51	A	C4-C5-C6	6.88	120.44	117.00
35	E	1864	C	N3-C4-N4	6.88	122.82	118.00
35	E	1873	G	C4-N9-C1'	-6.88	117.55	126.50
35	E	309	G	C5-C6-O6	-6.88	124.47	128.60
35	E	99	U	O4'-C1'-N1	6.88	113.71	108.20
35	E	137	C	N3-C4-N4	6.88	122.82	118.00
35	E	1706	A	C4-C5-C6	6.88	120.44	117.00
35	E	1906	C	C6-N1-C1'	-6.88	112.54	120.80
35	E	1873	G	C8-N9-C1'	6.88	135.94	127.00
35	E	2136	A	C5-C6-N6	-6.88	118.20	123.70
35	E	2280	A	C4-C5-C6	6.88	120.44	117.00
35	E	267	U	O4'-C1'-N1	6.88	113.70	108.20
35	E	327	U	O4'-C1'-N1	6.88	113.70	108.20
35	E	570	U	O4'-C1'-N1	6.88	113.70	108.20
35	E	729	C	O4'-C1'-N1	6.88	113.70	108.20
35	E	948	U	O4'-C1'-N1	6.88	113.70	108.20
35	E	1757	U	O4'-C1'-N1	6.88	113.70	108.20
35	E	301	U	O4'-C1'-N1	6.87	113.70	108.20
35	E	446	A	C4-C5-C6	6.87	120.44	117.00
35	E	511	G	C5-C6-O6	-6.87	124.48	128.60
35	E	2212	G	C5-C6-O6	-6.87	124.48	128.60
35	E	362	C	O4'-C1'-N1	6.87	113.69	108.20
35	E	2303	U	O4'-C1'-N1	6.86	113.69	108.20
35	E	592	A	C4-C5-C6	6.86	120.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	797	G	C5-C6-O6	-6.86	124.48	128.60
35	E	1321	G	C5-C6-O6	-6.86	124.48	128.60
35	E	160	A	C5-C6-N6	-6.86	118.21	123.70
35	E	247	U	O4'-C1'-N1	6.85	113.68	108.20
35	E	2025	U	O4'-C1'-N1	6.85	113.68	108.20
35	E	2276	U	O4'-C1'-N1	6.85	113.68	108.20
35	E	2010	G	C5-C6-O6	-6.85	124.49	128.60
35	E	1172	C	O4'-C1'-N1	6.85	113.68	108.20
35	E	52	U	O4'-C1'-N1	6.85	113.68	108.20
35	E	163	C	O4'-C1'-N1	6.85	113.68	108.20
35	E	714	G	C5-C6-O6	-6.85	124.49	128.60
35	E	1770	U	O4'-C1'-N1	6.85	113.68	108.20
35	E	1780	G	C5-C6-O6	-6.85	124.49	128.60
35	E	1969	G	C5-C6-O6	-6.85	124.49	128.60
35	E	1819	U	O4'-C1'-N1	6.85	113.68	108.20
35	E	1556	C	N3-C4-N4	6.84	122.79	118.00
35	E	1672	C	O4'-C1'-N1	6.84	113.67	108.20
35	E	342	U	O4'-C1'-N1	6.84	113.67	108.20
35	E	1632	G	C5-C6-O6	-6.84	124.49	128.60
35	E	1813	G	C5-C6-O6	-6.84	124.49	128.60
35	E	2177	U	O4'-C1'-N1	6.84	113.67	108.20
35	E	20	G	C5-C6-O6	-6.84	124.50	128.60
35	E	1253	G	C5-C6-O6	-6.84	124.50	128.60
35	E	1915	G	C5-C6-O6	-6.84	124.50	128.60
35	E	154	U	O4'-C1'-N1	6.84	113.67	108.20
35	E	1856	G	O4'-C1'-N9	6.84	113.67	108.20
35	E	40	A	C4-C5-C6	6.84	120.42	117.00
35	E	1754	U	O4'-C1'-N1	6.84	113.67	108.20
35	E	2091	U	O4'-C1'-N1	6.84	113.67	108.20
35	E	171	U	O4'-C1'-N1	6.83	113.67	108.20
35	E	947	U	O4'-C1'-N1	6.83	113.67	108.20
35	E	1617	G	C5-C6-O6	-6.83	124.50	128.60
35	E	1621	U	O4'-C1'-N1	6.83	113.67	108.20
35	E	2012	C	N3-C4-N4	6.83	122.78	118.00
35	E	2185	U	O4'-C1'-N1	6.83	113.67	108.20
35	E	937	C	N3-C4-N4	6.83	122.78	118.00
35	E	775	A	P-O3'-C3'	6.82	127.89	119.70
35	E	1297	C	O4'-C1'-N1	6.82	113.66	108.20
35	E	1631	A	O4'-C1'-N9	6.82	113.66	108.20
35	E	88	G	C5-C6-O6	-6.82	124.51	128.60
35	E	895	A	C4-C5-C6	6.82	120.41	117.00
35	E	973	G	C5-C6-O6	-6.82	124.51	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1204	U	O4'-C1'-N1	6.82	113.66	108.20
35	E	551	U	O4'-C1'-N1	6.82	113.66	108.20
35	E	924	G	C5-C6-O6	-6.82	124.51	128.60
35	E	934	C	O4'-C1'-N1	6.82	113.65	108.20
35	E	2030	G	C5-C6-O6	-6.82	124.51	128.60
35	E	631	G	C5-C6-O6	-6.82	124.51	128.60
35	E	806	C	O4'-C1'-N1	6.82	113.65	108.20
35	E	965	C	O4'-C1'-N1	6.82	113.65	108.20
35	E	2027	C	C2-N1-C1'	6.81	126.29	118.80
35	E	128	U	O4'-C1'-N1	6.81	113.65	108.20
35	E	308	C	O4'-C1'-N1	6.81	113.65	108.20
35	E	574	U	O4'-C1'-N1	6.81	113.65	108.20
35	E	630	G	C5-C6-O6	-6.81	124.52	128.60
35	E	1696	G	C5-C6-O6	-6.81	124.51	128.60
35	E	1221	U	O4'-C1'-N1	6.81	113.65	108.20
35	E	1720	C	O4'-C1'-N1	6.81	113.65	108.20
35	E	1972	G	C5-C6-O6	-6.81	124.52	128.60
35	E	1998	A	C5-C6-N6	-6.81	118.25	123.70
35	E	899	G	C5-C6-O6	-6.80	124.52	128.60
35	E	1993	G	C5-C6-O6	-6.80	124.52	128.60
35	E	998	C	O4'-C1'-N1	6.80	113.64	108.20
35	E	896	U	O4'-C1'-N1	6.80	113.64	108.20
35	E	1187	C	N3-C4-C5	-6.80	119.18	121.90
35	E	2076	A	O4'-C1'-N9	6.80	113.64	108.20
35	E	2213	G	C5-C6-O6	-6.80	124.52	128.60
35	E	29	U	O4'-C1'-N1	6.80	113.64	108.20
35	E	372	U	O4'-C1'-N1	6.80	113.64	108.20
35	E	727	C	O4'-C1'-N1	6.80	113.64	108.20
35	E	1281	U	O4'-C1'-N1	6.80	113.64	108.20
35	E	116	G	C5-C6-O6	-6.80	124.52	128.60
35	E	252	G	C5-C6-O6	-6.80	124.52	128.60
35	E	1691	G	C5-C6-O6	-6.80	124.52	128.60
35	E	1883	C	O4'-C1'-N1	6.80	113.64	108.20
35	E	1913	U	O4'-C1'-N1	6.80	113.64	108.20
35	E	1933	G	C5-C6-O6	-6.80	124.52	128.60
35	E	2099	G	N1-C6-O6	6.80	123.98	119.90
35	E	397	G	C5-C6-O6	-6.79	124.52	128.60
35	E	688	G	C5-C6-O6	-6.79	124.52	128.60
35	E	437	G	O4'-C1'-N9	6.79	113.64	108.20
35	E	500	A	C4-C5-C6	6.79	120.40	117.00
35	E	893	G	C5-C6-O6	-6.79	124.52	128.60
35	E	1963	G	C5-C6-O6	-6.79	124.53	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2145	A	C4-C5-C6	6.79	120.39	117.00
35	E	1825	A	C4-C5-C6	6.79	120.39	117.00
35	E	759	C	O4'-C1'-N1	6.79	113.63	108.20
35	E	819	G	C5-C6-O6	-6.79	124.53	128.60
35	E	909	G	C5-C6-O6	-6.79	124.53	128.60
35	E	90	A	C4-C5-C6	6.78	120.39	117.00
35	E	693	G	C5-C6-O6	-6.78	124.53	128.60
35	E	2243	U	O4'-C1'-N1	6.78	113.62	108.20
35	E	379	G	C5-C6-O6	-6.78	124.53	128.60
3	r	135	TRP	C-N-CA	6.78	136.53	122.30
35	E	144	A	C5-C6-N6	-6.78	118.28	123.70
35	E	966	C	O4'-C1'-N1	6.78	113.62	108.20
35	E	2017	G	C5-C6-O6	-6.78	124.53	128.60
35	E	2022	A	O4'-C1'-N9	6.78	113.62	108.20
35	E	426	U	O4'-C1'-N1	6.78	113.62	108.20
35	E	1688	C	N3-C4-N4	6.78	122.74	118.00
35	E	1717	U	O4'-C1'-N1	6.78	113.62	108.20
35	E	2235	C	N3-C4-N4	6.77	122.74	118.00
35	E	981	G	C5-C6-O6	-6.77	124.54	128.60
35	E	2298	G	C5-C6-O6	-6.77	124.54	128.60
35	E	1942	A	O4'-C1'-N9	6.77	113.62	108.20
35	E	252	G	O4'-C1'-N9	6.77	113.61	108.20
35	E	772	U	C4'-C3'-C2'	-6.77	95.83	102.60
35	E	1304	C	O4'-C1'-N1	6.77	113.61	108.20
35	E	1531	G	C5-C6-O6	-6.77	124.54	128.60
35	E	2101	G	C5-C6-O6	-6.77	124.54	128.60
35	E	1722	C	O4'-C1'-N1	6.77	113.61	108.20
35	E	2229	A	C5-C6-N6	-6.77	118.29	123.70
35	E	302	U	O4'-C1'-N1	6.77	113.61	108.20
35	E	1941	C	N3-C4-N4	6.77	122.74	118.00
35	E	2073	G	C5-C6-O6	-6.77	124.54	128.60
5	u	43	TYR	CB-CG-CD2	-6.76	116.94	121.00
35	E	172	A	C4-C5-C6	6.76	120.38	117.00
35	E	2291	U	O4'-C1'-N1	6.76	113.61	108.20
35	E	170	C	O4'-C1'-N1	6.76	113.61	108.20
35	E	1550	C	N3-C4-N4	6.76	122.73	118.00
35	E	1698	A	C4-C5-C6	6.76	120.38	117.00
35	E	2155	U	O4'-C1'-N1	6.76	113.61	108.20
35	E	1227	U	O4'-C1'-N1	6.76	113.61	108.20
35	E	2280	A	C5-C6-N6	-6.76	118.30	123.70
35	E	1954	C	O4'-C1'-N1	6.75	113.60	108.20
35	E	621	A	C4-C5-C6	6.75	120.38	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1765	G	C5-C6-O6	-6.75	124.55	128.60
35	E	819	G	P-O3'-C3'	6.75	127.80	119.70
35	E	687	U	O4'-C1'-N1	6.75	113.60	108.20
35	E	1902	G	C5-C6-O6	-6.75	124.55	128.60
35	E	419	G	C5-C6-O6	-6.75	124.55	128.60
35	E	919	G	C5-C6-O6	-6.75	124.55	128.60
35	E	461	C	O4'-C1'-N1	6.75	113.60	108.20
35	E	16	G	C5-C6-O6	-6.74	124.55	128.60
35	E	557	U	O4'-C1'-N1	6.74	113.59	108.20
35	E	629	C	O4'-C1'-N1	6.74	113.59	108.20
35	E	1191	G	C2'-C3'-O3'	6.74	124.49	113.70
35	E	839	C	O4'-C1'-N1	6.74	113.59	108.20
35	E	1977	G	C5-C6-O6	-6.74	124.56	128.60
35	E	494	U	O4'-C1'-N1	6.74	113.59	108.20
35	E	776	G	C5-C6-O6	-6.74	124.56	128.60
35	E	1287	A	C5-C6-N6	-6.74	118.31	123.70
35	E	1580	G	C5-C6-O6	-6.74	124.56	128.60
35	E	1875	G	C5-C6-O6	-6.74	124.56	128.60
35	E	400	G	C5-C6-O6	-6.74	124.56	128.60
35	E	834	G	C5-C6-O6	-6.74	124.56	128.60
35	E	274	C	N3-C4-N4	6.74	122.72	118.00
35	E	697	G	C5-C6-O6	-6.73	124.56	128.60
35	E	1167	C	N3-C4-N4	6.73	122.71	118.00
35	E	1588	U	O4'-C1'-N1	6.73	113.59	108.20
35	E	84	C	N3-C4-N4	6.73	122.71	118.00
35	E	984	A	C5-C6-N6	-6.73	118.31	123.70
35	E	985	G	O4'-C1'-N9	6.73	113.59	108.20
35	E	261	A	C5-C6-N6	-6.73	118.32	123.70
35	E	2031	A	C4-C5-C6	6.73	120.36	117.00
35	E	2109	G	C5-C6-O6	-6.73	124.56	128.60
35	E	1829	C	O4'-C1'-N1	6.73	113.58	108.20
35	E	298	C	O4'-C1'-N1	6.73	113.58	108.20
35	E	1358	G	C5-C6-O6	-6.72	124.56	128.60
35	E	2308	C	N3-C4-N4	6.72	122.71	118.00
25	i	116	PHE	CB-CG-CD1	6.72	125.51	120.80
35	E	194	U	O4'-C1'-N1	6.72	113.58	108.20
35	E	354	U	O4'-C1'-N1	6.72	113.58	108.20
35	E	923	A	C4-C5-C6	6.72	120.36	117.00
35	E	1849	U	O4'-C1'-N1	6.72	113.58	108.20
35	E	2191	G	O4'-C1'-N9	6.72	113.58	108.20
35	E	561	A	C5-C6-N6	-6.72	118.33	123.70
35	E	987	G	C5-C6-O6	-6.72	124.57	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1987	A	C4-C5-C6	6.72	120.36	117.00
35	E	259	C	N3-C4-N4	6.71	122.70	118.00
35	E	871	G	C5-C6-O6	-6.71	124.57	128.60
35	E	1599	A	C4-C5-C6	6.71	120.36	117.00
35	E	2230	C	N3-C4-N4	6.71	122.70	118.00
35	E	474	C	O4'-C1'-N1	6.71	113.57	108.20
35	E	801	C	N3-C4-N4	6.71	122.70	118.00
35	E	997	G	C5-C6-O6	-6.71	124.57	128.60
35	E	1641	C	O4'-C1'-N1	6.71	113.57	108.20
35	E	2144	G	C5-C6-O6	-6.71	124.57	128.60
35	E	443	G	C5-C6-O6	-6.71	124.57	128.60
35	E	1383	G	C5-C6-O6	-6.71	124.58	128.60
35	E	1542	U	O4'-C1'-N1	6.71	113.57	108.20
35	E	1912	U	O4'-C1'-N1	6.71	113.57	108.20
35	E	737	U	O4'-C1'-N1	6.71	113.56	108.20
35	E	1084	G	C5-C6-O6	-6.71	124.58	128.60
35	E	341	U	O4'-C1'-N1	6.71	113.56	108.20
35	E	559	U	O4'-C1'-N1	6.71	113.56	108.20
35	E	175	A	C4-C5-C6	6.70	120.35	117.00
35	E	248	G	C5-C6-O6	-6.70	124.58	128.60
35	E	522	A	C5-C6-N1	-6.70	114.35	117.70
35	E	1528	C	O4'-C1'-N1	6.70	113.56	108.20
35	E	903	G	C5-C6-O6	-6.70	124.58	128.60
35	E	930	G	C5-C6-O6	-6.70	124.58	128.60
35	E	1236	G	C5-C6-O6	-6.70	124.58	128.60
35	E	58	C	N3-C4-N4	6.70	122.69	118.00
35	E	95	U	O4'-C1'-N1	6.70	113.56	108.20
35	E	460	U	O4'-C1'-N1	6.70	113.56	108.20
35	E	129	U	O4'-C1'-N1	6.69	113.56	108.20
35	E	1296	U	O4'-C1'-N1	6.69	113.55	108.20
35	E	33	U	O4'-C1'-N1	6.69	113.55	108.20
35	E	172	A	C5-C6-N1	-6.69	114.36	117.70
35	E	505	A	C4-C5-C6	6.69	120.34	117.00
35	E	613	C	N3-C4-N4	6.69	122.68	118.00
35	E	791	G	C5-C6-O6	-6.69	124.59	128.60
35	E	1615	A	C4-C5-C6	6.69	120.34	117.00
35	E	1768	A	C5-C6-N1	-6.68	114.36	117.70
35	E	1924	G	C5-C6-O6	-6.68	124.59	128.60
35	E	461	C	N3-C4-N4	6.68	122.68	118.00
35	E	1741	G	C5-C6-O6	-6.68	124.59	128.60
35	E	2020	G	C5-C6-O6	-6.68	124.59	128.60
35	E	591	G	O4'-C1'-N9	6.68	113.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1805	G	C5-C6-O6	-6.68	124.59	128.60
35	E	1930	U	O4'-C1'-N1	6.68	113.54	108.20
35	E	1995	G	C5-C6-O6	-6.68	124.59	128.60
35	E	2106	G	C5-C6-O6	-6.68	124.59	128.60
35	E	2311	G	C5-C6-O6	-6.67	124.60	128.60
35	E	69	C	N3-C4-N4	6.67	122.67	118.00
35	E	70	U	O4'-C1'-N1	6.67	113.54	108.20
35	E	359	U	O4'-C1'-N1	6.67	113.54	108.20
35	E	768	G	C5-C6-O6	-6.67	124.60	128.60
35	E	991	C	O4'-C1'-N1	6.67	113.53	108.20
35	E	2307	G	C5-C6-O6	-6.67	124.60	128.60
35	E	759	C	N3-C4-C5	-6.67	119.23	121.90
35	E	849	U	O4'-C1'-N1	6.67	113.53	108.20
35	E	982	G	C5-C6-O6	-6.67	124.60	128.60
35	E	224	C	N3-C4-N4	6.67	122.67	118.00
35	E	236	C	N3-C4-N4	6.66	122.67	118.00
35	E	1328	A	C4-C5-C6	6.66	120.33	117.00
35	E	496	U	O4'-C1'-N1	6.66	113.53	108.20
35	E	1967	U	O4'-C1'-N1	6.66	113.53	108.20
35	E	213	G	C5-C6-O6	-6.66	124.61	128.60
35	E	1334	U	O4'-C1'-N1	6.66	113.53	108.20
35	E	1612	U	O4'-C1'-N1	6.66	113.53	108.20
35	E	1759	G	C5-C6-O6	-6.66	124.60	128.60
35	E	593	G	C5-C6-O6	-6.66	124.61	128.60
35	E	602	G	C5-C6-O6	-6.66	124.61	128.60
35	E	808	G	C5-C6-O6	-6.66	124.61	128.60
35	E	1276	G	C5-C6-O6	-6.66	124.61	128.60
35	E	2269	G	C5-C6-O6	-6.66	124.61	128.60
35	E	2293	U	O4'-C1'-N1	6.66	113.52	108.20
35	E	1	G	O4'-C1'-N9	6.65	113.52	108.20
35	E	591	G	C5-C6-O6	-6.65	124.61	128.60
35	E	920	A	C5-C6-N6	-6.65	118.38	123.70
35	E	1174	C	O4'-C1'-N1	6.65	113.52	108.20
35	E	1214	G	C5-C6-O6	-6.65	124.61	128.60
35	E	1923	U	O4'-C1'-N1	6.65	113.52	108.20
35	E	1980	C	N3-C4-N4	6.65	122.66	118.00
35	E	634	A	C5-C6-N6	-6.65	118.38	123.70
35	E	857	G	O4'-C1'-N9	6.65	113.52	108.20
35	E	181	A	C4-C5-C6	6.65	120.32	117.00
35	E	1603	U	O4'-C1'-N1	6.64	113.51	108.20
35	E	609	A	C4-C5-C6	6.64	120.32	117.00
35	E	634	A	C4-C5-C6	6.64	120.32	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	140	C	O4'-C1'-N1	6.64	113.51	108.20
35	E	2134	A	C4-C5-C6	6.64	120.32	117.00
35	E	1278	C	N3-C4-N4	6.63	122.64	118.00
35	E	216	A	O4'-C1'-N9	6.63	113.51	108.20
35	E	583	C	O4'-C1'-N1	6.63	113.51	108.20
35	E	726	C	N3-C4-C5	-6.63	119.25	121.90
35	E	701	C	O4'-C1'-N1	6.63	113.50	108.20
35	E	368	G	C5-C6-O6	-6.63	124.62	128.60
35	E	805	C	O4'-C1'-N1	6.63	113.50	108.20
35	E	1198	G	O4'-C1'-N9	6.63	113.50	108.20
35	E	1567	C	N3-C4-N4	6.63	122.64	118.00
35	E	834	G	O4'-C1'-N9	6.63	113.50	108.20
35	E	868	U	O4'-C1'-N1	6.63	113.50	108.20
35	E	1534	A	C5-C6-N1	-6.63	114.39	117.70
35	E	1582	G	C5-C6-O6	-6.63	124.62	128.60
35	E	1590	G	C5-C6-O6	-6.63	124.62	128.60
35	E	2305	C	O4'-C1'-N1	6.63	113.50	108.20
35	E	375	C	N3-C4-N4	6.62	122.64	118.00
35	E	1682	U	O4'-C1'-N1	6.62	113.50	108.20
35	E	2179	G	C5-C6-O6	-6.62	124.63	128.60
35	E	1272	C	N3-C4-N4	6.62	122.63	118.00
35	E	25	C	O4'-C1'-N1	6.62	113.50	108.20
35	E	1583	U	O4'-C1'-N1	6.62	113.50	108.20
35	E	1767	G	C5-C6-O6	-6.62	124.63	128.60
35	E	901	A	O4'-C1'-N9	6.62	113.49	108.20
35	E	1200	A	C5-C6-N6	-6.62	118.41	123.70
35	E	1551	G	C5-C6-O6	-6.62	124.63	128.60
35	E	1738	G	C5-C6-O6	-6.62	124.63	128.60
35	E	937	C	O4'-C1'-N1	6.61	113.49	108.20
35	E	965	C	N3-C4-N4	6.61	122.63	118.00
35	E	1989	G	C5-C6-O6	-6.61	124.63	128.60
35	E	2188	G	C5-C6-O6	-6.61	124.63	128.60
35	E	237	A	O4'-C1'-N9	6.61	113.49	108.20
35	E	691	U	O4'-C1'-N1	6.61	113.49	108.20
35	E	1799	A	C4-C5-C6	6.61	120.30	117.00
35	E	1868	G	O4'-C1'-N9	6.61	113.48	108.20
35	E	2316	U	O4'-C1'-N1	6.61	113.48	108.20
35	E	2204	A	C4-C5-C6	6.60	120.30	117.00
35	E	411	G	C5-C6-O6	-6.60	124.64	128.60
35	E	1545	U	O4'-C1'-N1	6.60	113.48	108.20
35	E	1643	U	O4'-C1'-N1	6.60	113.48	108.20
35	E	2054	G	C5-C6-O6	-6.60	124.64	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	418	G	C5-C6-O6	-6.60	124.64	128.60
35	E	1318	U	O4'-C1'-N1	6.60	113.48	108.20
35	E	2092	A	C5-C6-N6	-6.60	118.42	123.70
35	E	524	G	O4'-C1'-N9	6.60	113.48	108.20
35	E	749	C	N3-C4-C5	-6.60	119.26	121.90
35	E	1276	G	O4'-C1'-N9	6.60	113.48	108.20
35	E	1659	U	O4'-C1'-N1	6.60	113.48	108.20
35	E	1688	C	O4'-C1'-N1	6.60	113.48	108.20
35	E	2147	U	C2-N1-C1'	6.60	125.62	117.70
35	E	843	U	O4'-C1'-N1	6.60	113.48	108.20
35	E	24	U	O4'-C1'-N1	6.59	113.47	108.20
35	E	1858	U	O4'-C1'-N1	6.59	113.47	108.20
35	E	80	G	C5-C6-O6	-6.59	124.64	128.60
35	E	734	G	C6-C5-N7	-6.59	126.44	130.40
35	E	2249	A	C4-C5-C6	6.59	120.30	117.00
35	E	218	C	N3-C4-N4	6.59	122.61	118.00
35	E	462	U	O4'-C1'-N1	6.59	113.47	108.20
35	E	2014	C	O4'-C1'-N1	6.59	113.47	108.20
35	E	2166	C	O4'-C1'-N1	6.59	113.47	108.20
35	E	1804	A	C5-C6-N6	-6.58	118.43	123.70
35	E	114	C	N3-C4-N4	6.58	122.61	118.00
35	E	650	C	N3-C4-N4	6.58	122.61	118.00
35	E	856	U	O4'-C1'-N1	6.58	113.47	108.20
35	E	1831	C	O4'-C1'-N1	6.58	113.47	108.20
35	E	685	G	C5-C6-O6	-6.58	124.65	128.60
35	E	1587	U	O4'-C1'-N1	6.58	113.46	108.20
35	E	2022	A	C5-C6-N6	-6.58	118.44	123.70
35	E	119	G	C5-C6-O6	-6.58	124.65	128.60
35	E	1300	C	N3-C4-C5	-6.58	119.27	121.90
35	E	87	C	N3-C4-N4	6.58	122.60	118.00
35	E	1647	G	C5-C6-O6	-6.58	124.65	128.60
35	E	1873	G	C6-N1-C2	-6.58	121.15	125.10
35	E	2079	G	C5-C6-O6	-6.58	124.65	128.60
35	E	743	C	O4'-C1'-N1	6.57	113.46	108.20
35	E	1848	U	O4'-C1'-N1	6.57	113.46	108.20
35	E	831	A	C4-C5-C6	6.57	120.28	117.00
35	E	1669	G	N1-C6-O6	6.57	123.84	119.90
35	E	832	G	C5-C6-O6	-6.57	124.66	128.60
35	E	1704	A	C5-C6-N6	-6.57	118.45	123.70
35	E	1709	G	C5-C6-O6	-6.57	124.66	128.60
35	E	1964	U	O4'-C1'-N1	6.57	113.45	108.20
35	E	560	C	N3-C4-N4	6.56	122.59	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	996	G	O4'-C1'-N9	6.56	113.45	108.20
35	E	1166	C	N3-C4-N4	6.56	122.59	118.00
35	E	1199	G	C5-C6-O6	-6.56	124.66	128.60
35	E	957	U	O4'-C1'-N1	6.56	113.45	108.20
35	E	1885	U	O4'-C1'-N1	6.56	113.45	108.20
35	E	1969	G	O4'-C1'-N9	6.56	113.45	108.20
35	E	1986	A	C5-C6-N6	-6.56	118.45	123.70
35	E	884	A	C4-C5-C6	6.55	120.28	117.00
35	E	2068	C	O4'-C1'-N1	6.55	113.44	108.20
35	E	778	A	C4-C5-C6	6.55	120.28	117.00
35	E	862	A	O4'-C1'-N9	6.55	113.44	108.20
35	E	985	G	C5-C6-O6	-6.55	124.67	128.60
35	E	1646	G	C5-C6-O6	-6.55	124.67	128.60
35	E	226	A	C5-C6-N6	-6.55	118.46	123.70
35	E	338	U	O4'-C1'-N1	6.55	113.44	108.20
35	E	18	C	N3-C4-N4	6.55	122.58	118.00
35	E	483	A	C5-C6-N6	-6.55	118.46	123.70
35	E	2142	C	N3-C4-N4	6.55	122.58	118.00
35	E	774	C	N3-C4-N4	6.54	122.58	118.00
35	E	815	G	C5-C6-O6	-6.54	124.67	128.60
35	E	820	U	O4'-C1'-N1	6.54	113.43	108.20
35	E	863	A	C4-C5-C6	6.54	120.27	117.00
35	E	1860	U	O4'-C1'-N1	6.54	113.43	108.20
35	E	47	A	C4-C5-C6	6.54	120.27	117.00
35	E	603	G	C5-C6-O6	-6.54	124.68	128.60
35	E	1801	C	O4'-C1'-N1	6.54	113.43	108.20
35	E	1802	C	O4'-C1'-N1	6.54	113.43	108.20
35	E	828	G	C5-C6-O6	-6.53	124.68	128.60
35	E	847	U	O4'-C1'-N1	6.53	113.42	108.20
35	E	596	A	O4'-C1'-N9	6.53	113.42	108.20
35	E	708	G	C5-C6-O6	-6.53	124.68	128.60
35	E	1249	G	C5-C6-O6	-6.53	124.68	128.60
35	E	1790	A	C4-C5-C6	6.53	120.27	117.00
35	E	2232	U	O4'-C1'-N1	6.53	113.42	108.20
35	E	198	U	O4'-C1'-N1	6.53	113.42	108.20
35	E	445	G	C5-C6-O6	-6.53	124.68	128.60
35	E	2248	G	C5-C6-O6	-6.53	124.68	128.60
35	E	2317	U	O4'-C1'-N1	6.53	113.42	108.20
35	E	851	U	O4'-C1'-N1	6.53	113.42	108.20
35	E	1570	U	O4'-C1'-N1	6.52	113.42	108.20
35	E	2096	G	C5-C6-O6	-6.52	124.69	128.60
35	E	222	U	O4'-C1'-N1	6.52	113.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	804	U	O4'-C1'-N1	6.52	113.42	108.20
35	E	1593	A	C5-C6-N1	-6.52	114.44	117.70
35	E	2153	C	O4'-C1'-N1	6.52	113.42	108.20
35	E	489	C	N3-C4-N4	6.52	122.56	118.00
35	E	226	A	C4-C5-C6	6.52	120.26	117.00
35	E	954	G	C5-C6-O6	-6.52	124.69	128.60
35	E	1239	G	C5-C6-O6	-6.52	124.69	128.60
35	E	1637	G	C5-C6-O6	-6.52	124.69	128.60
35	E	2036	A	C4-C5-C6	6.52	120.26	117.00
35	E	2215	C	N3-C4-N4	6.52	122.56	118.00
35	E	1192	A	C4-C5-C6	6.52	120.26	117.00
35	E	1918	C	N3-C4-N4	6.52	122.56	118.00
35	E	1925	A	C5-C6-N6	-6.51	118.49	123.70
35	E	677	G	C5-C6-O6	-6.51	124.69	128.60
35	E	219	U	O4'-C1'-N1	6.51	113.41	108.20
35	E	1941	C	O4'-C1'-N1	6.51	113.41	108.20
35	E	2095	G	C5-C6-O6	-6.51	124.69	128.60
35	E	761	G	C5-C6-O6	-6.51	124.70	128.60
35	E	1852	G	O4'-C1'-N9	6.51	113.41	108.20
35	E	1882	G	C5-C6-O6	-6.51	124.70	128.60
35	E	1218	A	C5-C6-N6	-6.50	118.50	123.70
35	E	2051	C	N3-C4-N4	6.50	122.55	118.00
35	E	665	U	O4'-C1'-N1	6.50	113.40	108.20
35	E	1177	C	P-O3'-C3'	6.50	127.50	119.70
35	E	1212	G	C5-C6-O6	-6.50	124.70	128.60
35	E	2081	G	C5-C6-O6	-6.50	124.70	128.60
35	E	881	G	C5-C6-O6	-6.50	124.70	128.60
35	E	340	U	O4'-C1'-N1	6.50	113.40	108.20
35	E	1822	A	C4-C5-C6	6.50	120.25	117.00
35	E	558	U	O4'-C1'-N1	6.50	113.40	108.20
35	E	1553	A	C4-C5-C6	6.50	120.25	117.00
35	E	21	U	O4'-C1'-N1	6.50	113.40	108.20
35	E	577	A	C4-C5-C6	6.49	120.25	117.00
35	E	1364	G	O4'-C1'-N9	6.49	113.39	108.20
35	E	696	G	C5-C6-O6	-6.49	124.71	128.60
35	E	2055	A	C4-C5-C6	6.49	120.25	117.00
35	E	2144	G	N3-C2-N2	6.49	124.44	119.90
35	E	209	C	N3-C4-N4	6.49	122.54	118.00
35	E	1711	G	C5-C6-O6	-6.49	124.71	128.60
35	E	2024	C	O4'-C1'-N1	6.49	113.39	108.20
35	E	17	C	N3-C4-N4	6.49	122.54	118.00
35	E	660	U	O4'-C1'-N1	6.49	113.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1525	C	O4'-C1'-N1	6.49	113.39	108.20
35	E	1615	A	C5-C6-N6	-6.49	118.51	123.70
35	E	1270	A	C4-C5-C6	6.48	120.24	117.00
35	E	1604	U	O4'-C1'-N1	6.48	113.39	108.20
35	E	243	U	O4'-C1'-N1	6.48	113.39	108.20
35	E	333	C	N3-C4-N4	6.48	122.54	118.00
35	E	477	G	O4'-C1'-N9	6.48	113.39	108.20
35	E	510	U	O4'-C1'-N1	6.48	113.38	108.20
35	E	929	U	O4'-C1'-N1	6.48	113.38	108.20
35	E	1323	A	C4-C5-C6	6.48	120.24	117.00
35	E	1664	A	C4-C5-C6	6.48	120.24	117.00
35	E	2043	G	O4'-C1'-N9	6.48	113.38	108.20
35	E	2132	U	O4'-C1'-N1	6.48	113.38	108.20
35	E	251	A	O4'-C1'-N9	6.48	113.38	108.20
35	E	1350	U	O4'-C1'-N1	6.48	113.38	108.20
35	E	1704	A	C4-C5-C6	6.48	120.24	117.00
35	E	82	A	O4'-C1'-N9	6.47	113.38	108.20
35	E	1625	A	C4-C5-C6	6.47	120.24	117.00
35	E	1850	C	N3-C4-N4	6.47	122.53	118.00
35	E	1934	G	C5-C6-O6	-6.47	124.72	128.60
35	E	748	G	P-O3'-C3'	6.47	127.47	119.70
35	E	1271	G	C5-C6-O6	-6.47	124.72	128.60
35	E	1865	A	C4-C5-C6	6.47	120.24	117.00
35	E	2099	G	O4'-C1'-N9	6.47	113.38	108.20
35	E	1945	U	O4'-C1'-N1	6.47	113.38	108.20
35	E	2268	A	C5-C6-N6	-6.47	118.52	123.70
35	E	1327	A	C5-C6-N1	-6.47	114.47	117.70
35	E	499	A	C4-C5-C6	6.47	120.23	117.00
35	E	2223	U	O4'-C1'-N1	6.47	113.37	108.20
35	E	722	C	N3-C4-N4	6.46	122.53	118.00
35	E	2076	A	C4-C5-C6	6.46	120.23	117.00
35	E	83	U	O4'-C1'-N1	6.46	113.37	108.20
35	E	278	A	C5-C6-N6	-6.46	118.53	123.70
35	E	540	U	O4'-C1'-N1	6.46	113.37	108.20
35	E	1809	C	N3-C4-N4	6.46	122.52	118.00
35	E	44	C	O4'-C1'-N1	6.46	113.36	108.20
35	E	483	A	C4-C5-C6	6.46	120.23	117.00
35	E	1642	G	C5-C6-O6	-6.46	124.73	128.60
35	E	611	G	O4'-C1'-N9	6.45	113.36	108.20
35	E	715	U	O4'-C1'-N1	6.45	113.36	108.20
35	E	1761	U	O4'-C1'-N1	6.45	113.36	108.20
35	E	2231	U	O4'-C1'-N1	6.45	113.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1259	A	C5-C6-N1	-6.45	114.47	117.70
35	E	294	G	C5-C6-O6	-6.45	124.73	128.60
35	E	1544	U	P-O3'-C3'	6.45	127.44	119.70
35	E	1866	A	C5-C6-N1	-6.45	114.47	117.70
35	E	1890	C	N3-C4-N4	6.45	122.52	118.00
35	E	279	A	C4-C5-C6	6.45	120.22	117.00
35	E	390	C	N3-C4-N4	6.45	122.51	118.00
35	E	1363	C	O4'-C1'-N1	6.45	113.36	108.20
35	E	1708	U	O4'-C1'-N1	6.45	113.36	108.20
35	E	2126	A	C4-C5-C6	6.45	120.22	117.00
35	E	695	G	C5-C6-O6	-6.45	124.73	128.60
35	E	1262	C	N3-C4-N4	6.45	122.51	118.00
35	E	183	C	O4'-C1'-N1	6.45	113.36	108.20
35	E	1541	U	O4'-C1'-N1	6.45	113.36	108.20
35	E	2125	C	N3-C4-N4	6.45	122.51	118.00
35	E	2288	A	C5-C6-N6	-6.45	118.54	123.70
5	u	84	PHE	CB-CG-CD1	6.44	125.31	120.80
35	E	1732	A	C4-C5-C6	6.44	120.22	117.00
35	E	264	C	N3-C4-C5	-6.44	119.32	121.90
35	E	2048	A	C4-C5-C6	6.44	120.22	117.00
35	E	940	U	O4'-C1'-N1	6.44	113.35	108.20
35	E	1343	A	C4-C5-C6	6.44	120.22	117.00
35	E	682	G	C5-C6-O6	-6.44	124.74	128.60
35	E	769	A	C4-C5-C6	6.44	120.22	117.00
35	E	1167	C	O4'-C1'-N1	6.44	113.35	108.20
35	E	1537	U	O4'-C1'-N1	6.44	113.35	108.20
35	E	206	C	N3-C4-N4	6.44	122.50	118.00
35	E	1078	U	P-O3'-C3'	6.44	127.42	119.70
35	E	1168	U	O4'-C1'-N1	6.44	113.35	108.20
35	E	1250	A	C4-C5-C6	6.44	120.22	117.00
35	E	754	G	C5-C6-O6	-6.43	124.74	128.60
35	E	1988	U	O4'-C1'-N1	6.43	113.34	108.20
35	E	2152	C	N3-C4-N4	6.43	122.50	118.00
35	E	519	G	C5-C6-O6	-6.43	124.74	128.60
35	E	739	G	C5-C6-O6	-6.43	124.74	128.60
35	E	923	A	C5-C6-N6	-6.43	118.56	123.70
35	E	1197	A	C4-C5-C6	6.43	120.22	117.00
35	E	453	U	O4'-C1'-N1	6.43	113.34	108.20
35	E	756	G	O4'-C1'-N9	6.43	113.34	108.20
35	E	257	A	C4-C5-C6	6.42	120.21	117.00
35	E	1376	G	C5-C6-O6	-6.42	124.75	128.60
35	E	271	C	N3-C4-N4	6.42	122.50	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	989	G	C5-C6-O6	-6.42	124.75	128.60
35	E	1921	G	O4'-C1'-N9	6.42	113.34	108.20
35	E	9	U	O4'-C1'-N1	6.42	113.34	108.20
35	E	96	C	N3-C4-N4	6.42	122.50	118.00
35	E	1186	U	O4'-C1'-N1	6.42	113.34	108.20
35	E	1965	U	O4'-C1'-N1	6.42	113.34	108.20
35	E	2251	A	C5-C6-N6	-6.42	118.56	123.70
35	E	1351	C	N3-C4-N4	6.42	122.49	118.00
35	E	1360	A	C4-C5-C6	6.42	120.21	117.00
35	E	2277	C	N3-C4-N4	6.42	122.49	118.00
35	E	1524	U	O4'-C1'-N1	6.42	113.33	108.20
35	E	2052	C	C1'-O4'-C4'	-6.42	104.77	109.90
35	E	328	U	O4'-C1'-N1	6.42	113.33	108.20
35	E	1952	U	O4'-C1'-N1	6.42	113.33	108.20
35	E	1748	C	N3-C4-N4	6.41	122.49	118.00
35	E	1821	C	O4'-C1'-N1	6.41	113.33	108.20
35	E	105	A	C4-C5-C6	6.41	120.20	117.00
35	E	521	A	C4-C5-C6	6.41	120.20	117.00
35	E	2218	U	O4'-C1'-N1	6.41	113.33	108.20
35	E	2281	A	C5-C6-N6	-6.41	118.57	123.70
35	E	1074	C	N3-C4-N4	6.41	122.49	118.00
35	E	1676	A	C4-C5-C6	6.41	120.20	117.00
35	E	2306	A	C4-C5-C6	6.41	120.20	117.00
35	E	1797	A	C4-C5-C6	6.41	120.20	117.00
35	E	2003	G	C5-C6-O6	-6.41	124.76	128.60
35	E	73	A	C5-C6-N6	-6.40	118.58	123.70
35	E	81	A	C4-C5-C6	6.40	120.20	117.00
35	E	284	C	O4'-C1'-N1	6.40	113.32	108.20
35	E	689	A	C4-C5-C6	6.40	120.20	117.00
35	E	699	C	N3-C4-N4	6.40	122.48	118.00
35	E	337	G	C5-C6-O6	-6.40	124.76	128.60
35	E	1974	C	C6-N1-C1'	-6.40	113.12	120.80
35	E	371	A	C4-C5-C6	6.40	120.20	117.00
35	E	1927	A	C4-C5-C6	6.40	120.20	117.00
35	E	1078	U	O4'-C1'-N1	6.39	113.32	108.20
35	E	738	G	N1-C2-N3	-6.39	120.06	123.90
35	E	1649	U	O4'-C1'-N1	6.39	113.31	108.20
35	E	2077	C	O4'-C1'-N1	6.39	113.31	108.20
35	E	2114	U	C6-N1-C1'	-6.39	112.25	121.20
35	E	568	G	O4'-C1'-N9	6.39	113.31	108.20
35	E	1601	A	C4-C5-C6	6.39	120.20	117.00
35	E	2035	A	C4-C5-C6	6.39	120.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1171	C	N3-C4-N4	6.39	122.47	118.00
35	E	1261	A	C5-C6-N6	-6.39	118.59	123.70
35	E	1374	A	C5-C6-N6	-6.39	118.59	123.70
35	E	2164	U	O4'-C1'-N1	6.39	113.31	108.20
35	E	307	C	O4'-C1'-N1	6.39	113.31	108.20
35	E	538	A	C5-C6-N6	-6.39	118.59	123.70
35	E	1962	U	O4'-C1'-N1	6.39	113.31	108.20
35	E	875	A	C4-C5-C6	6.39	120.19	117.00
35	E	1554	A	C5-C6-N6	-6.39	118.59	123.70
35	E	2150	G	O4'-C1'-N9	6.39	113.31	108.20
35	E	2286	G	C5-C6-O6	-6.39	124.77	128.60
35	E	711	A	O3'-P-O5'	-6.38	91.87	104.00
35	E	1790	A	C5-C6-N6	-6.38	118.59	123.70
35	E	776	G	P-O5'-C5'	6.38	131.11	120.90
35	E	713	G	O4'-C1'-N9	6.38	113.31	108.20
35	E	1785	C	N3-C4-N4	6.38	122.47	118.00
35	E	1374	A	C4-C5-C6	6.38	120.19	117.00
35	E	1732	A	C5-C6-N6	-6.38	118.60	123.70
35	E	672	U	O4'-C1'-N1	6.38	113.30	108.20
35	E	744	C	C6-N1-C2	-6.38	117.75	120.30
35	E	526	A	C5-C6-N6	-6.38	118.60	123.70
35	E	641	C	N3-C4-N4	6.38	122.46	118.00
35	E	1870	G	O4'-C1'-N9	6.38	113.30	108.20
35	E	476	G	C5-C6-O6	-6.37	124.78	128.60
35	E	589	U	O4'-C1'-N1	6.37	113.30	108.20
35	E	1533	U	O4'-C1'-N1	6.37	113.30	108.20
35	E	2279	U	O4'-C1'-N1	6.37	113.30	108.20
25	i	116	PHE	CB-CG-CD2	-6.37	116.34	120.80
35	E	1527	G	C5-C6-O6	-6.37	124.78	128.60
35	E	100	A	C4-C5-C6	6.37	120.18	117.00
35	E	468	G	C5-C6-O6	-6.37	124.78	128.60
35	E	484	A	C4-C5-C6	6.37	120.18	117.00
35	E	2001	A	C5-C6-N6	-6.37	118.61	123.70
1	p	105	PHE	CB-CG-CD2	6.36	125.25	120.80
35	E	2214	A	C4-C5-C6	6.36	120.18	117.00
35	E	131	C	N3-C4-N4	6.36	122.45	118.00
35	E	285	A	O4'-C1'-N9	6.36	113.29	108.20
35	E	423	C	N3-C4-N4	6.36	122.45	118.00
35	E	2083	A	C4-C5-C6	6.36	120.18	117.00
35	E	502	A	C4-C5-C6	6.36	120.18	117.00
35	E	1244	U	O4'-C1'-N1	6.36	113.29	108.20
35	E	1734	U	O4'-C1'-N1	6.36	113.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1775	U	C2-N1-C1'	6.36	125.33	117.70
35	E	1887	U	C3'-C2'-C1'	6.36	106.59	101.50
35	E	576	A	C4-C5-C6	6.36	120.18	117.00
35	E	2022	A	C4-C5-C6	6.36	120.18	117.00
35	E	2040	G	C5-C6-O6	-6.36	124.78	128.60
35	E	537	C	N3-C4-N4	6.36	122.45	118.00
35	E	1201	G	C5-C6-O6	-6.36	124.79	128.60
35	E	1282	C	N3-C4-N4	6.36	122.45	118.00
35	E	2004	A	C5-C6-N6	-6.36	118.61	123.70
35	E	525	A	C4-C5-C6	6.35	120.18	117.00
35	E	2042	G	C5-C6-O6	-6.35	124.79	128.60
35	E	1179	C	N3-C4-C5	-6.35	119.36	121.90
35	E	1689	A	C4-C5-C6	6.35	120.18	117.00
35	E	2246	C	N3-C4-N4	6.35	122.45	118.00
35	E	447	A	C4-C5-C6	6.35	120.17	117.00
35	E	105	A	C5-C6-N6	-6.35	118.62	123.70
35	E	225	C	N3-C4-N4	6.35	122.44	118.00
35	E	153	C	N3-C4-N4	6.34	122.44	118.00
35	E	515	C	N3-C4-N4	6.34	122.44	118.00
35	E	151	A	O4'-C1'-N9	6.34	113.27	108.20
35	E	1248	A	C4-C5-C6	6.34	120.17	117.00
35	E	527	A	C4-C5-C6	6.34	120.17	117.00
35	E	626	C	N3-C4-N4	6.34	122.44	118.00
35	E	1815	A	C4-C5-C6	6.34	120.17	117.00
35	E	721	C	N3-C4-N4	6.34	122.44	118.00
35	E	1787	U	O4'-C1'-N1	6.34	113.27	108.20
35	E	1940	G	O4'-C1'-N9	6.34	113.27	108.20
35	E	920	A	C4-C5-C6	6.34	120.17	117.00
35	E	191	U	O4'-C1'-N1	6.34	113.27	108.20
35	E	278	A	C4-C5-C6	6.34	120.17	117.00
35	E	774	C	N3-C4-C5	-6.34	119.37	121.90
35	E	1321	G	O4'-C1'-N9	6.34	113.27	108.20
35	E	1611	A	C4-C5-C6	6.33	120.17	117.00
35	E	19	A	O4'-C1'-N9	6.33	113.27	108.20
35	E	1336	A	C5-C6-N6	-6.33	118.63	123.70
35	E	1751	U	O4'-C1'-N1	6.33	113.27	108.20
35	E	2020	G	P-O3'-C3'	6.33	127.30	119.70
35	E	2294	A	C4-C5-C6	6.33	120.17	117.00
35	E	867	G	C5-C6-O6	-6.33	124.80	128.60
35	E	1986	A	C4-C5-C6	6.33	120.17	117.00
35	E	82	A	C4-C5-C6	6.33	120.17	117.00
35	E	1242	A	C4-C5-C6	6.33	120.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1792	G	C5-C6-O6	-6.33	124.80	128.60
35	E	732	C	O4'-C1'-N1	6.33	113.26	108.20
35	E	1207	U	O4'-C1'-N1	6.33	113.26	108.20
35	E	1791	C	N3-C4-N4	6.33	122.43	118.00
35	E	2077	C	N3-C4-N4	6.33	122.43	118.00
35	E	864	A	C5-C6-N6	-6.33	118.64	123.70
35	E	1359	C	O4'-C1'-N1	6.33	113.26	108.20
35	E	2301	C	N3-C4-N4	6.33	122.43	118.00
35	E	381	A	C4-C5-C6	6.33	120.16	117.00
35	E	437	G	C5-C6-O6	-6.33	124.81	128.60
35	E	1319	G	O4'-C1'-N9	6.33	113.26	108.20
35	E	2008	A	C4-C5-C6	6.33	120.16	117.00
35	E	927	U	O4'-C1'-N1	6.32	113.26	108.20
35	E	1293	C	N3-C4-N4	6.32	122.42	118.00
35	E	935	A	C4-C5-C6	6.32	120.16	117.00
35	E	1320	G	O4'-C1'-N9	6.32	113.26	108.20
35	E	1903	A	C5'-C4'-C3'	6.32	126.11	116.00
35	E	2024	C	N3-C4-N4	6.32	122.42	118.00
35	E	506	A	C4-C5-C6	6.32	120.16	117.00
35	E	1638	G	C5-C6-O6	-6.32	124.81	128.60
35	E	2110	A	C4-C5-C6	6.32	120.16	117.00
35	E	130	G	O4'-C1'-N9	6.32	113.25	108.20
35	E	480	C	N3-C4-N4	6.32	122.42	118.00
35	E	936	C	N3-C4-N4	6.32	122.42	118.00
35	E	1330	A	C4-C5-C6	6.32	120.16	117.00
35	E	221	C	N3-C4-N4	6.32	122.42	118.00
35	E	586	A	C4-C5-C6	6.32	120.16	117.00
35	E	1187	C	O3'-P-O5'	6.32	116.00	104.00
35	E	933	C	N3-C4-N4	6.31	122.42	118.00
35	E	1202	G	C5-C6-O6	-6.31	124.81	128.60
35	E	1273	G	C5-C6-O6	-6.31	124.81	128.60
35	E	2255	C	N3-C4-N4	6.31	122.42	118.00
35	E	1	G	C5-C6-O6	-6.31	124.81	128.60
35	E	1707	U	O4'-C1'-N1	6.31	113.25	108.20
35	E	2148	A	O4'-C1'-N9	6.31	113.25	108.20
35	E	2191	G	C5-C6-O6	-6.31	124.81	128.60
35	E	1686	G	C5-C6-O6	-6.31	124.81	128.60
35	E	1294	C	N3-C4-N4	6.31	122.42	118.00
35	E	1560	G	C5-C6-O6	-6.31	124.81	128.60
35	E	1561	A	C4-C5-C6	6.31	120.15	117.00
35	E	996	G	P-O3'-C3'	-6.31	112.13	119.70
35	E	1269	C	N3-C4-N4	6.30	122.41	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1828	G	C5-C6-O6	-6.30	124.82	128.60
35	E	2239	A	C4-C5-C6	6.30	120.15	117.00
35	E	159	G	C5-C6-O6	-6.30	124.82	128.60
35	E	900	A	C4-C5-C6	6.30	120.15	117.00
35	E	1534	A	C5-C6-N6	-6.30	118.66	123.70
35	E	2234	A	O4'-C1'-N9	6.30	113.24	108.20
35	E	144	A	C4-C5-C6	6.30	120.15	117.00
35	E	984	A	O4'-C1'-N9	6.30	113.24	108.20
35	E	2258	C	N3-C4-N4	6.30	122.41	118.00
35	E	2115	C	N3-C4-N4	6.29	122.41	118.00
35	E	312	C	N3-C4-N4	6.29	122.41	118.00
35	E	1225	G	O4'-C1'-N9	6.29	113.23	108.20
35	E	2058	C	N3-C4-N4	6.29	122.41	118.00
35	E	454	A	C5-C6-N1	-6.29	114.55	117.70
35	E	1706	A	C5-C6-N1	-6.29	114.56	117.70
35	E	1703	C	N3-C4-N4	6.29	122.40	118.00
35	E	1958	U	O4'-C1'-N1	6.29	113.23	108.20
35	E	509	A	C4-C5-C6	6.29	120.14	117.00
35	E	1189	A	C4-C5-C6	6.29	120.14	117.00
35	E	1568	A	C4-C5-C6	6.29	120.14	117.00
35	E	1937	A	C4-C5-C6	6.29	120.14	117.00
35	E	264	C	N3-C4-N4	6.29	122.40	118.00
35	E	647	A	C5-C6-N6	-6.29	118.67	123.70
35	E	68	A	C4-C5-C6	6.28	120.14	117.00
35	E	548	C	N3-C4-N4	6.28	122.40	118.00
35	E	674	A	C4-C5-C6	6.28	120.14	117.00
35	E	2129	U	O4'-C1'-N1	6.28	113.23	108.20
35	E	954	G	C5-C6-N1	-6.28	108.36	111.50
35	E	1878	A	C4-C5-C6	6.28	120.14	117.00
35	E	55	A	C4-C5-C6	6.28	120.14	117.00
35	E	873	C	C6-N1-C1'	-6.28	113.26	120.80
35	E	1190	G	C5-C6-O6	-6.28	124.83	128.60
35	E	2002	A	C5-C6-N6	-6.28	118.68	123.70
35	E	96	C	O4'-C1'-N1	6.28	113.22	108.20
35	E	261	A	O4'-C1'-N9	6.28	113.22	108.20
35	E	357	C	N3-C4-N4	6.28	122.39	118.00
35	E	2131	A	C4-C5-C6	6.28	120.14	117.00
35	E	2274	A	C4-C5-C6	6.28	120.14	117.00
35	E	161	A	C4-C5-C6	6.28	120.14	117.00
35	E	383	U	O4'-C1'-N1	6.28	113.22	108.20
35	E	1265	A	C4-C5-C6	6.28	120.14	117.00
35	E	2085	U	O4'-C1'-N1	6.28	113.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	358	C	N3-C4-N4	6.27	122.39	118.00
35	E	472	A	C5-C6-N6	-6.27	118.68	123.70
35	E	1960	A	C4-C5-C6	6.27	120.14	117.00
35	E	1552	A	C4-C5-C6	6.27	120.14	117.00
35	E	2124	G	C5-C6-O6	-6.27	124.84	128.60
35	E	1641	C	N3-C4-N4	6.27	122.39	118.00
35	E	1832	A	C4-C5-C6	6.27	120.14	117.00
35	E	43	A	C4-C5-C6	6.27	120.13	117.00
35	E	297	U	O4'-C1'-N1	6.27	113.21	108.20
35	E	784	A	C4-C5-C6	6.27	120.13	117.00
35	E	111	A	C5-C6-N6	-6.27	118.69	123.70
35	E	2245	A	C5-C6-N6	-6.27	118.69	123.70
35	E	232	C	N3-C4-N4	6.26	122.39	118.00
35	E	345	A	C4-C5-C6	6.26	120.13	117.00
35	E	596	A	C4-C5-C6	6.26	120.13	117.00
35	E	906	U	O4'-C1'-N1	6.26	113.21	108.20
35	E	1589	C	N3-C4-N4	6.26	122.39	118.00
35	E	2119	U	O4'-C1'-N1	6.26	113.21	108.20
35	E	2120	A	C4-C5-C6	6.26	120.13	117.00
35	E	62	A	C4-C5-C6	6.26	120.13	117.00
35	E	587	A	C4-C5-C6	6.26	120.13	117.00
35	E	49	C	N3-C4-N4	6.26	122.38	118.00
35	E	54	C	N3-C4-N4	6.26	122.38	118.00
35	E	239	C	N3-C4-N4	6.26	122.38	118.00
35	E	1223	C	N3-C4-N4	6.26	122.38	118.00
35	E	1596	G	C5-C6-O6	-6.26	124.84	128.60
5	u	84	PHE	CB-CG-CD2	-6.26	116.42	120.80
35	E	104	C	N3-C4-N4	6.26	122.38	118.00
35	E	373	G	C5-C6-O6	-6.26	124.85	128.60
35	E	735	A	C6-N1-C2	-6.26	114.85	118.60
35	E	1246	U	O4'-C1'-N1	6.26	113.21	108.20
35	E	1650	U	O4'-C1'-N1	6.26	113.21	108.20
35	E	1884	U	P-O3'-C3'	6.26	127.21	119.70
35	E	78	A	C4-C5-C6	6.25	120.13	117.00
35	E	251	A	C5-C6-N6	-6.25	118.70	123.70
35	E	1571	C	N3-C4-N4	6.25	122.38	118.00
35	E	1673	U	O4'-C1'-N1	6.25	113.20	108.20
35	E	1951	A	C5-C6-N6	-6.25	118.70	123.70
35	E	434	A	C5-C6-N6	-6.25	118.70	123.70
35	E	444	A	C4-C5-C6	6.25	120.13	117.00
35	E	833	A	C4-C5-C6	6.25	120.13	117.00
35	E	1611	A	C5-C6-N1	-6.25	114.58	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1939	A	C4-C5-C6	6.25	120.12	117.00
35	E	2137	C	N3-C4-N4	6.25	122.38	118.00
35	E	216	A	C4-C5-C6	6.25	120.12	117.00
35	E	478	C	N3-C4-N4	6.25	122.37	118.00
35	E	750	C	N3-C4-N4	6.25	122.37	118.00
35	E	1532	U	O4'-C1'-N1	6.25	113.20	108.20
35	E	1710	A	C4-C5-C6	6.25	120.12	117.00
35	E	1859	U	O4'-C1'-N1	6.25	113.20	108.20
35	E	2229	A	C4-C5-C6	6.25	120.12	117.00
35	E	1252	C	N3-C4-N4	6.24	122.37	118.00
35	E	1818	A	C5-C6-N1	-6.24	114.58	117.70
35	E	281	A	C4-C5-C6	6.24	120.12	117.00
35	E	2216	A	C5-C6-N1	-6.24	114.58	117.70
35	E	1310	C	N3-C4-N4	6.24	122.37	118.00
35	E	2186	C	N3-C4-N4	6.24	122.37	118.00
35	E	2238	A	C4-C5-C6	6.24	120.12	117.00
35	E	339	C	N3-C4-N4	6.24	122.37	118.00
35	E	386	A	C4-C5-C6	6.24	120.12	117.00
35	E	475	A	C5-C6-N6	-6.24	118.71	123.70
35	E	713	G	C5-C6-O6	-6.24	124.86	128.60
35	E	1360	A	C5-C6-N6	-6.23	118.71	123.70
35	E	2221	A	C5-C6-N6	-6.23	118.71	123.70
35	E	777	A	C4-C5-C6	6.23	120.12	117.00
35	E	1313	A	O4'-C1'-N9	6.23	113.19	108.20
35	E	1847	C	N3-C4-N4	6.23	122.36	118.00
35	E	235	C	N3-C4-N4	6.23	122.36	118.00
35	E	872	A	C4-C5-C6	6.23	120.11	117.00
35	E	1586	G	C5-C6-O6	-6.23	124.86	128.60
35	E	1196	A	C5-C6-N1	-6.23	114.59	117.70
35	E	1336	A	C4-C5-C6	6.22	120.11	117.00
35	E	2075	G	O4'-C1'-N9	6.22	113.18	108.20
35	E	501	A	C4-C5-C6	6.22	120.11	117.00
35	E	1585	C	N3-C4-N4	6.22	122.36	118.00
35	E	491	C	O4'-C1'-N1	6.22	113.18	108.20
35	E	166	C	N3-C4-N4	6.22	122.35	118.00
35	E	250	A	C4-C5-C6	6.22	120.11	117.00
35	E	1259	A	C4-C5-C6	6.22	120.11	117.00
35	E	2189	A	C5-C6-N1	-6.22	114.59	117.70
35	E	503	A	C4-C5-C6	6.22	120.11	117.00
35	E	808	G	O4'-C1'-N9	6.22	113.17	108.20
35	E	911	U	O4'-C1'-N1	6.22	113.17	108.20
35	E	1660	C	O4'-C1'-N1	6.22	113.17	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1861	A	C4-C5-C6	6.22	120.11	117.00
35	E	149	A	C4-C5-C6	6.21	120.11	117.00
35	E	840	C	N3-C4-N4	6.21	122.35	118.00
35	E	1549	G	O4'-C1'-N9	6.21	113.17	108.20
35	E	2	A	O4'-C1'-N9	6.21	113.17	108.20
35	E	1662	A	C4-C5-C6	6.21	120.11	117.00
35	E	658	A	C5-C6-N6	-6.21	118.73	123.70
35	E	894	A	C4-C5-C6	6.21	120.10	117.00
35	E	2199	A	C4-C5-C6	6.21	120.11	117.00
4	t	60	ALA	N-CA-CB	6.21	118.79	110.10
35	E	1193	A	C4-C5-C6	6.21	120.10	117.00
35	E	1305	A	C5-C6-N1	-6.21	114.60	117.70
35	E	64	A	C4-C5-C6	6.20	120.10	117.00
35	E	162	A	C5-C6-N1	-6.20	114.60	117.70
35	E	785	A	C4-C5-C6	6.20	120.10	117.00
35	E	1268	A	C5-C6-N6	-6.20	118.74	123.70
35	E	1865	A	C5-C6-N6	-6.20	118.74	123.70
35	E	504	A	C4-C5-C6	6.20	120.10	117.00
35	E	561	A	C4-C5-C6	6.20	120.10	117.00
35	E	457	A	C5-C6-N6	-6.20	118.74	123.70
35	E	705	G	O4'-C1'-N9	6.20	113.16	108.20
35	E	936	C	N3-C4-C5	-6.20	119.42	121.90
35	E	1286	A	C5-C6-N1	-6.20	114.60	117.70
35	E	1342	C	N3-C4-N4	6.20	122.34	118.00
35	E	1539	A	C4-C5-C6	6.20	120.10	117.00
35	E	588	A	C4-C5-C6	6.20	120.10	117.00
35	E	645	A	C4-C5-C6	6.20	120.10	117.00
35	E	658	A	C4-C5-C6	6.20	120.10	117.00
35	E	829	C	O4'-C1'-N1	6.20	113.16	108.20
35	E	959	A	C4-C5-C6	6.20	120.10	117.00
35	E	2182	G	O4'-C1'-N9	6.20	113.16	108.20
35	E	1825	A	C5-C6-N1	-6.20	114.60	117.70
35	E	381	A	C5-C6-N6	-6.20	118.74	123.70
35	E	694	A	C4-C5-C6	6.20	120.10	117.00
35	E	905	A	C5-C6-N1	-6.20	114.60	117.70
35	E	942	C	C6-N1-C1'	-6.20	113.36	120.80
35	E	2026	A	C4-C5-C6	6.20	120.10	117.00
35	E	759	C	N3-C4-N4	6.19	122.34	118.00
35	E	584	C	O4'-C1'-N1	6.19	113.15	108.20
35	E	932	G	O4'-C1'-N9	6.19	113.15	108.20
35	E	22	A	C4-C5-C6	6.19	120.10	117.00
35	E	125	A	C4-C5-C6	6.19	120.09	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	356	C	O4'-C1'-N1	6.19	113.15	108.20
35	E	562	A	C4-C5-C6	6.19	120.09	117.00
35	E	1309	A	C5-C6-N6	-6.19	118.75	123.70
35	E	1218	A	C4-C5-C6	6.19	120.09	117.00
35	E	295	A	C4-C5-C6	6.19	120.09	117.00
35	E	961	A	C4-C5-C6	6.19	120.09	117.00
35	E	2305	C	N3-C4-N4	6.19	122.33	118.00
35	E	872	A	C5-C6-N6	-6.19	118.75	123.70
35	E	1966	C	O4'-C1'-N1	6.19	113.15	108.20
35	E	972	A	C4-C5-C6	6.18	120.09	117.00
35	E	1241	A	C4-C5-C6	6.18	120.09	117.00
35	E	2178	C	N3-C4-N4	6.18	122.33	118.00
35	E	2315	A	C4-C5-C6	6.18	120.09	117.00
35	E	696	G	O4'-C1'-N9	6.18	113.14	108.20
35	E	741	G	C5-C6-O6	-6.18	124.89	128.60
35	E	1170	C	N3-C4-N4	6.18	122.33	118.00
35	E	210	A	C4-C5-C6	6.18	120.09	117.00
35	E	1609	A	C4-C5-C6	6.18	120.09	117.00
35	E	22	A	C5-C6-N6	-6.18	118.76	123.70
35	E	185	A	C4-C5-C6	6.18	120.09	117.00
35	E	2069	A	C4-C5-C6	6.18	120.09	117.00
35	E	14	C	N3-C4-N4	6.18	122.32	118.00
35	E	265	C	N3-C4-N4	6.18	122.32	118.00
35	E	425	A	C4-C5-C6	6.18	120.09	117.00
35	E	538	A	C4-C5-C6	6.18	120.09	117.00
35	E	863	A	C5-C6-N1	-6.18	114.61	117.70
35	E	1308	A	C4-C5-C6	6.18	120.09	117.00
35	E	1652	A	C5-C6-N6	-6.18	118.76	123.70
35	E	1973	A	C4-C5-C6	6.18	120.09	117.00
35	E	1258	A	C4-C5-C6	6.17	120.09	117.00
35	E	1681	A	C4-C5-C6	6.17	120.09	117.00
35	E	1795	C	N3-C4-N4	6.17	122.32	118.00
35	E	1312	A	C4-C5-C6	6.17	120.09	117.00
35	E	287	A	C4-C5-C6	6.17	120.08	117.00
35	E	1639	A	C4-C5-C6	6.17	120.09	117.00
35	E	2234	A	C5-C6-N6	-6.17	118.76	123.70
35	E	1702	A	C4-C5-C6	6.17	120.08	117.00
35	E	78	A	C5-C6-N6	-6.17	118.77	123.70
35	E	299	A	C4-C5-C6	6.17	120.08	117.00
35	E	450	A	C4-C5-C6	6.17	120.08	117.00
35	E	2128	C	N3-C4-C5	-6.17	119.43	121.90
35	E	1795	C	O4'-C1'-N1	6.17	113.13	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	595	A	C4-C5-C6	6.16	120.08	117.00
35	E	744	C	N3-C4-C5	-6.16	119.44	121.90
35	E	1235	A	C4-C5-C6	6.16	120.08	117.00
35	E	2289	G	O4'-C1'-N9	6.16	113.13	108.20
35	E	140	C	N3-C4-N4	6.16	122.31	118.00
35	E	251	A	C4-C5-C6	6.16	120.08	117.00
35	E	316	A	C4-C5-C6	6.16	120.08	117.00
4	t	122	TYR	CB-CG-CD2	-6.16	117.31	121.00
35	E	205	G	O4'-C1'-N9	6.16	113.13	108.20
35	E	503	A	O4'-C1'-N9	6.16	113.13	108.20
35	E	2290	C	N3-C4-N4	6.16	122.31	118.00
35	E	1799	A	C5-C6-N6	-6.16	118.78	123.70
35	E	429	C	N3-C4-N4	6.15	122.31	118.00
35	E	1779	U	O4'-C1'-N1	6.15	113.12	108.20
35	E	2157	C	N3-C4-N4	6.15	122.31	118.00
35	E	2266	G	O4'-C1'-N9	6.15	113.12	108.20
35	E	1197	A	O4'-C1'-N9	6.15	113.12	108.20
35	E	1314	A	C4-C5-C6	6.15	120.08	117.00
35	E	2206	G	O4'-C1'-N9	6.15	113.12	108.20
35	E	2282	C	N3-C4-N4	6.15	122.31	118.00
35	E	1088	A	C4-C5-C6	6.15	120.07	117.00
35	E	1302	A	C5-C6-N6	-6.15	118.78	123.70
35	E	2219	C	N3-C4-N4	6.15	122.30	118.00
35	E	926	C	N3-C4-N4	6.15	122.30	118.00
35	E	1722	C	N3-C4-N4	6.15	122.30	118.00
35	E	168	A	C4-C5-C6	6.14	120.07	117.00
35	E	1526	A	C4-C5-C6	6.14	120.07	117.00
35	E	1613	U	O4'-C1'-N1	6.14	113.12	108.20
35	E	1633	A	C4-C5-C6	6.14	120.07	117.00
35	E	138	C	N3-C4-N4	6.14	122.30	118.00
35	E	1602	C	N3-C4-N4	6.14	122.30	118.00
35	E	1674	U	O4'-C1'-N1	6.14	113.11	108.20
35	E	259	C	C6-N1-C2	-6.14	117.84	120.30
35	E	273	G	C5-C6-O6	-6.14	124.92	128.60
35	E	450	A	C5-C6-N6	-6.14	118.79	123.70
35	E	1326	G	N3-C2-N2	6.14	124.20	119.90
35	E	1328	A	O4'-C1'-N9	6.14	113.11	108.20
35	E	2209	A	C4-C5-C6	6.14	120.07	117.00
35	E	45	U	O4'-C1'-N1	6.14	113.11	108.20
35	E	102	A	C4-C5-C6	6.14	120.07	117.00
35	E	281	A	C5-C6-N6	-6.14	118.79	123.70
35	E	527	A	O4'-C1'-N9	6.14	113.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	664	G	O4'-C1'-N9	6.14	113.11	108.20
35	E	753	U	C4'-C3'-C2'	-6.14	96.46	102.60
35	E	853	C	N3-C4-N4	6.14	122.30	118.00
35	E	915	A	C4-C5-C6	6.14	120.07	117.00
35	E	1264	A	C4-C5-C6	6.14	120.07	117.00
35	E	1285	C	N3-C4-N4	6.14	122.30	118.00
35	E	2002	A	C4-C5-C6	6.14	120.07	117.00
35	E	2302	C	N3-C4-N4	6.14	122.30	118.00
35	E	2175	C	N3-C4-N4	6.14	122.30	118.00
35	E	16	G	O4'-C1'-N9	6.14	113.11	108.20
35	E	170	C	N3-C4-N4	6.14	122.30	118.00
35	E	1226	G	O4'-C1'-N9	6.14	113.11	108.20
35	E	2083	A	C5-C6-N6	-6.14	118.79	123.70
35	E	2088	A	C5-C6-N6	-6.14	118.79	123.70
35	E	230	G	O4'-C1'-N9	6.13	113.11	108.20
35	E	242	A	C4-C5-C6	6.13	120.07	117.00
35	E	406	A	C4-C5-C6	6.13	120.07	117.00
35	E	844	G	C5-C6-O6	-6.13	124.92	128.60
35	E	1572	U	O4'-C1'-N1	6.13	113.11	108.20
35	E	1724	A	C4-C5-C6	6.13	120.07	117.00
35	E	2047	A	O4'-C1'-N9	6.13	113.11	108.20
35	E	960	A	C4-C5-C6	6.13	120.07	117.00
35	E	1195	G	C5-C6-O6	-6.13	124.92	128.60
35	E	1378	A	C4-C5-C6	6.13	120.06	117.00
35	E	176	C	N3-C4-N4	6.13	122.29	118.00
35	E	215	A	C4-C5-C6	6.13	120.06	117.00
35	E	356	C	N3-C4-N4	6.13	122.29	118.00
35	E	374	G	C5-C6-O6	-6.13	124.92	128.60
35	E	676	G	C5-C6-O6	-6.12	124.92	128.60
35	E	1981	A	C4-C5-C6	6.12	120.06	117.00
35	E	2061	G	C8-N9-C1'	-6.12	119.04	127.00
35	E	2263	G	C5-C6-O6	-6.12	124.92	128.60
35	E	768	G	P-O3'-C3'	6.12	127.05	119.70
35	E	1607	A	C4-C5-C6	6.12	120.06	117.00
35	E	1759	G	O4'-C1'-N9	6.12	113.10	108.20
35	E	2221	A	C4-C5-C6	6.12	120.06	117.00
35	E	2264	A	C5-C6-N6	-6.12	118.80	123.70
35	E	1087	A	C4-C5-C6	6.12	120.06	117.00
35	E	363	A	C4-C5-C6	6.12	120.06	117.00
35	E	2047	A	C4-C5-C6	6.12	120.06	117.00
35	E	2205	G	O4'-C1'-N9	6.12	113.10	108.20
35	E	319	C	N3-C4-N4	6.12	122.28	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	456	C	N3-C4-N4	6.12	122.28	118.00
35	E	790	G	O4'-C1'-N9	6.12	113.09	108.20
35	E	1219	C	N3-C4-N4	6.12	122.28	118.00
35	E	1286	A	O4'-C1'-N9	6.12	113.09	108.20
35	E	1920	A	C4-C5-C6	6.12	120.06	117.00
35	E	2202	A	C4-C5-C6	6.12	120.06	117.00
35	E	2234	A	C4-C5-C6	6.12	120.06	117.00
35	E	1998	A	O4'-C1'-N9	6.12	113.09	108.20
35	E	1200	A	C4-C5-C6	6.11	120.06	117.00
35	E	1592	A	C4-C5-C6	6.11	120.06	117.00
35	E	1597	U	O4'-C1'-N1	6.11	113.09	108.20
35	E	2247	C	N3-C4-N4	6.11	122.28	118.00
35	E	1371	C	N3-C4-N4	6.11	122.28	118.00
35	E	2268	A	C4-C5-C6	6.11	120.06	117.00
35	E	432	A	C5-C6-N1	-6.11	114.64	117.70
35	E	434	A	C4-C5-C6	6.11	120.06	117.00
35	E	1177	C	N3-C4-N4	6.11	122.28	118.00
35	E	392	A	C5-C6-N1	-6.11	114.65	117.70
35	E	783	A	C4-C5-C6	6.11	120.05	117.00
35	E	1559	U	O4'-C1'-N1	6.11	113.08	108.20
35	E	531	A	C4-C5-C6	6.10	120.05	117.00
35	E	1974	C	N3-C4-N4	6.10	122.27	118.00
35	E	349	A	C5-C6-N6	-6.10	118.82	123.70
35	E	646	A	C5-C6-N6	-6.10	118.82	123.70
35	E	1079	U	O4'-C1'-N1	6.10	113.08	108.20
35	E	352	A	C4-C5-C6	6.10	120.05	117.00
35	E	430	G	O4'-C1'-N9	6.10	113.08	108.20
35	E	520	A	C5-C6-N6	-6.10	118.82	123.70
35	E	1076	C	N3-C4-N4	6.10	122.27	118.00
35	E	1716	C	N3-C4-N4	6.10	122.27	118.00
35	E	1920	A	O4'-C1'-N9	6.10	113.08	108.20
35	E	865	A	C4-C5-C6	6.10	120.05	117.00
35	E	1306	A	C4-C5-C6	6.10	120.05	117.00
35	E	1619	A	C5-C6-N1	-6.10	114.65	117.70
35	E	1702	A	C5-C6-N6	-6.10	118.82	123.70
35	E	196	U	O4'-C1'-N1	6.10	113.08	108.20
35	E	1222	A	C4-C5-C6	6.10	120.05	117.00
35	E	314	A	C4-C5-C6	6.09	120.05	117.00
35	E	1233	A	C4-C5-C6	6.09	120.05	117.00
35	E	1369	C	N3-C4-N4	6.09	122.27	118.00
35	E	1695	A	C4-C5-C6	6.09	120.05	117.00
35	E	2009	C	N3-C4-N4	6.09	122.27	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	442	U	O4'-C1'-N1	6.09	113.07	108.20
35	E	637	C	N3-C4-N4	6.09	122.27	118.00
35	E	1330	A	C5-C6-N1	-6.09	114.65	117.70
35	E	1743	A	C5-C6-N6	-6.09	118.83	123.70
35	E	745	C	N3-C4-C5	-6.09	119.46	121.90
35	E	1999	A	C4-C5-C6	6.09	120.05	117.00
35	E	2133	C	N3-C4-N4	6.09	122.27	118.00
35	E	2262	A	C4-C5-C6	6.09	120.05	117.00
35	E	326	U	O4'-C1'-N1	6.09	113.07	108.20
35	E	1215	A	C4-C5-C6	6.09	120.05	117.00
35	E	1240	A	C5-C6-N6	-6.09	118.83	123.70
35	E	1595	A	C5-C6-N6	-6.09	118.83	123.70
35	E	1656	G	O4'-C1'-N9	6.09	113.07	108.20
35	E	1745	G	N1-C6-O6	6.09	123.55	119.90
35	E	1764	A	C4-C5-C6	6.09	120.05	117.00
35	E	817	A	C4-C5-C6	6.09	120.04	117.00
35	E	1268	A	C4-C5-C6	6.09	120.04	117.00
35	E	1313	A	C4-C5-C6	6.09	120.04	117.00
35	E	1710	A	C5-C6-N1	-6.09	114.66	117.70
35	E	1957	C	N3-C4-N4	6.09	122.26	118.00
35	E	300	A	C4-C5-C6	6.09	120.04	117.00
35	E	701	C	C6-N1-C2	-6.09	117.86	120.30
35	E	852	A	C4-C5-C6	6.09	120.04	117.00
35	E	967	A	C4-C5-C6	6.09	120.04	117.00
35	E	1340	A	C4-C5-C6	6.09	120.04	117.00
35	E	1373	C	N3-C4-N4	6.09	122.26	118.00
35	E	1630	A	C4-C5-C6	6.09	120.04	117.00
35	E	2088	A	C4-C5-C6	6.09	120.04	117.00
35	E	2192	A	C4-C5-C6	6.09	120.04	117.00
35	E	1784	C	N3-C4-N4	6.08	122.26	118.00
35	E	414	A	C4-C5-C6	6.08	120.04	117.00
35	E	741	G	O4'-C1'-N9	6.08	113.07	108.20
35	E	958	U	O4'-C1'-N1	6.08	113.07	108.20
35	E	1810	C	N3-C4-N4	6.08	122.26	118.00
35	E	2074	G	N3-C2-N2	6.08	124.16	119.90
35	E	392	A	C4-C5-C6	6.08	120.04	117.00
35	E	455	C	N3-C4-N4	6.08	122.26	118.00
35	E	977	A	C5-C6-N6	-6.08	118.84	123.70
35	E	1175	A	C4-C5-C6	6.08	120.04	117.00
35	E	1306	A	O4'-C1'-N9	6.08	113.06	108.20
35	E	1996	A	C4-C5-C6	6.08	120.04	117.00
35	E	365	C	N3-C4-N4	6.08	122.25	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	505	A	C5-C6-N6	-6.08	118.84	123.70
35	E	1355	A	C5-C6-N1	-6.08	114.66	117.70
35	E	2011	A	C4-C5-C6	6.08	120.04	117.00
35	E	161	A	O4'-C1'-N9	6.08	113.06	108.20
35	E	1896	C	N3-C4-N4	6.08	122.25	118.00
35	E	440	C	N3-C4-N4	6.08	122.25	118.00
35	E	508	G	O4'-C1'-N9	6.08	113.06	108.20
35	E	1624	C	N3-C4-N4	6.08	122.25	118.00
35	E	556	U	O4'-C1'-N1	6.07	113.06	108.20
35	E	1362	A	C4-C5-C6	6.07	120.04	117.00
35	E	1661	A	C4-C5-C6	6.07	120.04	117.00
35	E	1758	C	N3-C4-N4	6.07	122.25	118.00
35	E	490	C	N3-C4-N4	6.07	122.25	118.00
35	E	864	A	C4-C5-C6	6.07	120.04	117.00
35	E	2103	A	C4-C5-C6	6.07	120.04	117.00
35	E	124	A	C4-C5-C6	6.07	120.03	117.00
35	E	402	C	N3-C4-N4	6.07	122.25	118.00
35	E	536	A	C4-C5-C6	6.07	120.03	117.00
35	E	1370	A	O4'-C1'-N9	6.07	113.06	108.20
35	E	432	A	C4-C5-C6	6.07	120.03	117.00
35	E	485	A	C4-C5-C6	6.07	120.03	117.00
35	E	497	C	N3-C4-N4	6.07	122.25	118.00
35	E	1981	A	C5-C6-N6	-6.07	118.84	123.70
35	E	255	A	C4-C5-C6	6.07	120.03	117.00
35	E	549	A	C5-C6-N6	-6.07	118.85	123.70
35	E	624	A	C4-C5-C6	6.07	120.03	117.00
35	E	1211	G	C5-C6-O6	-6.07	124.96	128.60
35	E	2115	C	N3-C4-C5	-6.07	119.47	121.90
35	E	304	A	C4-C5-C6	6.07	120.03	117.00
35	E	588	A	C5-C6-N6	-6.07	118.85	123.70
35	E	800	C	N3-C4-C5	-6.07	119.47	121.90
35	E	904	C	N3-C4-N4	6.07	122.25	118.00
35	E	1984	A	C4-C5-C6	6.07	120.03	117.00
35	E	599	A	C4-C5-C6	6.06	120.03	117.00
35	E	681	C	N3-C4-N4	6.06	122.25	118.00
35	E	604	A	C5-C6-N6	-6.06	118.85	123.70
35	E	655	A	C4-C5-C6	6.06	120.03	117.00
35	E	763	G	C5-C6-O6	-6.06	124.96	128.60
35	E	917	A	C4-C5-C6	6.06	120.03	117.00
35	E	1087	A	C5-C6-N1	-6.06	114.67	117.70
35	E	1180	A	C4-C5-C6	6.06	120.03	117.00
35	E	1325	C	N3-C4-N4	6.06	122.24	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1645	C	N3-C4-N4	6.06	122.24	118.00
35	E	2300	A	C4-C5-C6	6.06	120.03	117.00
35	E	764	A	C5-C6-N6	-6.06	118.85	123.70
35	E	1258	A	C5-C6-N6	-6.06	118.85	123.70
35	E	167	A	C4-C5-C6	6.06	120.03	117.00
35	E	180	A	O4'-C1'-N9	6.06	113.05	108.20
35	E	952	U	O4'-C1'-N1	6.06	113.05	108.20
35	E	766	C	N3-C4-N4	6.06	122.24	118.00
35	E	1628	A	C5-C6-N6	-6.06	118.86	123.70
35	E	742	A	C5-C6-N1	-6.06	114.67	117.70
35	E	1925	A	C4-C5-C6	6.06	120.03	117.00
35	E	1998	A	C4-C5-C6	6.06	120.03	117.00
35	E	2251	A	C4-C5-C6	6.06	120.03	117.00
35	E	2299	A	C4-C5-C6	6.06	120.03	117.00
35	E	916	A	C4-C5-C6	6.05	120.03	117.00
35	E	1677	C	N3-C4-N4	6.05	122.24	118.00
35	E	2008	A	O4'-C1'-N9	6.05	113.04	108.20
35	E	306	U	O4'-C1'-N1	6.05	113.04	108.20
35	E	757	G	P-O3'-C3'	6.05	126.96	119.70
35	E	1309	A	C4-C5-C6	6.05	120.03	117.00
35	E	1657	A	C4-C5-C6	6.05	120.03	117.00
35	E	1333	A	C4-C5-C6	6.05	120.03	117.00
35	E	371	A	C5-C6-N6	-6.05	118.86	123.70
35	E	2059	A	C5-C6-N1	-6.05	114.68	117.70
35	E	882	U	O4'-C1'-N1	6.05	113.04	108.20
35	E	2065	A	O4'-C1'-N9	6.05	113.04	108.20
35	E	121	A	C5-C6-N6	-6.05	118.86	123.70
35	E	782	A	C4-C5-C6	6.05	120.02	117.00
35	E	1938	C	N3-C4-N4	6.05	122.23	118.00
35	E	147	G	O4'-C1'-N9	6.04	113.03	108.20
35	E	877	A	C4-C5-C6	6.04	120.02	117.00
35	E	913	A	C4-C5-C6	6.04	120.02	117.00
35	E	1680	G	C5-C6-O6	-6.04	124.97	128.60
35	E	2039	A	C4-C5-C6	6.04	120.02	117.00
35	E	2139	G	O4'-C1'-N9	6.04	113.03	108.20
35	E	2159	A	C4-C5-C6	6.04	120.02	117.00
35	E	180	A	C4-C5-C6	6.04	120.02	117.00
35	E	348	A	C4-C5-C6	6.04	120.02	117.00
35	E	406	A	C5-C6-N6	-6.04	118.87	123.70
35	E	417	A	C4-C5-C6	6.04	120.02	117.00
35	E	743	C	C6-N1-C2	-6.04	117.88	120.30
35	E	777	A	C5-C6-N1	-6.04	114.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1216	G	O4'-C1'-N9	6.04	113.03	108.20
35	E	1287	A	C4-C5-C6	6.04	120.02	117.00
35	E	1679	A	C5-C6-N1	-6.04	114.68	117.70
35	E	2148	A	C4-C5-C6	6.04	120.02	117.00
35	E	571	A	C4-C5-C6	6.04	120.02	117.00
35	E	1536	C	N3-C4-C5	-6.04	119.48	121.90
35	E	36	U	O4'-C1'-N1	6.04	113.03	108.20
35	E	82	A	P-O3'-C3'	6.04	126.95	119.70
35	E	1633	A	C5-C6-N1	-6.04	114.68	117.70
35	E	1781	A	C4-C5-C6	6.04	120.02	117.00
35	E	2194	G	O4'-C1'-N9	6.04	113.03	108.20
35	E	608	C	O4'-C1'-N1	6.04	113.03	108.20
35	E	989	G	C5'-C4'-C3'	-6.04	106.34	116.00
35	E	122	A	C4-C5-C6	6.04	120.02	117.00
35	E	826	A	C4-C5-C6	6.04	120.02	117.00
35	E	1804	A	C4-C5-C6	6.04	120.02	117.00
35	E	701	C	N3-C4-C5	-6.03	119.49	121.90
35	E	1554	A	C5-C6-N1	-6.03	114.68	117.70
35	E	2284	A	C4-C5-C6	6.03	120.02	117.00
35	E	410	G	O4'-C1'-N9	6.03	113.02	108.20
35	E	889	A	C5-C6-N1	-6.03	114.68	117.70
35	E	2080	A	C5-C6-N6	-6.03	118.88	123.70
35	E	2143	C	N3-C4-N4	6.03	122.22	118.00
35	E	2226	U	O4'-C1'-N1	6.03	113.03	108.20
35	E	1723	G	O4'-C1'-N9	6.03	113.02	108.20
35	E	1876	G	O4'-C1'-N9	6.03	113.02	108.20
35	E	1979	G	O4'-C1'-N9	6.03	113.02	108.20
35	E	111	A	C4-C5-C6	6.03	120.01	117.00
35	E	569	A	C4-C5-C6	6.03	120.01	117.00
35	E	1238	U	O4'-C1'-N1	6.03	113.02	108.20
35	E	2070	C	N3-C4-C5	-6.03	119.49	121.90
35	E	2111	A	C4-C5-C6	6.03	120.01	117.00
35	E	2015	U	P-O3'-C3'	6.03	126.93	119.70
35	E	2037	A	C4-C5-C6	6.02	120.01	117.00
35	E	11	A	C5-C6-N1	-6.02	114.69	117.70
35	E	576	A	C5-C6-N6	-6.02	118.88	123.70
35	E	692	U	O4'-C1'-N1	6.02	113.02	108.20
35	E	839	C	N3-C4-C5	-6.02	119.49	121.90
35	E	992	A	C4-C5-C6	6.02	120.01	117.00
35	E	1200	A	C5-C6-N1	-6.02	114.69	117.70
35	E	190	A	C4-C5-C6	6.02	120.01	117.00
35	E	1815	A	C5-C6-N6	-6.02	118.88	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	646	A	C5-C6-N1	-6.02	114.69	117.70
35	E	901	A	C5-C6-N6	-6.02	118.89	123.70
35	E	1174	C	N3-C4-N4	6.02	122.21	118.00
35	E	1632	G	O4'-C1'-N9	6.02	113.02	108.20
35	E	1701	G	C5-C6-O6	-6.02	124.99	128.60
35	E	690	A	C4-C5-C6	6.02	120.01	117.00
35	E	845	A	C4-C5-C6	6.02	120.01	117.00
35	E	1242	A	O4'-C1'-N9	6.02	113.02	108.20
35	E	1275	A	O4'-C1'-N9	6.02	113.01	108.20
35	E	1380	U	O4'-C1'-N1	6.02	113.02	108.20
35	E	439	G	O4'-C1'-N9	6.02	113.01	108.20
35	E	454	A	C4-C5-C6	6.02	120.01	117.00
35	E	858	A	C4-C5-C6	6.02	120.01	117.00
35	E	1176	A	C4-C5-C6	6.02	120.01	117.00
35	E	1547	A	C4-C5-C6	6.01	120.01	117.00
35	E	1591	C	O4'-C1'-N1	6.01	113.01	108.20
35	E	118	C	N3-C4-N4	6.01	122.21	118.00
35	E	121	A	C4-C5-C6	6.01	120.01	117.00
35	E	653	A	C4-C5-C6	6.01	120.01	117.00
35	E	728	A	C4-C5-C6	6.01	120.01	117.00
35	E	743	C	N3-C4-C5	-6.01	119.50	121.90
35	E	889	A	C5-C6-N6	-6.01	118.89	123.70
35	E	1187	C	N3-C4-N4	6.01	122.21	118.00
35	E	2006	A	C4-C5-C6	6.01	120.01	117.00
30	m	143	GLY	C-N-CA	6.01	136.72	121.70
35	E	28	A	C4-C5-C6	6.01	120.00	117.00
35	E	195	C	N3-C4-N4	6.01	122.21	118.00
35	E	269	A	C4-C5-C6	6.01	120.00	117.00
35	E	400	G	N3-C2-N2	6.01	124.11	119.90
35	E	781	A	C4-C5-C6	6.01	120.00	117.00
35	E	1769	U	O4'-C1'-N1	6.01	113.01	108.20
35	E	241	A	C4-C5-C6	6.01	120.00	117.00
35	E	608	C	N3-C4-N4	6.01	122.21	118.00
35	E	993	A	C4-C5-C6	6.01	120.00	117.00
35	E	1240	A	C4-C5-C6	6.01	120.00	117.00
35	E	1764	A	C5-C6-N6	-6.01	118.89	123.70
35	E	2065	A	C4-C5-C6	6.01	120.00	117.00
35	E	2080	A	C4-C5-C6	6.01	120.00	117.00
35	E	751	C	P-O3'-C3'	6.01	126.91	119.70
35	E	1269	C	N3-C4-C5	-6.01	119.50	121.90
35	E	1802	C	N3-C4-N4	6.01	122.20	118.00
35	E	414	A	C5-C6-N6	-6.00	118.90	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1891	C	N3-C4-N4	6.00	122.20	118.00
35	E	72	C	N3-C4-N4	6.00	122.20	118.00
35	E	402	C	N3-C4-C5	-6.00	119.50	121.90
35	E	774	C	O3'-P-O5'	6.00	115.41	104.00
35	E	1771	U	O4'-C1'-N1	6.00	113.00	108.20
35	E	2118	G	O4'-C1'-N9	6.00	113.00	108.20
35	E	2136	A	C4-C5-C6	6.00	120.00	117.00
35	E	785	A	C5-C6-N6	-6.00	118.90	123.70
35	E	876	A	C4-C5-C6	6.00	120.00	117.00
1	p	105	PHE	CB-CG-CD1	-6.00	116.60	120.80
35	E	734	G	C8-N9-C4	6.00	108.80	106.40
35	E	789	C	N3-C4-N4	6.00	122.20	118.00
35	E	794	G	O4'-C1'-N9	6.00	113.00	108.20
35	E	2053	G	O4'-C1'-N9	6.00	113.00	108.20
35	E	2063	A	O4'-C1'-N9	6.00	113.00	108.20
35	E	349	A	C4-C5-C6	6.00	120.00	117.00
35	E	2111	A	O4'-C1'-N9	6.00	113.00	108.20
35	E	360	A	C4-C5-C6	5.99	120.00	117.00
35	E	481	G	O4'-C1'-N9	5.99	113.00	108.20
35	E	1201	G	O4'-C1'-N9	5.99	112.99	108.20
35	E	2200	A	C5-C6-N6	-5.99	118.91	123.70
35	E	575	A	C4-C5-C6	5.99	120.00	117.00
35	E	1301	A	C4-C5-C6	5.99	120.00	117.00
35	E	1720	C	N3-C4-C5	-5.99	119.50	121.90
35	E	1794	A	C4-C5-C6	5.99	120.00	117.00
35	E	2092	A	C4-C5-C6	5.99	120.00	117.00
35	E	2135	A	C4-C5-C6	5.99	120.00	117.00
35	E	498	A	C4-C5-C6	5.99	120.00	117.00
35	E	1301	A	C5-C6-N6	-5.99	118.91	123.70
35	E	861	A	C5-C6-N1	-5.99	114.71	117.70
35	E	990	A	C4-C5-C6	5.99	119.99	117.00
35	E	1205	A	C4-C5-C6	5.99	119.99	117.00
35	E	1314	A	C5-C6-N6	-5.99	118.91	123.70
35	E	516	A	C4-C5-C6	5.99	119.99	117.00
35	E	581	A	C5-C6-N6	-5.99	118.91	123.70
35	E	607	A	C4-C5-C6	5.99	119.99	117.00
35	E	1854	G	O4'-C1'-N9	5.99	112.99	108.20
35	E	1349	G	O4'-C1'-N9	5.98	112.99	108.20
35	E	2015	U	O4'-C1'-N1	5.98	112.99	108.20
35	E	350	C	N3-C4-N4	5.98	122.19	118.00
35	E	549	A	C4-C5-C6	5.98	119.99	117.00
35	E	1690	G	C5-C6-O6	-5.98	125.01	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1732	A	O4'-C1'-N9	5.98	112.99	108.20
35	E	577	A	O4'-C1'-N9	5.98	112.98	108.20
35	E	582	U	O4'-C1'-N1	5.98	112.98	108.20
35	E	1354	C	N3-C4-N4	5.98	122.19	118.00
35	E	1631	A	C4-C5-C6	5.98	119.99	117.00
35	E	1919	A	C4-C5-C6	5.98	119.99	117.00
14	V	57	ALA	N-CA-CB	5.98	118.47	110.10
35	E	231	A	C5-C6-N1	-5.98	114.71	117.70
35	E	1345	U	O4'-C1'-N1	5.98	112.98	108.20
35	E	659	A	C4-C5-C6	5.98	119.99	117.00
35	E	1657	A	C5-C6-N6	-5.98	118.92	123.70
35	E	2265	G	O4'-C1'-N9	5.98	112.98	108.20
35	E	2034	A	C4-C5-C6	5.98	119.99	117.00
35	E	655	A	C5-C6-N6	-5.97	118.92	123.70
35	E	1228	G	O4'-C1'-N9	5.97	112.98	108.20
35	E	1353	A	C4-C5-C6	5.97	119.99	117.00
35	E	1592	A	C5-C6-N1	-5.97	114.71	117.70
35	E	1679	A	C4-C5-C6	5.97	119.99	117.00
35	E	1730	U	O4'-C1'-N1	5.97	112.98	108.20
35	E	838	G	C5-C6-O6	-5.97	125.02	128.60
35	E	954	G	C6-C5-N7	-5.97	126.82	130.40
35	E	1377	A	C4-C5-C6	5.97	119.99	117.00
35	E	1829	C	N3-C4-N4	5.97	122.18	118.00
35	E	2005	A	C4-C5-C6	5.97	119.99	117.00
35	E	2187	C	N3-C4-N4	5.97	122.18	118.00
35	E	1311	C	N3-C4-N4	5.97	122.18	118.00
35	E	2260	A	C4-C5-C6	5.97	119.99	117.00
35	E	311	G	O4'-C1'-N9	5.97	112.97	108.20
35	E	598	A	C4-C5-C6	5.97	119.98	117.00
35	E	1302	A	C4-C5-C6	5.97	119.98	117.00
35	E	2312	A	C4-C5-C6	5.97	119.98	117.00
35	E	525	A	C5-C6-N1	-5.97	114.72	117.70
35	E	1185	A	C4-C5-C6	5.97	119.98	117.00
35	E	2244	C	N3-C4-N4	5.97	122.18	118.00
35	E	62	A	C5-C6-N6	-5.97	118.93	123.70
35	E	184	A	C4-C5-C6	5.97	119.98	117.00
35	E	587	A	O4'-C1'-N9	5.96	112.97	108.20
35	E	721	C	O4'-C1'-N1	5.96	112.97	108.20
35	E	780	C	N3-C4-C5	-5.96	119.51	121.90
35	E	1209	C	N3-C4-N4	5.96	122.17	118.00
35	E	2083	A	O4'-C1'-N9	5.96	112.97	108.20
35	E	195	C	O4'-C1'-N1	5.96	112.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1304	C	N3-C4-N4	5.96	122.17	118.00
35	E	2166	C	N3-C4-N4	5.96	122.17	118.00
35	E	809	A	C4-C5-C6	5.96	119.98	117.00
35	E	165	C	N3-C4-N4	5.96	122.17	118.00
35	E	562	A	O4'-C1'-N9	5.96	112.97	108.20
35	E	638	C	N3-C4-N4	5.96	122.17	118.00
35	E	812	A	C4-C5-C6	5.96	119.98	117.00
35	E	866	A	C5-C6-N1	-5.96	114.72	117.70
35	E	2202	A	C5-C6-N6	-5.96	118.93	123.70
35	E	913	A	C5-C6-N1	-5.96	114.72	117.70
35	E	1705	G	O4'-C1'-N9	5.96	112.97	108.20
35	E	1954	C	N3-C4-N4	5.96	122.17	118.00
35	E	2288	A	C4-C5-C6	5.96	119.98	117.00
21	d	81	SER	N-CA-CB	5.96	119.43	110.50
35	E	448	A	C4-C5-C6	5.96	119.98	117.00
35	E	1981	A	C5-C6-N1	-5.96	114.72	117.70
20	f	172	TYR	CB-CG-CD2	-5.95	117.43	121.00
35	E	4	C	N3-C4-N4	5.95	122.17	118.00
35	E	143	C	N3-C4-N4	5.95	122.17	118.00
35	E	520	A	C4-C5-C6	5.95	119.98	117.00
35	E	521	A	O4'-C1'-N9	5.95	112.96	108.20
35	E	553	U	O4'-C1'-N1	5.95	112.96	108.20
35	E	684	A	C4-C5-C6	5.95	119.98	117.00
35	E	1229	C	N3-C4-N4	5.95	122.17	118.00
35	E	1573	C	N3-C4-N4	5.95	122.17	118.00
35	E	2027	C	N3-C4-C5	-5.95	119.52	121.90
35	E	2127	G	O4'-C1'-N9	5.95	112.96	108.20
35	E	2171	C	O4'-C1'-N1	5.95	112.96	108.20
35	E	789	C	N3-C4-C5	-5.95	119.52	121.90
35	E	1973	A	C5-C6-N6	-5.95	118.94	123.70
35	E	2004	A	C4-C5-C6	5.95	119.98	117.00
35	E	2047	A	C5-C6-N1	-5.95	114.72	117.70
35	E	581	A	C4-C5-C6	5.95	119.98	117.00
35	E	585	A	C4-C5-C6	5.95	119.97	117.00
35	E	2046	A	C5-C6-N6	-5.95	118.94	123.70
35	E	332	C	N3-C4-N4	5.95	122.16	118.00
35	E	989	G	O4'-C1'-N9	5.95	112.96	108.20
35	E	1235	A	C5-C6-N1	-5.95	114.73	117.70
35	E	1275	A	C5-C6-N6	-5.95	118.94	123.70
35	E	1939	A	O4'-C1'-N9	5.95	112.96	108.20
35	E	1984	A	O4'-C1'-N9	5.95	112.96	108.20
35	E	2010	G	O4'-C1'-N9	5.95	112.96	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	31	C	N3-C4-N4	5.95	122.16	118.00
35	E	127	C	O4'-C1'-N1	5.95	112.96	108.20
35	E	393	U	O4'-C1'-N1	5.95	112.96	108.20
35	E	645	A	C5-C6-N6	-5.95	118.94	123.70
35	E	1566	A	C4-C5-C6	5.95	119.97	117.00
35	E	2273	A	C4-C5-C6	5.95	119.97	117.00
35	E	1385	A	C5-C6-N6	-5.94	118.94	123.70
35	E	1936	A	C5-C6-N6	-5.94	118.94	123.70
35	E	156	G	O4'-C1'-N9	5.94	112.95	108.20
35	E	464	C	O4'-C1'-N1	5.94	112.95	108.20
35	E	1254	C	N3-C4-N4	5.94	122.16	118.00
35	E	2079	G	O4'-C1'-N9	5.94	112.95	108.20
35	E	898	A	C4-C5-C6	5.94	119.97	117.00
35	E	245	A	C4-C5-C6	5.94	119.97	117.00
35	E	2004	A	O4'-C1'-N9	5.94	112.95	108.20
35	E	1361	A	C4-C5-C6	5.94	119.97	117.00
35	E	249	A	C4-C5-C6	5.93	119.97	117.00
35	E	2262	A	C5-C6-N1	-5.93	114.73	117.70
35	E	1087	A	O4'-C1'-N9	5.93	112.94	108.20
35	E	1593	A	C5-C6-N6	-5.93	118.95	123.70
35	E	2298	G	O4'-C1'-N9	5.93	112.95	108.20
35	E	837	C	N3-C4-C5	-5.93	119.53	121.90
35	E	1332	G	O4'-C1'-N9	5.93	112.94	108.20
35	E	709	C	N3-C4-N4	5.93	122.15	118.00
35	E	912	A	C4-C5-C6	5.93	119.96	117.00
35	E	1179	C	N3-C4-N4	5.93	122.15	118.00
35	E	793	A	C5-C6-N1	-5.93	114.74	117.70
35	E	1561	A	C5-C6-N1	-5.93	114.74	117.70
35	E	703	A	C5-C6-N1	-5.93	114.74	117.70
35	E	744	C	N3-C4-N4	5.93	122.15	118.00
35	E	1373	C	N3-C4-C5	-5.93	119.53	121.90
35	E	1574	A	C4-C5-C6	5.93	119.96	117.00
35	E	2240	A	C5-C6-N6	-5.93	118.96	123.70
35	E	604	A	C4-C5-C6	5.92	119.96	117.00
35	E	1256	C	N3-C4-N4	5.92	122.15	118.00
35	E	507	A	C5-C6-N6	-5.92	118.96	123.70
35	E	523	A	C5-C6-N1	-5.92	114.74	117.70
35	E	799	A	C5-C6-N6	-5.92	118.96	123.70
35	E	1301	A	C5-C6-N1	-5.92	114.74	117.70
35	E	1874	C	N3-C4-C5	-5.92	119.53	121.90
35	E	287	A	C5-C6-N6	-5.92	118.96	123.70
35	E	598	A	O4'-C1'-N9	5.92	112.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1888	A	C4-C5-C6	5.92	119.96	117.00
35	E	1992	A	C4-C5-C6	5.92	119.96	117.00
35	E	231	A	C4-C5-C6	5.92	119.96	117.00
35	E	275	A	C4-C5-C6	5.92	119.96	117.00
35	E	531	A	C5-C6-N6	-5.92	118.97	123.70
35	E	925	C	N3-C4-N4	5.92	122.14	118.00
35	E	1316	U	O4'-C1'-N1	5.92	112.93	108.20
35	E	1629	C	N3-C4-N4	5.92	122.14	118.00
35	E	1917	G	O4'-C1'-N9	5.92	112.93	108.20
35	E	2260	A	O4'-C1'-N9	5.92	112.94	108.20
35	E	751	C	N3-C4-C5	-5.92	119.53	121.90
35	E	891	U	O4'-C1'-N1	5.92	112.93	108.20
35	E	1382	G	O4'-C1'-N9	5.92	112.93	108.20
35	E	1609	A	C5-C6-N6	-5.92	118.97	123.70
35	E	1818	A	C4-C5-C6	5.92	119.96	117.00
35	E	2200	A	C4-C5-C6	5.92	119.96	117.00
35	E	1297	C	N3-C4-C5	-5.92	119.53	121.90
35	E	2	A	C4-C5-C6	5.91	119.96	117.00
35	E	245	A	C5-C6-N1	-5.91	114.74	117.70
35	E	526	A	C4-C5-C6	5.91	119.96	117.00
35	E	639	A	C4-C5-C6	5.91	119.96	117.00
35	E	734	G	N3-C4-C5	5.91	131.56	128.60
35	E	1610	A	C4-C5-C6	5.91	119.96	117.00
35	E	1740	U	O4'-C1'-N1	5.91	112.93	108.20
35	E	1191	G	C5-C6-O6	-5.91	125.05	128.60
35	E	509	A	C5-C6-N6	-5.91	118.97	123.70
35	E	1368	A	C4-C5-C6	5.91	119.95	117.00
35	E	2087	C	N3-C4-N4	5.91	122.14	118.00
35	E	107	A	C4-C5-C6	5.91	119.95	117.00
35	E	313	G	C4-N9-C1'	5.91	134.18	126.50
35	E	610	A	C5-C6-N1	-5.91	114.75	117.70
35	E	512	A	C4-C5-C6	5.91	119.95	117.00
35	E	967	A	C5-C6-N1	-5.91	114.75	117.70
35	E	1733	A	C4-C5-C6	5.91	119.95	117.00
35	E	703	A	C4-C5-C6	5.91	119.95	117.00
35	E	999	U	O4'-C1'-N1	5.91	112.92	108.20
35	E	1085	G	O4'-C1'-N9	5.91	112.92	108.20
35	E	1355	A	C4-C5-C6	5.91	119.95	117.00
35	E	1385	A	C4-C5-C6	5.91	119.95	117.00
35	E	2039	A	O4'-C1'-N9	5.91	112.92	108.20
35	E	2245	A	C4-C5-C6	5.91	119.95	117.00
35	E	2259	A	C4-C5-C6	5.90	119.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1180	A	O4'-C1'-N9	5.90	112.92	108.20
35	E	2271	A	C4-C5-C6	5.90	119.95	117.00
35	E	285	A	C4-C5-C6	5.90	119.95	117.00
35	E	330	A	C4-C5-C6	5.90	119.95	117.00
35	E	901	A	C4-C5-C6	5.90	119.95	117.00
35	E	2046	A	C4-C5-C6	5.90	119.95	117.00
35	E	26	A	C4-C5-C6	5.90	119.95	117.00
35	E	64	A	C5-C6-N1	-5.90	114.75	117.70
35	E	192	G	O4'-C1'-N9	5.90	112.92	108.20
35	E	1266	C	N3-C4-N4	5.90	122.13	118.00
35	E	1308	A	C5-C6-N6	-5.90	118.98	123.70
35	E	141	A	O4'-C1'-N9	5.89	112.92	108.20
35	E	1271	G	O4'-C1'-N9	5.89	112.92	108.20
35	E	2089	A	C4-C5-C6	5.89	119.95	117.00
35	E	2169	A	C4-C5-C6	5.89	119.95	117.00
35	E	25	C	N3-C4-N4	5.89	122.12	118.00
35	E	1794	A	C5-C6-N6	-5.89	118.99	123.70
35	E	1961	A	O4'-C1'-N9	5.89	112.91	108.20
35	E	492	A	O4'-C1'-N9	5.89	112.91	108.20
35	E	2272	A	C4-C5-C6	5.89	119.94	117.00
35	E	1333	A	O4'-C1'-N9	5.89	112.91	108.20
35	E	2267	A	C4-C5-C6	5.89	119.94	117.00
35	E	962	A	C4-C5-C6	5.89	119.94	117.00
35	E	2027	C	O4'-C1'-N1	5.89	112.91	108.20
35	E	241	A	C5-C6-N6	-5.89	118.99	123.70
35	E	248	G	N3-C2-N2	5.89	124.02	119.90
35	E	451	G	O4'-C1'-N9	5.89	112.91	108.20
35	E	1951	A	O4'-C1'-N9	5.89	112.91	108.20
35	E	2269	G	O4'-C1'-N9	5.89	112.91	108.20
35	E	583	C	N3-C4-N4	5.88	122.12	118.00
35	E	764	A	C4-C5-C6	5.88	119.94	117.00
35	E	788	A	C4-C5-C6	5.88	119.94	117.00
35	E	1370	A	C4-C5-C6	5.88	119.94	117.00
35	E	1814	U	O4'-C1'-N1	5.88	112.91	108.20
35	E	1888	A	C5-C6-N1	-5.88	114.76	117.70
35	E	1973	A	C5-C6-N1	-5.88	114.76	117.70
35	E	2063	A	C4-C5-C6	5.88	119.94	117.00
35	E	2281	A	C4-C5-C6	5.88	119.94	117.00
35	E	704	A	C4-C5-C6	5.88	119.94	117.00
35	E	1667	G	C5-C6-O6	-5.88	125.07	128.60
35	E	653	A	C5-C6-N6	-5.88	118.99	123.70
35	E	1290	A	C5-C6-N1	-5.88	114.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2089	A	C5-C6-N1	-5.88	114.76	117.70
35	E	2098	C	N3-C4-C5	-5.88	119.55	121.90
35	E	472	A	C4-C5-C6	5.88	119.94	117.00
35	E	523	A	C4-C5-C6	5.88	119.94	117.00
35	E	765	A	C4-C5-C6	5.88	119.94	117.00
35	E	775	A	C5-C6-N6	-5.88	119.00	123.70
35	E	1217	A	C4-C5-C6	5.88	119.94	117.00
35	E	463	A	C4-C5-C6	5.88	119.94	117.00
35	E	491	C	N3-C4-N4	5.88	122.11	118.00
35	E	866	A	C4-C5-C6	5.88	119.94	117.00
35	E	912	A	C5-C6-N1	-5.88	114.76	117.70
35	E	1241	A	C5-C6-N6	-5.88	119.00	123.70
35	E	1245	C	N3-C4-N4	5.88	122.11	118.00
35	E	1290	A	C5-C6-N6	-5.88	119.00	123.70
35	E	1352	C	N3-C4-N4	5.88	122.11	118.00
35	E	1375	U	O4'-C1'-N1	5.88	112.90	108.20
35	E	1971	C	N3-C4-N4	5.88	122.11	118.00
35	E	2135	A	C5-C6-N1	-5.88	114.76	117.70
35	E	786	A	C4-C5-C6	5.88	119.94	117.00
35	E	1646	G	O4'-C1'-N9	5.88	112.90	108.20
35	E	464	C	N3-C4-N4	5.87	122.11	118.00
35	E	467	A	C4-C5-C6	5.87	119.94	117.00
35	E	645	A	C5-C6-N1	-5.87	114.76	117.70
35	E	1927	A	O4'-C1'-N9	5.87	112.90	108.20
35	E	81	A	O4'-C1'-N9	5.87	112.90	108.20
35	E	303	C	N3-C4-N4	5.87	122.11	118.00
35	E	1285	C	N3-C4-C5	-5.87	119.55	121.90
35	E	1975	A	C4-C5-C6	5.87	119.94	117.00
35	E	11	A	C4-C5-C6	5.87	119.94	117.00
35	E	902	A	C4-C5-C6	5.87	119.93	117.00
35	E	995	C	N3-C4-N4	5.87	122.11	118.00
35	E	1615	A	O4'-C1'-N9	5.87	112.89	108.20
35	E	1956	C	N3-C4-N4	5.87	122.11	118.00
35	E	2128	C	N3-C4-N4	5.87	122.11	118.00
35	E	646	A	C4-C5-C6	5.87	119.93	117.00
35	E	1338	A	C4-C5-C6	5.87	119.93	117.00
35	E	1584	A	C4-C5-C6	5.87	119.93	117.00
35	E	1663	C	N3-C4-N4	5.87	122.11	118.00
35	E	2100	C	N3-C4-C5	-5.86	119.55	121.90
35	E	647	A	C4-C5-C6	5.86	119.93	117.00
35	E	578	C	N3-C4-N4	5.86	122.10	118.00
35	E	889	A	C4-C5-C6	5.86	119.93	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2021	G	O4'-C1'-N9	5.86	112.89	108.20
35	E	2059	A	C5-C6-N6	-5.86	119.01	123.70
35	E	19	A	C4-C5-C6	5.86	119.93	117.00
35	E	649	G	O4'-C1'-N9	5.86	112.89	108.20
35	E	732	C	C2-N1-C1'	5.86	125.24	118.80
35	E	734	G	O4'-C1'-N9	5.86	112.89	108.20
35	E	1985	C	N3-C4-N4	5.86	122.10	118.00
35	E	2009	C	N3-C4-C5	-5.86	119.56	121.90
35	E	2056	A	C4-C5-C6	5.86	119.93	117.00
35	E	2209	A	C5-C6-N1	-5.86	114.77	117.70
35	E	1083	G	O4'-C1'-N9	5.86	112.89	108.20
35	E	1362	A	C5-C6-N6	-5.86	119.02	123.70
35	E	2042	G	O4'-C1'-N9	5.86	112.89	108.20
35	E	2103	A	C5-C6-N1	-5.86	114.77	117.70
35	E	2179	G	O4'-C1'-N9	5.86	112.89	108.20
35	E	2209	A	C5-C6-N6	-5.86	119.02	123.70
35	E	593	G	O4'-C1'-N9	5.85	112.88	108.20
35	E	800	C	O4'-C1'-N1	5.85	112.88	108.20
1	p	301	TYR	CB-CG-CD2	-5.85	117.49	121.00
35	E	173	A	C4-C5-C6	5.85	119.92	117.00
35	E	800	C	N3-C4-N4	5.85	122.09	118.00
35	E	1634	C	C5-C4-N4	-5.85	116.11	120.20
35	E	2018	U	O4'-C1'-N1	5.85	112.88	108.20
35	E	2259	A	O4'-C1'-N9	5.85	112.88	108.20
35	E	401	A	C4-C5-C6	5.85	119.92	117.00
35	E	592	A	C5-C6-N1	-5.85	114.78	117.70
35	E	1187	C	C4'-C3'-C2'	-5.85	96.75	102.60
35	E	1333	A	C5-C6-N6	-5.85	119.02	123.70
35	E	1774	U	O4'-C1'-N1	5.85	112.88	108.20
35	E	1942	A	C4-C5-C6	5.85	119.92	117.00
35	E	2170	C	N3-C4-N4	5.85	122.09	118.00
35	E	280	C	N3-C4-N4	5.85	122.09	118.00
35	E	852	A	C5-C6-N1	-5.85	114.78	117.70
35	E	246	A	C5-C6-N1	-5.84	114.78	117.70
35	E	991	C	N3-C4-N4	5.84	122.09	118.00
35	E	1290	A	C4-C5-C6	5.84	119.92	117.00
35	E	1728	C	O4'-C1'-N1	5.84	112.88	108.20
35	E	1747	C	N3-C4-N4	5.84	122.09	118.00
35	E	123	A	C5-C6-N6	-5.84	119.03	123.70
35	E	905	A	C4-C5-C6	5.84	119.92	117.00
35	E	1595	A	C4-C5-C6	5.84	119.92	117.00
35	E	844	G	O4'-C1'-N9	5.84	112.87	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1526	A	C5-C6-N6	-5.84	119.03	123.70
35	E	2059	A	C4-C5-C6	5.84	119.92	117.00
35	E	190	A	C5-C6-N6	-5.84	119.03	123.70
35	E	1955	U	O4'-C1'-N1	5.84	112.87	108.20
35	E	2271	A	C5-C6-N1	-5.84	114.78	117.70
35	E	2192	A	O4'-C1'-N9	5.83	112.87	108.20
35	E	760	C	N3-C4-N4	5.83	122.08	118.00
35	E	2068	C	N3-C4-N4	5.83	122.08	118.00
35	E	810	U	O4'-C1'-N1	5.83	112.86	108.20
35	E	2117	C	N3-C4-N4	5.83	122.08	118.00
35	E	805	C	N3-C4-N4	5.83	122.08	118.00
35	E	1853	C	N3-C4-N4	5.83	122.08	118.00
35	E	39	A	C4-C5-C6	5.83	119.91	117.00
35	E	1346	G	C5-C6-O6	-5.83	125.10	128.60
35	E	457	A	C4-C5-C6	5.83	119.91	117.00
35	E	1742	C	N3-C4-N4	5.83	122.08	118.00
35	E	1801	C	N3-C4-N4	5.83	122.08	118.00
35	E	2263	G	N3-C2-N2	5.83	123.98	119.90
35	E	1616	C	N3-C4-N4	5.82	122.08	118.00
35	E	1177	C	O4'-C1'-N1	5.82	112.86	108.20
35	E	2281	A	C5-C6-N1	-5.82	114.79	117.70
35	E	65	A	C5-C6-N6	-5.82	119.04	123.70
35	E	351	A	C4-C5-C6	5.82	119.91	117.00
35	E	1298	C	N3-C4-N4	5.82	122.07	118.00
35	E	1797	A	C5-C6-N6	-5.82	119.04	123.70
35	E	1939	A	C5-C6-N1	-5.82	114.79	117.70
35	E	2274	A	O4'-C1'-N9	5.82	112.86	108.20
35	E	1803	A	C4-C5-C6	5.82	119.91	117.00
35	E	2080	A	C5-C6-N1	-5.82	114.79	117.70
35	E	98	U	O4'-C1'-N1	5.82	112.85	108.20
35	E	502	A	O4'-C1'-N9	5.82	112.85	108.20
35	E	547	G	C5'-C4'-C3'	5.82	125.31	116.00
35	E	1591	C	N3-C4-N4	5.82	122.07	118.00
35	E	1665	C	N3-C4-N4	5.82	122.07	118.00
35	E	177	A	C4-C5-C6	5.82	119.91	117.00
35	E	1529	A	C4-C5-C6	5.82	119.91	117.00
35	E	1832	A	C5-C6-N6	-5.82	119.05	123.70
35	E	2070	C	N3-C4-N4	5.82	122.07	118.00
35	E	884	A	C5-C6-N6	-5.81	119.05	123.70
35	E	1335	U	C2-N1-C1'	5.81	124.68	117.70
35	E	431	G	O4'-C1'-N9	5.81	112.85	108.20
35	E	839	C	N3-C4-N4	5.81	122.07	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	845	A	C5-C6-N6	-5.81	119.05	123.70
35	E	975	U	O4'-C1'-N1	5.81	112.85	108.20
35	E	1086	A	C5-C6-N1	-5.81	114.79	117.70
35	E	1363	C	N3-C4-N4	5.81	122.07	118.00
35	E	1936	A	C4-C5-C6	5.81	119.91	117.00
35	E	648	A	C5-C6-N1	-5.81	114.80	117.70
35	E	507	A	C4-C5-C6	5.81	119.90	117.00
35	E	1302	A	O4'-C1'-N9	5.81	112.85	108.20
35	E	1750	C	N3-C4-N4	5.81	122.07	118.00
35	E	4	C	O4'-C1'-N1	5.81	112.84	108.20
35	E	2	A	C5-C6-N6	-5.80	119.06	123.70
35	E	273	G	O4'-C1'-N9	5.80	112.84	108.20
35	E	321	G	O4'-C1'-N9	5.80	112.84	108.20
35	E	609	A	C5-C6-N1	-5.80	114.80	117.70
35	E	47	A	C5-C6-N1	-5.80	114.80	117.70
35	E	382	G	C5-C6-O6	-5.80	125.12	128.60
35	E	543	U	O4'-C1'-N1	5.80	112.84	108.20
35	E	1260	G	O4'-C1'-N9	5.80	112.84	108.20
35	E	1652	A	C5-C6-N1	-5.80	114.80	117.70
35	E	1653	U	O4'-C1'-N1	5.80	112.84	108.20
35	E	1222	A	C5-C6-N6	-5.80	119.06	123.70
35	E	1756	G	O4'-C1'-N9	5.80	112.84	108.20
35	E	367	A	O4'-C1'-N9	5.80	112.84	108.20
35	E	1205	A	C5-C6-N6	-5.80	119.06	123.70
35	E	1883	C	N3-C4-N4	5.80	122.06	118.00
35	E	65	A	C4-C5-C6	5.80	119.90	117.00
35	E	257	A	C5-C6-N1	-5.80	114.80	117.70
35	E	684	A	O4'-C1'-N9	5.80	112.84	108.20
35	E	826	A	C5-C6-N6	-5.80	119.06	123.70
35	E	1985	C	N3-C4-C5	-5.80	119.58	121.90
35	E	2111	A	C5-C6-N6	-5.80	119.06	123.70
35	E	215	A	C5-C6-N6	-5.79	119.06	123.70
35	E	438	A	C5-C6-N1	-5.79	114.80	117.70
35	E	817	A	C5-C6-N1	-5.79	114.80	117.70
35	E	1181	C	N3-C4-C5	-5.79	119.58	121.90
35	E	1806	C	N3-C4-C5	-5.79	119.58	121.90
35	E	2014	C	N3-C4-N4	5.79	122.06	118.00
35	E	831	A	C5-C6-N6	-5.79	119.06	123.70
35	E	840	C	N3-C4-C5	-5.79	119.58	121.90
35	E	1280	U	O4'-C1'-N1	5.79	112.83	108.20
35	E	1346	G	N3-C2-N2	5.79	123.95	119.90
35	E	458	C	N3-C4-N4	5.79	122.05	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	706	G	O4'-C1'-N9	5.79	112.83	108.20
35	E	830	C	N3-C4-N4	5.79	122.05	118.00
35	E	939	U	O4'-C1'-N1	5.79	112.83	108.20
35	E	1365	A	C4-C5-C6	5.79	119.90	117.00
35	E	1574	A	C5-C6-N6	-5.79	119.07	123.70
35	E	1627	C	N3-C4-N4	5.79	122.06	118.00
35	E	186	C	N3-C4-N4	5.79	122.05	118.00
35	E	643	C	N3-C4-N4	5.79	122.05	118.00
35	E	1652	A	C4-C5-C6	5.79	119.89	117.00
35	E	1669	G	O4'-C1'-N9	5.79	112.83	108.20
35	E	161	A	C5-C6-N1	-5.79	114.81	117.70
35	E	396	C	N3-C4-N4	5.79	122.05	118.00
35	E	867	G	N3-C2-N2	5.79	123.95	119.90
35	E	1681	A	C5-C6-N6	-5.79	119.07	123.70
35	E	1881	C	N3-C4-C5	-5.79	119.58	121.90
35	E	2058	C	N3-C4-C5	-5.79	119.58	121.90
35	E	898	A	C5-C6-N1	-5.79	114.81	117.70
35	E	1620	A	C4-C5-C6	5.79	119.89	117.00
35	E	88	G	O4'-C1'-N9	5.79	112.83	108.20
35	E	330	A	O4'-C1'-N9	5.79	112.83	108.20
35	E	336	C	N3-C4-N4	5.79	122.05	118.00
35	E	941	U	O4'-C1'-N1	5.79	112.83	108.20
35	E	1292	A	C5-C6-N6	-5.79	119.07	123.70
35	E	1948	G	C5-C6-O6	-5.79	125.13	128.60
35	E	428	C	N3-C4-N4	5.78	122.05	118.00
35	E	546	U	C6-N1-C1'	-5.78	113.10	121.20
35	E	2295	G	O4'-C1'-N9	5.78	112.83	108.20
35	E	63	G	O4'-C1'-N9	5.78	112.83	108.20
35	E	242	A	C5-C6-N6	-5.78	119.08	123.70
35	E	1222	A	C5-C6-N1	-5.78	114.81	117.70
35	E	2292	G	O4'-C1'-N9	5.78	112.82	108.20
35	E	1822	A	C5-C6-N1	-5.78	114.81	117.70
35	E	704	A	C5-C6-N6	-5.78	119.08	123.70
35	E	1847	C	N3-C4-C5	-5.78	119.59	121.90
35	E	164	G	O4'-C1'-N9	5.78	112.82	108.20
35	E	260	A	C5-C6-N6	-5.78	119.08	123.70
35	E	307	C	N3-C4-N4	5.78	122.04	118.00
35	E	348	A	O4'-C1'-N9	5.78	112.82	108.20
35	E	1372	C	N3-C4-N4	5.78	122.04	118.00
35	E	1903	A	C5-C6-N6	-5.78	119.08	123.70
35	E	495	G	O4'-C1'-N9	5.77	112.82	108.20
35	E	499	A	O4'-C1'-N9	5.77	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	529	A	C4-C5-C6	5.77	119.89	117.00
35	E	646	A	O4'-C1'-N9	5.77	112.82	108.20
35	E	1086	A	O4'-C1'-N9	5.77	112.82	108.20
35	E	324	U	O4'-C1'-N1	5.77	112.82	108.20
35	E	142	A	C4-C5-C6	5.77	119.89	117.00
35	E	149	A	C5-C6-N6	-5.77	119.08	123.70
35	E	417	A	C5-C6-N6	-5.77	119.08	123.70
35	E	519	G	N3-C2-N2	5.77	123.94	119.90
35	E	590	C	N3-C4-N4	5.77	122.04	118.00
35	E	783	A	O4'-C1'-N9	5.77	112.82	108.20
35	E	1800	U	O4'-C1'-N1	5.77	112.82	108.20
35	E	1932	G	O4'-C1'-N9	5.77	112.81	108.20
35	E	2078	C	N3-C4-N4	5.77	122.04	118.00
35	E	39	A	C5-C6-N1	-5.77	114.82	117.70
35	E	1698	A	O4'-C1'-N9	5.77	112.81	108.20
35	E	890	C	N3-C4-C5	-5.77	119.59	121.90
35	E	2045	A	C4-C5-C6	5.77	119.88	117.00
35	E	288	A	C4-C5-C6	5.76	119.88	117.00
35	E	304	A	C5-C6-N6	-5.76	119.09	123.70
35	E	471	C	N3-C4-N4	5.76	122.03	118.00
35	E	2173	C	N3-C4-C5	-5.76	119.59	121.90
35	E	1356	C	N3-C4-N4	5.76	122.03	118.00
35	E	2159	A	O4'-C1'-N9	5.76	112.81	108.20
35	E	1600	A	C5-C6-N1	-5.76	114.82	117.70
35	E	2134	A	C5-C6-N1	-5.76	114.82	117.70
35	E	94	C	N3-C4-N4	5.76	122.03	118.00
35	E	974	A	C4-C5-C6	5.76	119.88	117.00
35	E	1184	C	N3-C4-N4	5.76	122.03	118.00
35	E	254	A	C4-C5-C6	5.76	119.88	117.00
35	E	386	A	C5-C6-N1	-5.76	114.82	117.70
35	E	387	C	N3-C4-N4	5.76	122.03	118.00
35	E	710	A	C5-C6-N6	-5.76	119.10	123.70
35	E	1176	A	C5-C6-N6	-5.76	119.09	123.70
35	E	1231	U	O4'-C1'-N1	5.76	112.80	108.20
35	E	1830	C	N3-C4-N4	5.76	122.03	118.00
35	E	778	A	C5-C6-N1	-5.75	114.82	117.70
35	E	934	C	N3-C4-C5	-5.75	119.60	121.90
35	E	493	A	C5-C6-N6	-5.75	119.10	123.70
35	E	518	C	N3-C4-N4	5.75	122.03	118.00
35	E	666	U	O4'-C1'-N1	5.75	112.80	108.20
35	E	977	A	C4-C5-C6	5.75	119.88	117.00
35	E	1261	A	C4-C5-C6	5.75	119.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	26	A	C5-C6-N6	-5.75	119.10	123.70
35	E	427	U	O4'-C1'-N1	5.75	112.80	108.20
35	E	531	A	O4'-C1'-N9	5.75	112.80	108.20
35	E	788	A	C5-C6-N6	-5.75	119.10	123.70
35	E	1251	C	N3-C4-N4	5.75	122.03	118.00
35	E	1661	A	C5-C6-N6	-5.75	119.10	123.70
35	E	2069	A	C5-C6-N1	-5.75	114.82	117.70
