



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:02 PM GMT

PDB ID : 3V29  
Title : Crystal structure of HPF bound to the 70S ribosome. This entry contains the 50S subunit of the 2nd molecule in the ASU.  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-12  
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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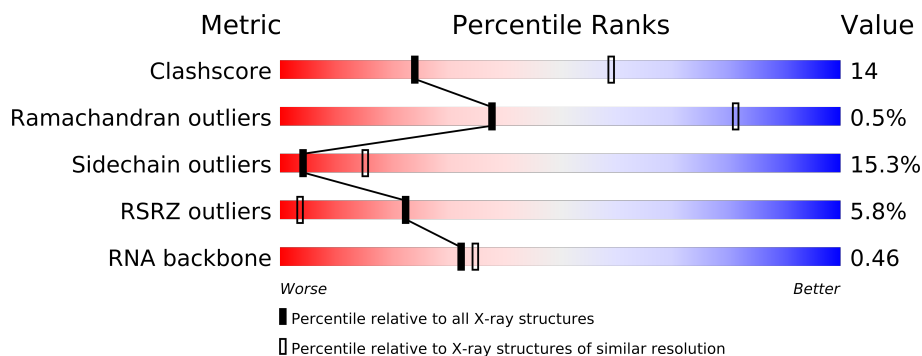
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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












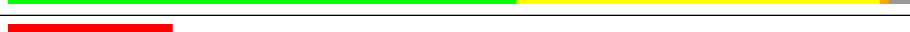

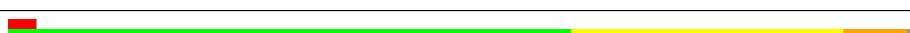


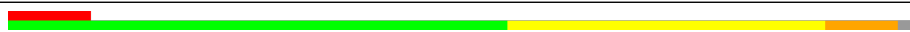


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	2913	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	
13	R	118	
14	S	112	

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Mol	Chain	Length	Quality of chain
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 91682 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2814	Total	C	N	O	P	0	0	0
			60621	26978	11351	19479	2813			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	U	DELETION	GB AP008226.1
A	?	-	U	DELETION	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			953	608	168	176	1			

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	110	Total	C	N	O	S	0	0	0
			865	544	172	149				

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	W	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	X	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Y	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	1	Total	Mg	0	0
			1	1		
32	O	2	Total	Mg	0	0
			2	2		
32	Q	2	Total	Mg	0	0
			2	2		
32	D	2	Total	Mg	0	0
			2	2		
32	E	4	Total	Mg	0	0
			4	4		
32	B	8	Total	Mg	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	595	Total 595	Mg 595	0	0
32	8	2	Total 2	Mg 2	0	0
32	O	1	Total 1	Mg 1	0	0
32	R	3	Total 3	Mg 3	0	0
32	F	1	Total 1	Mg 1	0	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	1	Total 1	Zn 1	0	0
33	Y	1	Total 1	Zn 1	0	0
33	4	1	Total 1	Zn 1	0	0
33	6	1	Total 1	Zn 1	0	0
33	5	1	Total 1	Zn 1	0	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	1166	Total 1166	O 1166	0	0
34	B	19	Total 19	O 19	0	0
34	D	8	Total 8	O 8	0	0
34	E	10	Total 10	O 10	0	0
34	F	6	Total 6	O 6	0	0
34	N	1	Total 1	O 1	0	0
34	P	9	Total 9	O 9	0	0

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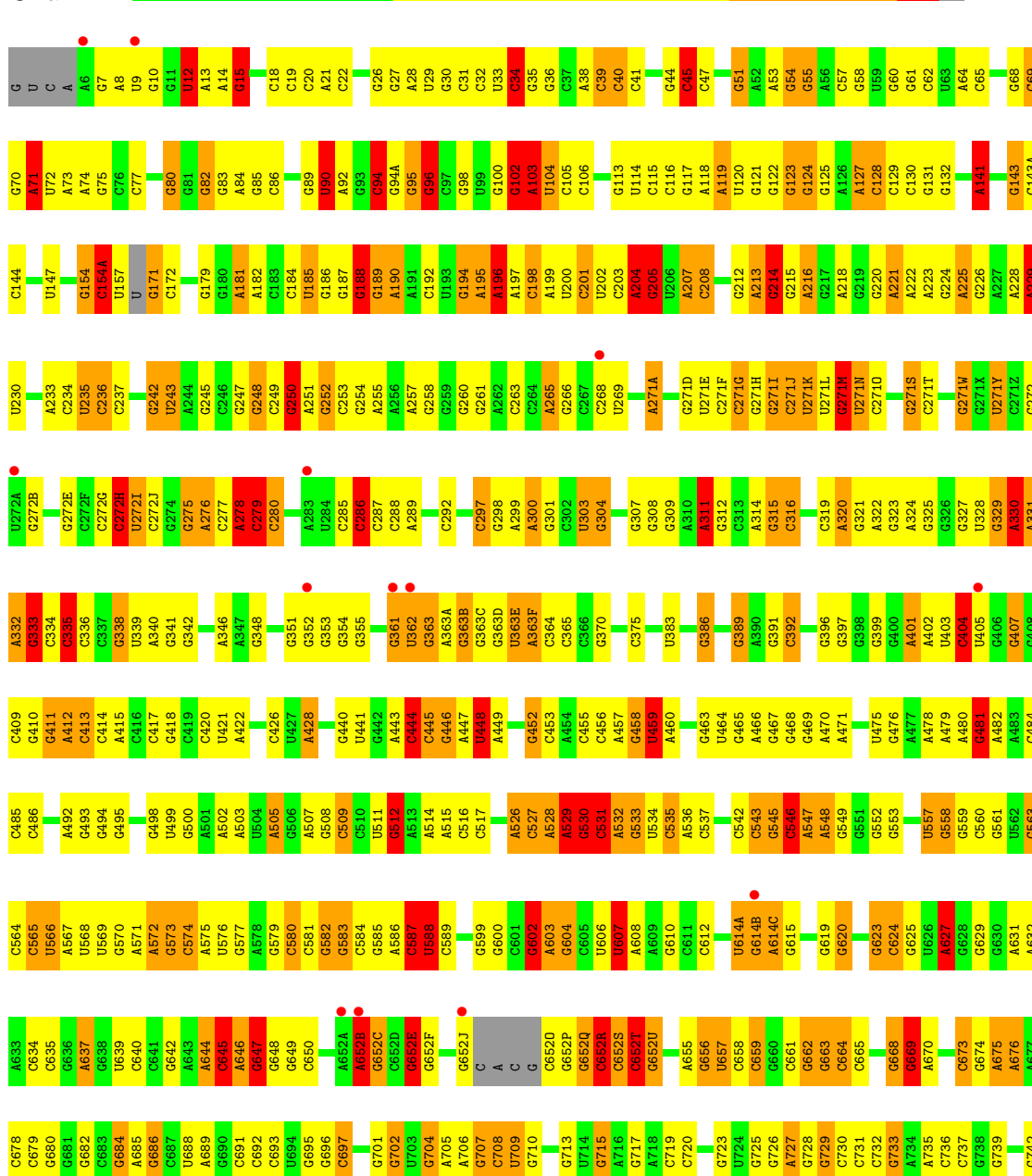
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	Q	3	Total 3	O 3	0	0
34	R	2	Total 2	O 2	0	0
34	T	2	Total 2	O 2	0	0
34	U	4	Total 4	O 4	0	0
34	V	2	Total 2	O 2	0	0
34	W	2	Total 2	O 2	0	0
34	X	2	Total 2	O 2	0	0
34	Y	1	Total 1	O 1	0	0
34	0	1	Total 1	O 1	0	0
34	1	4	Total 4	O 4	0	0
34	3	1	Total 1	O 1	0	0
34	7	3	Total 3	O 3	0	0
34	8	1	Total 1	O 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 23S Ribosomal RNA

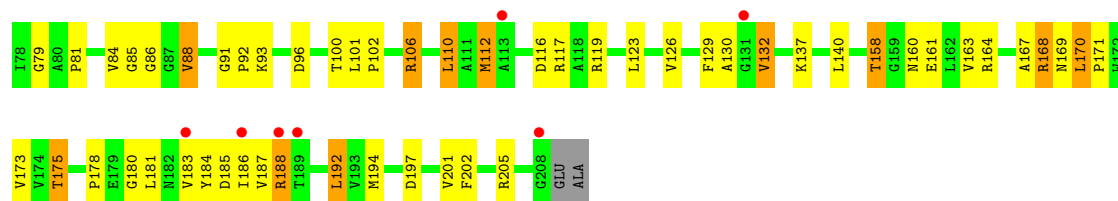
Chain A:



A1722	G1568	A1439	G1277	G1206	A1128	C1006	A941	A878	G808	G743
U1739	A1569	U1420	A1278	C1207	A1129	C1007	G944	G879	G809	G744
A1741	A1570	G1421	G1279	G1208	U1130	C1008	G945	G880	U810	A746
G1742	C1575	G1422	G1280	G1209	G1131		G946	G881	U811	
C1743	U1576	G1423	U1281	A1210	U1132	G1011	G947	G882	C812	U747
G1746	U1577	G1424	G1282	G1211	U1133	U1012	G948	G	C815	G748
G1750	C1578	G1425	G1283	G1212	U1135	C1013		C	C816	C749
G1751	U1579	G1426	C1284	A1213	G1136	U1014		C	C817	A750
A1755	A1580	A1427	U1287	G1216	G1137	G1015	C951	C	C818	A751
G1756	G1581	G1428	U1288	G1219	G1138	U1016	G952	C	A752	
U1757	C1582	C1429	C1289	A1220	G1139	G1017	G953	C	A753	
G1758	U1583	U1430	U1290	U1221	U1140	C1018	G954	C	C820	C754
A1759	C1584	C1431	C1291	U1222	U1141	U1019	C955	A	A821	C755
A1760	A1586	U1432	U1292	C1223	U1142	A1020	G956	G	U822	C756
C1761	U1587	A1433	C1293	G1224	A1142A	A1021	A957	C993	A823	U757
A1762	C1588	G1434	C1294	G1225		U1022	A958	C894	A824	
G1763	G1589	G1435	U1295	G1226	C1153	U1023	A959	U895	C825	G760
G1764	U1594	U1436	G1296	A1226	U1154	U1024	A960	A896	U826	G761
A1668	A1365	A1366	C1297	U1227	U1155	G1025	C961	C997	U827	U762
A1669	A1367	A1368	U1298	C1230	A1156	U1026		A900	U828	
A1670	G1369	U1370	U1300	G1231	U1159	A1027	C965	A901	G763	
U1671	C1370	G1371	A1301	U1232	G1160	A1028	G968	C902	A764	
G1772	U1372	U1372	U1302	G1236	C1161	G1030	C970	C903	G765	
G1773	A1373	A1373	C1303	A1237	G1162	G1031	C971	C904	C766	
U1774	G1374	G1374	C1304	G1238	G1163	A1032	G972	U905	U767	
U1775	C1375	U1375	C1305	G1239	G1164	U1033	A973	G906	G768	
U1776	G1376	U1376	A1308	U1240	U1165	G1034	G974	U907	G769	
U1777	G1377	G1377	A1309	A1241	C1166	U1035	G975	C908	A841	
U1778	A1378	U1378	G1310	G1243	U1169	G1036	G976	A909	C842	
U1779	U1379	U1379	G1311	G1244	G1170	G1037	G977	A910	G843	U773
U1780	G1380	G1380	U1312		G1171	C1038	G978	A911	G844	
A1689	C1381	U1381	C1313	A1247	G	G1039	G979	C912	G845	A774
U1692	G1382	G1382	C1314	U1248	A	C1040	G980	U913	C846	A775
U1693	C1383	U1383	C1315	U1249	U	G1041	A981	C914	U847	
U1694	A1384	U1384	U1316	G1250	G	G1042	A982	C915	C848	
U1695	G1385	G1385	A1317	C1251	A	C1043	C982	G916	A849	
U1696	C1386	U1386	C1318	G1252	C1178	G1044	C983	A917	C850	A782
U1697	G1387	U1387	G1319	A1253	C1179	A1045	A984	A918	A783	
U1698	U1388	G1388	A1320	U1254	C1180	G1047	C985	G920	A784	
A1698	U1391	U1391	A1321	U1255	C1181	A1048	C986	G921	G785	
G1699			A1322	G1256		C1049	G987	U922	C856	U787
A1700	U1394	U1394	G1325	C1257	C1185	A1050	A988	C923	U858	A788
A1701	A1395	U1395	U1326	C1258	G1186	G1051	G989	C924	C859	A789
G1702	U1396	U1396	G1327	C1261	G1187	C1052	A990	C925	U860	C790
G1703	C1403	U1403	U1328	G1264	U1188	C	C991	A926	A861	C791
U1709	U1404	U1404	G1329	U1265	U1189	G	C992	G927	G862	G792
C1710	U1405	U1405	C1330	G1266	G1190	C	G993	G928	A863	A793
C1711	C1406	U1406	A1331	U1267	G1191	A	C994	U930	C864	G794
C1712	C1407	U1407	G1332	G1268	G1192	G	C995	G931	C865	C795
U1713	U1408	U1408	C1333	U1269	G1193	U	A996	A932	A866	C796
G1714	U1415	U1415	U1336	C1270	U1199	U	G997	G933	C867	C797
U1717	G1416	U1416	G1337	G1271	C1200	G	A1001	C934	U868	A802
G1718	U1417	U1417	U1338	A1272	C1201	C	G1002	C935	C869	U803
A1803	U1418	U1418	G1339	U1273	C1202	U	G1003	C936	A870	A804
C1804	U1419	U1419	U1340	U1274	G1203	C	C1004	G937	G874	G805
U1805	C1493	A1494	U1341	U1276	U1205	U	C1005	C938		U807

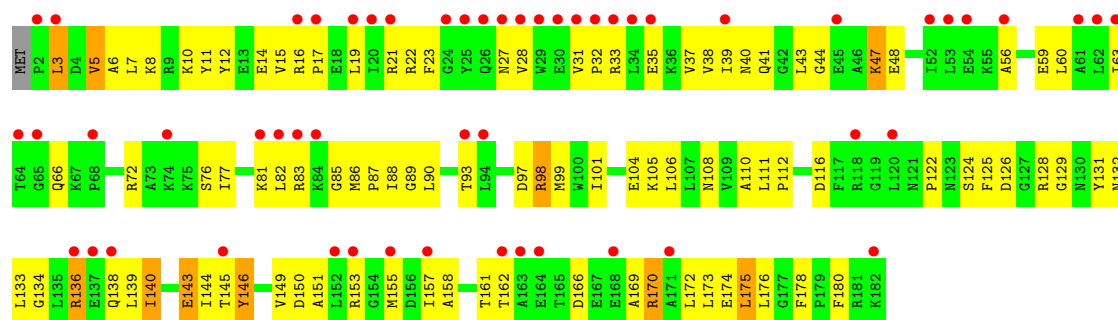
A2705	G2630	C2568	C2499	A2352	G2290	A2225	G2155	U2092	A2019	C1957	A1890	C1806
G2706	G2631	G2569	U2500	G2353	U2291	C2225	G2156	G2093	A2020	C1958	G1891	G1807
G2707	A2632	G2570	C2501	G2354	C2292	A2227	G2157	U2096	C2021	C1959	C1892	U1808
G2708	C2571	G2572	G2502	G2355	C2293	G2228	A2158	A2158	U2022	G1960	C1893	A1809
G2709	U2637	A2573	A2503	G2356	G2294	C2229	G2159	U2098	G2023	U1963	C1894	A1810
G2710	U2638	C2574	U2504	G2357	G2295	U2232	G2160	U2098	G2023	U1963	C1895	A1811
A2711	U2639	C2575	G2505	G2358	U2296	U2233	C2161	U2099	C2026	G1964	G1896	A1812
U2712	G2641	G2576	U2506	C2359	C2297	U2234	G2162	U2099	C2027	G1965	G1897	A1813
A2712A	G2644	A2577	C2510	G2360	A2298	U2235	C2163	G2101	U2028	C1966	U1998	G1814
G2713	G2645	G2578	U2513	A2361	G2299	G2235	G2164	U2102	G2029	C1967	G1989	A1815
G2714	U2647	U2580	U2514	G2362	G2300	G2236	G2165	U2103	A2030	C1968	A1900	G1816
C2715	C2648	G2581	C2515	G2363	G2301	G2237	G2166	G2104	G2031	A1969	U1970	G1817
G2718	U2649	G2582	G2516	G2364	G2302	G2238	U2167	C2105	G2032	A1970	G1903	U1818
G2719	U2652	G2583	C2517	G2365	G2303	G2239	G2168	G2106	A2033	A1971	G1904	A1819
G2722	A2654	G2584	G2518	G2371	G2304	C2240	A2169	C2107	U2034	A1972	G1906	U1820
G2723	U2584	G2585	C2519	G2372	A2305	A2241	A2170	C2108	U2034	C1973	C1905	A1821
C2724	A2657	U2586	U2519	G2373	G2306	G2242	A2171	U2109	G2036	C1974	G1910	G1822
A2725	U2587	C2586	C2520	G2374	G2307	U2243	A2172	U2109	C2037	C1975	G1911	G1823
U2726	G2661	G2588	C2521	G2375	G2308	U2244	A2173	C2111	G2038	U1976	U1911	G1824
G2727	A2662	G2589	U2522	G2376	A2309	U2245	C2174	G2112	C2039	A1977	A1912	G1825
U2728	G2663	A2590	G2523	A2377	A2310	A2247	C2175	U2113	U2041	A1978	A1913	G1826
G2729	G2664	G2591	G2524	A2378	A2311	C2248	A2176	A2114	A2042	C1979	C1914	G1827
A2730	A2665	G2592	G2525	G2379	G2312	U2249	C2177	G2115	U1915	C1980	A1829	G1828
G2731	U2593	G2593	G2526	G2380	G2313	U2250	C2178	G2116	C2043	A1981	U1915	C1830
G2732	G2594	G2594	G2527	C2381	G2315	G2251	U2180	U2118	U2047	C1982	A1918	G1833
A2733	G2595	G2595	U2528	G2382	G2316	G2252	U2181	A2119	G2048	C1983	A1919	U1834
G2739	G2672	U2596	C2529	G2383	C2317	G2253	G2182	G2120	G2049	G1984	G1920	G1835
A2740	G2673	U2597	A2530	G2384	G2318	C2254	C2183	G2121	G2052	A1986	U1926	G1838
A2741	G2674	A2598	G2535	G2385	G2319	U2255	C2184	U2122	G2053	G1987	G1927	G1839
A2742	A2675	U2600	U2536	G2386	A2320	C2256	G2185	G2123	A2054	C1988	A1928	C1843
C2743	G2677	G2601	C2537	G2387	G2321	C2257	G2186	G2124	G2055	C1989	A1929	G1844
G2744	G2678	A2602	C2538	G2388	A2322	C2258	G2187	G2125	G2056	U1991	G1930	G1845
G2745	A2679	G2603	C2539	G2389	G2323	C2259	U2188	A2126	A2057	C1992	A1931	G1846
U2746	G2680	U2604	U2544	G2390	C2324	C2260	C2189	G2127	A2058	U1993	A1932	A1847
G2747	C2681	U2605	G2545	G2391	G2325	C2261	G2190	C2128	A2059	U1994	G1933	A1848
A2748	U2682	G2606	G2546	G2392	C2326	C2262	G2191	C2129	A2060	U1995	C1934	G1849
A2749	G2683	G2607	U2547	G2393	A2327	U2265	G2192	U2130	G2061	C1996	G1935	G1850
A2750	U2684	U2608	G2548	G2394	A2328	A2266	G2193	U2131	A2062	C1997	A1936	G1851
G2751	G2685	U2609	G2549	G2395	G2329	A2267	C2194	G2132	C2063	G1998	A1937	G1852
G2752	G2686	G2610	U2550	G2396	G2330	A2268	C2195	A2134	C2064	C1999	A1937	G1853
A2753	U2687	U2611	C2551	G2400	U2331	U2271	U2197	C2135	C2065	G2000	A1938	G1854
U2754	U2688	G2612	U2552	U2406	A2332	U2272	A2198	C2136	G2069	A2001	U1939	G1863
U2755	U2689	G2613	G2553	G2407	A2333	A2273	A2199	C2137	G2070	C2005	C1941	U1864
A2756	G2690	U2615	U2554	U2408	A2336	A2274	C2200	C2138	A2071	G2006	C1942	G1865
G2757	C2691	C2616	U2555	G2409	G2337	G2275	C2202	C2139	U2074	C2007	U1943	C1866
G2758	U2692	G2617	C2556	G2410	G2338	G2276	U2203	C2140	G2075	G2008	U1944	A1876
G2759	G2693	G2618	G2557	A2411	G2339	A2278	U2205	U2144	U2076	G2009	G1945	A1877
C2760	G2694	C2619	C2558	A2412	G2340	G2279	G2206	G2145	A2077	G2010	U1946	G1878
G2761	U2696	G2622	C2559	G2413	C2343	U2282	G2207	C2146	G2077	U2011	G1948	C1881
G2762	G2697	U2491	U2560	G2414	U2344	C2283	U2208	G2147	A2082	G2012	G1949	C1882
G2763	U2698	U2492	A2561	U2417	G2345	C2284	G2219	G2148	G2083	A2013	G1950	G1883
A2764	G2699	U2493	U2562	G2418	A2346	C2285	G2220	U2149	C2084	A2014	U1951	A1884
A2765	C2700	G2494	U2563	A2418	A2347	A2286	G2221	G2151	G2087	A2015	A1952	A1885
G2766	G2701	G2495	A2564	U2419	C2347	A2287	G2222	G2152	U2091	U2016	U1955	C1886
G2767	U2702	G2496	A2565	G2420	C2350	A2288	G2223	G2153	U2091	U2017	U1956	G1887
C2768	C2703	A2497	A2566	A2421	G2351	G2289	G2224	G2154				