35	E	2130	C	N3-C4-N4	5.75	122.03	118.00
35	E	781	A	C5-C6-N6	-5.75	119.10	123.70
35	E	894	A	C5-C6-N6	-5.75	119.10	123.70
35	E	1601	A	C5-C6-N6	-5.75	119.10	123.70
35	E	2102	C	N3-C4-N4	5.75	122.03	118.00
35	E	2123	C	N3-C4-N4	5.75	122.03	118.00
35	E	14	C	N3-C4-C5	-5.75	119.60	121.90
35	E	246	A	C4-C5-C6	5.75	119.87	117.00
35	E	1279	A	C5-C6-N1	-5.75	114.83	117.70
35	E	1553	A	C5-C6-N6	-5.75	119.10	123.70
35	E	1581	A	C4-C5-C6	5.75	119.87	117.00
35	E	1772	G	N3-C2-N2	5.75	123.92	119.90
35	E	1830	C	N3-C4-C5	-5.75	119.60	121.90
35	E	2294	A	C5-C6-N6	-5.75	119.10	123.70
35	E	295	A	C5-C6-N6	-5.75	119.10	123.70
35	E	873	C	N3-C4-C5	-5.75	119.60	121.90
35	E	1817	G	O4'-C1'-N9	5.75	112.80	108.20
35	E	214	C	N3-C4-N4	5.74	122.02	118.00
35	E	675	A	C5-C6-N1	-5.74	114.83	117.70
35	E	1716	C	N3-C4-C5	-5.74	119.60	121.90
35	E	624	A	C5-C6-N1	-5.74	114.83	117.70
35	E	640	G	O4'-C1'-N9	5.74	112.79	108.20
35	E	1171	C	N3-C4-C5	-5.74	119.60	121.90
35	E	1629	C	N3-C4-C5	-5.74	119.60	121.90
35	E	1651	A	C5-C6-N6	-5.74	119.11	123.70
35	E	2145	A	C5-C6-N6	-5.74	119.11	123.70
35	E	2283	A	C4-C5-C6	5.74	119.87	117.00
35	E	599	A	C5-C6-N1	-5.74	114.83	117.70
35	E	1628	A	C4-C5-C6	5.74	119.87	117.00
35	E	2174	C	N3-C4-N4	5.74	122.02	118.00
35	E	438	A	C4-C5-C6	5.74	119.87	117.00
35	E	529	A	C5-C6-N1	-5.74	114.83	117.70
35	E	619	C	N3-C4-N4	5.74	122.02	118.00
35	E	1217	A	C5-C6-N6	-5.74	119.11	123.70
35	E	2228	C	N3-C4-C5	-5.74	119.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	504	A	O4'-C1'-N9	5.74	112.79	108.20
35	E	659	A	C5-C6-N6	-5.74	119.11	123.70
35	E	1265	A	C5-C6-N6	-5.74	119.11	123.70
35	E	1279	A	C5-C6-N6	-5.74	119.11	123.70
35	E	1875	G	O4'-C1'-N9	5.74	112.79	108.20
35	E	167	A	C5-C6-N6	-5.73	119.11	123.70
35	E	369	C	O4'-C1'-N1	5.73	112.79	108.20
35	E	618	G	O4'-C1'-N9	5.73	112.79	108.20
35	E	775	A	C4-C5-C6	5.73	119.87	117.00
35	E	1235	A	C5-C6-N6	-5.73	119.11	123.70
35	E	1240	A	C5-C6-N1	-5.73	114.83	117.70
35	E	1812	A	C4-C5-C6	5.73	119.87	117.00
35	E	28	A	O4'-C1'-N9	5.73	112.79	108.20
35	E	552	G	O4'-C1'-N9	5.73	112.79	108.20
35	E	773	U	O4'-C1'-N1	5.73	112.78	108.20
35	E	787	C	N3-C4-N4	5.73	122.01	118.00
35	E	791	G	O4'-C1'-N9	5.73	112.78	108.20
35	E	1255	A	C4-C5-C6	5.73	119.87	117.00
35	E	2031	A	C5-C6-N1	-5.73	114.83	117.70
35	E	28	A	C5-C6-N6	-5.73	119.12	123.70
35	E	516	A	O4'-C1'-N9	5.73	112.78	108.20
35	E	694	A	P-O3'-C3'	5.73	126.58	119.70
35	E	701	C	N3-C4-N4	5.73	122.01	118.00
35	E	783	A	C5-C6-N6	-5.73	119.12	123.70
35	E	142	A	C5-C6-N6	-5.73	119.12	123.70
35	E	1368	A	C5-C6-N6	-5.73	119.12	123.70
35	E	1616	C	N3-C4-C5	-5.73	119.61	121.90
35	E	114	C	N3-C4-C5	-5.72	119.61	121.90
35	E	978	U	O4'-C1'-N1	5.72	112.78	108.20
35	E	1175	A	C5-C6-N6	-5.72	119.12	123.70
35	E	1671	A	C5-C6-N6	-5.72	119.12	123.70
35	E	1781	A	C5-C6-N6	-5.72	119.12	123.70
35	E	1984	A	C5-C6-N1	-5.72	114.84	117.70
35	E	2237	G	O4'-C1'-N9	5.72	112.78	108.20
35	E	249	A	C5-C6-N6	-5.72	119.12	123.70
35	E	408	C	N3-C4-N4	5.72	122.01	118.00
35	E	507	A	O4'-C1'-N9	5.72	112.78	108.20
35	E	639	A	C5-C6-N1	-5.72	114.84	117.70
35	E	1289	G	O4'-C1'-N9	5.72	112.78	108.20
35	E	1974	C	N3-C4-C5	-5.72	119.61	121.90
35	E	2122	G	O4'-C1'-N9	5.72	112.78	108.20
35	E	916	A	C5-C6-N6	-5.72	119.12	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1553	A	C5-C6-N1	-5.72	114.84	117.70
35	E	875	A	C5-C6-N6	-5.72	119.12	123.70
35	E	942	C	C2'-C3'-O3'	5.72	122.85	113.70
35	E	974	A	C5-C6-N6	-5.72	119.12	123.70
35	E	1862	C	N3-C4-N4	5.72	122.00	118.00
35	E	2238	A	C5-C6-N1	-5.72	114.84	117.70
35	E	20	G	O4'-C1'-N9	5.72	112.77	108.20
35	E	809	A	C5-C6-N6	-5.72	119.13	123.70
35	E	822	A	C4-C5-C6	5.72	119.86	117.00
35	E	1172	C	N3-C4-N4	5.72	122.00	118.00
35	E	1248	A	O4'-C1'-N9	5.72	112.77	108.20
35	E	1370	A	C5-C6-N6	-5.72	119.13	123.70
35	E	1681	A	C5-C6-N1	-5.72	114.84	117.70
35	E	1966	C	C2-N1-C1'	5.72	125.09	118.80
35	E	2167	A	C5-C6-N6	-5.72	119.13	123.70
35	E	288	A	O4'-C1'-N9	5.71	112.77	108.20
35	E	984	A	C4-C5-C6	5.71	119.86	117.00
35	E	2145	A	C5-C6-N1	-5.71	114.84	117.70
35	E	2165	A	C4-C5-C6	5.71	119.86	117.00
35	E	466	G	O4'-C1'-N9	5.71	112.77	108.20
35	E	873	C	O4'-C1'-N1	5.71	112.77	108.20
35	E	1210	G	O4'-C1'-N9	5.71	112.77	108.20
35	E	261	A	C4-C5-C6	5.71	119.86	117.00
35	E	1167	C	N3-C4-C5	-5.71	119.61	121.90
35	E	2001	A	C4-C5-C6	5.71	119.86	117.00
35	E	2273	A	C5-C6-N1	-5.71	114.84	117.70
35	E	73	A	C4-C5-C6	5.71	119.86	117.00
35	E	148	G	O4'-C1'-N9	5.71	112.77	108.20
35	E	182	C	N3-C4-N4	5.71	122.00	118.00
35	E	1086	A	C4-C5-C6	5.71	119.86	117.00
35	E	2216	A	C4-C5-C6	5.71	119.86	117.00
35	E	711	A	C4-C5-C6	5.71	119.85	117.00
35	E	2005	A	C5-C6-N6	-5.71	119.13	123.70
35	E	2167	A	C4-C5-C6	5.71	119.85	117.00
35	E	1076	C	N3-C4-C5	-5.71	119.62	121.90
35	E	532	G	O4'-C1'-N9	5.70	112.76	108.20
35	E	718	A	O4'-C1'-N9	5.70	112.76	108.20
35	E	883	C	O4'-C1'-N1	5.70	112.76	108.20
35	E	1672	C	N3-C4-N4	5.70	121.99	118.00
35	E	596	A	C5-C6-N6	-5.70	119.14	123.70
35	E	1250	A	C5-C6-N1	-5.70	114.85	117.70
35	E	1292	A	C4-C5-C6	5.70	119.85	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1534	A	C4-C5-C6	5.70	119.85	117.00
35	E	610	A	C4-C5-C6	5.70	119.85	117.00
35	E	861	A	C4-C5-C6	5.70	119.85	117.00
35	E	915	A	C5-C6-N6	-5.70	119.14	123.70
35	E	1088	A	C5-C6-N1	-5.70	114.85	117.70
35	E	1192	A	C5-C6-N6	-5.70	119.14	123.70
35	E	469	G	O4'-C1'-N9	5.70	112.76	108.20
35	E	1077	C	O4'-C1'-N1	5.70	112.76	108.20
35	E	1263	G	O4'-C1'-N9	5.70	112.76	108.20
35	E	1529	A	O4'-C1'-N9	5.70	112.76	108.20
35	E	1676	A	C5-C6-N1	-5.70	114.85	117.70
35	E	1866	A	C5-C6-N6	-5.70	119.14	123.70
35	E	1966	C	N3-C4-N4	5.70	121.99	118.00
35	E	2211	C	N3-C4-N4	5.70	121.99	118.00
35	E	152	A	C4-C5-C6	5.70	119.85	117.00
35	E	742	A	C4-C5-C6	5.70	119.85	117.00
35	E	934	C	N3-C4-N4	5.70	121.99	118.00
35	E	569	A	C5-C6-N6	-5.69	119.14	123.70
35	E	745	C	C6-N1-C2	-5.69	118.02	120.30
35	E	935	A	C5-C6-N1	-5.69	114.85	117.70
35	E	123	A	C4-C5-C6	5.69	119.85	117.00
35	E	168	A	C5-C6-N6	-5.69	119.15	123.70
35	E	498	A	C5-C6-N6	-5.69	119.15	123.70
35	E	586	A	C5-C6-N6	-5.69	119.15	123.70
35	E	723	C	N3-C4-N4	5.69	121.98	118.00
35	E	1568	A	C5-C6-N6	-5.69	119.15	123.70
35	E	1595	A	C5-C6-N1	-5.69	114.85	117.70
35	E	1799	A	C5-C6-N1	-5.69	114.85	117.70
35	E	1845	C	N3-C4-N4	5.69	121.98	118.00
35	E	227	U	O4'-C1'-N1	5.69	112.75	108.20
35	E	1627	C	O4'-C1'-N1	5.69	112.75	108.20
35	E	1926	G	O4'-C1'-N9	5.69	112.75	108.20
35	E	542	C	N3-C4-N4	5.69	121.98	118.00
35	E	668	C	N3-C4-N4	5.69	121.98	118.00
35	E	1896	C	N3-C4-C5	-5.69	119.62	121.90
35	E	2090	U	O4'-C1'-N1	5.69	112.75	108.20
35	E	1275	A	C4-C5-C6	5.69	119.84	117.00
35	E	639	A	C5-C6-N6	-5.68	119.15	123.70
35	E	1257	C	N3-C4-N4	5.68	121.98	118.00
35	E	68	A	C5-C6-N6	-5.68	119.16	123.70
35	E	1205	A	O4'-C1'-N9	5.68	112.75	108.20
35	E	1539	A	C5-C6-N6	-5.68	119.16	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	112	A	C4-C5-C6	5.68	119.84	117.00
35	E	479	G	O4'-C1'-N9	5.68	112.74	108.20
35	E	1807	U	O4'-C1'-N1	5.68	112.74	108.20
35	E	1811	C	N3-C4-N4	5.68	121.97	118.00
35	E	2032	U	C2-N1-C1'	5.68	124.52	117.70
35	E	2149	C	N3-C4-N4	5.68	121.98	118.00
35	E	945	C	N3-C4-N4	5.68	121.97	118.00
35	E	2245	A	O4'-C1'-N9	5.68	112.74	108.20
35	E	256	A	C5-C6-N6	-5.68	119.16	123.70
35	E	522	A	C4-C5-C6	5.68	119.84	117.00
35	E	735	A	C5-C6-N6	-5.68	119.16	123.70
35	E	2047	A	C5-C6-N6	-5.68	119.16	123.70
35	E	2245	A	C5-C6-N1	-5.68	114.86	117.70
35	E	417	A	O4'-C1'-N9	5.67	112.74	108.20
35	E	467	A	C5-C6-N1	-5.67	114.86	117.70
35	E	2267	A	O4'-C1'-N9	5.67	112.74	108.20
35	E	782	A	C5-C6-N6	-5.67	119.16	123.70
35	E	2048	A	O4'-C1'-N9	5.67	112.74	108.20
35	E	44	C	N3-C4-C5	-5.67	119.63	121.90
35	E	314	A	C5-C6-N6	-5.67	119.16	123.70
35	E	598	A	C5-C6-N6	-5.67	119.16	123.70
35	E	698	C	N3-C4-N4	5.67	121.97	118.00
35	E	732	C	P-O3'-C3'	5.67	126.51	119.70
35	E	1987	A	O4'-C1'-N9	5.67	112.74	108.20
35	E	690	A	C5-C6-N1	-5.67	114.86	117.70
35	E	860	U	O4'-C1'-N1	5.67	112.74	108.20
35	E	362	C	N3-C4-C5	-5.67	119.63	121.90
35	E	1915	G	O4'-C1'-N9	5.67	112.73	108.20
35	E	492	A	C4-C5-C6	5.67	119.83	117.00
35	E	500	A	C5-C6-N6	-5.67	119.17	123.70
35	E	1529	A	C5-C6-N6	-5.67	119.17	123.70
35	E	994	G	O4'-C1'-N9	5.67	112.73	108.20
35	E	1815	A	C5-C6-N1	-5.67	114.87	117.70
35	E	1942	A	C5-C6-N6	-5.67	119.17	123.70
35	E	2048	A	C5-C6-N6	-5.67	119.17	123.70
35	E	293	U	O4'-C1'-N1	5.66	112.73	108.20
35	E	516	A	C5-C6-N6	-5.66	119.17	123.70
35	E	858	A	C5-C6-N1	-5.66	114.87	117.70
35	E	861	A	O4'-C1'-N9	5.66	112.73	108.20
35	E	959	A	C5-C6-N1	-5.66	114.87	117.70
35	E	1270	A	C5-C6-N1	-5.66	114.87	117.70
35	E	1959	C	N3-C4-C5	-5.66	119.63	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	62	A	O4'-C1'-N9	5.66	112.73	108.20
35	E	174	U	O4'-C1'-N1	5.66	112.73	108.20
35	E	366	C	N3-C4-C5	-5.66	119.64	121.90
35	E	2011	A	C5-C6-N6	-5.66	119.17	123.70
35	E	2098	C	N3-C4-N4	5.66	121.96	118.00
35	E	765	A	C5-C6-N1	-5.66	114.87	117.70
35	E	1086	A	C5-C6-N6	-5.66	119.17	123.70
35	E	1181	C	N3-C4-N4	5.66	121.96	118.00
35	E	1922	G	O4'-C1'-N9	5.66	112.73	108.20
35	E	2065	A	C5-C6-N1	-5.66	114.87	117.70
35	E	434	A	C5-C6-N1	-5.66	114.87	117.70
35	E	571	A	C5-C6-N1	-5.66	114.87	117.70
35	E	707	C	N3-C4-N4	5.66	121.96	118.00
35	E	990	A	C5-C6-N6	-5.66	119.17	123.70
35	E	852	A	C5-C6-N6	-5.66	119.18	123.70
35	E	1733	A	C5-C6-N6	-5.66	119.18	123.70
35	E	2236	C	N3-C4-C5	-5.66	119.64	121.90
35	E	910	A	C4-C5-C6	5.65	119.83	117.00
35	E	1299	U	O4'-C1'-N1	5.65	112.72	108.20
35	E	2141	G	O4'-C1'-N9	5.65	112.72	108.20
35	E	2236	C	N3-C4-N4	5.65	121.96	118.00
35	E	2299	A	C5-C6-N6	-5.65	119.18	123.70
35	E	300	A	C5-C6-N1	-5.65	114.88	117.70
35	E	647	A	O4'-C1'-N9	5.65	112.72	108.20
35	E	728	A	C5-C6-N6	-5.65	119.18	123.70
35	E	771	A	C5-C6-N6	-5.65	119.18	123.70
35	E	1279	A	C4-C5-C6	5.65	119.83	117.00
35	E	2173	C	N3-C4-N4	5.65	121.95	118.00
35	E	1999	A	O4'-C1'-N9	5.65	112.72	108.20
35	E	2264	A	C5-C6-N1	-5.65	114.88	117.70
35	E	1215	A	C5-C6-N6	-5.65	119.18	123.70
35	E	1383	G	O4'-C1'-N9	5.65	112.72	108.20
35	E	2039	A	C5-C6-N1	-5.65	114.88	117.70
35	E	141	A	C5-C6-N1	-5.65	114.88	117.70
35	E	2169	A	C5-C6-N6	-5.65	119.18	123.70
35	E	237	A	C4-C5-C6	5.64	119.82	117.00
35	E	633	A	C4-C5-C6	5.64	119.82	117.00
35	E	941	U	P-O3'-C3'	5.64	126.47	119.70
35	E	2105	C	N3-C4-N4	5.64	121.95	118.00
35	E	348	A	C5-C6-N1	-5.64	114.88	117.70
35	E	629	C	N3-C4-N4	5.64	121.95	118.00
35	E	282	C	N3-C4-N4	5.64	121.95	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	447	A	C5-C6-N6	-5.64	119.19	123.70
35	E	503	A	C5-C6-N6	-5.64	119.19	123.70
35	E	754	G	O4'-C1'-N9	5.64	112.71	108.20
35	E	1637	G	N3-C2-N2	5.64	123.85	119.90
35	E	407	G	O4'-C1'-N9	5.64	112.71	108.20
35	E	865	A	C5-C6-N6	-5.64	119.19	123.70
35	E	880	A	C4-C5-C6	5.64	119.82	117.00
35	E	1355	A	C5-C6-N6	-5.64	119.19	123.70
35	E	1574	A	C5-C6-N1	-5.64	114.88	117.70
35	E	1793	G	O4'-C1'-N9	5.64	112.71	108.20
35	E	1904	U	O4'-C1'-N1	5.64	112.71	108.20
35	E	1982	C	N3-C4-N4	5.63	121.94	118.00
35	E	40	A	C5-C6-N6	-5.63	119.19	123.70
35	E	348	A	C5-C6-N6	-5.63	119.19	123.70
35	E	157	G	O4'-C1'-N9	5.63	112.70	108.20
35	E	954	G	O4'-C1'-N9	5.63	112.70	108.20
35	E	1343	A	C5-C6-N1	-5.63	114.88	117.70
35	E	1232	C	N3-C4-N4	5.63	121.94	118.00
35	E	1261	A	O4'-C1'-N9	5.63	112.70	108.20
35	E	355	G	O4'-C1'-N9	5.63	112.70	108.20
35	E	1237	G	O4'-C1'-N9	5.63	112.70	108.20
35	E	1357	U	O4'-C1'-N1	5.63	112.70	108.20
35	E	1679	A	C5-C6-N6	-5.63	119.20	123.70
35	E	1833	U	O4'-C1'-N1	5.63	112.70	108.20
35	E	2037	A	O4'-C1'-N9	5.63	112.70	108.20
35	E	2137	C	N3-C4-C5	-5.63	119.65	121.90
35	E	1869	G	O4'-C1'-N9	5.63	112.70	108.20
35	E	2036	A	C5-C6-N6	-5.63	119.20	123.70
35	E	2166	C	N3-C4-C5	-5.63	119.65	121.90
35	E	662	C	N3-C4-N4	5.62	121.94	118.00
4	t	122	TYR	CB-CG-CD1	5.62	124.37	121.00
35	E	160	A	O4'-C1'-N9	5.62	112.70	108.20
35	E	444	A	C5-C6-N6	-5.62	119.20	123.70
35	E	1241	A	C5-C6-N1	-5.62	114.89	117.70
35	E	2199	A	C5-C6-N6	-5.62	119.20	123.70
35	E	727	C	N3-C4-N4	5.62	121.94	118.00
35	E	771	A	C4-C5-C6	5.62	119.81	117.00
35	E	1203	G	O4'-C1'-N9	5.62	112.70	108.20
35	E	1987	A	C5-C6-N6	-5.62	119.20	123.70
35	E	2035	A	O4'-C1'-N9	5.62	112.70	108.20
35	E	2198	C	N3-C4-N4	5.62	121.93	118.00
35	E	499	A	C5-C6-N6	-5.62	119.20	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	781	A	O4'-C1'-N9	5.62	112.70	108.20
30	m	144	GLN	N-CA-CB	5.62	120.71	110.60
35	E	180	A	C5-C6-N6	-5.62	119.20	123.70
35	E	367	A	C4-C5-C6	5.62	119.81	117.00
35	E	760	C	N3-C4-C5	-5.62	119.65	121.90
35	E	928	C	N3-C4-N4	5.62	121.93	118.00
35	E	1789	A	C4-C5-C6	5.62	119.81	117.00
35	E	2050	C	O4'-C1'-N1	5.62	112.69	108.20
35	E	1907	C	N3-C4-N4	5.62	121.93	118.00
35	E	151	A	C4-C5-C6	5.62	119.81	117.00
35	E	648	A	C4-C5-C6	5.62	119.81	117.00
35	E	1170	C	N3-C4-C5	-5.62	119.65	121.90
35	E	1268	A	C5-C6-N1	-5.62	114.89	117.70
35	E	1824	A	C4-C5-C6	5.62	119.81	117.00
35	E	2044	G	O4'-C1'-N9	5.62	112.69	108.20
35	E	44	C	N3-C4-N4	5.61	121.93	118.00
35	E	1605	A	C5-C6-N1	-5.61	114.89	117.70
35	E	1651	A	C4-C5-C6	5.61	119.81	117.00
35	E	2278	G	O4'-C1'-N9	5.61	112.69	108.20
35	E	2297	U	O4'-C1'-N1	5.61	112.69	108.20
35	E	414	A	C5-C6-N1	-5.61	114.89	117.70
35	E	433	G	O4'-C1'-N9	5.61	112.69	108.20
35	E	816	C	N3-C4-N4	5.61	121.93	118.00
35	E	990	A	O4'-C1'-N9	5.61	112.69	108.20
35	E	1312	A	C5-C6-N6	-5.61	119.21	123.70
35	E	1552	A	C5-C6-N1	-5.61	114.89	117.70
35	E	504	A	C5-C6-N6	-5.61	119.21	123.70
35	E	586	A	O4'-C1'-N9	5.61	112.69	108.20
35	E	599	A	C5-C6-N6	-5.61	119.21	123.70
35	E	2260	A	C5-C6-N1	-5.61	114.89	117.70
2	q	30	ALA	N-CA-CB	5.61	117.95	110.10
35	E	1865	A	O4'-C1'-N9	5.61	112.69	108.20
35	E	1881	C	N3-C4-N4	5.61	121.93	118.00
35	E	254	A	P-O3'-C3'	5.61	126.43	119.70
35	E	268	C	N3-C4-N4	5.61	121.92	118.00
35	E	879	C	N3-C4-N4	5.61	121.92	118.00
35	E	1863	C	N3-C4-C5	-5.61	119.66	121.90
35	E	2049	C	N3-C4-C5	-5.61	119.66	121.90
35	E	2192	A	C5-C6-N1	-5.61	114.90	117.70
35	E	57	G	O4'-C1'-N9	5.61	112.68	108.20
35	E	501	A	C5-C6-N6	-5.61	119.22	123.70
35	E	506	A	C5-C6-N6	-5.61	119.22	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	821	C	O4'-C1'-N1	5.61	112.69	108.20
35	E	992	A	C5-C6-N6	-5.61	119.22	123.70
35	E	1248	A	C5-C6-N6	-5.61	119.22	123.70
35	E	2272	A	C5-C6-N6	-5.61	119.22	123.70
3	r	85	TYR	CB-CG-CD2	-5.60	117.64	121.00
35	E	1619	A	C4-C5-C6	5.60	119.80	117.00
35	E	1919	A	O4'-C1'-N9	5.60	112.68	108.20
35	E	2027	C	C6-N1-C1'	-5.60	114.08	120.80
35	E	159	G	N3-C2-N2	5.60	123.82	119.90
35	E	747	U	O4'-C1'-N1	5.60	112.68	108.20
35	E	750	C	N3-C4-C5	-5.60	119.66	121.90
35	E	874	C	N3-C4-N4	5.60	121.92	118.00
35	E	922	C	N3-C4-C5	-5.60	119.66	121.90
35	E	1829	C	N3-C4-C5	-5.60	119.66	121.90
35	E	1919	A	C5-C6-N1	-5.60	114.90	117.70
35	E	2076	A	C5-C6-N1	-5.60	114.90	117.70
35	E	2270	C	N3-C4-N4	5.60	121.92	118.00
35	E	352	A	C5-C6-N6	-5.60	119.22	123.70
35	E	1211	G	O4'-C1'-N9	5.60	112.68	108.20
35	E	1845	C	N3-C4-C5	-5.60	119.66	121.90
35	E	577	A	C5-C6-N6	-5.60	119.22	123.70
35	E	779	A	C5-C6-N6	-5.60	119.22	123.70
35	E	1784	C	N3-C4-C5	-5.60	119.66	121.90
35	E	2283	A	C5-C6-N6	-5.60	119.22	123.70
35	E	107	A	C5-C6-N6	-5.60	119.22	123.70
35	E	217	C	N3-C4-N4	5.60	121.92	118.00
35	E	569	A	C5-C6-N1	-5.60	114.90	117.70
35	E	810	U	C2'-C3'-O3'	5.60	122.66	113.70
35	E	1823	G	O4'-C1'-N9	5.60	112.68	108.20
35	E	2172	G	O4'-C1'-N9	5.60	112.68	108.20
35	E	314	A	C5-C6-N1	-5.59	114.90	117.70
35	E	318	C	N3-C4-N4	5.59	121.92	118.00
35	E	376	C	N3-C4-N4	5.59	121.92	118.00
35	E	2104	A	C5-C6-N1	-5.59	114.90	117.70
35	E	56	U	O4'-C1'-N1	5.59	112.67	108.20
35	E	364	G	O4'-C1'-N9	5.59	112.67	108.20
35	E	587	A	C5-C6-N6	-5.59	119.23	123.70
35	E	778	A	C5-C6-N6	-5.59	119.23	123.70
35	E	1706	A	O4'-C1'-N9	5.59	112.67	108.20
35	E	208	G	O4'-C1'-N9	5.59	112.67	108.20
35	E	474	C	N3-C4-N4	5.59	121.91	118.00
35	E	1196	A	C5-C6-N6	-5.59	119.23	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1323	A	C5-C6-N1	-5.59	114.91	117.70
35	E	2026	A	C5-C6-N6	-5.59	119.23	123.70
35	E	879	C	O4'-C1'-N1	5.59	112.67	108.20
35	E	1255	A	C5-C6-N6	-5.59	119.23	123.70
35	E	1698	A	C5-C6-N1	-5.59	114.91	117.70
35	E	256	A	C5-C6-N1	-5.59	114.91	117.70
35	E	101	C	N3-C4-N4	5.58	121.91	118.00
35	E	139	G	O4'-C1'-N9	5.58	112.67	108.20
35	E	452	C	N3-C4-N4	5.58	121.91	118.00
35	E	942	C	N3-C4-N4	5.58	121.91	118.00
35	E	81	A	C5-C6-N1	-5.58	114.91	117.70
35	E	112	A	C5-C6-N6	-5.58	119.23	123.70
35	E	595	A	C5-C6-N6	-5.58	119.23	123.70
35	E	1180	A	C5-C6-N6	-5.58	119.23	123.70
35	E	1626	C	N3-C4-C5	-5.58	119.67	121.90
35	E	788	A	C5-C6-N1	-5.58	114.91	117.70
35	E	995	C	N3-C4-C5	-5.58	119.67	121.90
35	E	1312	A	O4'-C1'-N9	5.58	112.67	108.20
35	E	43	A	C5-C6-N6	-5.58	119.24	123.70
35	E	1878	A	C5-C6-N6	-5.58	119.24	123.70
35	E	2060	C	N3-C4-N4	5.58	121.91	118.00
35	E	124	A	C5-C6-N1	-5.58	114.91	117.70
35	E	675	A	C4-C5-C6	5.58	119.79	117.00
35	E	833	A	C5-C6-N1	-5.58	114.91	117.70
35	E	2274	A	C5-C6-N6	-5.58	119.24	123.70
35	E	100	A	C5-C6-N1	-5.58	114.91	117.70
35	E	158	C	N3-C4-N4	5.58	121.90	118.00
35	E	1684	C	N3-C4-C5	-5.58	119.67	121.90
35	E	2048	A	C5-C6-N1	-5.58	114.91	117.70
35	E	2107	A	C4-C5-C6	5.58	119.79	117.00
35	E	2130	C	N3-C4-C5	-5.58	119.67	121.90
35	E	837	C	N3-C4-N4	5.57	121.90	118.00
35	E	1215	A	C5-C6-N1	-5.57	114.91	117.70
35	E	1781	A	C5-C6-N1	-5.57	114.91	117.70
35	E	1812	A	C5-C6-N1	-5.57	114.91	117.70
35	E	1574	A	O4'-C1'-N9	5.57	112.66	108.20
35	E	2259	A	C5-C6-N6	-5.57	119.24	123.70
35	E	279	A	C5-C6-N1	-5.57	114.92	117.70
20	f	172	TYR	CB-CG-CD1	5.57	124.34	121.00
35	E	446	A	C5-C6-N1	-5.57	114.92	117.70
35	E	1670	A	C5-C6-N6	-5.57	119.25	123.70
35	E	425	A	C5-C6-N6	-5.57	119.25	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	577	A	C5-C6-N1	-5.57	114.92	117.70
35	E	1528	C	N3-C4-N4	5.57	121.90	118.00
35	E	1631	A	C5-C6-N6	-5.57	119.25	123.70
35	E	257	A	C5-C6-N6	-5.56	119.25	123.70
35	E	960	A	C5-C6-N6	-5.56	119.25	123.70
35	E	821	C	N3-C4-N4	5.56	121.89	118.00
35	E	1287	A	O4'-C1'-N9	5.56	112.65	108.20
35	E	1960	A	C5-C6-N6	-5.56	119.25	123.70
35	E	2066	C	N3-C4-C5	-5.56	119.67	121.90
35	E	161	A	C5-C6-N6	-5.56	119.25	123.70
35	E	1530	C	N3-C4-N4	5.56	121.89	118.00
35	E	1610	A	C5-C6-N1	-5.56	114.92	117.70
35	E	231	A	O4'-C1'-N9	5.56	112.65	108.20
35	E	1999	A	C5-C6-N6	-5.56	119.25	123.70
35	E	2000	C	N3-C4-C5	-5.56	119.68	121.90
35	E	82	A	C5-C6-N6	-5.56	119.25	123.70
35	E	362	C	N3-C4-N4	5.56	121.89	118.00
35	E	1255	A	O4'-C1'-N9	5.56	112.65	108.20
35	E	1676	A	C5-C6-N6	-5.56	119.25	123.70
35	E	1866	A	O4'-C1'-N9	5.56	112.65	108.20
35	E	251	A	P-O3'-C3'	5.56	126.37	119.70
35	E	1877	U	O4'-C1'-N1	5.56	112.64	108.20
35	E	1991	C	N3-C4-N4	5.56	121.89	118.00
35	E	2036	A	C5-C6-N1	-5.56	114.92	117.70
35	E	177	A	C5-C6-N1	-5.55	114.92	117.70
35	E	644	C	O4'-C1'-N1	5.55	112.64	108.20
35	E	724	A	C5'-C4'-O4'	5.55	115.77	109.10
35	E	951	U	O4'-C1'-N1	5.55	112.64	108.20
35	E	1689	A	C5-C6-N1	-5.55	114.92	117.70
35	E	704	A	C5-C6-N1	-5.55	114.92	117.70
35	E	873	C	N3-C4-N4	5.55	121.89	118.00
35	E	1217	A	O4'-C1'-N9	5.55	112.64	108.20
35	E	1670	A	C4-C5-C6	5.55	119.78	117.00
35	E	1925	A	O4'-C1'-N9	5.55	112.64	108.20
35	E	623	C	N3-C4-N4	5.55	121.89	118.00
35	E	902	A	C5-C6-N6	-5.55	119.26	123.70
35	E	1523	C	N3-C4-N4	5.55	121.89	118.00
35	E	1607	A	O4'-C1'-N9	5.55	112.64	108.20
35	E	59	C	N3-C4-N4	5.55	121.89	118.00
35	E	102	A	O4'-C1'-N9	5.55	112.64	108.20
35	E	384	G	O4'-C1'-N9	5.55	112.64	108.20
35	E	392	A	C5-C6-N6	-5.55	119.26	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	561	A	O4'-C1'-N9	5.55	112.64	108.20
35	E	1525	C	N3-C4-N4	5.55	121.89	118.00
35	E	1687	A	C4-C5-C6	5.55	119.77	117.00
35	E	124	A	C5-C6-N6	-5.55	119.26	123.70
35	E	1724	A	C5-C6-N1	-5.55	114.93	117.70
35	E	2126	A	C5-C6-N6	-5.55	119.26	123.70
35	E	380	U	O4'-C1'-N1	5.55	112.64	108.20
35	E	438	A	C5-C6-N6	-5.55	119.26	123.70
35	E	1192	A	C5-C6-N1	-5.55	114.93	117.70
35	E	1308	A	C5-C6-N1	-5.55	114.93	117.70
35	E	1662	A	C5-C6-N6	-5.55	119.26	123.70
35	E	1831	C	N3-C4-N4	5.55	121.88	118.00
35	E	2050	C	N3-C4-C5	-5.55	119.68	121.90
35	E	2195	G	O4'-C1'-N9	5.55	112.64	108.20
35	E	511	G	O4'-C1'-N9	5.54	112.64	108.20
35	E	549	A	C5-C6-N1	-5.54	114.93	117.70
35	E	187	C	N3-C4-N4	5.54	121.88	118.00
35	E	1264	A	C5-C6-N6	-5.54	119.27	123.70
35	E	1622	G	O4'-C1'-N9	5.54	112.64	108.20
35	E	1728	C	N3-C4-N4	5.54	121.88	118.00
35	E	2063	A	C5-C6-N1	-5.54	114.93	117.70
35	E	2189	A	O4'-C1'-N9	5.54	112.64	108.20
35	E	19	A	C5-C6-N1	-5.54	114.93	117.70
35	E	831	A	C5-C6-N1	-5.54	114.93	117.70
35	E	2097	U	C2-N1-C1'	5.54	124.35	117.70
35	E	2100	C	N3-C4-N4	5.54	121.88	118.00
35	E	2117	C	O4'-C1'-N1	5.54	112.63	108.20
35	E	2267	A	C5-C6-N6	-5.54	119.27	123.70
35	E	527	A	C5-C6-N1	-5.54	114.93	117.70
35	E	972	A	C5-C6-N6	-5.54	119.27	123.70
35	E	61	C	N3-C4-N4	5.54	121.88	118.00
35	E	107	A	O4'-C1'-N9	5.54	112.63	108.20
35	E	215	A	C5-C6-N1	-5.54	114.93	117.70
35	E	793	A	C4-C5-C6	5.54	119.77	117.00
35	E	1317	G	O4'-C1'-N9	5.54	112.63	108.20
35	E	1951	A	C4-C5-C6	5.54	119.77	117.00
35	E	216	A	C5-C6-N6	-5.54	119.27	123.70
35	E	735	A	C5-C6-N1	-5.54	114.93	117.70
35	E	2124	G	O4'-C1'-N9	5.54	112.63	108.20
35	E	125	A	O4'-C1'-N9	5.54	112.63	108.20
35	E	475	A	C4-C5-C6	5.54	119.77	117.00
35	E	562	A	C5-C6-N6	-5.54	119.27	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	799	A	C4-C5-C6	5.54	119.77	117.00
35	E	1241	A	O4'-C1'-N9	5.54	112.63	108.20
35	E	1353	A	C5-C6-N6	-5.54	119.27	123.70
35	E	1749	G	O4'-C1'-N9	5.54	112.63	108.20
35	E	1822	A	C5-C6-N6	-5.54	119.27	123.70
35	E	1996	A	C5-C6-N1	-5.54	114.93	117.70
35	E	2000	C	N3-C4-N4	5.54	121.88	118.00
35	E	2007	A	C4-C5-C6	5.54	119.77	117.00
35	E	2031	A	C5-C6-N6	-5.54	119.27	123.70
35	E	2076	A	C5-C6-N6	-5.54	119.27	123.70
35	E	914	C	N3-C4-C5	-5.53	119.69	121.90
35	E	968	U	O4'-C1'-N1	5.53	112.63	108.20
35	E	1975	A	C5-C6-N6	-5.53	119.27	123.70
35	E	246	A	O4'-C1'-N9	5.53	112.62	108.20
35	E	280	C	N3-C4-C5	-5.53	119.69	121.90
35	E	363	A	C5-C6-N1	-5.53	114.94	117.70
35	E	1818	A	C5-C6-N6	-5.53	119.28	123.70
35	E	1992	A	C5-C6-N6	-5.53	119.28	123.70
35	E	2126	A	C5-C6-N1	-5.53	114.94	117.70
35	E	580	C	N3-C4-N4	5.53	121.87	118.00
35	E	832	G	O4'-C1'-N9	5.53	112.62	108.20
35	E	1695	A	C5-C6-N6	-5.53	119.28	123.70
35	E	2088	A	O4'-C1'-N9	5.53	112.62	108.20
35	E	1600	A	O4'-C1'-N9	5.53	112.62	108.20
35	E	1620	A	C5-C6-N1	-5.53	114.94	117.70
35	E	1863	C	N3-C4-N4	5.53	121.87	118.00
35	E	2168	C	N3-C4-N4	5.53	121.87	118.00
35	E	2300	A	C5-C6-N1	-5.53	114.94	117.70
35	E	183	C	N3-C4-N4	5.53	121.87	118.00
35	E	1624	C	N3-C4-C5	-5.53	119.69	121.90
35	E	2037	A	C5-C6-N6	-5.53	119.28	123.70
35	E	2267	A	C5-C6-N1	-5.53	114.94	117.70
35	E	627	C	N3-C4-N4	5.52	121.87	118.00
35	E	644	C	N3-C4-C5	-5.52	119.69	121.90
35	E	1270	A	C5-C6-N6	-5.52	119.28	123.70
35	E	1374	A	C5-C6-N1	-5.52	114.94	117.70
35	E	1791	C	N3-C4-C5	-5.52	119.69	121.90
35	E	630	G	O4'-C1'-N9	5.52	112.62	108.20
35	E	674	A	C5-C6-N1	-5.52	114.94	117.70
35	E	1229	C	N3-C4-C5	-5.52	119.69	121.90
35	E	1323	A	O4'-C1'-N9	5.52	112.62	108.20
35	E	2035	A	C5-C6-N6	-5.52	119.28	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2098	C	O4'-C1'-N1	5.52	112.62	108.20
35	E	277	U	O4'-C1'-N1	5.52	112.62	108.20
35	E	833	A	C5-C6-N6	-5.52	119.28	123.70
35	E	1275	A	C5-C6-N1	-5.52	114.94	117.70
35	E	1628	A	C5-C6-N1	-5.52	114.94	117.70
35	E	40	A	O4'-C1'-N9	5.52	112.61	108.20
35	E	122	A	C5-C6-N6	-5.52	119.29	123.70
35	E	270	C	N3-C4-N4	5.52	121.86	118.00
35	E	464	C	N3-C4-C5	-5.52	119.69	121.90
35	E	1605	A	C4-C5-C6	5.52	119.76	117.00
35	E	418	G	O4'-C1'-N9	5.52	112.61	108.20
35	E	369	C	N3-C4-C5	-5.51	119.69	121.90
35	E	607	A	C5-C6-N6	-5.51	119.29	123.70
35	E	2037	A	C5-C6-N1	-5.51	114.94	117.70
35	E	1688	C	N3-C4-C5	-5.51	119.69	121.90
35	E	2315	A	O4'-C1'-N9	5.51	112.61	108.20
35	E	728	A	C5-C6-N1	-5.51	114.94	117.70
35	E	786	A	C5-C6-N6	-5.51	119.29	123.70
35	E	1189	A	C5-C6-N6	-5.51	119.29	123.70
35	E	1297	C	N3-C4-N4	5.51	121.86	118.00
35	E	1978	C	N3-C4-N4	5.51	121.86	118.00
35	E	2056	A	O4'-C1'-N9	5.51	112.61	108.20
35	E	106	G	O4'-C1'-N9	5.51	112.61	108.20
35	E	637	C	N3-C4-C5	-5.51	119.70	121.90
35	E	1249	G	N3-C2-N2	5.51	123.75	119.90
35	E	135	C	N3-C4-N4	5.51	121.86	118.00
35	E	300	A	O4'-C1'-N9	5.51	112.61	108.20
35	E	655	A	O4'-C1'-N9	5.51	112.61	108.20
35	E	1851	C	N3-C4-N4	5.51	121.86	118.00
35	E	1977	G	O4'-C1'-N9	5.51	112.61	108.20
35	E	2026	A	C5-C6-N1	-5.51	114.95	117.70
35	E	2136	A	C5-C6-N1	-5.51	114.95	117.70
35	E	255	A	O4'-C1'-N9	5.50	112.60	108.20
35	E	1702	A	C5-C6-N1	-5.50	114.95	117.70
35	E	438	A	O4'-C1'-N9	5.50	112.60	108.20
35	E	961	A	C5-C6-N6	-5.50	119.30	123.70
35	E	1313	A	C5-C6-N6	-5.50	119.30	123.70
35	E	1667	G	O4'-C1'-N9	5.50	112.60	108.20
35	E	1959	C	N3-C4-N4	5.50	121.85	118.00
35	E	38	C	N3-C4-C5	-5.50	119.70	121.90
35	E	120	C	N3-C4-N4	5.50	121.85	118.00
35	E	250	A	C5-C6-N6	-5.50	119.30	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	270	C	N3-C4-C5	-5.50	119.70	121.90
35	E	870	U	O4'-C1'-N1	5.50	112.60	108.20
35	E	993	A	C5-C6-N6	-5.50	119.30	123.70
35	E	1353	A	C5-C6-N1	-5.50	114.95	117.70
35	E	1548	C	N3-C4-C5	-5.50	119.70	121.90
35	E	2033	C	N3-C4-N4	5.50	121.85	118.00
35	E	806	C	N3-C4-N4	5.50	121.85	118.00
35	E	1328	A	C5-C6-N6	-5.50	119.30	123.70
35	E	197	C	N3-C4-N4	5.50	121.85	118.00
35	E	846	U	O4'-C1'-N1	5.50	112.60	108.20
35	E	1265	A	C5-C6-N1	-5.50	114.95	117.70
35	E	1286	A	C4-C5-C6	5.50	119.75	117.00
35	E	2049	C	N3-C4-N4	5.50	121.85	118.00
35	E	345	A	O4'-C1'-N9	5.50	112.60	108.20
35	E	685	G	O4'-C1'-N9	5.50	112.60	108.20
35	E	841	C	N3-C4-N4	5.50	121.85	118.00
35	E	132	G	O4'-C1'-N9	5.50	112.60	108.20
35	E	133	G	O4'-C1'-N9	5.50	112.60	108.20
35	E	387	C	N3-C4-C5	-5.50	119.70	121.90
35	E	984	A	C5-C6-N1	-5.50	114.95	117.70
35	E	1681	A	O4'-C1'-N9	5.50	112.60	108.20
35	E	184	A	C5-C6-N1	-5.49	114.95	117.70
35	E	233	G	O4'-C1'-N9	5.49	112.59	108.20
35	E	749	C	N3-C4-N4	5.49	121.85	118.00
35	E	1671	A	C4-C5-C6	5.49	119.75	117.00
35	E	1920	A	C5-C6-N6	-5.49	119.31	123.70
35	E	2105	C	N3-C4-C5	-5.49	119.70	121.90
35	E	1937	A	C5-C6-N6	-5.49	119.31	123.70
35	E	769	A	C5-C6-N6	-5.49	119.31	123.70
35	E	1887	U	C5'-C4'-C3'	-5.49	107.22	116.00
35	E	102	A	C5-C6-N1	-5.49	114.96	117.70
35	E	123	A	C5-C6-N1	-5.49	114.96	117.70
35	E	163	C	N3-C4-N4	5.49	121.84	118.00
35	E	351	A	O4'-C1'-N9	5.49	112.59	108.20
35	E	734	G	N1-C2-N2	5.49	121.14	116.20
35	E	1217	A	C5-C6-N1	-5.49	114.96	117.70
35	E	258	C	N3-C4-N4	5.49	121.84	118.00
35	E	703	A	C5-C6-N6	-5.49	119.31	123.70
35	E	780	C	N3-C4-N4	5.49	121.84	118.00
35	E	1309	A	O4'-C1'-N9	5.49	112.59	108.20
35	E	2133	C	N3-C4-C5	-5.49	119.70	121.90
35	E	62	A	C5-C6-N1	-5.49	114.96	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	621	A	C5-C6-N6	-5.49	119.31	123.70
35	E	1566	A	C5-C6-N6	-5.49	119.31	123.70
35	E	1738	G	O4'-C1'-N9	5.49	112.59	108.20
35	E	1866	A	C4-C5-C6	5.49	119.74	117.00
35	E	1906	C	N3-C4-C5	-5.49	119.71	121.90
35	E	2060	C	N3-C4-C5	-5.49	119.70	121.90
35	E	2262	A	C5-C6-N6	-5.49	119.31	123.70
35	E	254	A	C5-C6-N1	-5.48	114.96	117.70
35	E	2176	G	O4'-C1'-N9	5.48	112.59	108.20
35	E	787	C	N3-C4-C5	-5.48	119.71	121.90
35	E	890	C	N3-C4-N4	5.48	121.84	118.00
35	E	917	A	C5-C6-N6	-5.48	119.31	123.70
35	E	1348	A	C5-C6-N1	-5.48	114.96	117.70
35	E	2159	A	C5-C6-N6	-5.48	119.31	123.70
35	E	526	A	O4'-C1'-N9	5.48	112.58	108.20
35	E	935	A	C5-C6-N6	-5.48	119.31	123.70
35	E	595	A	C5-C6-N1	-5.48	114.96	117.70
35	E	2248	G	O4'-C1'-N9	5.48	112.58	108.20
35	E	97	A	C5-C6-N6	-5.48	119.32	123.70
35	E	403	G	O4'-C1'-N9	5.48	112.58	108.20
35	E	673	A	C5-C6-N6	-5.48	119.32	123.70
35	E	732	C	C6-N1-C1'	-5.48	114.23	120.80
35	E	2283	A	C5-C6-N1	-5.48	114.96	117.70
35	E	2299	A	C5-C6-N1	-5.48	114.96	117.70
35	E	425	A	O4'-C1'-N9	5.48	112.58	108.20
35	E	181	A	C5-C6-N6	-5.47	119.32	123.70
35	E	585	A	C5-C6-N6	-5.47	119.32	123.70
35	E	2225	C	N3-C4-N4	5.47	121.83	118.00
3	r	121	TYR	CB-CG-CD2	-5.47	117.72	121.00
35	E	184	A	C5-C6-N6	-5.47	119.32	123.70
35	E	185	A	C5-C6-N6	-5.47	119.32	123.70
35	E	428	C	N3-C4-C5	-5.47	119.71	121.90
35	E	482	C	N3-C4-N4	5.47	121.83	118.00
35	E	269	A	C5-C6-N6	-5.47	119.32	123.70
35	E	859	C	N3-C4-N4	5.47	121.83	118.00
35	E	1599	A	C5-C6-N1	-5.47	114.97	117.70
35	E	1996	A	C5-C6-N6	-5.47	119.32	123.70
35	E	97	A	C5-C6-N1	-5.47	114.97	117.70
35	E	853	C	N3-C4-C5	-5.47	119.71	121.90
35	E	1934	G	O4'-C1'-N9	5.47	112.58	108.20
35	E	2163	G	O4'-C1'-N9	5.47	112.58	108.20
35	E	181	A	C5-C6-N1	-5.47	114.97	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	604	A	C5-C6-N1	-5.47	114.97	117.70
35	E	1255	A	C5-C6-N1	-5.47	114.97	117.70
35	E	2260	A	C5-C6-N6	-5.47	119.33	123.70
35	E	2284	A	C5-C6-N6	-5.47	119.33	123.70
35	E	619	C	N3-C4-C5	-5.46	119.71	121.90
35	E	673	A	C4-C5-C6	5.46	119.73	117.00
35	E	506	A	C5-C6-N1	-5.46	114.97	117.70
35	E	805	C	N3-C4-C5	-5.46	119.72	121.90
35	E	723	C	N3-C4-C5	-5.46	119.72	121.90
35	E	1286	A	C5-C6-N6	-5.46	119.33	123.70
35	E	7	G	O4'-C1'-N9	5.46	112.57	108.20
35	E	55	A	C5-C6-N6	-5.46	119.33	123.70
35	E	141	A	C5-C6-N6	-5.46	119.33	123.70
35	E	482	C	N3-C4-C5	-5.46	119.72	121.90
35	E	709	C	N3-C4-C5	-5.46	119.72	121.90
35	E	1584	A	C5-C6-N6	-5.46	119.33	123.70
35	E	1609	A	C5-C6-N1	-5.46	114.97	117.70
35	E	1961	A	C5-C6-N6	-5.46	119.33	123.70
35	E	345	A	C5-C6-N1	-5.46	114.97	117.70
35	E	502	A	C5-C6-N6	-5.46	119.33	123.70
35	E	769	A	C5-C6-N1	-5.46	114.97	117.70
35	E	930	G	O4'-C1'-N9	5.46	112.57	108.20
35	E	1561	A	C5-C6-N6	-5.46	119.33	123.70
35	E	1824	A	C5-C6-N1	-5.46	114.97	117.70
35	E	2251	A	O4'-C1'-N9	5.46	112.56	108.20
5	u	43	TYR	CB-CG-CD1	5.46	124.27	121.00
35	E	173	A	C5-C6-N1	-5.46	114.97	117.70
35	E	806	C	N3-C4-C5	-5.46	119.72	121.90
35	E	816	C	N3-C4-C5	-5.46	119.72	121.90
35	E	1578	G	O4'-C1'-N9	5.46	112.56	108.20
35	E	1710	A	C5-C6-N6	-5.46	119.34	123.70
35	E	2014	C	N3-C4-C5	-5.45	119.72	121.90
35	E	812	A	C5-C6-N6	-5.45	119.34	123.70
35	E	2055	A	C5-C6-N1	-5.45	114.97	117.70
35	E	330	A	C5-C6-N6	-5.45	119.34	123.70
35	E	493	A	C4-C5-C6	5.45	119.73	117.00
35	E	841	C	N3-C4-C5	-5.45	119.72	121.90
35	E	1180	A	C5-C6-N1	-5.45	114.97	117.70
35	E	1920	A	C5-C6-N1	-5.45	114.97	117.70
35	E	2199	A	O4'-C1'-N9	5.45	112.56	108.20
35	E	170	C	N3-C4-C5	-5.45	119.72	121.90
35	E	1189	A	C5-C6-N1	-5.45	114.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1664	A	O4'-C1'-N9	5.45	112.56	108.20
35	E	2008	A	C5-C6-N6	-5.45	119.34	123.70
35	E	2272	A	C5-C6-N1	-5.45	114.98	117.70
35	E	503	A	C5-C6-N1	-5.45	114.98	117.70
35	E	168	A	C5-C6-N1	-5.45	114.98	117.70
35	E	300	A	C5-C6-N6	-5.45	119.34	123.70
35	E	917	A	C5-C6-N1	-5.45	114.98	117.70
35	E	1683	C	N3-C4-N4	5.45	121.81	118.00
35	E	2126	A	O4'-C1'-N9	5.45	112.56	108.20
35	E	2167	A	C5-C6-N1	-5.45	114.98	117.70
35	E	502	A	C5-C6-N1	-5.44	114.98	117.70
35	E	644	C	N3-C4-N4	5.44	121.81	118.00
35	E	1661	A	C5-C6-N1	-5.44	114.98	117.70
35	E	2009	C	O4'-C1'-N1	5.44	112.56	108.20
35	E	6	G	O4'-C1'-N9	5.44	112.55	108.20
35	E	61	C	N3-C4-C5	-5.44	119.72	121.90
35	E	578	C	N3-C4-C5	-5.44	119.72	121.90
35	E	688	G	O4'-C1'-N9	5.44	112.55	108.20
35	E	710	A	C5-C6-N1	-5.44	114.98	117.70
35	E	1826	U	O4'-C1'-N1	5.44	112.55	108.20
35	E	1960	A	C5-C6-N1	-5.44	114.98	117.70
35	E	2052	C	P-O3'-C3'	5.44	126.23	119.70
35	E	587	A	C5-C6-N1	-5.44	114.98	117.70
35	E	1330	A	C5-C6-N6	-5.44	119.35	123.70
35	E	2005	A	O4'-C1'-N9	5.44	112.55	108.20
35	E	3	U	O4'-C1'-N1	5.44	112.55	108.20
35	E	51	A	C5-C6-N6	-5.44	119.35	123.70
35	E	97	A	O4'-C1'-N9	5.44	112.55	108.20
35	E	330	A	C1'-O4'-C4'	-5.44	105.55	109.90
35	E	117	C	N3-C4-N4	5.44	121.81	118.00
35	E	120	C	N3-C4-C5	-5.44	119.72	121.90
35	E	592	A	C5-C6-N6	-5.44	119.35	123.70
35	E	694	A	C5-C6-N1	-5.44	114.98	117.70
35	E	858	A	C5-C6-N6	-5.44	119.35	123.70
35	E	1806	C	N3-C4-N4	5.44	121.81	118.00
35	E	1851	C	N3-C4-C5	-5.44	119.72	121.90
35	E	304	A	C5-C6-N1	-5.44	114.98	117.70
35	E	391	C	N3-C4-N4	5.44	121.81	118.00
35	E	2171	C	N3-C4-N4	5.44	121.81	118.00
35	E	483	A	C5-C6-N1	-5.43	114.98	117.70
35	E	766	C	N3-C4-C5	-5.43	119.73	121.90
35	E	825	C	N3-C4-N4	5.43	121.81	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1596	G	O4'-C1'-N9	5.43	112.55	108.20
35	E	2080	A	O4'-C1'-N9	5.43	112.55	108.20
35	E	86	G	O4'-C1'-N9	5.43	112.55	108.20
35	E	190	A	C5-C6-N1	-5.43	114.98	117.70
35	E	457	A	C5-C6-N1	-5.43	114.98	117.70
35	E	799	A	C5-C6-N1	-5.43	114.98	117.70
35	E	1259	A	O4'-C1'-N9	5.43	112.55	108.20
35	E	2040	G	O4'-C1'-N9	5.43	112.55	108.20
35	E	562	A	C5-C6-N1	-5.43	114.98	117.70
35	E	81	A	C5-C6-N6	-5.43	119.36	123.70
35	E	694	A	C5-C6-N6	-5.43	119.36	123.70
35	E	2315	A	C5-C6-N1	-5.43	114.98	117.70
35	E	195	C	P-O3'-C3'	5.43	126.21	119.70
35	E	765	A	C5-C6-N6	-5.43	119.36	123.70
35	E	1657	A	C5-C6-N1	-5.43	114.99	117.70
35	E	2027	C	N3-C4-N4	5.43	121.80	118.00
35	E	480	C	N3-C4-C5	-5.43	119.73	121.90
35	E	527	A	C5-C6-N6	-5.43	119.36	123.70
35	E	1883	C	N3-C4-C5	-5.43	119.73	121.90
35	E	2030	G	O4'-C1'-N9	5.43	112.54	108.20
35	E	177	A	O4'-C1'-N9	5.42	112.54	108.20
35	E	187	C	N3-C4-C5	-5.42	119.73	121.90
35	E	900	A	C5-C6-N6	-5.42	119.36	123.70
35	E	1579	G	O4'-C1'-N9	5.42	112.54	108.20
35	E	1644	G	O4'-C1'-N9	5.42	112.54	108.20
35	E	1792	G	O4'-C1'-N9	5.42	112.54	108.20
35	E	1265	A	O4'-C1'-N9	5.42	112.54	108.20
35	E	564	G	O4'-C1'-N9	5.42	112.54	108.20
35	E	566	G	O4'-C1'-N9	5.42	112.54	108.20
35	E	2019	C	N3-C4-C5	-5.42	119.73	121.90
35	E	2111	A	C5-C6-N1	-5.42	114.99	117.70
35	E	504	A	C5-C6-N1	-5.42	114.99	117.70
35	E	829	C	N3-C4-N4	5.42	121.79	118.00
35	E	942	C	N3-C4-C5	-5.42	119.73	121.90
35	E	2008	A	C5-C6-N1	-5.42	114.99	117.70
35	E	2055	A	C5-C6-N6	-5.42	119.36	123.70
35	E	203	C	N3-C4-C5	-5.42	119.73	121.90
35	E	743	C	N3-C4-N4	5.42	121.79	118.00
35	E	1196	A	C4-C5-C6	5.42	119.71	117.00
35	E	1298	C	N3-C4-C5	-5.42	119.73	121.90
35	E	1531	G	O4'-C1'-N9	5.42	112.53	108.20
35	E	2186	C	N3-C4-C5	-5.42	119.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	38	C	N3-C4-N4	5.42	121.79	118.00
35	E	89	C	N3-C4-N4	5.42	121.79	118.00
35	E	607	A	C5-C6-N1	-5.42	114.99	117.70
35	E	1197	A	C5-C6-N1	-5.42	114.99	117.70
35	E	1660	C	N3-C4-N4	5.42	121.79	118.00
35	E	1907	C	N3-C4-C5	-5.42	119.73	121.90
35	E	675	A	C5-C6-N6	-5.42	119.37	123.70
35	E	1378	A	C5-C6-N6	-5.42	119.37	123.70
35	E	1686	G	P-O5'-C5'	-5.42	112.24	120.90
35	E	2068	C	N3-C4-C5	-5.42	119.73	121.90
35	E	19	A	C5-C6-N6	-5.41	119.37	123.70
35	E	141	A	C4-C5-C6	5.41	119.71	117.00
35	E	175	A	C5-C6-N1	-5.41	114.99	117.70
35	E	1197	A	C5-C6-N6	-5.41	119.37	123.70
35	E	1857	U	O4'-C1'-N1	5.41	112.53	108.20
35	E	1984	A	C5-C6-N6	-5.41	119.37	123.70
35	E	2034	A	C5-C6-N6	-5.41	119.37	123.70
35	E	2147	U	C6-N1-C1'	-5.41	113.62	121.20
35	E	386	A	C5-C6-N6	-5.41	119.37	123.70
35	E	689	A	C5-C6-N6	-5.41	119.37	123.70
35	E	1803	A	C5-C6-N6	-5.41	119.37	123.70
35	E	1610	A	C5-C6-N6	-5.41	119.37	123.70
35	E	1742	C	N3-C4-C5	-5.41	119.74	121.90
35	E	1850	C	N3-C4-C5	-5.41	119.74	121.90
35	E	90	A	C5-C6-N1	-5.41	115.00	117.70
35	E	450	A	C5-C6-N1	-5.41	115.00	117.70
35	E	1177	C	N3-C4-C5	-5.41	119.74	121.90
35	E	367	A	C5-C6-N6	-5.41	119.38	123.70
35	E	585	A	C5-C6-N1	-5.41	115.00	117.70
35	E	641	C	N3-C4-C5	-5.41	119.74	121.90
35	E	945	C	N3-C4-C5	-5.41	119.74	121.90
35	E	1689	A	C5-C6-N6	-5.41	119.38	123.70
35	E	2065	A	C5-C6-N6	-5.41	119.38	123.70
35	E	2067	C	N3-C4-C5	-5.41	119.74	121.90
35	E	2259	A	C5-C6-N1	-5.41	115.00	117.70
35	E	1292	A	C5-C6-N1	-5.40	115.00	117.70
35	E	1340	A	C5-C6-N6	-5.40	119.38	123.70
35	E	1729	C	N3-C4-N4	5.40	121.78	118.00
35	E	182	C	N3-C4-C5	-5.40	119.74	121.90
35	E	254	A	C5-C6-N6	-5.40	119.38	123.70
35	E	499	A	C5-C6-N1	-5.40	115.00	117.70
35	E	707	C	N3-C4-C5	-5.40	119.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1343	A	C5-C6-N6	-5.40	119.38	123.70
35	E	1658	C	N3-C4-C5	-5.40	119.74	121.90
35	E	2315	A	C5-C6-N6	-5.40	119.38	123.70
35	E	241	A	O4'-C1'-N9	5.40	112.52	108.20
35	E	2204	A	O4'-C1'-N9	5.40	112.52	108.20
35	E	51	A	C5-C6-N1	-5.40	115.00	117.70
35	E	214	C	N3-C4-C5	-5.40	119.74	121.90
35	E	101	C	N3-C4-C5	-5.40	119.74	121.90
35	E	444	A	C5-C6-N1	-5.40	115.00	117.70
35	E	586	A	C5-C6-N1	-5.40	115.00	117.70
35	E	966	C	N3-C4-C5	-5.40	119.74	121.90
35	E	1182	G	O4'-C1'-N9	5.40	112.52	108.20
35	E	2092	A	C5-C6-N1	-5.40	115.00	117.70
35	E	2225	C	N3-C4-C5	-5.40	119.74	121.90
35	E	467	A	C5-C6-N6	-5.40	119.38	123.70
35	E	547	G	O4'-C1'-N9	5.40	112.52	108.20
35	E	168	A	O4'-C1'-N9	5.39	112.52	108.20
35	E	177	A	C5-C6-N6	-5.39	119.39	123.70
35	E	245	A	O4'-C1'-N9	5.39	112.52	108.20
35	E	405	G	O4'-C1'-N9	5.39	112.52	108.20
35	E	615	G	O4'-C1'-N9	5.39	112.52	108.20
35	E	1214	G	O4'-C1'-N9	5.39	112.52	108.20
35	E	1264	A	C5-C6-N1	-5.39	115.00	117.70
35	E	1797	A	C5-C6-N1	-5.39	115.00	117.70
35	E	2240	A	C4-C5-C6	5.39	119.70	117.00
35	E	142	A	C5-C6-N1	-5.39	115.00	117.70
35	E	345	A	C5-C6-N6	-5.39	119.39	123.70
35	E	887	C	N3-C4-N4	5.39	121.78	118.00
35	E	960	A	C5-C6-N1	-5.39	115.00	117.70
35	E	1172	C	N3-C4-C5	-5.39	119.74	121.90
35	E	1233	A	C5-C6-N1	-5.39	115.00	117.70
35	E	1338	A	O4'-C1'-N9	5.39	112.51	108.20
35	E	1678	C	N3-C4-C5	-5.39	119.74	121.90
35	E	2052	C	N3-C4-C5	-5.39	119.74	121.90
35	E	2192	A	C5-C6-N6	-5.39	119.39	123.70
35	E	1077	C	N3-C4-N4	5.39	121.77	118.00
35	E	1251	C	N3-C4-C5	-5.39	119.74	121.90
35	E	1536	C	N3-C4-N4	5.39	121.77	118.00
35	E	485	A	C5-C6-N1	-5.39	115.01	117.70
35	E	784	A	C5-C6-N6	-5.39	119.39	123.70
35	E	1790	A	C5-C6-N1	-5.39	115.00	117.70
35	E	360	A	C5-C6-N1	-5.39	115.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	894	A	C5-C6-N1	-5.39	115.01	117.70
35	E	1995	G	O4'-C1'-N9	5.39	112.51	108.20
35	E	30	G	O4'-C1'-N9	5.38	112.51	108.20
35	E	962	A	C5-C6-N1	-5.38	115.01	117.70
35	E	990	A	C5-C6-N1	-5.38	115.01	117.70
35	E	1720	C	N3-C4-N4	5.38	121.77	118.00
35	E	350	C	N3-C4-C5	-5.38	119.75	121.90
35	E	976	U	O4'-C1'-N1	5.38	112.51	108.20
35	E	1684	C	N3-C4-N4	5.38	121.77	118.00
35	E	2099	G	C5-C6-O6	-5.38	125.37	128.60
35	E	2200	A	C5-C6-N1	-5.38	115.01	117.70
35	E	22	A	C5-C6-N1	-5.38	115.01	117.70
35	E	926	C	N3-C4-C5	-5.38	119.75	121.90
35	E	1174	C	N3-C4-C5	-5.38	119.75	121.90
35	E	1576	G	C5-C6-O6	-5.38	125.37	128.60
35	E	2239	A	C5-C6-N1	-5.38	115.01	117.70
35	E	160	A	C4-C5-C6	5.38	119.69	117.00
35	E	330	A	C5-C6-N1	-5.38	115.01	117.70
35	E	555	G	O4'-C1'-N9	5.38	112.50	108.20
35	E	127	C	N3-C4-C5	-5.38	119.75	121.90
35	E	373	G	O4'-C1'-N9	5.38	112.50	108.20
35	E	936	C	C6-N1-C2	-5.38	118.15	120.30
35	E	2158	C	N3-C4-N4	5.38	121.77	118.00
35	E	309	G	O4'-C1'-N9	5.38	112.50	108.20
35	E	1606	A	C4-C5-C6	5.38	119.69	117.00
35	E	125	A	C5-C6-N1	-5.38	115.01	117.70
35	E	2312	A	C5-C6-N1	-5.38	115.01	117.70
35	E	158	C	N3-C4-C5	-5.37	119.75	121.90
35	E	704	A	O4'-C1'-N9	5.37	112.50	108.20
35	E	1173	U	O4'-C1'-N1	5.37	112.50	108.20
35	E	1288	G	O4'-C1'-N9	5.37	112.50	108.20
35	E	2089	A	C5-C6-N6	-5.37	119.40	123.70
35	E	125	A	C5-C6-N6	-5.37	119.40	123.70
35	E	244	G	O4'-C1'-N9	5.37	112.50	108.20
35	E	259	C	O4'-C1'-N1	5.37	112.50	108.20
35	E	449	U	O4'-C1'-N1	5.37	112.50	108.20
35	E	633	A	C5-C6-N1	-5.37	115.01	117.70
35	E	859	C	N3-C4-C5	-5.37	119.75	121.90
35	E	864	A	C5-C6-N1	-5.37	115.01	117.70
35	E	1803	A	C5-C6-N1	-5.37	115.02	117.70
35	E	2107	A	C5-C6-N6	-5.37	119.40	123.70
35	E	2197	G	O4'-C1'-N9	5.37	112.50	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	855	G	O4'-C1'-N9	5.37	112.50	108.20
35	E	916	A	C5-C6-N1	-5.37	115.02	117.70
35	E	1372	C	N3-C4-C5	-5.37	119.75	121.90
35	E	784	A	C5-C6-N1	-5.37	115.02	117.70
35	E	960	A	O4'-C1'-N9	5.37	112.50	108.20
35	E	1239	G	O4'-C1'-N9	5.37	112.49	108.20
35	E	1991	C	N3-C4-C5	-5.37	119.75	121.90
35	E	121	A	C5-C6-N1	-5.37	115.02	117.70
35	E	1176	A	C5-C6-N1	-5.37	115.02	117.70
35	E	1724	A	C5-C6-N6	-5.37	119.41	123.70
35	E	258	C	N3-C4-C5	-5.37	119.75	121.90
35	E	432	A	C5-C6-N6	-5.37	119.41	123.70
35	E	1662	A	C5-C6-N1	-5.37	115.02	117.70
34	h	218	SER	N-CA-CB	5.36	118.54	110.50
35	E	28	A	C5-C6-N1	-5.36	115.02	117.70
35	E	107	A	C5-C6-N1	-5.36	115.02	117.70
35	E	608	C	N3-C4-C5	-5.36	119.75	121.90
35	E	653	A	O4'-C1'-N9	5.36	112.49	108.20
35	E	726	C	N3-C4-N4	5.36	121.75	118.00
35	E	1861	A	C5-C6-N1	-5.36	115.02	117.70
35	E	2026	A	O4'-C1'-N9	5.36	112.49	108.20
35	E	2033	C	N3-C4-C5	-5.36	119.75	121.90
35	E	11	A	C5-C6-N6	-5.36	119.41	123.70
35	E	571	A	C5-C6-N6	-5.36	119.41	123.70
35	E	1274	A	O4'-C1'-N9	5.36	112.49	108.20
35	E	245	A	C5-C6-N6	-5.36	119.41	123.70
35	E	284	C	N3-C4-C5	-5.36	119.76	121.90
35	E	624	A	O4'-C1'-N9	5.36	112.49	108.20
35	E	1697	G	O4'-C1'-N9	5.36	112.49	108.20
35	E	2148	A	C5-C6-N1	-5.36	115.02	117.70
35	E	4	C	N3-C4-C5	-5.36	119.76	121.90
35	E	246	A	C5-C6-N6	-5.36	119.41	123.70
35	E	682	G	N3-C2-N2	5.36	123.65	119.90
35	E	1313	A	C5-C6-N1	-5.36	115.02	117.70
35	E	1592	A	C5-C6-N6	-5.36	119.41	123.70
35	E	2097	U	O4'-C1'-N1	5.36	112.49	108.20
35	E	638	C	N3-C4-C5	-5.36	119.76	121.90
35	E	814	C	N3-C4-C5	-5.36	119.76	121.90
35	E	998	C	N3-C4-N4	5.36	121.75	118.00
35	E	1304	C	N3-C4-C5	-5.36	119.76	121.90
35	E	1658	C	O4'-C1'-N1	5.36	112.48	108.20
35	E	2056	A	C5-C6-N1	-5.36	115.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	260	A	C4-C5-C6	5.35	119.68	117.00
35	E	673	A	C5-C6-N1	-5.35	115.02	117.70
35	E	742	A	C5-C6-N6	-5.35	119.42	123.70
35	E	1365	A	C5-C6-N6	-5.35	119.42	123.70
3	r	135	TRP	CA-C-N	5.35	126.90	116.20
20	f	206	PHE	CB-CG-CD1	5.35	124.55	120.80
35	E	82	A	C5-C6-N1	-5.35	115.02	117.70
35	E	92	G	O4'-C1'-N9	5.35	112.48	108.20
35	E	397	G	O4'-C1'-N9	5.35	112.48	108.20
35	E	854	U	O4'-C1'-N1	5.35	112.48	108.20
35	E	1975	A	C5-C6-N1	-5.35	115.02	117.70
35	E	59	C	N3-C4-C5	-5.35	119.76	121.90
35	E	183	C	N3-C4-C5	-5.35	119.76	121.90
35	E	2102	C	N3-C4-C5	-5.35	119.76	121.90
35	E	250	A	C5-C6-N1	-5.35	115.03	117.70
35	E	404	G	O4'-C1'-N9	5.35	112.48	108.20
35	E	689	A	C5-C6-N1	-5.35	115.03	117.70
35	E	727	C	N3-C4-C5	-5.35	119.76	121.90
35	E	1314	A	C5-C6-N1	-5.35	115.03	117.70
35	E	2202	A	C5-C6-N1	-5.35	115.03	117.70
35	E	108	C	N3-C4-N4	5.35	121.74	118.00
35	E	179	G	O4'-C1'-N9	5.35	112.48	108.20
35	E	220	G	O4'-C1'-N9	5.35	112.48	108.20
35	E	285	A	C5-C6-N6	-5.35	119.42	123.70
35	E	509	A	C5-C6-N1	-5.35	115.03	117.70
35	E	830	C	N3-C4-C5	-5.35	119.76	121.90
35	E	875	A	C5-C6-N1	-5.35	115.03	117.70
35	E	1546	C	N3-C4-N4	5.35	121.74	118.00
35	E	1627	C	N3-C4-C5	-5.35	119.76	121.90
35	E	889	A	O4'-C1'-N9	5.35	112.48	108.20
35	E	1360	A	C5-C6-N1	-5.35	115.03	117.70
35	E	1999	A	C5-C6-N1	-5.35	115.03	117.70
35	E	463	A	C5-C6-N6	-5.34	119.42	123.70
35	E	484	A	C5-C6-N1	-5.34	115.03	117.70
35	E	812	A	C5-C6-N1	-5.34	115.03	117.70
35	E	1205	A	C5-C6-N1	-5.34	115.03	117.70
35	E	1322	G	O4'-C1'-N9	5.34	112.48	108.20
35	E	1706	A	C5-C6-N6	-5.34	119.42	123.70
35	E	1731	G	O4'-C1'-N9	5.34	112.47	108.20
35	E	25	C	N3-C4-C5	-5.34	119.76	121.90
35	E	417	A	C5-C6-N1	-5.34	115.03	117.70
35	E	1525	C	N3-C4-C5	-5.34	119.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1546	C	N3-C4-C5	-5.34	119.76	121.90
35	E	1631	A	C5-C6-N1	-5.34	115.03	117.70
35	E	1678	C	N3-C4-N4	5.34	121.74	118.00
35	E	1766	U	O4'-C1'-N1	5.34	112.47	108.20
35	E	783	A	C5-C6-N1	-5.34	115.03	117.70
35	E	1377	A	C5-C6-N6	-5.34	119.43	123.70
35	E	2239	A	C5-C6-N6	-5.34	119.43	123.70
35	E	2308	C	N3-C4-C5	-5.34	119.76	121.90
35	E	108	C	N3-C4-C5	-5.34	119.77	121.90
35	E	260	A	C6-C5-N7	-5.34	128.56	132.30
35	E	315	A	C4-C5-C6	5.34	119.67	117.00
35	E	530	G	O4'-C1'-N9	5.34	112.47	108.20
35	E	1338	A	C5-C6-N1	-5.34	115.03	117.70
35	E	1794	A	C5-C6-N1	-5.34	115.03	117.70
35	E	998	C	N3-C4-C5	-5.34	119.77	121.90
35	E	1832	A	C5-C6-N1	-5.34	115.03	117.70
35	E	444	A	O4'-C1'-N9	5.34	112.47	108.20
35	E	632	U	O4'-C1'-N1	5.34	112.47	108.20
35	E	643	C	N3-C4-C5	-5.34	119.77	121.90
35	E	1552	A	O4'-C1'-N9	5.34	112.47	108.20
35	E	1743	A	O4'-C1'-N9	5.34	112.47	108.20
35	E	2035	A	C5-C6-N1	-5.34	115.03	117.70
35	E	529	A	C5-C6-N6	-5.33	119.43	123.70
35	E	974	A	C5-C6-N1	-5.33	115.03	117.70
35	E	1302	A	C5-C6-N1	-5.33	115.03	117.70
35	E	1620	A	C5-C6-N6	-5.33	119.43	123.70
35	E	1919	A	C5-C6-N6	-5.33	119.43	123.70
35	E	2156	G	O4'-C1'-N9	5.33	112.47	108.20
21	d	223	TYR	CB-CG-CD2	-5.33	117.80	121.00
35	E	40	A	C5-C6-N1	-5.33	115.03	117.70
35	E	1223	C	N3-C4-C5	-5.33	119.77	121.90
35	E	1325	C	N3-C4-C5	-5.33	119.77	121.90
35	E	2110	A	C5-C6-N6	-5.33	119.43	123.70
35	E	2312	A	C5-C6-N6	-5.33	119.44	123.70
35	E	116	G	O4'-C1'-N9	5.33	112.46	108.20
35	E	269	A	C5-C6-N1	-5.33	115.03	117.70
35	E	316	A	C5-C6-N1	-5.33	115.03	117.70
35	E	659	A	C5-C6-N1	-5.33	115.03	117.70
35	E	690	A	C5-C6-N6	-5.33	119.44	123.70
35	E	11	A	O4'-C1'-N9	5.33	112.46	108.20
35	E	2066	C	N3-C4-N4	5.33	121.73	118.00
35	E	2238	A	C5-C6-N6	-5.33	119.44	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	135	C	N3-C4-C5	-5.33	119.77	121.90
35	E	779	A	O4'-C1'-N9	5.33	112.46	108.20
35	E	1329	G	O4'-C1'-N9	5.33	112.46	108.20
35	E	509	A	O4'-C1'-N9	5.32	112.46	108.20
35	E	1352	C	N3-C4-C5	-5.32	119.77	121.90
35	E	1630	A	C5-C6-N6	-5.32	119.44	123.70
35	E	2203	C	N3-C4-N4	5.32	121.73	118.00
35	E	429	C	N3-C4-C5	-5.32	119.77	121.90
35	E	1861	A	O4'-C1'-N9	5.32	112.46	108.20
35	E	610	A	C5-C6-N6	-5.32	119.44	123.70
35	E	760	C	O4'-C1'-N1	5.32	112.46	108.20
35	E	809	A	C5-C6-N1	-5.32	115.04	117.70
35	E	1323	A	C5-C6-N6	-5.32	119.44	123.70
35	E	1938	C	N3-C4-C5	-5.32	119.77	121.90
35	E	2168	C	N3-C4-C5	-5.32	119.77	121.90
35	E	2214	A	O4'-C1'-N9	5.32	112.46	108.20
35	E	351	A	C5-C6-N6	-5.32	119.44	123.70
35	E	770	C	N3-C4-C5	-5.32	119.77	121.90
35	E	959	A	C5-C6-N6	-5.32	119.44	123.70
35	E	1963	G	O4'-C1'-N9	5.32	112.45	108.20
35	E	89	C	N3-C4-C5	-5.32	119.77	121.90
35	E	185	A	C5-C6-N1	-5.32	115.04	117.70
35	E	1348	A	C5-C6-N6	-5.32	119.45	123.70
35	E	1348	A	O4'-C1'-N9	5.32	112.45	108.20
35	E	2011	A	C5-C6-N1	-5.32	115.04	117.70
35	E	2305	C	N3-C4-C5	-5.32	119.77	121.90
35	E	46	U	C2-N1-C1'	5.32	124.08	117.70
35	E	84	C	N3-C4-C5	-5.32	119.77	121.90
35	E	241	A	C5-C6-N1	-5.32	115.04	117.70
35	E	278	A	O4'-C1'-N9	5.32	112.45	108.20
35	E	1736	G	O4'-C1'-N9	5.32	112.45	108.20
35	E	102	A	C5-C6-N6	-5.31	119.45	123.70
35	E	440	C	N3-C4-C5	-5.31	119.78	121.90
35	E	662	C	N3-C4-C5	-5.31	119.78	121.90
35	E	979	G	C6-C5-N7	-5.31	127.21	130.40
35	E	2077	C	N3-C4-C5	-5.31	119.77	121.90
35	E	2135	A	C5-C6-N6	-5.31	119.45	123.70
35	E	366	C	N3-C4-N4	5.31	121.72	118.00
35	E	1584	A	O4'-C1'-N9	5.31	112.45	108.20
35	E	1697	G	C4-N9-C1'	5.31	133.41	126.50
35	E	55	A	C5-C6-N1	-5.31	115.05	117.70
35	E	304	A	O4'-C1'-N9	5.31	112.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	580	C	N3-C4-C5	-5.31	119.78	121.90
35	E	1959	C	O4'-C1'-N1	5.31	112.45	108.20
35	E	1677	C	N3-C4-C5	-5.31	119.78	121.90
35	E	1916	C	N3-C4-N4	5.31	121.72	118.00
35	E	80	G	O4'-C1'-N9	5.31	112.44	108.20
35	E	127	C	N3-C4-N4	5.31	121.72	118.00
35	E	581	A	C5-C6-N1	-5.31	115.05	117.70
35	E	1599	A	C5-C6-N6	-5.31	119.45	123.70
35	E	2268	A	C5-C6-N1	-5.31	115.05	117.70
35	E	467	A	O4'-C1'-N9	5.30	112.44	108.20
35	E	597	C	N3-C4-N4	5.30	121.71	118.00
35	E	1936	A	C5-C6-N1	-5.30	115.05	117.70
35	E	1966	C	N3-C4-C5	-5.30	119.78	121.90
35	E	2273	A	C5-C6-N6	-5.30	119.46	123.70
35	E	369	C	N3-C4-N4	5.30	121.71	118.00
35	E	876	A	C5-C6-N1	-5.30	115.05	117.70
35	E	878	G	O4'-C1'-N9	5.30	112.44	108.20
35	E	1619	A	C5-C6-N6	-5.30	119.46	123.70
35	E	1726	C	N3-C4-C5	-5.30	119.78	121.90
35	E	212	G	O4'-C1'-N9	5.30	112.44	108.20
35	E	351	A	C5-C6-N1	-5.30	115.05	117.70
35	E	153	C	N3-C4-C5	-5.30	119.78	121.90
35	E	203	C	N3-C4-N4	5.30	121.71	118.00
35	E	288	A	C5-C6-N6	-5.30	119.46	123.70
35	E	961	A	C5-C6-N1	-5.30	115.05	117.70
35	E	1728	C	N3-C4-C5	-5.30	119.78	121.90
35	E	1788	C	N3-C4-C5	-5.30	119.78	121.90
35	E	2142	C	N3-C4-C5	-5.30	119.78	121.90
35	E	55	A	O4'-C1'-N9	5.29	112.44	108.20
35	E	287	A	C5-C6-N1	-5.29	115.05	117.70
35	E	441	C	N3-C4-C5	-5.29	119.78	121.90
35	E	476	G	O4'-C1'-N9	5.29	112.44	108.20
35	E	571	A	O4'-C1'-N9	5.29	112.44	108.20
35	E	1647	G	O4'-C1'-N9	5.29	112.44	108.20
35	E	2215	C	N3-C4-C5	-5.29	119.78	121.90
35	E	352	A	C5-C6-N1	-5.29	115.05	117.70
35	E	425	A	C5-C6-N1	-5.29	115.05	117.70
35	E	521	A	C5-C6-N1	-5.29	115.05	117.70
35	E	898	A	C5-C6-N6	-5.29	119.47	123.70
35	E	1378	A	C5-C6-N1	-5.29	115.05	117.70
35	E	1902	G	N3-C2-N2	5.29	123.60	119.90
35	E	1529	A	C5-C6-N1	-5.29	115.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1620	A	O4'-C1'-N9	5.29	112.43	108.20
35	E	1961	A	C5-C6-N1	-5.29	115.06	117.70
20	f	206	PHE	CB-CG-CD2	-5.29	117.10	120.80
35	E	47	A	C5-C6-N6	-5.29	119.47	123.70
35	E	424	G	O4'-C1'-N9	5.29	112.43	108.20
35	E	653	A	C5-C6-N1	-5.29	115.06	117.70
35	E	1178	U	O4'-C1'-N1	5.29	112.43	108.20
35	E	1664	A	C5-C6-N6	-5.29	119.47	123.70
35	E	1709	G	O4'-C1'-N9	5.29	112.43	108.20
35	E	1862	C	N3-C4-C5	-5.29	119.78	121.90
35	E	1992	A	C5-C6-N1	-5.29	115.06	117.70
35	E	2294	A	C5-C6-N1	-5.29	115.06	117.70
35	E	1188	C	C5-C4-N4	-5.29	116.50	120.20
35	E	163	C	N3-C4-C5	-5.29	119.78	121.90
35	E	1175	A	C5-C6-N1	-5.29	115.06	117.70
35	E	549	A	O4'-C1'-N9	5.28	112.43	108.20
35	E	624	A	C5-C6-N6	-5.28	119.47	123.70
35	E	1927	A	C5-C6-N1	-5.28	115.06	117.70
35	E	2007	A	C5-C6-N1	-5.28	115.06	117.70
35	E	1307	G	O4'-C1'-N9	5.28	112.43	108.20
35	E	2054	G	O4'-C1'-N9	5.28	112.43	108.20
35	E	826	A	O4'-C1'-N9	5.28	112.42	108.20
35	E	877	A	C5-C6-N6	-5.28	119.48	123.70
35	E	1523	C	N3-C4-C5	-5.28	119.79	121.90
35	E	1726	C	N3-C4-N4	5.28	121.70	118.00
35	E	2052	C	N3-C4-N4	5.28	121.70	118.00
35	E	2104	A	C5-C6-N6	-5.28	119.48	123.70
35	E	2170	C	O4'-C1'-N1	5.28	112.42	108.20
35	E	2314	C	N3-C4-N4	5.28	121.70	118.00
35	E	902	A	C5-C6-N1	-5.28	115.06	117.70
35	E	1630	A	C5-C6-N1	-5.28	115.06	117.70
35	E	699	C	P-O3'-C3'	5.28	126.03	119.70
35	E	1608	G	O4'-C1'-N9	5.28	112.42	108.20
35	E	1700	U	O4'-C1'-N1	5.28	112.42	108.20
35	E	1746	G	O4'-C1'-N9	5.28	112.42	108.20
35	E	50	C	N3-C4-C5	-5.28	119.79	121.90
35	E	1282	C	N3-C4-C5	-5.28	119.79	121.90
35	E	1733	A	C5-C6-N1	-5.28	115.06	117.70
35	E	1811	C	N3-C4-C5	-5.28	119.79	121.90
35	E	2092	A	O4'-C1'-N9	5.28	112.42	108.20
35	E	2294	A	O4'-C1'-N9	5.28	112.42	108.20
35	E	516	A	C5-C6-N1	-5.27	115.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	545	U	O4'-C1'-N1	5.27	112.42	108.20
35	E	605	G	O4'-C1'-N9	5.27	112.42	108.20
35	E	771	A	O4'-C1'-N9	5.27	112.42	108.20
35	E	884	A	C5-C6-N1	-5.27	115.06	117.70
35	E	186	C	N3-C4-C5	-5.27	119.79	121.90
35	E	622	G	O4'-C1'-N9	5.27	112.42	108.20
35	E	711	A	C5-C6-N6	-5.27	119.48	123.70
35	E	1308	A	O4'-C1'-N9	5.27	112.42	108.20
35	E	1789	A	C5-C6-N6	-5.27	119.48	123.70
35	E	1966	C	C6-N1-C1'	-5.27	114.47	120.80
35	E	501	A	C5-C6-N1	-5.27	115.06	117.70
35	E	1821	C	N3-C4-C5	-5.27	119.79	121.90
35	E	104	C	N3-C4-C5	-5.27	119.79	121.90
35	E	1553	A	O4'-C1'-N9	5.27	112.42	108.20
35	E	1580	G	O4'-C1'-N9	5.27	112.42	108.20
35	E	2199	A	C5-C6-N1	-5.27	115.06	117.70
35	E	255	A	C5-C6-N1	-5.27	115.07	117.70
35	E	374	G	O4'-C1'-N9	5.27	112.41	108.20
35	E	1626	C	N3-C4-N4	5.27	121.69	118.00
35	E	1660	C	N3-C4-C5	-5.27	119.79	121.90
35	E	1698	A	C5-C6-N6	-5.27	119.49	123.70
35	E	1831	C	N3-C4-C5	-5.27	119.79	121.90
35	E	2284	A	C5-C6-N1	-5.27	115.07	117.70
35	E	1371	C	N3-C4-C5	-5.26	119.79	121.90
35	E	912	A	C5-C6-N6	-5.26	119.49	123.70
35	E	1077	C	N3-C4-C5	-5.26	119.80	121.90
35	E	845	A	C5-C6-N1	-5.26	115.07	117.70
35	E	915	A	C5-C6-N1	-5.26	115.07	117.70
35	E	1290	A	O4'-C1'-N9	5.26	112.41	108.20
35	E	2039	A	C5-C6-N6	-5.26	119.49	123.70
35	E	2103	A	O4'-C1'-N9	5.26	112.41	108.20
35	E	2174	C	N3-C4-C5	-5.26	119.80	121.90
35	E	2221	A	C5-C6-N1	-5.26	115.07	117.70
35	E	1543	C	N3-C4-C5	-5.26	119.80	121.90
35	E	1953	G	O4'-C1'-N9	5.26	112.41	108.20
35	E	2209	A	O4'-C1'-N9	5.26	112.41	108.20
35	E	284	C	N3-C4-N4	5.26	121.68	118.00
35	E	1242	A	C5-C6-N1	-5.26	115.07	117.70
35	E	1528	C	N3-C4-C5	-5.26	119.80	121.90
35	E	1935	C	N3-C4-N4	5.26	121.68	118.00
35	E	1361	A	O4'-C1'-N9	5.25	112.40	108.20
35	E	1727	C	N3-C4-N4	5.25	121.68	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	26	A	C5-C6-N1	-5.25	115.07	117.70
35	E	207	G	O4'-C1'-N9	5.25	112.40	108.20
35	E	606	G	O4'-C1'-N9	5.25	112.40	108.20
35	E	887	C	N3-C4-C5	-5.25	119.80	121.90
35	E	928	C	N3-C4-C5	-5.25	119.80	121.90
35	E	179	G	N3-C2-N2	5.25	123.58	119.90
35	E	598	A	C5-C6-N1	-5.25	115.08	117.70
35	E	786	A	C5-C6-N1	-5.25	115.08	117.70
35	E	826	A	C5-C6-N1	-5.25	115.08	117.70
35	E	862	A	C4-C5-C6	5.25	119.62	117.00
35	E	900	A	C5-C6-N1	-5.25	115.07	117.70
35	E	142	A	O4'-C1'-N9	5.25	112.40	108.20
35	E	353	C	N3-C4-C5	-5.25	119.80	121.90
35	E	483	A	O4'-C1'-N9	5.25	112.40	108.20
35	E	533	C	N3-C4-N4	5.25	121.67	118.00
35	E	792	G	O4'-C1'-N9	5.25	112.40	108.20
35	E	122	A	C5-C6-N1	-5.25	115.08	117.70
35	E	166	C	N3-C4-C5	-5.25	119.80	121.90
35	E	169	G	O4'-C1'-N9	5.25	112.40	108.20
35	E	874	C	N3-C4-C5	-5.25	119.80	121.90
35	E	2002	A	C5-C6-N1	-5.25	115.08	117.70
35	E	240	G	O4'-C1'-N9	5.25	112.40	108.20
35	E	263	G	O4'-C1'-N9	5.25	112.40	108.20
35	E	35	U	O4'-C1'-N1	5.24	112.39	108.20
35	E	68	A	C5-C6-N1	-5.24	115.08	117.70
35	E	765	A	O4'-C1'-N9	5.24	112.39	108.20
35	E	1185	A	N1-C2-N3	5.24	131.92	129.30
35	E	1575	G	O4'-C1'-N9	5.24	112.39	108.20
35	E	2300	A	C5-C6-N6	-5.24	119.50	123.70
35	E	1539	A	C5-C6-N1	-5.24	115.08	117.70
35	E	1903	A	C5-C6-N1	-5.24	115.08	117.70
35	E	2056	A	C5-C6-N6	-5.24	119.51	123.70
35	E	825	C	N3-C4-C5	-5.24	119.80	121.90
35	E	1878	A	C5-C6-N1	-5.24	115.08	117.70
35	E	112	A	C5-C6-N1	-5.24	115.08	117.70
35	E	695	G	O4'-C1'-N9	5.24	112.39	108.20
35	E	795	U	C2'-C3'-O3'	5.24	122.08	113.70
35	E	842	G	O4'-C1'-N9	5.24	112.39	108.20
35	E	895	A	C5-C6-N1	-5.24	115.08	117.70
35	E	1683	C	N3-C4-C5	-5.24	119.81	121.90
35	E	2271	A	O4'-C1'-N9	5.24	112.39	108.20
35	E	785	A	C5-C6-N1	-5.24	115.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1888	A	C5-C6-N6	-5.24	119.51	123.70
35	E	1935	C	N3-C4-C5	-5.24	119.81	121.90
35	E	2078	C	N3-C4-C5	-5.24	119.81	121.90
35	E	228	G	O4'-C1'-N9	5.24	112.39	108.20
35	E	291	G	O4'-C1'-N9	5.24	112.39	108.20
35	E	463	A	C5-C6-N1	-5.24	115.08	117.70
35	E	648	A	C5-C6-N6	-5.24	119.51	123.70
35	E	793	A	C5-C6-N6	-5.24	119.51	123.70
35	E	2204	A	C5-C6-N6	-5.24	119.51	123.70
35	E	90	A	C5-C6-N6	-5.23	119.51	123.70
35	E	668	C	N3-C4-C5	-5.23	119.81	121.90
35	E	414	A	O4'-C1'-N9	5.23	112.39	108.20
35	E	432	A	O4'-C1'-N9	5.23	112.39	108.20
35	E	576	A	O4'-C1'-N9	5.23	112.39	108.20
35	E	682	G	O4'-C1'-N9	5.23	112.39	108.20
35	E	782	A	C5-C6-N1	-5.23	115.08	117.70
35	E	1309	A	C5-C6-N1	-5.23	115.08	117.70
35	E	1910	G	O4'-C1'-N9	5.23	112.39	108.20
35	E	798	U	O4'-C1'-N1	5.23	112.39	108.20
35	E	920	A	C5-C6-N1	-5.23	115.08	117.70
35	E	2050	C	C5'-C4'-O4'	5.23	115.38	109.10
35	E	1739	G	O4'-C1'-N9	5.23	112.38	108.20
35	E	123	A	O4'-C1'-N9	5.23	112.38	108.20
35	E	288	A	C5-C6-N1	-5.23	115.09	117.70
35	E	360	A	C5-C6-N6	-5.23	119.52	123.70
35	E	452	C	N3-C4-C5	-5.23	119.81	121.90
35	E	1877	U	C4'-C3'-C2'	5.23	107.83	102.60
35	E	1944	G	O4'-C1'-N9	5.23	112.38	108.20
35	E	2069	A	C5-C6-N6	-5.23	119.52	123.70
35	E	2103	A	C5-C6-N6	-5.23	119.52	123.70
35	E	1591	C	N3-C4-C5	-5.23	119.81	121.90
35	E	1846	C	N3-C4-C5	-5.23	119.81	121.90
35	E	2050	C	N3-C4-N4	5.23	121.66	118.00
35	E	295	A	C5-C6-N1	-5.22	115.09	117.70
35	E	1378	A	O4'-C1'-N9	5.22	112.38	108.20
35	E	347	G	O4'-C1'-N9	5.22	112.38	108.20
35	E	629	C	N3-C4-C5	-5.22	119.81	121.90
35	E	931	G	O4'-C1'-N9	5.22	112.38	108.20
35	E	992	A	C5-C6-N1	-5.22	115.09	117.70
35	E	1780	G	O4'-C1'-N9	5.22	112.38	108.20
35	E	2241	G	O4'-C1'-N9	5.22	112.38	108.20
35	E	2299	A	O4'-C1'-N9	5.22	112.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	94	C	N3-C4-C5	-5.22	119.81	121.90
35	E	1568	A	C5-C6-N1	-5.22	115.09	117.70
35	E	2314	C	N3-C4-C5	-5.22	119.81	121.90
35	E	281	A	C5-C6-N1	-5.22	115.09	117.70
35	E	308	C	N3-C4-N4	5.22	121.65	118.00
35	E	498	A	C5-C6-N1	-5.22	115.09	117.70
35	E	515	C	N3-C4-C5	-5.22	119.81	121.90
35	E	1264	A	O4'-C1'-N9	5.22	112.38	108.20
35	E	1361	A	C5-C6-N1	-5.22	115.09	117.70
35	E	1359	C	N3-C4-C5	-5.22	119.81	121.90
35	E	491	C	N3-C4-C5	-5.22	119.81	121.90
35	E	658	A	C5-C6-N1	-5.22	115.09	117.70
35	E	1206	G	O4'-C1'-N9	5.22	112.37	108.20
35	E	1743	A	C4-C5-C6	5.22	119.61	117.00
35	E	659	A	O4'-C1'-N9	5.21	112.37	108.20
35	E	991	C	N3-C4-C5	-5.21	119.81	121.90
35	E	1201	G	C5'-C4'-C3'	5.21	124.34	116.00
35	E	1273	G	O4'-C1'-N9	5.21	112.37	108.20
35	E	1312	A	C5-C6-N1	-5.21	115.09	117.70
35	E	1825	A	C5-C6-N6	-5.21	119.53	123.70
35	E	1946	C	N3-C4-N4	5.21	121.65	118.00
35	E	2275	G	O4'-C1'-N9	5.21	112.37	108.20
35	E	538	A	C5-C6-N1	-5.21	115.09	117.70
35	E	569	A	O4'-C1'-N9	5.21	112.37	108.20
35	E	1741	G	O4'-C1'-N9	5.21	112.37	108.20
35	E	2109	G	O4'-C1'-N9	5.21	112.37	108.20
35	E	64	A	C5-C6-N6	-5.21	119.53	123.70
35	E	1625	A	C5-C6-N6	-5.21	119.53	123.70
35	E	2046	A	C5-C6-N1	-5.21	115.09	117.70
35	E	72	C	N3-C4-C5	-5.21	119.82	121.90
35	E	454	A	C5-C6-N6	-5.21	119.53	123.70
35	E	626	C	N3-C4-C5	-5.21	119.82	121.90
35	E	1548	C	N3-C4-N4	5.21	121.65	118.00
35	E	2258	C	N3-C4-C5	-5.21	119.82	121.90
26	j	97	ALA	N-CA-CB	5.21	117.39	110.10
35	E	48	G	O4'-C1'-N9	5.21	112.36	108.20
35	E	1311	C	N3-C4-C5	-5.21	119.82	121.90
35	E	1601	A	O4'-C1'-N9	5.21	112.36	108.20
35	E	1812	A	C5-C6-N6	-5.21	119.53	123.70
35	E	2248	G	N3-C2-N2	5.21	123.54	119.90
35	E	180	A	C5-C6-N1	-5.21	115.10	117.70
35	E	65	A	C5-C6-N1	-5.20	115.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	533	C	N3-C4-C5	-5.20	119.82	121.90
35	E	1300	C	C6-N1-C2	-5.20	118.22	120.30
35	E	1359	C	N3-C4-N4	5.20	121.64	118.00
35	E	879	C	N3-C4-C5	-5.20	119.82	121.90
35	E	1633	A	C5-C6-N6	-5.20	119.54	123.70
35	E	501	A	O4'-C1'-N9	5.20	112.36	108.20
35	E	525	A	C5-C6-N6	-5.20	119.54	123.70
35	E	584	C	N3-C4-C5	-5.20	119.82	121.90
35	E	903	G	O4'-C1'-N9	5.20	112.36	108.20
35	E	2274	A	C5-C6-N1	-5.20	115.10	117.70
35	E	248	G	O4'-C1'-N9	5.20	112.36	108.20
35	E	505	A	C5-C6-N1	-5.20	115.10	117.70
35	E	801	C	N3-C4-C5	-5.20	119.82	121.90
35	E	922	C	N3-C4-N4	5.20	121.64	118.00
35	E	963	G	O4'-C1'-N9	5.20	112.36	108.20
35	E	1358	G	O4'-C1'-N9	5.20	112.36	108.20
35	E	1368	A	C5-C6-N1	-5.20	115.10	117.70
35	E	2234	A	C5-C6-N1	-5.20	115.10	117.70
35	E	389	G	O4'-C1'-N9	5.20	112.36	108.20
35	E	674	A	C5-C6-N6	-5.20	119.54	123.70
35	E	729	C	N3-C4-N4	5.20	121.64	118.00
35	E	1987	A	C5-C6-N1	-5.20	115.10	117.70
35	E	2251	A	C5-C6-N1	-5.20	115.10	117.70
35	E	268	C	N3-C4-C5	-5.20	119.82	121.90
35	E	904	C	N3-C4-C5	-5.20	119.82	121.90
35	E	1937	A	C5-C6-N1	-5.20	115.10	117.70
35	E	2255	C	N3-C4-C5	-5.20	119.82	121.90
35	E	561	A	C5-C6-N1	-5.19	115.10	117.70
35	E	972	A	C5-C6-N1	-5.19	115.10	117.70
35	E	325	U	O4'-C1'-N1	5.19	112.35	108.20
35	E	539	G	O4'-C1'-N9	5.19	112.35	108.20
35	E	925	C	N3-C4-C5	-5.19	119.82	121.90
35	E	1340	A	C5-C6-N1	-5.19	115.10	117.70
35	E	1581	A	C5-C6-N1	-5.19	115.10	117.70
35	E	1607	A	C5-C6-N1	-5.19	115.10	117.70
35	E	1727	C	N3-C4-C5	-5.19	119.82	121.90
35	E	2007	A	C5-C6-N6	-5.19	119.55	123.70
35	E	744	C	C2-N1-C1'	5.19	124.51	118.80
35	E	993	A	C5-C6-N1	-5.19	115.11	117.70
35	E	1266	C	N3-C4-C5	-5.19	119.82	121.90
35	E	1954	C	N3-C4-C5	-5.19	119.82	121.90
35	E	2013	U	P-O3'-C3'	5.19	125.93	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	237	A	C5-C6-N6	-5.19	119.55	123.70
35	E	575	A	C5-C6-N6	-5.19	119.55	123.70
35	E	1633	A	O4'-C1'-N9	5.19	112.35	108.20
35	E	2296	G	O4'-C1'-N9	5.19	112.35	108.20
35	E	590	C	N3-C4-C5	-5.19	119.83	121.90
35	E	966	C	N3-C4-N4	5.19	121.63	118.00
35	E	1218	A	C5-C6-N1	-5.19	115.11	117.70
35	E	1982	C	N3-C4-C5	-5.19	119.83	121.90
35	E	1658	C	N3-C4-N4	5.19	121.63	118.00
30	m	146	ALA	N-CA-CB	5.18	117.36	110.10
35	E	554	C	N3-C4-C5	-5.18	119.83	121.90
35	E	945	C	O4'-C1'-N1	5.18	112.35	108.20
35	E	751	C	N3-C4-N4	5.18	121.63	118.00
35	E	914	C	N3-C4-N4	5.18	121.63	118.00
35	E	1248	A	C5-C6-N1	-5.18	115.11	117.70
35	E	1292	A	O4'-C1'-N9	5.18	112.35	108.20
35	E	1903	A	C4-C5-C6	5.18	119.59	117.00
35	E	596	A	C5-C6-N1	-5.18	115.11	117.70
35	E	2087	C	N3-C4-C5	-5.18	119.83	121.90
35	E	450	A	O4'-C1'-N9	5.18	112.34	108.20
35	E	1599	A	O4'-C1'-N9	5.18	112.34	108.20
35	E	419	G	O4'-C1'-N9	5.18	112.34	108.20
35	E	923	A	C5-C6-N1	-5.18	115.11	117.70
35	E	1199	G	O4'-C1'-N9	5.18	112.34	108.20
35	E	1663	C	N3-C4-C5	-5.18	119.83	121.90
35	E	1946	C	N3-C4-C5	-5.18	119.83	121.90
35	E	2005	A	C5-C6-N1	-5.18	115.11	117.70
35	E	435	G	O4'-C1'-N9	5.17	112.34	108.20
35	E	1626	C	O4'-C1'-N1	5.17	112.34	108.20
35	E	1925	A	C5-C6-N1	-5.17	115.11	117.70
35	E	2114	U	O4'-C1'-N1	5.17	112.34	108.20
35	E	2134	A	C5-C6-N6	-5.17	119.56	123.70
35	E	210	A	C5-C6-N1	-5.17	115.11	117.70
35	E	392	A	O4'-C1'-N9	5.17	112.34	108.20
35	E	588	A	C5-C6-N1	-5.17	115.11	117.70
35	E	684	A	C5-C6-N1	-5.17	115.11	117.70
35	E	1087	A	C5-C6-N6	-5.17	119.56	123.70
35	E	1566	A	C5-C6-N1	-5.17	115.11	117.70
35	E	1611	A	C5-C6-N6	-5.17	119.56	123.70
35	E	834	G	P-O5'-C5'	5.17	129.17	120.90
35	E	863	A	C5-C6-N6	-5.17	119.56	123.70
35	E	821	C	N3-C4-C5	-5.17	119.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1526	A	C5-C6-N1	-5.17	115.12	117.70
35	E	1898	G	O4'-C1'-N9	5.17	112.33	108.20
35	E	2171	C	N3-C4-C5	-5.17	119.83	121.90
35	E	308	C	N3-C4-C5	-5.17	119.83	121.90
35	E	1543	C	C5-C4-N4	-5.17	116.58	120.20
35	E	1798	G	O4'-C1'-N9	5.17	112.33	108.20
35	E	303	C	N3-C4-C5	-5.16	119.83	121.90
35	E	379	G	O4'-C1'-N9	5.16	112.33	108.20
35	E	932	G	N1-C2-N3	-5.16	120.80	123.90
35	E	1665	C	N3-C4-C5	-5.16	119.83	121.90
35	E	2202	A	O4'-C1'-N9	5.16	112.33	108.20
35	E	463	A	O4'-C1'-N9	5.16	112.33	108.20
35	E	455	C	N3-C4-C5	-5.16	119.84	121.90
35	E	1184	C	N3-C4-C5	-5.16	119.84	121.90
35	E	1552	A	C5-C6-N6	-5.16	119.57	123.70
35	E	317	G	O4'-C1'-N9	5.16	112.33	108.20
35	E	658	A	O4'-C1'-N9	5.16	112.33	108.20
35	E	1377	A	C5-C6-N1	-5.16	115.12	117.70
35	E	2004	A	C5-C6-N1	-5.16	115.12	117.70
35	E	282	C	N3-C4-C5	-5.16	119.84	121.90
35	E	681	C	N3-C4-C5	-5.16	119.84	121.90
35	E	908	G	O4'-C1'-N9	5.16	112.32	108.20
35	E	493	A	O4'-C1'-N9	5.15	112.32	108.20
35	E	1367	G	O4'-C1'-N9	5.15	112.32	108.20
35	E	218	C	N3-C4-C5	-5.15	119.84	121.90
35	E	336	C	N3-C4-C5	-5.15	119.84	121.90
35	E	1209	C	N3-C4-C5	-5.15	119.84	121.90
35	E	1362	A	C5-C6-N1	-5.15	115.12	117.70
35	E	1530	C	N3-C4-C5	-5.15	119.84	121.90
35	E	1563	G	O4'-C1'-N9	5.15	112.32	108.20
35	E	447	A	C5-C6-N1	-5.15	115.12	117.70
35	E	738	G	C6-C5-N7	-5.15	127.31	130.40
35	E	1259	A	C5-C6-N6	-5.15	119.58	123.70
35	E	2234	A	C4'-C3'-C2'	-5.15	97.45	102.60
35	E	740	U	O4'-C1'-N1	5.15	112.32	108.20
35	E	117	C	N3-C4-C5	-5.15	119.84	121.90
35	E	367	A	C5-C6-N1	-5.15	115.13	117.70
35	E	746	A	C5-C6-N6	-5.15	119.58	123.70
35	E	1801	C	N3-C4-C5	-5.15	119.84	121.90
35	E	272	G	O4'-C1'-N9	5.14	112.32	108.20
35	E	917	A	O4'-C1'-N9	5.14	112.31	108.20
35	E	1301	A	O4'-C1'-N9	5.14	112.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	779	A	C5-C6-N1	-5.14	115.13	117.70
35	E	784	A	O4'-C1'-N9	5.14	112.31	108.20
35	E	1538	G	O4'-C1'-N9	5.14	112.31	108.20
35	E	2120	A	O4'-C1'-N9	5.14	112.31	108.20
35	E	2204	A	C5-C6-N1	-5.14	115.13	117.70
35	E	43	A	C5-C6-N1	-5.14	115.13	117.70
35	E	781	A	C5-C6-N1	-5.14	115.13	117.70
35	E	1666	G	O4'-C1'-N9	5.14	112.31	108.20
35	E	975	U	P-O3'-C3'	5.14	125.87	119.70
35	E	1642	G	O4'-C1'-N9	5.14	112.31	108.20
35	E	1956	C	N3-C4-C5	-5.14	119.84	121.90
35	E	1370	A	C5-C6-N1	-5.14	115.13	117.70
35	E	1894	C	N3-C4-N4	5.14	121.60	118.00
35	E	1986	A	C5-C6-N1	-5.14	115.13	117.70
35	E	2136	A	O4'-C1'-N9	5.14	112.31	108.20
35	E	401	A	C5-C6-N1	-5.14	115.13	117.70
35	E	475	A	O4'-C1'-N9	5.14	112.31	108.20
35	E	1190	G	O4'-C1'-N9	5.14	112.31	108.20
35	E	1287	A	C5-C6-N1	-5.14	115.13	117.70
35	E	1891	C	N3-C4-C5	-5.14	119.84	121.90
35	E	261	A	C5-C6-N1	-5.13	115.13	117.70
35	E	316	A	C5-C6-N6	-5.13	119.59	123.70
35	E	1916	C	N3-C4-C5	-5.13	119.85	121.90
35	E	2189	A	C5-C6-N6	-5.13	119.59	123.70
35	E	2229	A	O4'-C1'-N9	5.13	112.31	108.20
35	E	2288	A	O4'-C1'-N9	5.13	112.31	108.20
15	W	165	TRP	CA-CB-CG	5.13	123.45	113.70
35	E	406	A	C5-C6-N1	-5.13	115.13	117.70
35	E	861	A	C5-C6-N6	-5.13	119.59	123.70
35	E	865	A	C5-C6-N1	-5.13	115.13	117.70
35	E	2238	A	O4'-C1'-N9	5.13	112.31	108.20
35	E	526	A	C5-C6-N1	-5.13	115.13	117.70
35	E	905	A	C5-C6-N6	-5.13	119.59	123.70
35	E	67	C	N3-C4-N4	5.13	121.59	118.00
35	E	315	A	C5-C6-N6	-5.13	119.60	123.70
35	E	676	G	O4'-C1'-N9	5.13	112.30	108.20
35	E	965	C	N3-C4-C5	-5.13	119.85	121.90
35	E	2264	A	O4'-C1'-N9	5.13	112.30	108.20
35	E	203	C	P-O3'-C3'	5.13	125.85	119.70
35	E	1220	G	O4'-C1'-N9	5.13	112.30	108.20
35	E	1864	C	N3-C4-C5	-5.13	119.85	121.90
35	E	2071	U	O4'-C1'-N1	5.13	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2222	G	O4'-C1'-N9	5.13	112.30	108.20
35	E	54	C	N3-C4-C5	-5.12	119.85	121.90
35	E	446	A	C5-C6-N6	-5.12	119.60	123.70
35	E	485	A	C5-C6-N6	-5.12	119.60	123.70
35	E	537	C	N3-C4-C5	-5.12	119.85	121.90
35	E	759	C	C5'-C4'-O4'	-5.12	102.95	109.10
35	E	2063	A	C5-C6-N6	-5.12	119.60	123.70
35	E	2	A	C5-C6-N1	-5.12	115.14	117.70
35	E	78	A	C5-C6-N1	-5.12	115.14	117.70
35	E	237	A	C5-C6-N1	-5.12	115.14	117.70
35	E	445	G	O4'-C1'-N9	5.12	112.30	108.20
35	E	1242	A	C5-C6-N6	-5.12	119.60	123.70
35	E	1385	A	O4'-C1'-N9	5.12	112.30	108.20
35	E	1565	U	O4'-C1'-N1	5.12	112.30	108.20
35	E	1695	A	C5-C6-N1	-5.12	115.14	117.70
35	E	1729	C	N3-C4-C5	-5.12	119.85	121.90
35	E	2143	C	N3-C4-C5	-5.12	119.85	121.90
35	E	2208	G	O4'-C1'-N9	5.12	112.30	108.20
35	E	51	A	O4'-C1'-N9	5.12	112.30	108.20
35	E	517	G	O4'-C1'-N9	5.12	112.30	108.20
20	f	205	PHE	CB-CG-CD1	5.12	124.38	120.80
35	E	684	A	C5-C6-N6	-5.12	119.61	123.70
35	E	916	A	O4'-C1'-N9	5.12	112.30	108.20
35	E	1257	C	N3-C4-C5	-5.12	119.85	121.90
35	E	140	C	N3-C4-C5	-5.12	119.85	121.90
35	E	1336	A	C5-C6-N1	-5.12	115.14	117.70
35	E	143	C	N3-C4-C5	-5.12	119.85	121.90
35	E	848	U	O4'-C1'-N1	5.12	112.29	108.20
35	E	1165	G	O4'-C1'-N9	5.12	112.29	108.20
35	E	1232	C	N3-C4-C5	-5.12	119.85	121.90
35	E	1981	A	O4'-C1'-N9	5.12	112.29	108.20
35	E	2283	A	O4'-C1'-N9	5.12	112.29	108.20
35	E	53	G	O4'-C1'-N9	5.11	112.29	108.20
35	E	724	A	O4'-C1'-N9	5.11	112.29	108.20
35	E	1340	A	O4'-C1'-N9	5.11	112.29	108.20
35	E	2178	C	N3-C4-C5	-5.11	119.86	121.90
35	E	2203	C	N3-C4-C5	-5.11	119.86	121.90
35	E	1778	U	O4'-C1'-N1	5.11	112.29	108.20
35	E	732	C	N3-C4-N4	5.11	121.58	118.00
35	E	829	C	N3-C4-C5	-5.11	119.86	121.90
35	E	902	A	O4'-C1'-N9	5.11	112.29	108.20
35	E	1353	A	O4'-C1'-N9	5.11	112.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1873	G	O4'-C1'-N9	5.11	112.29	108.20
35	E	1240	A	O4'-C1'-N9	5.11	112.29	108.20
35	E	2215	C	P-O3'-C3'	5.11	125.83	119.70
35	E	87	C	N3-C4-C5	-5.11	119.86	121.90
35	E	588	A	O4'-C1'-N9	5.11	112.29	108.20
35	E	1623	G	O4'-C1'-N9	5.11	112.29	108.20
35	E	1760	G	O4'-C1'-N9	5.11	112.29	108.20
35	E	2059	A	O4'-C1'-N9	5.11	112.29	108.20
35	E	2216	A	C5-C6-N6	-5.11	119.61	123.70
24	a	104	PHE	CB-CG-CD1	5.11	124.37	120.80
34	h	206	ALA	N-CA-CB	5.11	117.25	110.10
35	E	49	C	N3-C4-C5	-5.11	119.86	121.90
35	E	523	A	C5-C6-N6	-5.11	119.61	123.70
35	E	603	G	O4'-C1'-N9	5.11	112.28	108.20
35	E	1360	A	O4'-C1'-N9	5.11	112.28	108.20
35	E	1799	A	O4'-C1'-N9	5.11	112.28	108.20
35	E	39	A	C5-C6-N6	-5.10	119.62	123.70
35	E	409	G	O4'-C1'-N9	5.10	112.28	108.20
35	E	1610	A	O4'-C1'-N9	5.10	112.28	108.20
35	E	209	C	N3-C4-C5	-5.10	119.86	121.90
35	E	1788	C	N3-C4-N4	5.10	121.57	118.00
35	E	242	A	O4'-C1'-N9	5.10	112.28	108.20
35	E	877	A	C5-C6-N1	-5.10	115.15	117.70
35	E	583	C	N3-C4-C5	-5.10	119.86	121.90
35	E	817	A	C5-C6-N6	-5.10	119.62	123.70
35	E	822	A	C5-C6-N1	-5.10	115.15	117.70
35	E	983	C	N3-C4-C5	-5.10	119.86	121.90
35	E	1365	A	C5-C6-N1	-5.10	115.15	117.70
35	E	214	C	O4'-C1'-N1	5.10	112.28	108.20
35	E	661	G	O4'-C1'-N9	5.10	112.28	108.20
35	E	1269	C	C2-N3-C4	5.10	122.45	119.90
35	E	1546	C	P-O5'-C5'	5.10	129.06	120.90
35	E	1878	A	O4'-C1'-N9	5.10	112.28	108.20
35	E	1936	A	O4'-C1'-N9	5.10	112.28	108.20
35	E	1976	C	N3-C4-C5	-5.10	119.86	121.90
35	E	2213	G	C2'-C3'-O3'	5.10	121.86	113.70
35	E	2220	G	O4'-C1'-N9	5.10	112.28	108.20
35	E	250	A	O4'-C1'-N9	5.10	112.28	108.20
35	E	711	A	C6-N1-C2	5.09	121.66	118.60
35	E	1274	A	C4-C5-C6	5.09	119.55	117.00
35	E	2214	A	C5-C6-N1	-5.09	115.15	117.70
35	E	1354	C	N3-C4-C5	-5.09	119.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2148	A	C5-C6-N6	-5.09	119.63	123.70
35	E	2158	C	N3-C4-C5	-5.09	119.86	121.90
35	E	764	A	C5-C6-N1	-5.09	115.15	117.70
35	E	1547	A	O4'-C1'-N9	5.09	112.27	108.20
35	E	2120	A	C5-C6-N6	-5.09	119.63	123.70
35	E	43	A	O4'-C1'-N9	5.09	112.27	108.20
35	E	352	A	O4'-C1'-N9	5.09	112.27	108.20
35	E	913	A	C5-C6-N6	-5.09	119.63	123.70
35	E	1827	U	O4'-C1'-N1	5.09	112.27	108.20
35	E	408	C	N3-C4-C5	-5.09	119.87	121.90
35	E	655	A	C5-C6-N1	-5.09	115.16	117.70
35	E	1222	A	O4'-C1'-N9	5.09	112.27	108.20
35	E	1808	G	O4'-C1'-N9	5.08	112.27	108.20
35	E	2152	C	N3-C4-C5	-5.08	119.87	121.90
35	E	131	C	N3-C4-C5	-5.08	119.87	121.90
35	E	294	G	O4'-C1'-N9	5.08	112.27	108.20
35	E	299	A	C5-C6-N6	-5.08	119.63	123.70
35	E	862	A	C5-C6-N6	-5.08	119.63	123.70
35	E	2159	A	C5-C6-N1	-5.08	115.16	117.70
35	E	231	A	C5-C6-N6	-5.08	119.64	123.70
35	E	381	A	C5-C6-N1	-5.08	115.16	117.70
35	E	1939	A	C5-C6-N6	-5.08	119.64	123.70
35	E	2200	A	O4'-C1'-N9	5.08	112.26	108.20
5	u	9	GLN	C-N-CA	5.08	134.39	121.70
35	E	734	G	N3-C4-N9	-5.08	122.95	126.00
35	E	1374	A	O4'-C1'-N9	5.08	112.26	108.20
35	E	2081	G	O4'-C1'-N9	5.08	112.26	108.20
35	E	137	C	N3-C4-C5	-5.08	119.87	121.90
35	E	406	A	O4'-C1'-N9	5.08	112.26	108.20
35	E	17	C	N3-C4-C5	-5.08	119.87	121.90
35	E	1338	A	C5-C6-N6	-5.08	119.64	123.70
35	E	349	A	C5-C6-N1	-5.07	115.16	117.70
35	E	518	C	N3-C4-C5	-5.07	119.87	121.90
35	E	1258	A	O4'-C1'-N9	5.07	112.26	108.20
35	E	1573	C	N3-C4-C5	-5.07	119.87	121.90
35	E	778	A	O4'-C1'-N9	5.07	112.26	108.20
35	E	2280	A	C5-C6-N1	-5.07	115.16	117.70
35	E	500	A	C5-C6-N1	-5.07	115.17	117.70
35	E	782	A	O4'-C1'-N9	5.07	112.26	108.20
35	E	1235	A	O4'-C1'-N9	5.07	112.26	108.20
35	E	1540	C	N3-C4-N4	5.07	121.55	118.00
35	E	1262	C	N3-C4-C5	-5.07	119.87	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1630	A	O4'-C1'-N9	5.07	112.25	108.20
11	S	53	SER	N-CA-CB	5.07	118.10	110.50
35	E	242	A	C5-C6-N1	-5.07	115.17	117.70
35	E	271	C	N3-C4-C5	-5.07	119.87	121.90
35	E	454	A	O4'-C1'-N9	5.07	112.25	108.20
35	E	575	A	C5-C6-N1	-5.07	115.17	117.70
35	E	1887	U	O4'-C1'-N1	5.07	112.25	108.20
35	E	2022	A	C5-C6-N1	-5.07	115.17	117.70
35	E	278	A	C5-C6-N1	-5.07	115.17	117.70
35	E	490	C	N3-C4-C5	-5.07	119.87	121.90
35	E	1368	A	O4'-C1'-N9	5.07	112.25	108.20
35	E	224	C	N3-C4-C5	-5.06	119.87	121.90
35	E	349	A	O4'-C1'-N9	5.06	112.25	108.20
35	E	2067	C	N3-C4-N4	5.06	121.55	118.00
35	E	1075	G	C5'-C4'-O4'	-5.06	103.03	109.10
35	E	2211	C	N3-C4-C5	-5.06	119.88	121.90
35	E	149	A	C3'-C2'-C1'	5.06	105.55	101.50
35	E	1606	A	O4'-C1'-N9	5.06	112.25	108.20
35	E	2006	A	C5-C6-N1	-5.06	115.17	117.70
35	E	2271	A	C5-C6-N6	-5.06	119.65	123.70
35	E	488	G	O4'-C1'-N9	5.06	112.25	108.20
35	E	763	G	O4'-C1'-N9	5.06	112.25	108.20
35	E	1639	A	C5-C6-N1	-5.06	115.17	117.70
35	E	472	A	O4'-C1'-N9	5.06	112.25	108.20
35	E	1569	G	O4'-C1'-N9	5.06	112.25	108.20
30	m	178	ALA	N-CA-CB	5.05	117.17	110.10
35	E	597	C	O4'-C1'-N1	5.05	112.24	108.20
35	E	1978	C	N3-C4-C5	-5.05	119.88	121.90
35	E	1586	G	O4'-C1'-N9	5.05	112.24	108.20
35	E	1237	G	N3-C2-N2	5.05	123.44	119.90
35	E	1326	G	O4'-C1'-N9	5.05	112.24	108.20
35	E	576	A	C5-C6-N1	-5.05	115.17	117.70
35	E	866	A	C5-C6-N6	-5.05	119.66	123.70
35	E	1702	A	O4'-C1'-N9	5.05	112.24	108.20
35	E	456	C	N3-C4-C5	-5.04	119.88	121.90
35	E	513	G	O4'-C1'-N9	5.04	112.24	108.20
35	E	575	A	O4'-C1'-N9	5.04	112.24	108.20
35	E	1245	C	N3-C4-C5	-5.04	119.88	121.90
35	E	1976	C	N3-C4-N4	5.04	121.53	118.00
35	E	2107	A	O4'-C1'-N9	5.04	112.24	108.20
35	E	1602	C	N3-C4-C5	-5.04	119.88	121.90
35	E	1651	A	C5-C6-N1	-5.04	115.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	2034	A	C5-C6-N1	-5.04	115.18	117.70
35	E	2302	C	N3-C4-C5	-5.04	119.88	121.90
35	E	1183	G	O4'-C1'-N9	5.04	112.23	108.20
35	E	299	A	O4'-C1'-N9	5.04	112.23	108.20
35	E	845	A	O4'-C1'-N9	5.04	112.23	108.20
35	E	1385	A	C5-C6-N1	-5.04	115.18	117.70
35	E	1595	A	O4'-C1'-N9	5.04	112.23	108.20
35	E	2038	G	O4'-C1'-N9	5.04	112.23	108.20
35	E	26	A	O4'-C1'-N9	5.04	112.23	108.20
35	E	1540	C	N3-C4-C5	-5.04	119.89	121.90
35	E	2131	A	C5-C6-N1	-5.04	115.18	117.70
35	E	813	U	O4'-C1'-N1	5.03	112.23	108.20
35	E	1699	U	O4'-C1'-N1	5.03	112.23	108.20
35	E	1768	A	C5-C6-N6	-5.03	119.67	123.70
35	E	1802	C	N3-C4-C5	-5.03	119.89	121.90
35	E	2149	C	N3-C4-C5	-5.03	119.89	121.90
35	E	2233	G	O4'-C1'-N9	5.03	112.23	108.20
35	E	216	A	C5-C6-N1	-5.03	115.18	117.70
35	E	249	A	C5-C6-N1	-5.03	115.19	117.70
35	E	600	U	O4'-C1'-N1	5.03	112.22	108.20
35	E	877	A	O4'-C1'-N9	5.03	112.22	108.20
35	E	1252	C	N3-C4-C5	-5.03	119.89	121.90
35	E	1547	A	C5-C6-N6	-5.03	119.68	123.70
35	E	721	C	N3-C4-C5	-5.03	119.89	121.90
35	E	2187	C	N3-C4-C5	-5.03	119.89	121.90
35	E	2247	C	N3-C4-C5	-5.03	119.89	121.90
35	E	983	C	N3-C4-N4	5.03	121.52	118.00
35	E	1261	A	C5-C6-N1	-5.03	115.19	117.70
35	E	1310	C	N3-C4-C5	-5.03	119.89	121.90
35	E	2287	U	O4'-C1'-N1	5.03	112.22	108.20
35	E	738	G	C5-C6-N1	-5.03	108.99	111.50
35	E	2012	C	N3-C4-C5	-5.03	119.89	121.90
35	E	2290	C	N3-C4-C5	-5.03	119.89	121.90
35	E	1580	G	N3-C2-N2	5.02	123.42	119.90
35	E	202	C	N3-C4-C5	-5.02	119.89	121.90
3	r	121	TYR	CB-CG-CD1	5.02	124.01	121.00
35	E	2095	G	C4-N9-C1'	5.02	133.02	126.50
35	E	211	G	O4'-C1'-N9	5.02	112.21	108.20
35	E	1254	C	N3-C4-C5	-5.02	119.89	121.90
35	E	436	G	O4'-C1'-N9	5.02	112.21	108.20
35	E	623	C	N3-C4-C5	-5.02	119.89	121.90
35	E	771	A	C5-C6-N1	-5.02	115.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	E	1250	A	O4'-C1'-N9	5.01	112.21	108.20
35	E	1589	C	N3-C4-C5	-5.01	119.89	121.90
35	E	206	C	N3-C4-C5	-5.01	119.89	121.90
35	E	616	G	O4'-C1'-N9	5.01	112.21	108.20
35	E	1074	C	N3-C4-C5	-5.01	119.89	121.90
35	E	2169	A	C5-C6-N1	-5.01	115.19	117.70
35	E	411	G	O4'-C1'-N9	5.01	112.21	108.20
35	E	2088	A	C5-C6-N1	-5.01	115.19	117.70
35	E	111	A	C5-C6-N1	-5.01	115.20	117.70
35	E	1980	C	N3-C4-C5	-5.01	119.90	121.90
35	E	313	G	C8-N9-C1'	-5.01	120.49	127.00
35	E	295	A	O4'-C1'-N9	5.00	112.20	108.20
35	E	1194	U	O4'-C1'-N1	5.00	112.20	108.20
35	E	522	A	C5-C6-N6	-5.00	119.70	123.70
35	E	534	C	N3-C4-C5	-5.00	119.90	121.90
35	E	542	C	N3-C4-C5	-5.00	119.90	121.90
35	E	1072	G	O4'-C1'-N9	5.00	112.20	108.20
35	E	1230	G	O4'-C1'-N9	5.00	112.20	108.20
35	E	1328	A	C5-C6-N1	-5.00	115.20	117.70
35	E	2023	C	N3-C4-N4	5.00	121.50	118.00
35	E	189	G	O4'-C1'-N9	5.00	112.20	108.20
35	E	232	C	N3-C4-C5	-5.00	119.90	121.90
35	E	271	C	P-O5'-C5'	5.00	128.90	120.90
35	E	484	A	C5-C6-N6	-5.00	119.70	123.70
35	E	1998	A	C5-C6-N1	-5.00	115.20	117.70
35	E	2121	G	O4'-C1'-N9	5.00	112.20	108.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	E	325	U	C3'
35	E	702	U	C1'
35	E	810	U	C3'
35	E	1903	A	C3'

All (180) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	E	1080	U	Sidechain
35	E	1084	G	Sidechain
35	E	1169	U	Sidechain
35	E	1170	C	Sidechain

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Mol	Chain	Res	Type	Group
35	E	1171	C	Sidechain
35	E	1182	G	Sidechain
35	E	1186	U	Sidechain
35	E	1187	C	Sidechain
35	E	1188	C	Sidechain
35	E	1190	G	Sidechain
35	E	1253	G	Sidechain
35	E	1271	G	Sidechain
35	E	1300	C	Sidechain
35	E	1358	G	Sidechain
35	E	1376	G	Sidechain
35	E	143	C	Sidechain
35	E	1542	U	Sidechain
35	E	1543	C	Sidechain
35	E	1559	U	Sidechain
35	E	1560	G	Sidechain
35	E	159	G	Sidechain
35	E	1625	A	Sidechain
35	E	1638	G	Sidechain
35	E	1651	A	Sidechain
35	E	1652	A	Sidechain
35	E	1667	G	Sidechain
35	E	1670	A	Sidechain
35	E	1686	G	Sidechain
35	E	1714	U	Sidechain
35	E	172	A	Sidechain
35	E	1735	G	Sidechain
35	E	1737	U	Sidechain
35	E	1825	A	Sidechain
35	E	1867	G	Sidechain
35	E	1870	G	Sidechain
35	E	1872	G	Sidechain
35	E	1873	G	Sidechain
35	E	1874	C	Sidechain
35	E	1876	G	Sidechain
35	E	1880	U	Sidechain
35	E	1886	G	Sidechain
35	E	1903	A	Sidechain
35	E	1924	G	Sidechain
35	E	1925	A	Sidechain
35	E	1928	U	Sidechain
35	E	1941	C	Sidechain