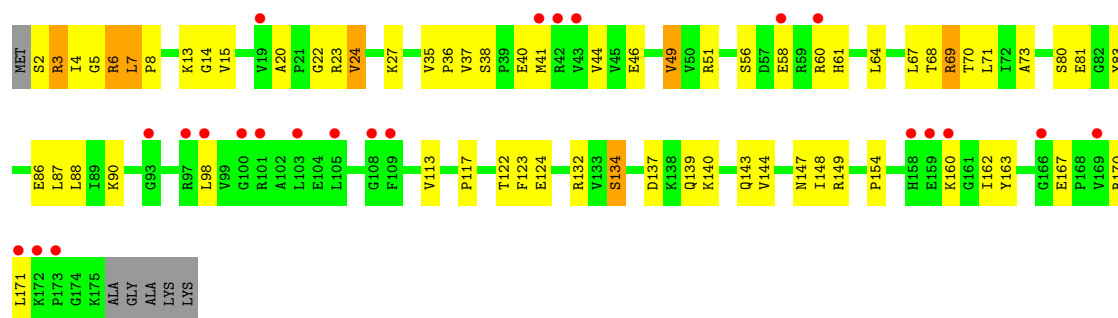
• Molecule 6: 50S Ribosomal Protein L5

Chain G:



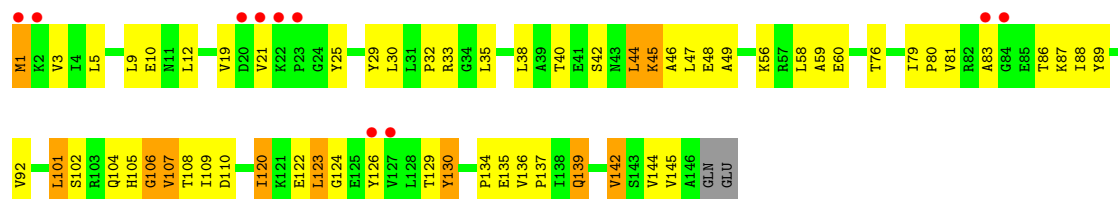
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



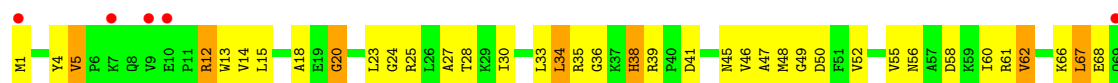
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



• Molecule 9: 50S Ribosomal Protein L13

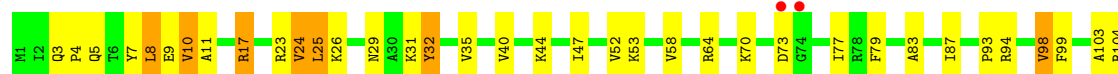
Chain N:





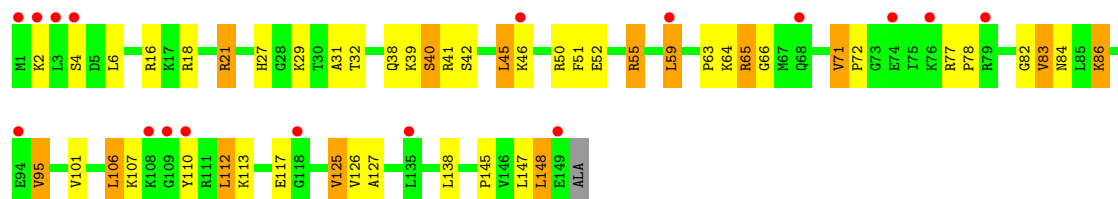
• Molecule 10: 50S Ribosomal Protein L14

Chain O:



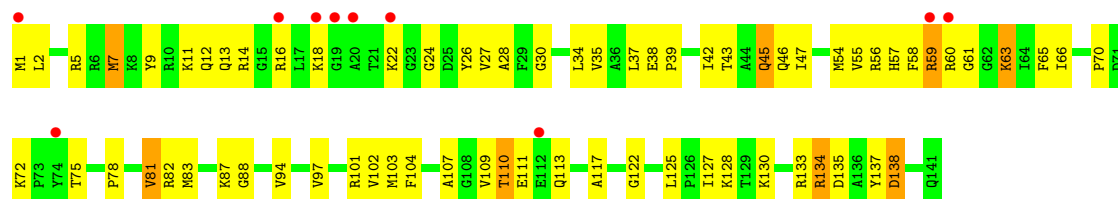
• Molecule 11: 50S Ribosomal Protein L15

Chain P:



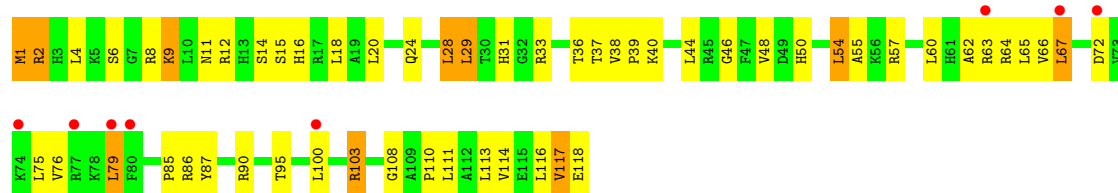
• Molecule 12: 50S Ribosomal Protein L16