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Mol	Chain	Res	Type	Group
35	E	1989	G	Sidechain
35	E	2003	G	Sidechain
35	E	2012	C	Sidechain
35	E	2019	C	Sidechain
35	E	202	C	Sidechain
35	E	2044	G	Sidechain
35	E	2075	G	Sidechain
35	E	2113	G	Sidechain
35	E	2129	U	Sidechain
35	E	213	G	Sidechain
35	E	2153	C	Sidechain
35	E	2215	C	Sidechain
35	E	2239	A	Sidechain
35	E	2240	A	Sidechain
35	E	226	A	Sidechain
35	E	228	G	Sidechain
35	E	2283	A	Sidechain
35	E	249	A	Sidechain
35	E	259	C	Sidechain
35	E	260	A	Sidechain
35	E	344	G	Sidechain
35	E	361	U	Sidechain
35	E	39	A	Sidechain
35	E	476	G	Sidechain
35	E	481	G	Sidechain
35	E	512	A	Sidechain
35	E	60	U	Sidechain
35	E	600	U	Sidechain
35	E	667	G	Sidechain
35	E	700	U	Sidechain
35	E	701	C	Sidechain
35	E	706	G	Sidechain
35	E	708	G	Sidechain
35	E	710	A	Sidechain
35	E	712	U	Sidechain
35	E	713	G	Sidechain
35	E	717	U	Sidechain
35	E	718	A	Sidechain
35	E	719	G	Sidechain
35	E	720	U	Sidechain
35	E	721	C	Sidechain
35	E	724	A	Sidechain