Chain Q:



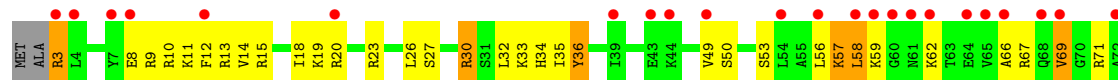
• Molecule 13: 50S Ribosomal Protein L17

Chain R:

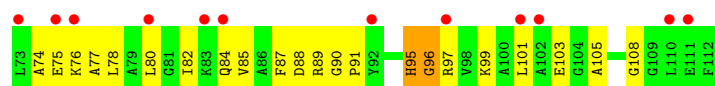


• Molecule 14: 50S Ribosomal Protein L18

Chain S:

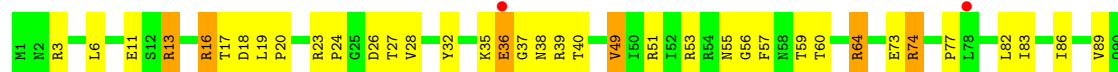






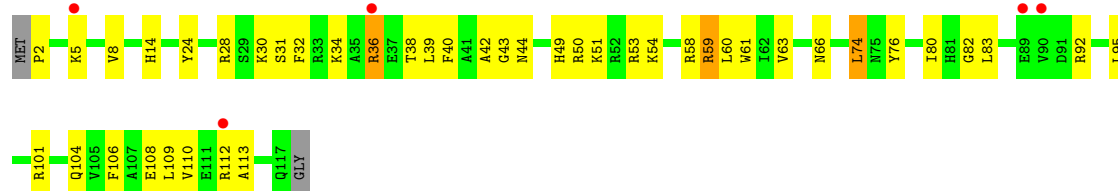
• Molecule 15: 50S Ribosomal Protein L19

Chain T:



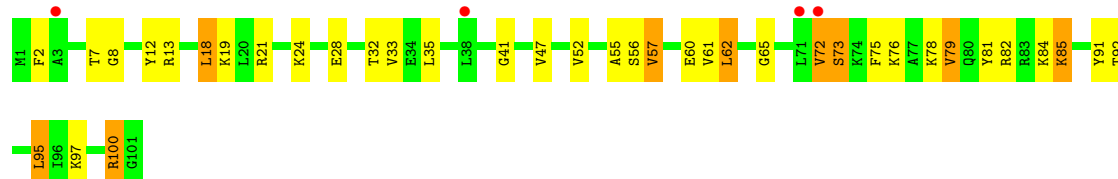
• Molecule 16: 50S Ribosomal Protein L20

Chain U:



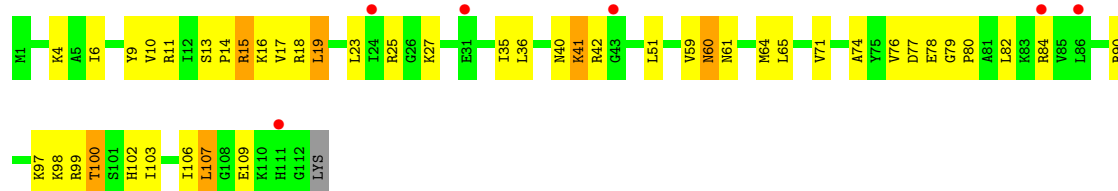
• Molecule 17: 50S Ribosomal Protein L21

Chain V:



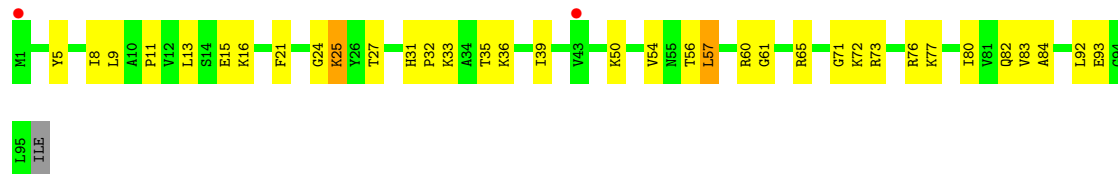
• Molecule 18: 50S Ribosomal Protein L22

Chain W:



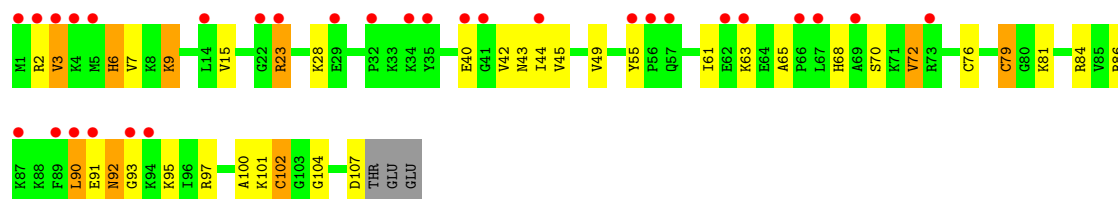
• Molecule 19: 50S Ribosomal Protein L23

Chain X:



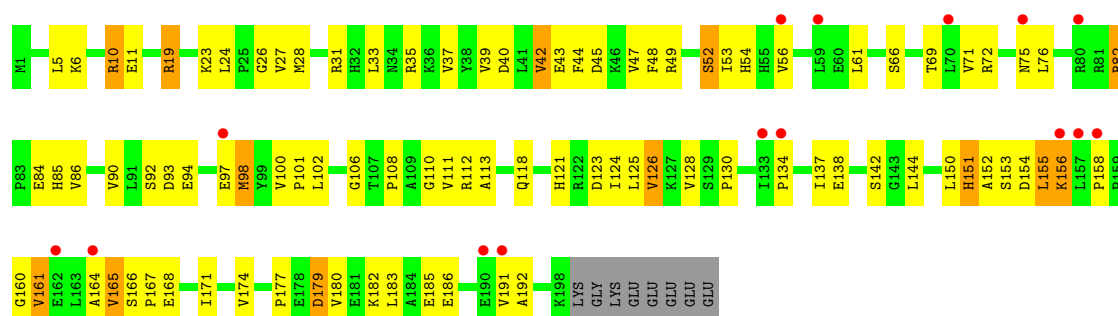
- Molecule 20: 50S Ribosomal Protein L24

Chain Y:



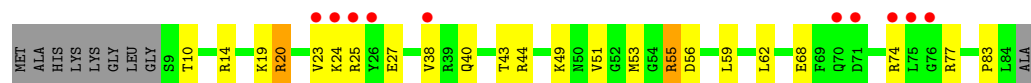
- Molecule 21: 50S Ribosomal Protein L25

Chain Z:



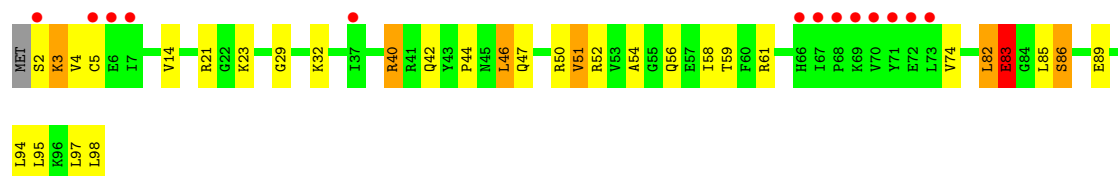
- Molecule 22: 50S Ribosomal Protein L27

Chain 0:



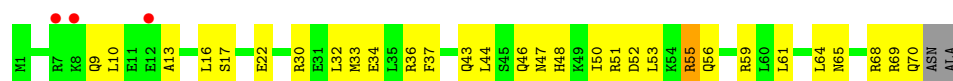
- Molecule 23: 50S Ribosomal Protein L28

Chain 1:



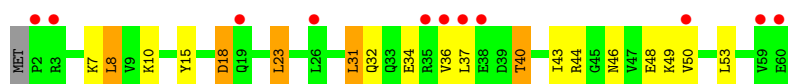
- Molecule 24: 50S Ribosomal Protein L29

Chain 2:



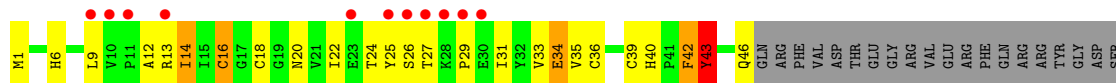
- Molecule 25: 50S Ribosomal Protein L30

Chain 3:



• Molecule 26: 50S Ribosomal Protein L31

Chain 4:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.216 , 0.258 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 993194 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.58	EDS
Total number of atoms	91682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	A	1.21	155/67893 (0.2%)	1.65	1848/105980 (1.7%)
2	B	1.13	2/2878 (0.1%)	1.52	49/4490 (1.1%)
3	D	0.82	0/2186	0.91	2/2944 (0.1%)
4	E	0.78	0/1588	0.92	3/2145 (0.1%)
5	F	0.74	0/1615	0.92	2/2188 (0.1%)
6	G	0.72	0/1393	0.81	0/1892
7	H	0.66	0/1343	0.81	0/1820
8	I	0.63	0/967	0.84	1/1334 (0.1%)
9	N	0.71	0/1139	0.89	1/1538 (0.1%)
10	O	0.73	0/933	0.83	1/1257 (0.1%)
11	P	0.73	0/1148	0.89	1/1529 (0.1%)
12	Q	0.74	0/1143	0.86	0/1527
13	R	0.75	0/982	0.92	1/1312 (0.1%)
14	S	0.69	0/875	0.87	1/1168 (0.1%)
15	T	0.73	0/1077	0.90	0/1444
16	U	0.79	0/977	0.86	0/1301
17	V	0.77	0/782	0.85	0/1049
18	W	0.87	0/891	0.91	1/1197 (0.1%)
19	X	0.78	0/756	0.86	1/1016 (0.1%)
20	Y	0.73	1/798 (0.1%)	0.89	0/1073
21	Z	0.72	0/1555	0.81	1/2118 (0.0%)
22	0	0.78	0/602	0.92	0/804
23	1	0.80	0/752	0.89	1/1003 (0.1%)
24	2	0.79	0/590	0.86	0/781
25	3	0.69	0/463	0.81	0/623
26	4	0.85	0/358	0.83	1/487 (0.2%)
27	5	0.86	1/469 (0.2%)	0.96	0/634
28	6	0.75	0/456	0.87	2/609 (0.3%)
29	7	0.88	0/426	1.01	1/561 (0.2%)
30	8	0.76	0/516	0.90	0/679
31	9	0.71	0/300	0.90	0/395
All	All	1.10	159/97851 (0.2%)	1.49	1918/146898 (1.3%)

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	A	0	1
4	E	0	1
5	F	0	1
8	I	0	1
12	Q	0	1
14	S	0	1
19	X	0	1
21	Z	0	1
23	1	0	1
26	4	0	1
All	All	0	10

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142(A)	A	N9-C4	-12.18	1.30	1.37
1	A	945	A	N9-C4	-11.74	1.30	1.37
1	A	528	A	N9-C4	-9.70	1.32	1.37
1	A	71	A	N9-C4	-8.63	1.32	1.37
1	A	1308	A	N7-C5	-8.57	1.34	1.39
1	A	1204	A	N9-C4	-8.45	1.32	1.37
1	A	1490	A	N3-C4	8.38	1.39	1.34
1	A	207	A	N9-C4	-8.37	1.32	1.37
1	A	251	A	N3-C4	-8.31	1.29	1.34
1	A	330	A	N9-C4	-8.27	1.32	1.37
1	A	652(B)	A	N9-C4	7.95	1.42	1.37
1	A	1788	C	N1-C6	-7.92	1.32	1.37
1	A	2725	A	N9-C4	-7.90	1.33	1.37
1	A	2296	U	C4-C5	7.73	1.50	1.43
1	A	1762	A	N9-C4	7.66	1.42	1.37
27	5	49	CYS	CB-SG	-7.48	1.69	1.82
1	A	676	A	N9-C8	7.30	1.43	1.37
1	A	746	A	N9-C4	-7.19	1.33	1.37
1	A	204	A	N3-C4	-7.12	1.30	1.34
1	A	1142(A)	A	N3-C4	-7.06	1.30	1.34
1	A	1045	A	N9-C4	7.04	1.42	1.37
1	A	2252	G	N3-C4	-6.89	1.30	1.35
1	A	1107	G	N9-C4	6.86	1.43	1.38
1	A	2335	A	C5-C4	-6.82	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2561	A	N3-C4	-6.82	1.30	1.34
1	A	2322	A	C6-N1	6.80	1.40	1.35
1	A	2790	A	N9-C4	6.77	1.42	1.37
1	A	960	A	N9-C4	-6.77	1.33	1.37
1	A	2826	A	N3-C4	-6.72	1.30	1.34
1	A	1257	C	N1-C6	-6.70	1.33	1.37
1	A	571	A	N9-C4	-6.64	1.33	1.37
1	A	190	A	N9-C4	-6.61	1.33	1.37
1	A	1960	A	N9-C4	-6.53	1.33	1.37
1	A	251	A	N9-C4	-6.52	1.33	1.37
1	A	1021	A	N9-C4	-6.45	1.33	1.37
1	A	2593	U	C2-N3	-6.35	1.33	1.37
1	A	676	A	C5-C6	-6.35	1.35	1.41
1	A	802	A	C6-N1	-6.30	1.31	1.35
2	B	102	A	N7-C5	6.29	1.43	1.39
1	A	981	A	N9-C4	-6.23	1.34	1.37
1	A	15	G	N7-C5	-6.07	1.35	1.39
1	A	789	A	N9-C4	-6.05	1.34	1.37
1	A	278	A	N3-C4	6.01	1.38	1.34
1	A	2320	A	N9-C4	6.00	1.41	1.37
1	A	1569	A	N7-C5	-5.94	1.35	1.39
1	A	2251	G	N7-C5	-5.94	1.35	1.39
1	A	1616	A	C5-C6	-5.91	1.35	1.41
1	A	1981	A	C6-N1	-5.90	1.31	1.35
1	A	945	A	N3-C4	-5.87	1.31	1.34
1	A	1378	A	N9-C4	-5.86	1.34	1.37
1	A	2031	A	C5-C6	-5.84	1.35	1.41
1	A	1998	G	N3-C4	-5.82	1.31	1.35
1	A	2032	G	N7-C5	-5.82	1.35	1.39
1	A	2803	C	N1-C6	5.81	1.40	1.37
1	A	1252	G	C5-C4	-5.80	1.34	1.38
1	A	57	C	N3-C4	-5.79	1.29	1.33
1	A	469	G	C5-C4	-5.78	1.34	1.38
1	A	1829	A	N3-C4	-5.77	1.31	1.34
1	A	1821	A	C5-C4	-5.76	1.34	1.38
1	A	2500	U	C4-O4	-5.75	1.19	1.23
1	A	1787	A	N9-C4	-5.75	1.34	1.37
1	A	2602	A	N9-C4	5.75	1.41	1.37
1	A	2352	A	N9-C4	-5.74	1.34	1.37
1	A	1649	G	C5-C4	-5.71	1.34	1.38
1	A	2049	G	N9-C4	-5.69	1.33	1.38
1	A	514	A	N3-C4	-5.69	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1772	G	N9-C4	-5.66	1.33	1.38
1	A	2791	C	N1-C2	5.65	1.45	1.40
1	A	1471	A	N9-C4	5.63	1.41	1.37
1	A	1698	A	N9-C4	-5.63	1.34	1.37
1	A	689	A	N9-C4	-5.61	1.34	1.37
1	A	2502	G	C5-C6	-5.58	1.36	1.42
1	A	1619	G	C2-N3	-5.58	1.28	1.32
1	A	2446	G	N3-C4	5.58	1.39	1.35
1	A	1308	A	N9-C8	-5.55	1.33	1.37
1	A	469	G	N9-C8	-5.55	1.33	1.37
1	A	1037	G	C6-N1	5.54	1.43	1.39
1	A	12	U	N1-C2	5.54	1.43	1.38
1	A	2607	G	C2-N3	5.54	1.37	1.32
1	A	746	A	N3-C4	-5.53	1.31	1.34
1	A	2296	U	N1-C2	5.53	1.43	1.38
1	A	1760	A	N3-C4	-5.52	1.31	1.34
1	A	1969	A	N9-C4	-5.51	1.34	1.37
1	A	1783	A	C5-C6	-5.50	1.36	1.41
1	A	1213	A	N9-C4	-5.50	1.34	1.37
1	A	2826	A	N9-C4	-5.50	1.34	1.37
1	A	1698	A	N7-C5	-5.50	1.35	1.39
1	A	2606	C	N1-C6	-5.50	1.33	1.37
1	A	786	C	C4-N4	-5.49	1.29	1.33
1	A	2151	G	C6-N1	5.49	1.43	1.39
1	A	1267	U	C2-N3	-5.48	1.33	1.37
1	A	2149	G	C6-N1	5.48	1.43	1.39
1	A	2791	C	N1-C6	5.47	1.40	1.37
1	A	1142(A)	A	C5-C6	-5.47	1.36	1.41
1	A	1669	A	N3-C4	-5.46	1.31	1.34
1	A	1927	A	N9-C4	-5.45	1.34	1.37
1	A	2487	G	N9-C4	-5.45	1.33	1.38
1	A	2561	A	N9-C4	-5.45	1.34	1.37
1	A	802	A	C6-N6	-5.44	1.29	1.33
1	A	2587	A	N7-C5	-5.43	1.35	1.39
1	A	580	C	N1-C6	-5.43	1.33	1.37
20	Y	79	CYS	CB-SG	-5.40	1.73	1.81
1	A	775	G	C6-N1	-5.40	1.35	1.39
1	A	676	A	N9-C4	-5.39	1.34	1.37
1	A	1567	A	N9-C4	-5.39	1.34	1.37
1	A	2058	A	C6-N1	-5.38	1.31	1.35
1	A	1314	C	C4-C5	-5.38	1.38	1.43
1	A	1142(A)	A	N7-C5	-5.37	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1826	G	N9-C8	-5.35	1.34	1.37
1	A	727	A	N7-C5	-5.33	1.36	1.39
1	A	2436	G	C2-N3	-5.32	1.28	1.32
1	A	1308	A	N3-C4	-5.31	1.31	1.34
1	A	531	C	N1-C6	-5.29	1.33	1.37
1	A	255	A	N9-C4	-5.28	1.34	1.37
1	A	251	A	C5-C4	-5.27	1.35	1.38
1	A	1026	U	N1-C2	5.25	1.43	1.38
1	A	38	A	C5-C4	-5.25	1.35	1.38
1	A	739	G	C5-C4	-5.25	1.34	1.38
1	A	980	A	N9-C4	-5.24	1.34	1.37
1	A	948	G	N3-C4	-5.24	1.31	1.35
1	A	254	G	N9-C4	-5.23	1.33	1.38
1	A	2286	A	N7-C5	-5.22	1.36	1.39
1	A	1309	G	C5-C4	-5.22	1.34	1.38
1	A	1490	A	C6-N1	5.22	1.39	1.35
1	A	530	G	C6-O6	-5.21	1.19	1.24
1	A	2028	U	C2-N3	-5.21	1.34	1.37
1	A	2424	C	N1-C6	-5.20	1.34	1.37
1	A	1933	G	C6-N1	-5.20	1.35	1.39
1	A	1257	C	N1-C2	-5.19	1.34	1.40
1	A	652(B)	A	N3-C4	5.17	1.38	1.34
1	A	750	A	N3-C4	-5.17	1.31	1.34
1	A	2589	A	N9-C4	-5.15	1.34	1.37
1	A	2577	A	N9-C4	-5.14	1.34	1.37
1	A	220	G	N7-C5	-5.14	1.36	1.39
1	A	1107	G	N3-C4	5.13	1.39	1.35
1	A	71	A	C3'-O3'	5.13	1.49	1.42
1	A	2322	A	C5-C6	5.13	1.45	1.41
2	B	53	A	N9-C4	5.12	1.41	1.37
1	A	1369	G	N3-C4	-5.12	1.31	1.35
1	A	245	G	N7-C5	-5.12	1.36	1.39
1	A	1301	A	N3-C4	-5.11	1.31	1.34
1	A	2437	U	N3-C4	-5.11	1.33	1.38
1	A	1989	G	N7-C5	-5.10	1.36	1.39
1	A	71	A	N9-C8	5.10	1.41	1.37
1	A	1419	A	N9-C4	-5.10	1.34	1.37
1	A	2730	C	N3-C4	-5.09	1.30	1.33
1	A	1022	G	N3-C4	-5.09	1.31	1.35
1	A	2027	G	N3-C4	-5.09	1.31	1.35
1	A	805	G	N9-C8	-5.08	1.34	1.37
1	A	2335	A	N9-C4	-5.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1021	A	N3-C4	-5.07	1.31	1.34
1	A	1787	A	N3-C4	-5.05	1.31	1.34
1	A	1981	A	N3-C4	-5.04	1.31	1.34
1	A	194	G	N9-C4	-5.04	1.33	1.38
1	A	585	G	N9-C4	-5.03	1.33	1.38
1	A	745	G	N7-C5	-5.03	1.36	1.39
1	A	1332	G	N7-C5	-5.02	1.36	1.39
1	A	1107	G	C2-N3	5.01	1.36	1.32
1	A	1829	A	N9-C4	-5.01	1.34	1.37