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Mol	Chain	Res	Type	Group
35	E	726	C	Sidechain
35	E	733	G	Sidechain
35	E	734	G	Sidechain
35	E	735	A	Sidechain
35	E	738	G	Sidechain
35	E	739	G	Sidechain
35	E	741	G	Sidechain
35	E	744	C	Sidechain
35	E	746	A	Sidechain
35	E	754	G	Sidechain
35	E	756	G	Sidechain
35	E	758	U	Sidechain
35	E	759	C	Sidechain
35	E	774	C	Sidechain
35	E	776	G	Sidechain
35	E	788	A	Sidechain
35	E	792	G	Sidechain
35	E	796	G	Sidechain
35	E	807	U	Sidechain
35	E	824	G	Sidechain
35	E	828	G	Sidechain
35	E	834	G	Sidechain
35	E	849	U	Sidechain
35	E	874	C	Sidechain
35	E	936	C	Sidechain
35	E	937	C	Sidechain
35	E	953	G	Sidechain
35	E	954	G	Sidechain
35	E	966	C	Sidechain
35	E	979	G	Sidechain
35	E	982	G	Sidechain
35	E	984	A	Sidechain
35	E	989	G	Sidechain
8	O	138	TYR	Sidechain
8	O	150	ARG	Peptide
8	O	57	ARG	Sidechain
27	P	44	ASP	Peptide
27	P	9	ARG	Peptide
9	Q	112	TYR	Sidechain
9	Q	119	ARG	Sidechain
9	Q	37	LYS	Peptide
15	W	81	ASP	Peptide