All (1918) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	U	N3-C4-O4	-25.95	101.23	119.40
1	A	2296	U	C2-N3-C4	-19.90	115.06	127.00
1	A	2296	U	C5-C6-N1	-19.31	113.05	122.70
1	A	2296	U	C2-N1-C1'	-18.94	94.97	117.70
1	A	2296	U	C5-C4-O4	18.26	136.86	125.90
1	A	945	A	C2-N3-C4	-14.96	103.12	110.60
1	A	1142(A)	A	C2-N3-C4	-14.54	103.33	110.60
1	A	676	A	C5-N7-C8	-14.08	96.86	103.90
1	A	528	A	N3-C4-N9	-13.69	116.45	127.40
2	B	115	G	C8-N9-C4	13.59	111.84	106.40
1	A	528	A	C2-N3-C4	-13.39	103.91	110.60
1	A	2296	U	C6-N1-C1'	13.36	139.90	121.20
1	A	945	A	C5-N7-C8	-13.20	97.30	103.90
1	A	2296	U	N1-C2-N3	12.91	122.65	114.90
1	A	330	A	C2-N3-C4	-12.81	104.19	110.60
1	A	2335	A	C5-C6-N1	12.79	124.10	117.70
1	A	571	A	C8-N9-C4	12.68	110.87	105.80
1	A	71	A	C5-N7-C8	-12.58	97.61	103.90
1	A	1565	C	C6-N1-C2	12.38	125.25	120.30
1	A	2296	U	N3-C4-C5	12.14	121.88	114.60
1	A	1359	A	N1-C6-N6	-12.01	111.39	118.60
1	A	2028	U	C6-N1-C2	11.88	128.13	121.00
1	A	676	A	C4-C5-N7	11.84	116.62	110.70
1	A	2447	G	N1-C6-O6	11.84	127.00	119.90
1	A	2371	G	N1-C6-O6	11.75	126.95	119.90
1	A	928	G	N1-C6-O6	11.66	126.89	119.90
1	A	2572	A	C8-N9-C4	11.60	110.44	105.80
1	A	945	A	N7-C8-N9	11.58	119.59	113.80
1	A	676	A	C2-N3-C4	-11.52	104.84	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2322	A	N9-C4-C5	11.48	110.39	105.80
1	A	1437	C	C6-N1-C2	-11.44	115.72	120.30
1	A	1021	A	C2-N3-C4	-11.32	104.94	110.60
1	A	1204	A	C5-N7-C8	-11.25	98.27	103.90
1	A	528	A	N3-C4-C5	11.19	134.63	126.80
1	A	2791	C	C6-N1-C2	-10.97	115.91	120.30
1	A	676	A	N7-C8-N9	10.90	119.25	113.80
1	A	2322	A	C6-N1-C2	-10.75	112.15	118.60
1	A	2028	U	N3-C4-C5	10.69	121.02	114.60
1	A	2363	C	C6-N1-C2	10.68	124.57	120.30
1	A	1107	G	N3-C4-N9	10.66	132.40	126.00
1	A	728	G	C8-N9-C4	10.66	110.66	106.40
1	A	2646	C	C6-N1-C2	10.35	124.44	120.30
2	B	104	U	C5-C6-N1	-10.32	117.54	122.70
1	A	2296	U	N3-C2-O2	-10.31	114.98	122.20
1	A	71	A	C2-N3-C4	-10.27	105.47	110.60
1	A	297	C	C6-N1-C2	-10.22	116.21	120.30
1	A	1762	A	C8-N9-C4	-10.20	101.72	105.80
1	A	154(A)	C	N1-C2-O2	10.19	125.01	118.90
1	A	2277	G	N1-C6-O6	-10.15	113.81	119.90
1	A	2036	C	N1-C2-O2	-10.15	112.81	118.90
1	A	1142(A)	A	C5-C6-N1	-10.10	112.65	117.70
1	A	2375	G	C8-N9-C4	10.07	110.43	106.40
1	A	2619	C	C6-N1-C2	10.05	124.32	120.30
1	A	205	G	N9-C4-C5	-10.04	101.38	105.40
1	A	2286	A	C6-C5-N7	-10.00	125.30	132.30
1	A	1123	C	C6-N1-C2	9.97	124.29	120.30
1	A	1254	A	N1-C2-N3	9.94	134.27	129.30
1	A	587	C	C6-N1-C2	-9.94	116.32	120.30
1	A	2689	U	N3-C4-O4	-9.94	112.44	119.40
1	A	2286	A	N1-C6-N6	9.92	124.55	118.60
1	A	1777	U	C5-C6-N1	-9.87	117.77	122.70
1	A	678	C	C6-N1-C2	9.85	124.24	120.30
1	A	1107	G	C4-N9-C1'	9.84	139.29	126.50
1	A	676	A	C8-N9-C4	-9.81	101.88	105.80
1	A	2619	C	C5-C6-N1	-9.80	116.10	121.00
1	A	978	G	C8-N9-C4	9.79	110.31	106.40
1	A	1107	G	C8-N9-C1'	-9.72	114.37	127.00
1	A	1022	G	N9-C4-C5	9.71	109.28	105.40
1	A	201	C	N3-C4-C5	9.70	125.78	121.90
1	A	1049	C	C5-C6-N1	9.68	125.84	121.00
1	A	2626	C	C6-N1-C2	9.66	124.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	856	C	C6-N1-C2	-9.63	116.45	120.30
1	A	1565	C	N3-C4-C5	9.60	125.74	121.90
1	A	1800	C	C6-N1-C2	9.60	124.14	120.30
1	A	62	C	C5-C6-N1	-9.56	116.22	121.00
1	A	915	C	C6-N1-C2	-9.55	116.48	120.30
1	A	2624	G	N1-C6-O6	9.55	125.63	119.90
1	A	2107	C	C2-N3-C4	9.52	124.66	119.90
1	A	2593	U	N3-C4-O4	-9.52	112.74	119.40
1	A	560	C	C6-N1-C2	9.48	124.09	120.30
1	A	735	A	C8-N9-C4	9.43	109.57	105.80
1	A	122	G	C5-C6-O6	-9.43	122.94	128.60
1	A	2591	C	N1-C2-O2	-9.39	113.27	118.90
1	A	123	G	C8-N9-C4	9.38	110.15	106.40
1	A	2322	A	N1-C6-N6	-9.36	112.98	118.60
1	A	645	C	N1-C2-O2	9.30	124.48	118.90
1	A	2447	G	C5-C6-O6	-9.30	123.02	128.60
1	A	2286	A	C2-N3-C4	-9.29	105.95	110.60
1	A	179	G	N1-C6-O6	9.29	125.47	119.90
1	A	1108	U	N3-C2-O2	-9.29	115.70	122.20
1	A	1616	A	N1-C6-N6	9.28	124.17	118.60
1	A	62	C	C6-N1-C2	9.27	124.01	120.30
1	A	928	G	C6-C5-N7	-9.27	124.84	130.40
1	A	1565	C	C5-C6-N1	-9.23	116.38	121.00
1	A	2828	C	C6-N1-C2	9.23	123.99	120.30
1	A	2322	A	C8-N9-C4	-9.22	102.11	105.80
1	A	1107	G	N3-C4-C5	-9.18	124.01	128.60
1	A	2676	C	C2-N3-C4	-9.13	115.33	119.90
1	A	2570	G	N1-C6-O6	9.13	125.38	119.90
1	A	2329	G	C8-N9-C4	9.12	110.05	106.40
1	A	2277	G	C5-C6-O6	9.11	134.07	128.60
1	A	1490	A	C8-N9-C4	9.11	109.44	105.80
1	A	141	A	N7-C8-N9	9.06	118.33	113.80
1	A	2755	C	C5-C6-N1	9.03	125.51	121.00
1	A	71	A	N7-C8-N9	9.01	118.31	113.80
1	A	1049	C	C6-N1-C2	-9.00	116.70	120.30
1	A	988	A	N1-C6-N6	8.96	123.97	118.60
1	A	764	A	N1-C2-N3	-8.95	124.82	129.30
1	A	2723	C	C5-C6-N1	-8.94	116.53	121.00
1	A	2393	A	C8-N9-C4	-8.94	102.22	105.80
1	A	141	A	C5-N7-C8	-8.92	99.44	103.90
1	A	945	A	N1-C2-N3	8.90	133.75	129.30
1	A	2615	U	N3-C4-O4	-8.90	113.17	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	G	N1-C6-O6	8.89	125.23	119.90
1	A	2624	G	C5-C6-O6	-8.87	123.28	128.60
1	A	1230	C	C6-N1-C2	8.86	123.84	120.30
1	A	1490	A	N9-C4-C5	-8.85	102.26	105.80
1	A	71	A	C4-C5-N7	8.84	115.12	110.70
1	A	571	A	N9-C4-C5	-8.83	102.27	105.80
1	A	1248	G	C8-N9-C4	8.83	109.93	106.40
1	A	1328	G	C8-N9-C4	8.77	109.91	106.40
1	A	128	C	C6-N1-C2	8.76	123.80	120.30
1	A	1325	G	C6-C5-N7	-8.74	125.15	130.40
1	A	2449	U	N3-C2-O2	8.74	128.32	122.20
1	A	1142(A)	A	N3-C4-C5	8.73	132.91	126.80
2	B	79	C	C6-N1-C2	-8.73	116.81	120.30
1	A	528	A	C5-C6-N1	-8.70	113.35	117.70
1	A	945	A	C8-N9-C4	-8.70	102.32	105.80
1	A	760	G	C5-C6-O6	-8.70	123.38	128.60
1	A	179	G	C5-C6-N1	-8.66	107.17	111.50
1	A	945	A	N3-C4-C5	8.66	132.86	126.80
1	A	665	C	C6-N1-C2	8.65	123.76	120.30
1	A	676	A	N3-C4-C5	8.65	132.86	126.80
1	A	1437	C	C5-C6-N1	8.61	125.31	121.00
1	A	915	C	N3-C2-O2	-8.60	115.88	121.90
1	A	1698	A	C5-N7-C8	-8.59	99.60	103.90
1	A	792	G	C8-N9-C4	8.59	109.83	106.40
1	A	1992	G	C4-C5-N7	-8.57	107.37	110.80
2	B	89	G	N1-C6-O6	8.56	125.04	119.90
1	A	2371	G	C5-C6-O6	-8.54	123.48	128.60
1	A	330	A	C5-N7-C8	-8.53	99.64	103.90
1	A	2821	A	C8-N9-C4	8.53	109.21	105.80
1	A	1207	C	C6-N1-C2	8.52	123.71	120.30
1	A	2087	G	C8-N9-C4	8.51	109.80	106.40
1	A	2521	C	C6-N1-C2	8.50	123.70	120.30
1	A	1204	A	C4-C5-N7	8.50	114.95	110.70
1	A	1977	A	C8-N9-C4	8.49	109.20	105.80
1	A	12	U	N1-C2-O2	8.48	128.73	122.80
2	B	104	U	C6-N1-C2	8.46	126.08	121.00
2	B	115	G	N7-C8-N9	-8.43	108.89	113.10
1	A	1022	G	C4-C5-N7	-8.42	107.43	110.80
1	A	2881	C	N1-C2-O2	-8.41	113.86	118.90
1	A	446	G	C8-N9-C4	8.40	109.76	106.40
1	A	2791	C	N1-C2-O2	8.40	123.94	118.90
1	A	154(A)	C	N3-C2-O2	-8.37	116.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2286	A	C4-C5-C6	8.35	121.18	117.00
1	A	2287	A	N1-C6-N6	8.35	123.61	118.60
2	B	83	G	N1-C6-O6	8.31	124.89	119.90
1	A	566	U	C6-N1-C2	8.31	125.98	121.00
1	A	1565	C	C2-N3-C4	-8.29	115.76	119.90
1	A	2498	C	C6-N1-C2	8.26	123.60	120.30
1	A	2572	A	N7-C8-N9	-8.24	109.68	113.80
1	A	568	U	C5-C4-O4	-8.24	120.96	125.90
1	A	2827	C	C6-N1-C2	8.23	123.59	120.30
1	A	1022	G	N3-C2-N2	-8.23	114.14	119.90
1	A	440	G	N1-C6-O6	-8.23	114.96	119.90
1	A	2040	C	C6-N1-C2	8.22	123.59	120.30
1	A	201	C	C6-N1-C2	8.22	123.59	120.30
1	A	945	A	C5-C6-N1	-8.22	113.59	117.70
1	A	2589	A	C2-N3-C4	-8.22	106.49	110.60
1	A	2606	C	N3-C4-C5	8.22	125.19	121.90
1	A	528	A	C5-C6-N6	8.22	130.27	123.70
1	A	2690	C	N3-C4-C5	-8.22	118.61	121.90
1	A	448	U	N1-C2-N3	8.21	119.83	114.90
1	A	271(S)	G	N1-C6-O6	8.21	124.82	119.90
1	A	1698	A	N7-C8-N9	8.20	117.90	113.80
1	A	945	A	N3-C4-N9	-8.20	120.84	127.40
1	A	789	A	C8-N9-C4	8.18	109.07	105.80
1	A	2371	G	N9-C4-C5	-8.14	102.14	105.40
1	A	413	C	N1-C2-O2	-8.13	114.02	118.90
1	A	1108	U	N1-C2-O2	8.12	128.48	122.80
1	A	1760	A	N1-C6-N6	-8.11	113.74	118.60
2	B	30	C	C6-N1-C2	-8.11	117.06	120.30
1	A	453	C	C6-N1-C2	8.10	123.54	120.30
1	A	2296	U	O4'-C1'-N1	8.10	114.68	108.20
1	A	1350	C	C6-N1-C2	8.09	123.54	120.30
1	A	933	A	C5-N7-C8	-8.08	99.86	103.90
1	A	1992	G	N9-C4-C5	8.04	108.62	105.40
1	A	1779	U	C6-N1-C1'	-8.04	109.95	121.20
1	A	39	C	C5-C6-N1	-8.02	116.99	121.00
1	A	2676	C	C5-C6-N1	-8.01	116.99	121.00
1	A	1608	A	C2-N3-C4	-8.00	106.60	110.60
1	A	2292	C	C5-C6-N1	-8.00	117.00	121.00
1	A	1377	G	N3-C4-C5	-7.99	124.61	128.60
1	A	826	U	N1-C2-N3	7.98	119.69	114.90
1	A	2306	C	C5-C6-N1	7.98	124.99	121.00
1	A	729	G	C5-C6-O6	-7.98	123.81	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	C	N3-C4-C5	7.96	125.08	121.90
1	A	736	C	N1-C2-O2	-7.96	114.12	118.90
1	A	468	G	C8-N9-C4	7.95	109.58	106.40
1	A	12	U	N3-C2-O2	-7.93	116.64	122.20
1	A	2100	G	N3-C4-N9	7.93	130.76	126.00
1	A	1967	C	C6-N1-C2	7.93	123.47	120.30
1	A	2250	G	C4-C5-N7	-7.92	107.63	110.80
1	A	1937	A	N1-C6-N6	7.92	123.35	118.60
1	A	1142(A)	A	N1-C6-N6	7.91	123.34	118.60
1	A	389	G	N9-C4-C5	-7.90	102.24	105.40
1	A	1993	U	N1-C2-O2	-7.90	117.27	122.80
1	A	2319	G	N3-C2-N2	-7.89	114.38	119.90
1	A	1021	A	C5-N7-C8	-7.89	99.95	103.90
1	A	652(E)	G	C6-N1-C2	7.88	129.83	125.10
1	A	1983	C	N1-C2-O2	-7.86	114.19	118.90
1	A	1006	C	N3-C4-N4	-7.83	112.52	118.00