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Mol	Chain	Res	Type	Group
18	Z	56	ARG	Sidechain
24	a	107	TYR	Sidechain
24	a	46	VAL	Peptide
33	c	62	PRO	Peptide
33	c	65	ALA	Peptide
22	e	57	ARG	Sidechain
34	h	111	ALA	Peptide
34	h	120	LEU	Peptide
34	h	139	THR	Peptide
34	h	147	ASN	Peptide
34	h	154	SER	Peptide
34	h	155	PRO	Peptide
34	h	157	PHE	Peptide
34	h	158	ARG	Peptide
34	h	159	ALA	Peptide
34	h	160	SER	Peptide
34	h	174	LYS	Peptide
34	h	179	ARG	Peptide
34	h	180	THR	Peptide
34	h	182	ARG	Peptide
34	h	183	ASN	Peptide
34	h	184	ASN	Peptide
34	h	203	LYS	Peptide
34	h	207	GLU	Peptide
34	h	217	LEU	Peptide
34	h	77	GLN	Peptide
34	h	93	VAL	Peptide
34	h	94	VAL	Peptide
26	j	99	LYS	Peptide
28	k	173	ARG	Sidechain
30	m	142	LYS	Peptide
30	m	145	ARG	Peptide
32	o	63	ALA	Peptide
32	o	89	TYR	Sidechain
1	p	110	LYS	Peptide
1	p	261	ARG	Sidechain
1	p	43	TRP	Peptide
3	r	120	LYS	Peptide
3	r	121	TYR	Peptide
3	r	141	ARG	Peptide
3	r	142	THR	Peptide
3	r	147	SER	Peptide

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Mol	Chain	Res	Type	Group
3	r	32	GLN	Peptide
3	r	42	VAL	Peptide
4	t	104	TYR	Sidechain
4	t	128	MET	Peptide
5	u	43	TYR	Sidechain
5	u	48	LYS	Peptide
5	u	56	ARG	Peptide
5	u	9	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	p	2405	0	2323	0	0
2	q	311	0	319	0	0
3	r	1113	0	1175	0	0
4	t	969	0	1003	0	0
5	u	981	0	1021	0	0
6	L	2038	0	2142	0	0
7	M	1116	0	1169	0	0
8	O	1493	0	1562	0	0
9	Q	1670	0	1778	1	0
10	R	1143	0	1226	1	0
11	S	630	0	630	0	0
12	T	829	0	866	0	0
13	U	526	0	550	0	0
14	V	1011	0	1019	0	0
15	W	1781	0	1853	0	0
16	X	1212	0	1250	0	0
17	Y	989	0	1065	0	0
18	Z	1404	0	1503	1	0
19	b	1365	0	1410	0	0
20	f	1658	0	1704	0	0
21	d	1726	0	1774	0	0
22	e	1019	0	1050	0	0
23	g	635	0	631	0	0
24	a	553	0	608	0	0
25	i	958	0	981	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	j	518	0	513	0	0
27	P	1983	0	2131	0	0
28	k	972	0	1031	0	0
29	l	784	0	848	0	0
30	m	1587	0	1662	0	0
31	n	780	0	771	0	0
32	o	1116	0	1166	0	0
33	c	480	0	532	0	0
34	h	1358	0	1419	0	0
35	E	43106	0	21756	87	0
All	All	82219	0	62441	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:E:725:U:H3	35:E:733:G:H1	1.12	0.96
35:E:1849:U:H3	35:E:1869:G:H1	1.26	0.83
35:E:207:G:H1	35:E:222:U:H3	1.30	0.78
35:E:2220:G:H1	35:E:2232:U:H3	1.32	0.77
35:E:711:A:N1	35:E:746:A:N1	2.33	0.77
35:E:1085:G:H1	35:E:1169:U:H3	1.33	0.76
35:E:322:G:H1	35:E:331:U:H3	1.31	0.76
35:E:546:U:H2'	35:E:547:G:H5'	1.68	0.75
35:E:539:G:H1	35:E:550:U:H3	1.35	0.74
35:E:259:C:N3	35:E:954:G:N1	2.35	0.73
35:E:724:A:C4	35:E:735:A:C2	2.80	0.70
35:E:216:A:H2'	35:E:217:C:H5'	1.74	0.69
35:E:1088:A:N1	35:E:1166:C:N3	2.41	0.69
35:E:532:G:H1	35:E:558:U:H3	1.38	0.69
35:E:1089:U:H3	35:E:1165:G:H1	1.39	0.68
35:E:1381:G:H1	35:E:1537:U:H3	1.40	0.67
35:E:880:A:H62	35:E:892:U:H3	1.43	0.64
35:E:546:U:C2'	35:E:547:G:H5'	2.28	0.63
35:E:724:A:C2	35:E:734:G:N1	2.65	0.63
35:E:259:C:C2	35:E:954:G:C2	2.88	0.62
35:E:2124:G:H22	35:E:2140:U:H3	1.48	0.61
35:E:1852:G:C2	35:E:1866:A:C2	2.93	0.57
35:E:216:A:C2'	35:E:217:C:H5'	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:E:1872:G:C6	35:E:1873:G:C6	2.94	0.55
35:E:724:A:C2	35:E:725:U:C2	2.96	0.54
35:E:2004:A:H61	35:E:2052:C:H41	1.57	0.53
35:E:259:C:N3	35:E:954:G:C6	2.77	0.53
35:E:817:A:C2	35:E:828:G:C2	2.97	0.52
35:E:1856:G:H3'	35:E:1857:U:H5"	1.92	0.52
35:E:989:G:H1	35:E:1177:C:H42	1.57	0.51
35:E:1689:A:H1'	35:E:1691:G:H1	1.74	0.51
35:E:718:A:C2	35:E:719:G:C2	2.99	0.51
35:E:1911:U:H3	35:E:1917:G:H1	1.59	0.50
35:E:1852:G:N1	35:E:1866:A:C2	2.80	0.50
35:E:1184:C:H2'	35:E:1185:A:C8	2.46	0.50
35:E:724:A:N1	35:E:734:G:C6	2.80	0.50
35:E:1866:A:C2	35:E:1867:G:C4	3.00	0.49
35:E:260:A:N1	35:E:953:G:C6	2.81	0.49
35:E:744:C:H2'	35:E:745:C:C6	2.47	0.49
35:E:259:C:C4	35:E:954:G:N1	2.81	0.48
35:E:202:C:N3	35:E:226:A:N1	2.61	0.48
35:E:1200:A:N1	35:E:1300:C:C4	2.81	0.48
35:E:1848:U:H3	35:E:1870:G:H1	1.60	0.48
35:E:1384:G:N1	35:E:1534:A:C2	2.82	0.48
35:E:2091:U:H3'	35:E:2092:A:H5"	1.96	0.48
35:E:1987:A:H3'	35:E:1988:U:H5'	1.96	0.47
35:E:260:A:C6	35:E:953:G:N1	2.82	0.47
35:E:711:A:C2	35:E:746:A:C2	3.03	0.47
35:E:120:C:H3'	35:E:121:A:H5"	1.97	0.47
35:E:1908:U:H3'	35:E:1909:U:H5'	1.98	0.46
35:E:734:G:C6	35:E:735:A:C6	3.04	0.46
35:E:1375:U:H3	35:E:1543:C:N4	2.13	0.45
35:E:774:C:H1'	35:E:775:A:H5"	1.98	0.45
35:E:259:C:C2	35:E:954:G:C4	3.05	0.45
35:E:2051:C:H3'	35:E:2052:C:H4'	1.99	0.45
35:E:1846:C:C2	35:E:1873:G:N2	2.85	0.44
35:E:1923:U:H3	35:E:1927:A:H62	1.66	0.44
35:E:156:G:H3'	35:E:157:G:H5"	1.99	0.44
35:E:1169:U:C4	35:E:1170:C:C4	3.05	0.44
35:E:743:C:H2'	35:E:744:C:C6	2.52	0.43
35:E:999:U:H3	35:E:1072:G:H1	1.66	0.43
35:E:1872:G:N1	35:E:1873:G:N1	2.66	0.43
35:E:824:G:H5"	35:E:825:C:H5"	1.99	0.43
35:E:711:A:C5	35:E:712:U:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:64:ASN:HD21	35:E:305:U:H2'	1.83	0.43
35:E:1380:U:H3	35:E:1538:G:H1	1.65	0.43
35:E:1542:U:H2'	35:E:1543:C:H5"	2.01	0.43
10:R:16:LEU:HD11	35:E:1196:A:H5"	2.01	0.43
35:E:711:A:N1	35:E:746:A:C2	2.86	0.42
35:E:1905:U:H3	35:E:1922:G:H22	1.68	0.42
35:E:714:G:H2'	35:E:718:A:H62	1.84	0.42
35:E:1629:C:H1'	35:E:2153:C:H41	1.84	0.42
35:E:1852:G:C6	35:E:1866:A:N1	2.88	0.42
35:E:260:A:C2	35:E:953:G:C2	3.08	0.42
35:E:1993:G:H21	35:E:1994:U:H2'	1.84	0.41
35:E:703:A:C2	35:E:704:A:C5	3.09	0.41
35:E:260:A:C2	35:E:953:G:C4	3.08	0.41
35:E:724:A:C6	35:E:735:A:N1	2.88	0.41
35:E:1825:A:C2	35:E:1879:U:O4	2.73	0.41
35:E:1852:G:N2	35:E:1866:A:C2	2.89	0.41
35:E:817:A:N1	35:E:828:G:N1	2.69	0.41
35:E:718:A:C2	35:E:744:C:O2	2.73	0.41
35:E:602:G:N1	35:E:645:A:N1	2.69	0.41
35:E:1856:G:C3'	35:E:1857:U:H5"	2.51	0.41
9:Q:103:LYS:HA	35:E:763:G:H1	1.85	0.41
35:E:1384:G:C2	35:E:1534:A:C2	3.09	0.40
35:E:216:A:C2	35:E:217:C:C6	3.10	0.40

There are no symmetry-related clashes.

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	p	308/318 (97%)	288 (94%)	18 (6%)	2 (1%)	25 63
2	q	36/57 (63%)	28 (78%)	6 (17%)	2 (6%)	2 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	r	138/149 (93%)	113 (82%)	18 (13%)	7 (5%)	2	22
4	t	117/152 (77%)	105 (90%)	8 (7%)	4 (3%)	3	30
5	u	118/153 (77%)	102 (86%)	13 (11%)	3 (2%)	5	35
6	L	256/273 (94%)	239 (93%)	16 (6%)	1 (0%)	34	71
7	M	140/143 (98%)	131 (94%)	8 (6%)	1 (1%)	22	61
8	O	188/190 (99%)	165 (88%)	16 (8%)	7 (4%)	3	28
9	Q	198/211 (94%)	178 (90%)	16 (8%)	4 (2%)	7	40
10	R	139/151 (92%)	127 (91%)	11 (8%)	1 (1%)	22	61
11	S	80/86 (93%)	73 (91%)	5 (6%)	2 (2%)	5	35
12	T	102/112 (91%)	90 (88%)	12 (12%)	0	100	100
13	U	66/112 (59%)	62 (94%)	3 (4%)	1 (2%)	10	45
14	V	133/144 (92%)	116 (87%)	16 (12%)	1 (1%)	19	58
15	W	215/261 (82%)	200 (93%)	13 (6%)	2 (1%)	17	55
16	X	146/173 (84%)	133 (91%)	11 (8%)	2 (1%)	11	46
17	Y	121/137 (88%)	113 (93%)	8 (7%)	0	100	100
18	Z	171/221 (77%)	157 (92%)	12 (7%)	2 (1%)	13	49
19	b	162/190 (85%)	143 (88%)	17 (10%)	2 (1%)	13	49
20	f	205/245 (84%)	190 (93%)	12 (6%)	3 (2%)	10	45
21	d	221/263 (84%)	205 (93%)	14 (6%)	2 (1%)	17	55
22	e	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	19	58
23	g	81/236 (34%)	78 (96%)	3 (4%)	0	100	100
24	a	68/110 (62%)	58 (85%)	6 (9%)	4 (6%)	1	19
25	i	119/141 (84%)	111 (93%)	7 (6%)	1 (1%)	19	58
26	j	62/150 (41%)	47 (76%)	11 (18%)	4 (6%)	1	18
27	P	247/250 (99%)	226 (92%)	21 (8%)	0	100	100
28	k	116/196 (59%)	102 (88%)	13 (11%)	1 (1%)	17	55
29	l	97/117 (83%)	82 (84%)	15 (16%)	0	100	100
30	m	198/214 (92%)	179 (90%)	14 (7%)	5 (2%)	5	35
31	n	91/161 (56%)	83 (91%)	5 (6%)	3 (3%)	4	30
32	o	138/167 (83%)	112 (81%)	21 (15%)	5 (4%)	3	28
33	c	58/66 (88%)	53 (91%)	4 (7%)	1 (2%)	9	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	h	171/257 (66%)	123 (72%)	31 (18%)	17 (10%)	0 9
All	All	4833/5936 (81%)	4330 (90%)	412 (8%)	91 (2%)	11 40

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	r	121	TYR
3	r	124	ILE
5	u	120	VAL
9	Q	138	CYS
21	d	81	SER
26	j	95	MET
26	j	97	ALA
30	m	144	GLN
34	h	77	GLN
34	h	121	PHE
34	h	155	PRO
34	h	158	ARG
34	h	162	THR
34	h	183	ASN
34	h	184	ASN
34	h	204	ASN
2	q	31	VAL
3	r	119	ASP
3	r	146	LYS
4	t	45	HIS
5	u	35	LYS
8	O	10	ASN
8	O	114	VAL
9	Q	122	THR
11	S	53	SER
11	S	71	LYS
19	b	136	ALA
24	a	101	SER
24	a	103	LYS
24	a	105	ARG
30	m	141	ILE
30	m	187	ILE
32	o	81	VAL
34	h	94	VAL
34	h	164	LYS
34	h	191	ASP

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Mol	Chain	Res	Type
1	p	131	ASN
2	q	30	ALA
3	r	127	PRO
8	O	155	LEU
9	Q	51	VAL
16	X	43	MET
18	Z	69	THR
20	f	36	ALA
20	f	116	GLN
26	j	105	GLU
26	j	115	ARG
32	o	13	ARG
32	o	15	ILE
34	h	128	GLY
34	h	163	LYS
4	t	60	ALA
4	t	128	MET
7	M	86	PRO
8	O	25	SER
8	O	39	ALA
10	R	134	GLN
13	U	108	ALA
14	V	57	ALA
18	Z	29	LEU
24	a	45	ALA
25	i	103	LEU
28	k	141	PRO
31	n	32	THR
31	n	36	SER
31	n	68	TRP
34	h	161	THR
1	p	122	ARG
3	r	143	ARG
5	u	9	GLN
8	O	2	SER
8	O	11	LYS
9	Q	39	LEU
15	W	56	ILE
19	b	137	LYS
20	f	9	LYS
21	d	238	ALA
32	o	77	ILE

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Mol	Chain	Res	Type
34	h	175	VAL
34	h	206	ALA
30	m	92	VAL
32	o	63	ALA
33	c	23	LYS
34	h	111	ALA
22	e	29	PRO
4	t	61	PRO
3	r	61	VAL
30	m	47	ILE
6	L	167	VAL
15	W	223	PRO
16	X	89	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	p	262/268 (98%)	260 (99%)	2 (1%)	81 89
2	q	34/49 (69%)	34 (100%)	0	100 100
3	r	113/121 (93%)	113 (100%)	0	100 100
4	t	102/131 (78%)	102 (100%)	0	100 100
5	u	104/132 (79%)	104 (100%)	0	100 100
6	L	217/230 (94%)	217 (100%)	0	100 100
7	M	116/117 (99%)	116 (100%)	0	100 100
8	O	160/160 (100%)	160 (100%)	0	100 100
9	Q	188/195 (96%)	188 (100%)	0	100 100
10	R	125/132 (95%)	124 (99%)	1 (1%)	81 89
11	S	70/73 (96%)	70 (100%)	0	100 100
12	T	87/93 (94%)	87 (100%)	0	100 100
13	U	57/97 (59%)	57 (100%)	0	100 100
14	V	103/112 (92%)	102 (99%)	1 (1%)	76 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	W	194/223 (87%)	192 (99%)	2 (1%)	76 86
16	X	137/157 (87%)	137 (100%)	0	100 100
17	Y	104/116 (90%)	104 (100%)	0	100 100
18	Z	143/184 (78%)	143 (100%)	0	100 100
19	b	148/165 (90%)	148 (100%)	0	100 100
20	f	182/211 (86%)	181 (100%)	1 (0%)	88 93
21	d	187/208 (90%)	187 (100%)	0	100 100
22	e	110/111 (99%)	109 (99%)	1 (1%)	78 88
23	g	68/186 (37%)	68 (100%)	0	100 100
24	a	64/96 (67%)	63 (98%)	1 (2%)	62 79
25	i	103/120 (86%)	99 (96%)	4 (4%)	32 58
26	j	55/123 (45%)	54 (98%)	1 (2%)	59 77
27	P	204/205 (100%)	204 (100%)	0	100 100
28	k	108/172 (63%)	108 (100%)	0	100 100
29	l	89/104 (86%)	89 (100%)	0	100 100
30	m	167/179 (93%)	166 (99%)	1 (1%)	86 92
31	n	84/125 (67%)	83 (99%)	1 (1%)	71 84
32	o	118/139 (85%)	117 (99%)	1 (1%)	81 89
33	c	49/53 (92%)	49 (100%)	0	100 100
34	h	138/191 (72%)	133 (96%)	5 (4%)	35 61
All	All	4190/4978 (84%)	4168 (100%)	22 (0%)	89 93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	p	29	ILE
1	p	175	ASP
10	R	16	LEU
14	V	44	GLU
15	W	89	VAL
15	W	165	TRP
20	f	72	GLU
22	e	57	ARG
24	a	106	LEU
25	i	69	GLU

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Mol	Chain	Res	Type
25	i	121	VAL
25	i	128	GLU
25	i	133	LEU
26	j	119	GLU
30	m	137	VAL
31	n	48	GLN
32	o	116	LEU
34	h	94	VAL
34	h	103	TYR
34	h	181	TYR
34	h	217	LEU
34	h	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	p	307	ASN
3	r	13	GLN
6	L	33	HIS
8	O	27	HIS
9	Q	36	HIS
9	Q	47	HIS
14	V	25	HIS
15	W	193	ASN
16	X	11	HIS
16	X	37	ASN
18	Z	64	ASN
20	f	121	GLN
30	m	163	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	E	2017/2319 (86%)	437 (21%)	86 (4%)

All (437) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	E	4	C
35	E	5	U

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Mol	Chain	Res	Type
35	E	17	C
35	E	25	C
35	E	26	A
35	E	34	G
35	E	35	U
35	E	45	U
35	E	46	U
35	E	47	A
35	E	56	U
35	E	65	A
35	E	74	U
35	E	75	U
35	E	76	G
35	E	82	A
35	E	83	U
35	E	90	A
35	E	111	A
35	E	121	A
35	E	137	C
35	E	143	C
35	E	144	A
35	E	145	U
35	E	157	G
35	E	163	C
35	E	170	C
35	E	184	A
35	E	191	U
35	E	193	U
35	E	194	U
35	E	196	U
35	E	198	U
35	E	199	G
35	E	200	U
35	E	202	C
35	E	203	C
35	E	204	G
35	E	227	U
35	E	228	G
35	E	249	A
35	E	252	G
35	E	253	U
35	E	255	A

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Mol	Chain	Res	Type
35	E	257	A
35	E	258	C
35	E	271	C
35	E	284	C
35	E	286	G
35	E	287	A
35	E	288	A
35	E	309	G
35	E	311	G
35	E	313	G
35	E	316	A
35	E	322	G
35	E	325	U
35	E	326	U
35	E	327	U
35	E	329	U
35	E	331	U
35	E	357	C
35	E	362	C
35	E	364	G
35	E	385	G
35	E	386	A
35	E	408	C
35	E	427	U
35	E	447	A
35	E	449	U
35	E	450	A
35	E	463	A
35	E	464	C
35	E	465	G
35	E	471	C
35	E	472	A
35	E	473	G
35	E	486	U
35	E	491	C
35	E	507	A
35	E	520	A
35	E	529	A
35	E	531	A
35	E	532	G
35	E	533	C
35	E	560	C

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Mol	Chain	Res	Type
35	E	564	G
35	E	570	U
35	E	571	A
35	E	585	A
35	E	586	A
35	E	590	C
35	E	592	A
35	E	593	G
35	E	596	A
35	E	613	C
35	E	634	A
35	E	648	A
35	E	665	U
35	E	673	A
35	E	674	A
35	E	676	G
35	E	677	G
35	E	678	G
35	E	698	C
35	E	699	C
35	E	702	U
35	E	703	A
35	E	704	A
35	E	705	G
35	E	706	G
35	E	707	C
35	E	708	G
35	E	710	A
35	E	713	G
35	E	714	G
35	E	717	U
35	E	718	A
35	E	720	U
35	E	721	C
35	E	726	C
35	E	727	C
35	E	728	A
35	E	729	C
35	E	730	U
35	E	731	U
35	E	732	C
35	E	733	G

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Mol	Chain	Res	Type
35	E	736	U
35	E	737	U
35	E	738	G
35	E	739	G
35	E	740	U
35	E	741	G
35	E	742	A
35	E	745	C
35	E	747	U
35	E	748	G
35	E	749	C
35	E	750	C
35	E	751	C
35	E	752	U
35	E	757	G
35	E	760	C
35	E	762	U
35	E	766	C
35	E	768	G
35	E	769	A
35	E	770	C
35	E	771	A
35	E	772	U
35	E	773	U
35	E	774	C
35	E	775	A
35	E	776	G
35	E	777	A
35	E	778	A
35	E	785	A
35	E	786	A
35	E	789	C
35	E	793	A
35	E	795	U
35	E	796	G
35	E	798	U
35	E	799	A
35	E	804	U
35	E	806	C
35	E	808	G
35	E	809	A
35	E	810	U

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Mol	Chain	Res	Type
35	E	811	U
35	E	812	A
35	E	813	U
35	E	814	C
35	E	815	G
35	E	821	C
35	E	822	A
35	E	823	U
35	E	824	G
35	E	825	C
35	E	827	U
35	E	829	C
35	E	830	C
35	E	834	G
35	E	835	G
35	E	836	G
35	E	844	G
35	E	847	U
35	E	848	U
35	E	858	A
35	E	861	A
35	E	871	G
35	E	872	A
35	E	877	A
35	E	880	A
35	E	881	G
35	E	884	A
35	E	885	U
35	E	886	U
35	E	887	C
35	E	888	G
35	E	889	A
35	E	891	U
35	E	892	U
35	E	893	G
35	E	895	A
35	E	901	A
35	E	919	G
35	E	920	A
35	E	921	G
35	E	922	C
35	E	923	A

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Mol	Chain	Res	Type
35	E	924	G
35	E	925	C
35	E	935	A
35	E	936	C
35	E	940	U
35	E	941	U
35	E	942	C
35	E	943	G
35	E	944	G
35	E	945	C
35	E	946	U
35	E	947	U
35	E	950	G
35	E	966	C
35	E	969	U
35	E	975	U
35	E	976	U
35	E	977	A
35	E	979	G
35	E	980	G
35	E	983	C
35	E	986	U
35	E	988	U
35	E	989	G
35	E	994	G
35	E	999	U
35	E	1074	C
35	E	1077	C
35	E	1078	U
35	E	1079	U
35	E	1081	G
35	E	1082	U
35	E	1083	G
35	E	1171	C
35	E	1172	C
35	E	1175	A
35	E	1177	C
35	E	1178	U
35	E	1187	C
35	E	1188	C
35	E	1189	A
35	E	1191	G

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Mol	Chain	Res	Type
35	E	1192	A
35	E	1193	A
35	E	1194	U
35	E	1195	G
35	E	1197	A
35	E	1207	U
35	E	1208	U
35	E	1211	G
35	E	1221	U
35	E	1247	U
35	E	1268	A
35	E	1270	A
35	E	1295	U
35	E	1301	A
35	E	1339	G
35	E	1340	A
35	E	1356	C
35	E	1359	C
35	E	1360	A
35	E	1361	A
35	E	1363	C
35	E	1375	U
35	E	1524	U
35	E	1541	U
35	E	1542	U
35	E	1543	C
35	E	1544	U
35	E	1545	U
35	E	1546	C
35	E	1547	A
35	E	1559	U
35	E	1560	G
35	E	1561	A
35	E	1606	A
35	E	1618	G
35	E	1626	C
35	E	1627	C
35	E	1628	A
35	E	1631	A
35	E	1638	G
35	E	1653	U
35	E	1659	U

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Mol	Chain	Res	Type
35	E	1661	A
35	E	1664	A
35	E	1668	G
35	E	1669	G
35	E	1671	A
35	E	1672	C
35	E	1685	G
35	E	1689	A
35	E	1690	G
35	E	1691	G
35	E	1695	A
35	E	1696	G
35	E	1701	G
35	E	1711	G
35	E	1712	U
35	E	1724	A
35	E	1725	U
35	E	1727	C
35	E	1738	G
35	E	1782	U
35	E	1783	U
35	E	1789	A
35	E	1813	G
35	E	1815	A
35	E	1829	C
35	E	1830	C
35	E	1831	C
35	E	1832	A
35	E	1833	U
35	E	1857	U
35	E	1872	G
35	E	1873	G
35	E	1874	C
35	E	1875	G
35	E	1876	G
35	E	1877	U
35	E	1878	A
35	E	1880	U
35	E	1881	C
35	E	1882	G
35	E	1883	C
35	E	1884	U

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Mol	Chain	Res	Type
35	E	1885	U
35	E	1886	G
35	E	1887	U
35	E	1903	A
35	E	1904	U
35	E	1905	U
35	E	1909	U
35	E	1910	G
35	E	1914	U
35	E	1927	A
35	E	1930	U
35	E	1943	G
35	E	1947	U
35	E	1950	G
35	E	1951	A
35	E	1955	U
35	E	1956	C
35	E	1959	C
35	E	1961	A
35	E	1965	U
35	E	1966	C
35	E	1974	C
35	E	1976	C
35	E	1977	G
35	E	1988	U
35	E	1990	U
35	E	1991	C
35	E	1992	A
35	E	1993	G
35	E	1994	U
35	E	2000	C
35	E	2002	A
35	E	2007	A
35	E	2008	A
35	E	2009	C
35	E	2010	G
35	E	2012	C
35	E	2013	U
35	E	2016	U
35	E	2018	U
35	E	2019	C
35	E	2020	G

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Mol	Chain	Res	Type
35	E	2021	G
35	E	2022	A
35	E	2030	G
35	E	2032	U
35	E	2033	C
35	E	2034	A
35	E	2048	A
35	E	2049	C
35	E	2050	C
35	E	2051	C
35	E	2052	C
35	E	2053	G
35	E	2054	G
35	E	2060	C
35	E	2061	G
35	E	2063	A
35	E	2064	G
35	E	2068	C
35	E	2070	C
35	E	2071	U
35	E	2072	U
35	E	2075	G
35	E	2077	C
35	E	2087	C
35	E	2090	U
35	E	2091	U
35	E	2092	A
35	E	2097	U
35	E	2099	G
35	E	2102	C
35	E	2103	A
35	E	2107	A
35	E	2108	G
35	E	2118	G
35	E	2135	A
35	E	2153	C
35	E	2165	A
35	E	2214	A
35	E	2216	A
35	E	2217	G
35	E	2218	U
35	E	2225	C

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Mol	Chain	Res	Type
35	E	2226	U
35	E	2228	C
35	E	2235	C
35	E	2275	G
35	E	2278	G
35	E	2280	A
35	E	2283	A
35	E	2284	A
35	E	2287	U
35	E	2288	A
35	E	2310	G
35	E	2311	G
35	E	2312	A
35	E	2314	C
35	E	2317	U

All (86) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	E	56	U
35	E	68	A
35	E	193	U
35	E	227	U
35	E	325	U
35	E	531	A
35	E	701	C
35	E	702	U
35	E	703	A
35	E	712	U
35	E	713	G
35	E	717	U
35	E	719	G
35	E	727	C
35	E	729	C
35	E	756	G
35	E	765	A
35	E	769	A
35	E	771	A
35	E	774	C
35	E	775	A
35	E	777	A
35	E	785	A

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Mol	Chain	Res	Type
35	E	788	A
35	E	792	G
35	E	795	U
35	E	797	G
35	E	807	U
35	E	808	G
35	E	810	U
35	E	812	A
35	E	813	U
35	E	814	C
35	E	822	A
35	E	828	G
35	E	829	C
35	E	847	U
35	E	885	U
35	E	890	C
35	E	891	U
35	E	892	U
35	E	918	G
35	E	919	G
35	E	921	G
35	E	922	C
35	E	923	A
35	E	935	A
35	E	939	U
35	E	940	U
35	E	942	C
35	E	968	U
35	E	975	U
35	E	982	G
35	E	988	U
35	E	998	C
35	E	1076	C
35	E	1186	U
35	E	1187	C
35	E	1188	C
35	E	1191	G
35	E	1192	A
35	E	1526	A
35	E	1545	U
35	E	1546	C
35	E	1695	A

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Mol	Chain	Res	Type
35	E	1712	U
35	E	1872	G
35	E	1875	G
35	E	1876	G
35	E	1882	G
35	E	1886	G
35	E	1903	A
35	E	1904	U
35	E	1913	U
35	E	2006	A
35	E	2017	G
35	E	2020	G
35	E	2048	A
35	E	2049	C
35	E	2050	C
35	E	2051	C
35	E	2052	C
35	E	2152	C
35	E	2213	G
35	E	2227	U
35	E	2234	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

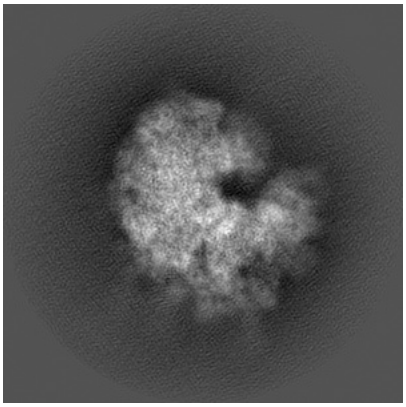
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3844. These allow visual inspection of the internal detail of the map and identification of artifacts.

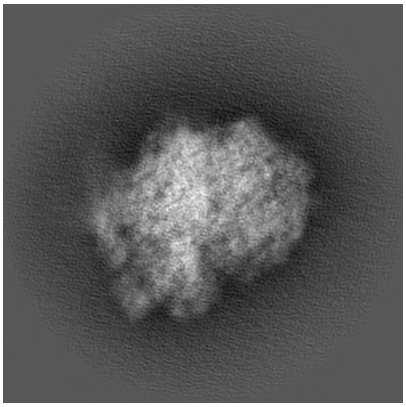
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

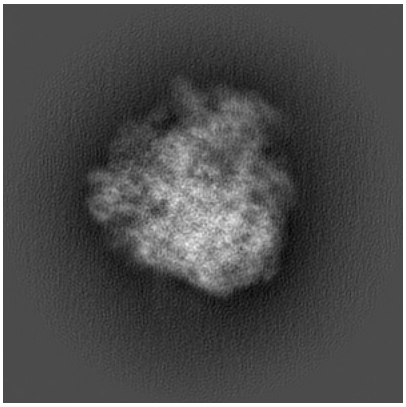
6.1.1 Primary map



X



Y

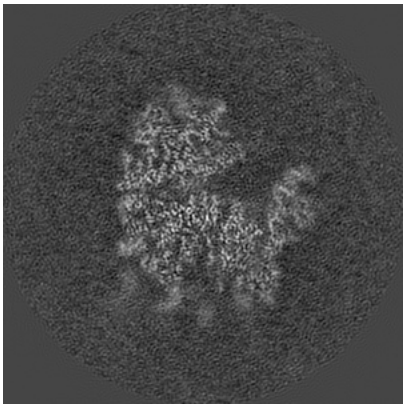


Z

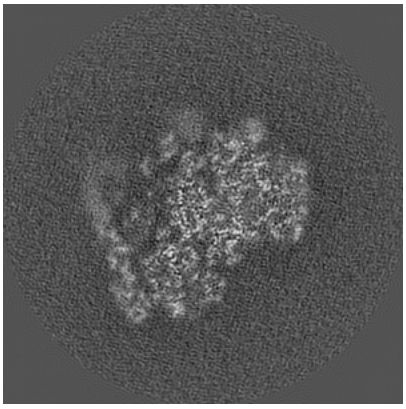
The images above show the map projected in three orthogonal directions.

6.2 Central slices

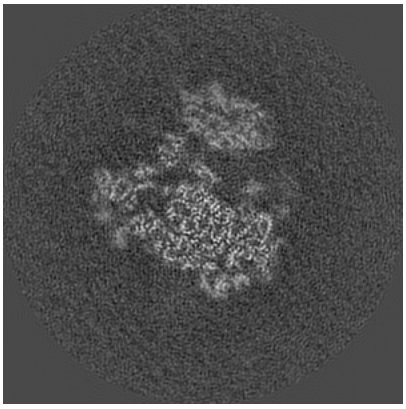
6.2.1 Primary map



X Index: 160



Y Index: 160

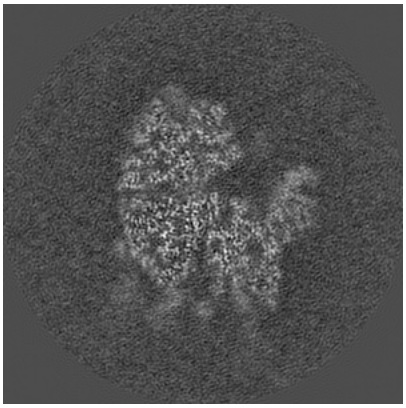


Z Index: 160

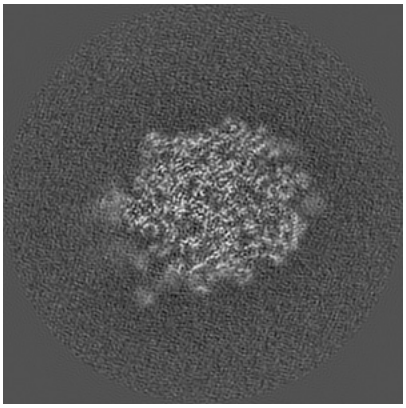
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

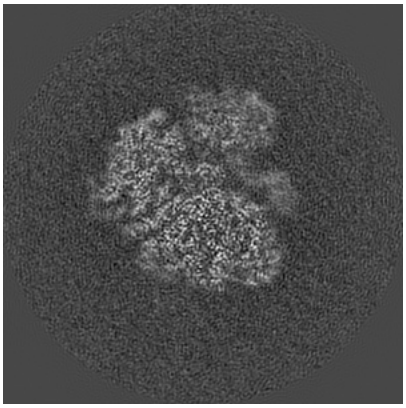
6.3.1 Primary map



X Index: 157



Y Index: 134



Z Index: 147

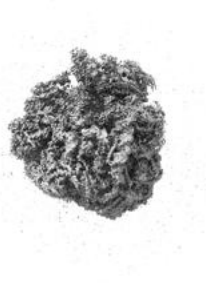
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0549. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

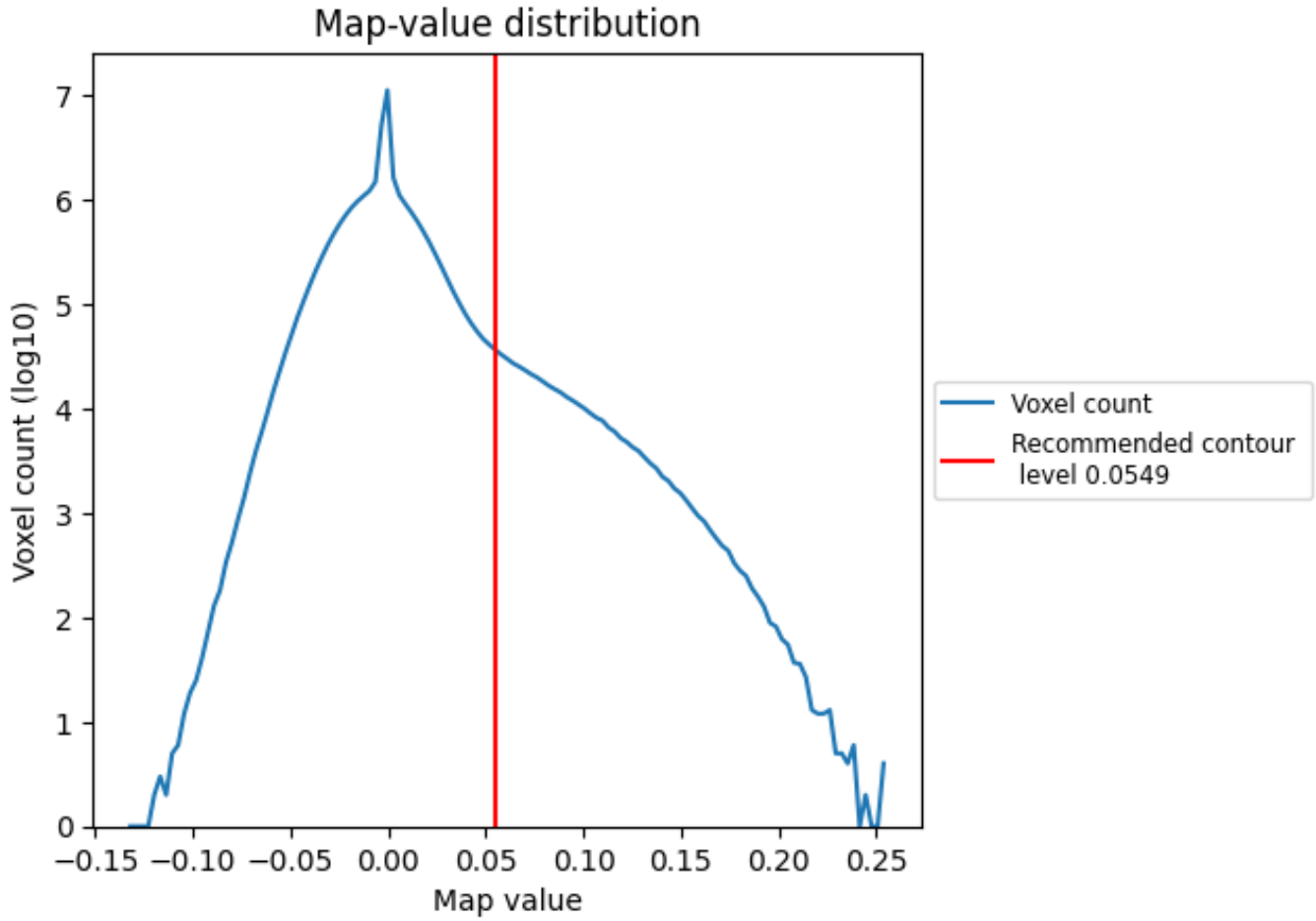
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

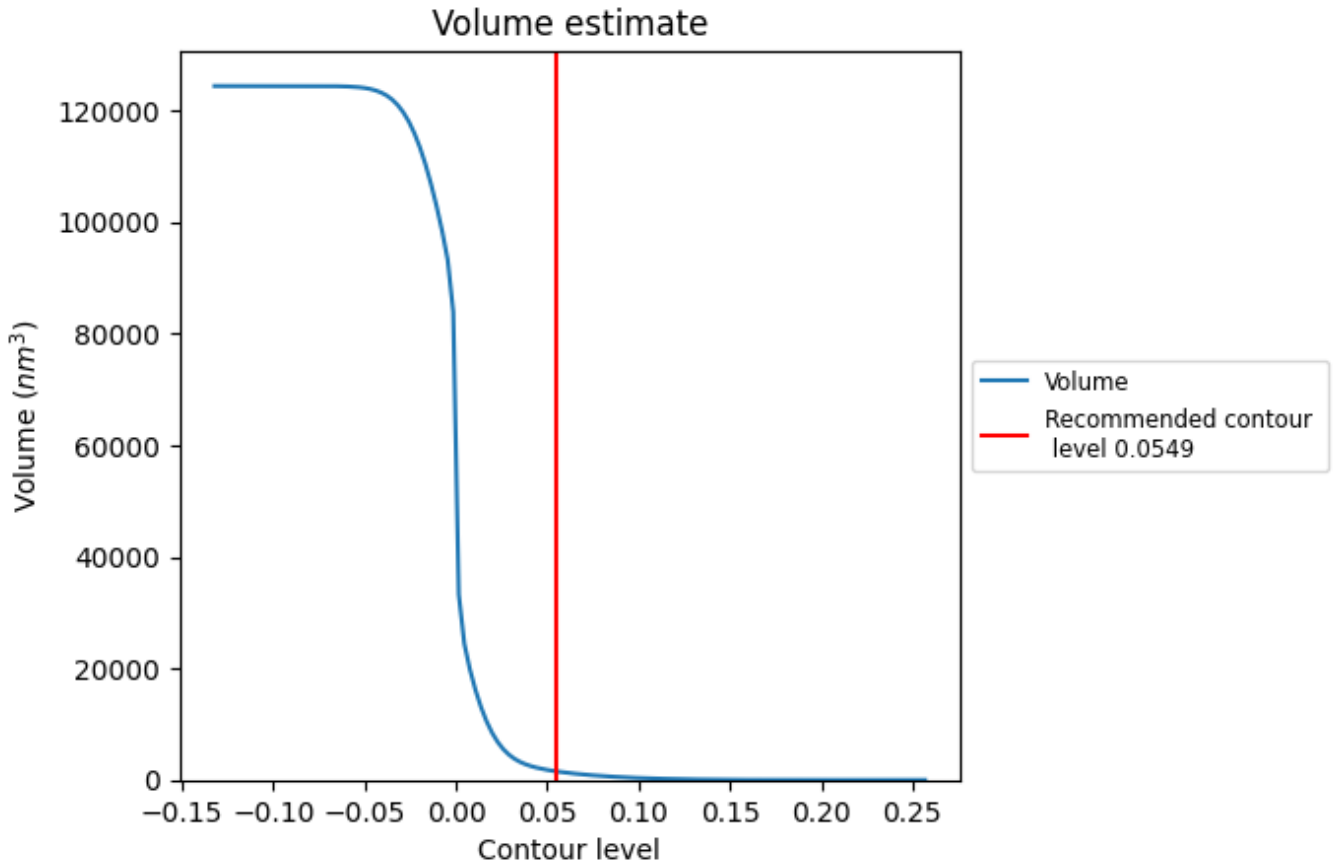
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

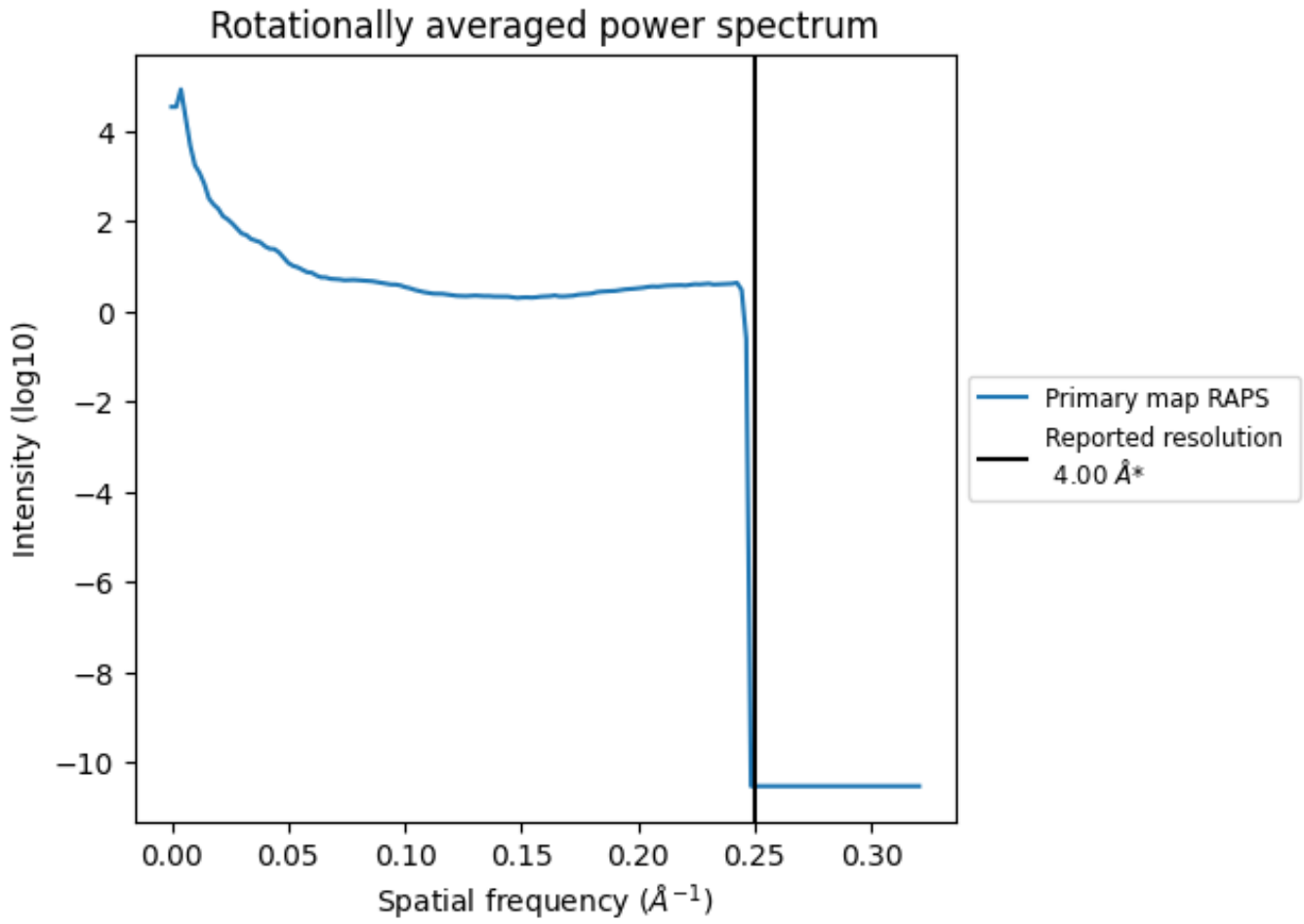
7.2 Volume estimate



The volume at the recommended contour level is 1549 nm^3; this corresponds to an approximate mass of 1400 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

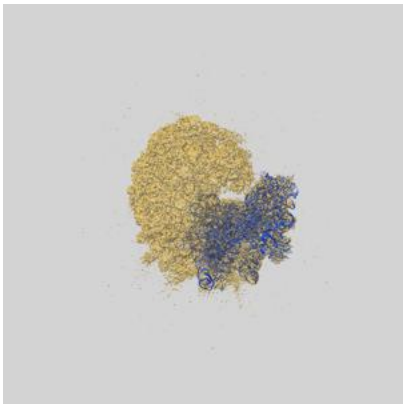
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

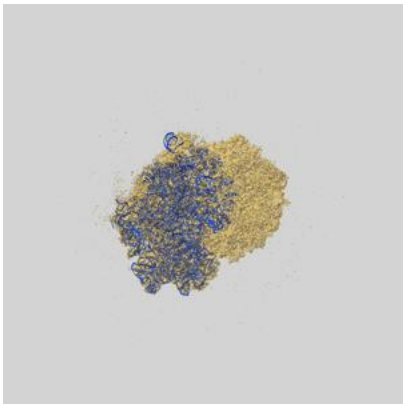
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3844 and PDB model 5OPT. Per-residue inclusion information can be found in section 3 on page 11.

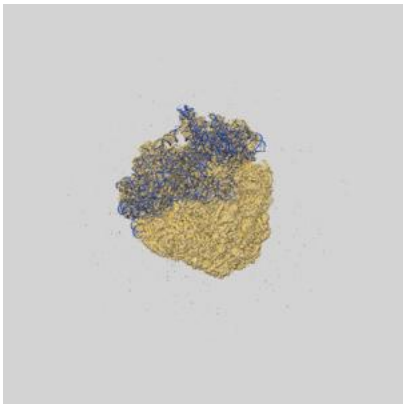
9.1 Map-model overlay



X



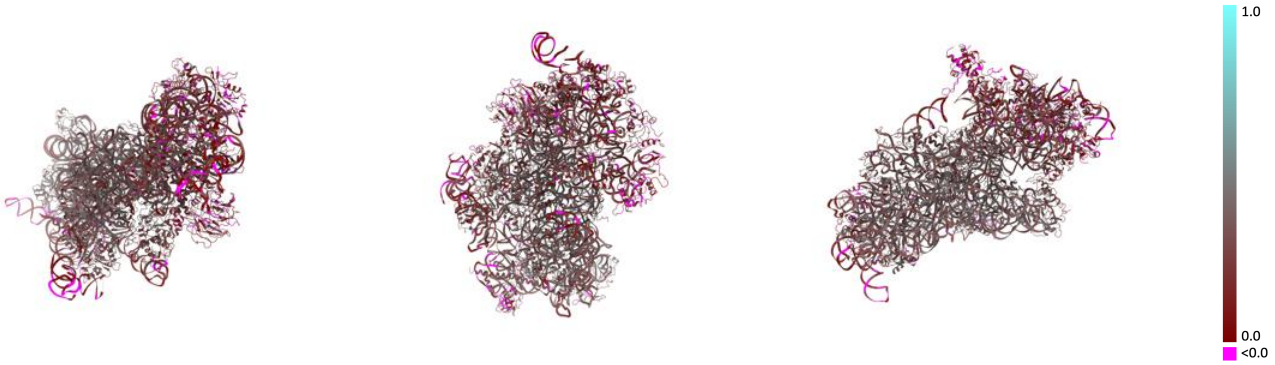
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0549 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

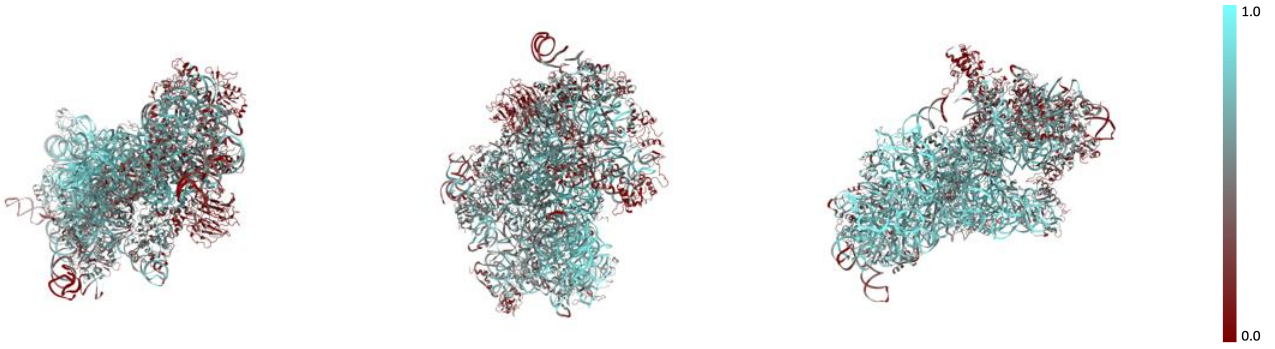
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

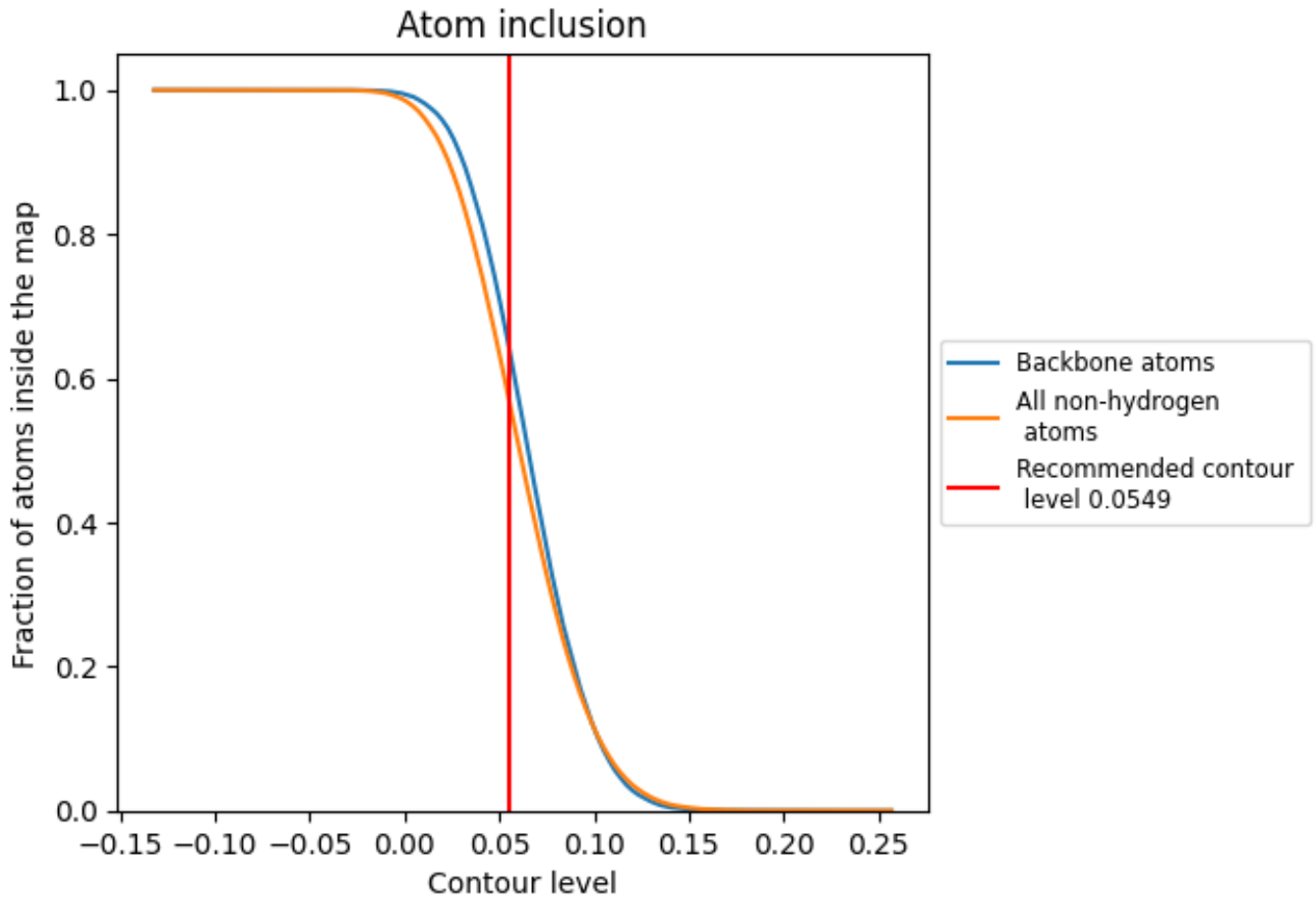
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0549).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0549) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5724	0.2840
E	0.6987	0.2970
L	0.5232	0.3590
M	0.5606	0.3500
O	0.3579	0.2240
P	0.5280	0.2910
Q	0.5311	0.3060
R	0.5204	0.3280
S	0.4421	0.3200
T	0.5044	0.3360
U	0.2609	0.2090
V	0.4923	0.3140
W	0.5513	0.3340
X	0.5149	0.3370
Y	0.5848	0.3250
Z	0.5968	0.3600
a	0.2983	0.1260
b	0.5505	0.3240
c	0.4765	0.2910
d	0.5234	0.3260
e	0.5473	0.3480
f	0.5207	0.3120
g	0.5169	0.3330
h	0.2966	0.1270
i	0.1113	0.0940
j	0.1861	0.1000
k	0.3771	0.2550
l	0.2936	0.2240
m	0.2931	0.2600
n	0.2964	0.2120
o	0.3843	0.1690
p	0.1712	0.1680
q	0.3767	0.2290
r	0.3924	0.2380
t	0.2790	0.1820
u	0.3231	0.1910