1	A	1284	A	N1-C6-N6	7.83	123.30	118.60
1	A	201	C	C2-N3-C4	-7.83	115.99	119.90
1	A	2335	A	C5-C6-N6	-7.83	117.44	123.70
1	A	928	G	C5-C6-O6	-7.82	123.91	128.60
1	A	1124	C	C6-N1-C2	7.81	123.42	120.30
1	A	1001	A	C8-N9-C4	7.80	108.92	105.80
1	A	2449	U	N1-C2-O2	-7.80	117.34	122.80
1	A	528	A	N9-C4-C5	7.79	108.92	105.80
1	A	1348	G	N1-C6-O6	7.79	124.57	119.90
1	A	1333	C	N3-C4-C5	7.79	125.01	121.90
1	A	205	G	C8-N9-C4	7.78	109.51	106.40
1	A	792	G	N9-C4-C5	-7.78	102.29	105.40
1	A	627	A	C8-N9-C4	7.78	108.91	105.80
1	A	1204	A	N7-C8-N9	7.78	117.69	113.80
1	A	2340	G	C8-N9-C4	7.78	109.51	106.40
1	A	121	G	C8-N9-C4	7.77	109.51	106.40
2	B	61	G	N3-C2-N2	-7.77	114.46	119.90
1	A	728	G	N7-C8-N9	-7.76	109.22	113.10
1	A	2607	G	N1-C2-N2	-7.75	109.22	116.20
1	A	2371	G	C4-C5-N7	7.75	113.90	110.80
1	A	2502	G	C4-C5-N7	7.75	113.90	110.80
1	A	2515	C	N3-C4-C5	7.75	125.00	121.90
1	A	1979	C	C6-N1-C2	-7.73	117.21	120.30
1	A	1659	U	C5-C6-N1	-7.73	118.83	122.70
1	A	1792	G	C8-N9-C4	7.73	109.49	106.40
1	A	1807	G	N1-C6-O6	7.73	124.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1022	G	N3-C4-N9	-7.73	121.36	126.00
1	A	2594	C	N1-C2-O2	-7.72	114.27	118.90
1	A	934	G	C8-N9-C4	7.72	109.49	106.40
28	6	40	CYS	CA-CB-SG	-7.72	100.11	114.00
1	A	1762	A	N7-C8-N9	7.72	117.66	113.80
1	A	1776	G	C8-N9-C4	7.71	109.48	106.40
1	A	759	G	N1-C6-O6	7.71	124.53	119.90
1	A	47	C	C6-N1-C2	7.71	123.38	120.30
1	A	572	A	N1-C2-N3	7.69	133.15	129.30
1	A	2856	C	C5-C6-N1	7.68	124.84	121.00
2	B	83	G	C5-C6-O6	-7.68	123.99	128.60
1	A	2324	C	N3-C4-C5	7.67	124.97	121.90
1	A	197	A	C6-N1-C2	-7.64	114.02	118.60
1	A	1603	A	C8-N9-C4	-7.63	102.75	105.80
1	A	13	A	N1-C6-N6	-7.62	114.03	118.60
1	A	1302	A	N1-C6-N6	-7.61	114.03	118.60
1	A	560	C	N3-C4-C5	7.61	124.94	121.90
1	A	202	U	C6-N1-C2	7.61	125.56	121.00
1	A	772	C	N1-C2-O2	-7.61	114.34	118.90
1	A	2704	C	C6-N1-C2	7.61	123.34	120.30
1	A	1314	C	C2-N1-C1'	7.60	127.16	118.80
1	A	452	G	C8-N9-C4	-7.60	103.36	106.40
1	A	729	G	N1-C6-O6	7.59	124.45	119.90
1	A	940	G	N1-C6-O6	7.58	124.45	119.90
1	A	818	G	C8-N9-C4	7.57	109.43	106.40
1	A	1821	A	C6-N1-C2	-7.57	114.06	118.60
1	A	1325	G	N1-C6-O6	7.56	124.44	119.90
1	A	2501	C	C5-C4-N4	-7.54	114.92	120.20
1	A	2789	C	C6-N1-C2	7.54	123.31	120.30
1	A	684	G	N3-C2-N2	-7.53	114.63	119.90
2	B	89	G	C5-C6-O6	-7.52	124.09	128.60
1	A	330	A	N3-C4-C5	7.51	132.06	126.80
1	A	2791	C	N3-C2-O2	-7.51	116.64	121.90
1	A	2241	A	C2-N3-C4	-7.50	106.85	110.60
1	A	2306	C	C2-N1-C1'	7.50	127.05	118.80
1	A	1950	G	C4-C5-N7	-7.50	107.80	110.80
1	A	1800	C	C5-C6-N1	-7.49	117.25	121.00
1	A	51	G	N1-C6-O6	-7.49	115.41	119.90
1	A	2206	G	C4-N9-C1'	-7.48	116.78	126.50
1	A	945	A	C4-C5-N7	7.47	114.44	110.70
1	A	2182	G	N3-C4-N9	-7.47	121.52	126.00
1	A	1415	U	C5-C6-N1	-7.47	118.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	A	N1-C6-N6	7.46	123.08	118.60
1	A	1021	A	C5-C6-N1	-7.46	113.97	117.70
1	A	2346	A	C6-N1-C2	-7.45	114.13	118.60
1	A	751	A	C8-N9-C4	7.44	108.78	105.80
1	A	1005	C	C6-N1-C2	7.44	123.28	120.30
1	A	2307	G	N7-C8-N9	7.42	116.81	113.10
1	A	727	A	N1-C6-N6	7.42	123.05	118.60
1	A	1026	U	N1-C2-O2	7.41	127.99	122.80
1	A	1779	U	C6-N1-C2	7.41	125.44	121.00
1	A	2013	A	C8-N9-C4	7.41	108.76	105.80
1	A	2322	A	C4-C5-N7	-7.41	107.00	110.70
1	A	1698	A	C8-N9-C4	-7.40	102.84	105.80
1	A	528	A	C6-N1-C2	7.40	123.04	118.60
1	A	2700	C	C6-N1-C2	7.40	123.26	120.30
1	A	769	G	C8-N9-C4	7.40	109.36	106.40
1	A	932	G	N3-C4-N9	-7.39	121.56	126.00
1	A	516	C	C6-N1-C2	-7.39	117.34	120.30
1	A	1325	G	C4-C5-N7	7.39	113.76	110.80
1	A	1251	C	N3-C4-C5	-7.38	118.95	121.90
1	A	2307	G	C8-N9-C4	-7.38	103.45	106.40
1	A	847	U	N3-C2-O2	-7.38	117.04	122.20
1	A	1663	C	C2-N3-C4	-7.37	116.21	119.90
1	A	1776	G	N9-C4-C5	-7.37	102.45	105.40
1	A	2077	A	C5-C6-N1	7.35	121.38	117.70
1	A	665	C	N3-C4-C5	7.35	124.84	121.90
1	A	787	U	C5-C4-O4	7.35	130.31	125.90
1	A	936	C	C6-N1-C2	7.35	123.24	120.30
1	A	569	U	C5-C4-O4	-7.34	121.49	125.90
1	A	2247	A	C2-N3-C4	-7.34	106.93	110.60
1	A	2593	U	C5-C4-O4	7.33	130.30	125.90
1	A	263	C	N1-C2-O2	7.33	123.30	118.90
1	A	764	A	C6-N1-C2	7.33	123.00	118.60
1	A	1974	C	C6-N1-C2	7.33	123.23	120.30
1	A	2375	G	N7-C8-N9	-7.33	109.44	113.10
1	A	570	G	C8-N9-C4	7.32	109.33	106.40
1	A	1655	A	C8-N9-C4	7.31	108.72	105.80
1	A	1405	U	C5-C6-N1	-7.30	119.05	122.70
1	A	2338	G	N1-C6-O6	7.29	124.28	119.90
1	A	2015	A	N1-C6-N6	-7.27	114.24	118.60
1	A	679	C	C2-N3-C4	-7.27	116.27	119.90
1	A	2070	G	C5-C6-N1	7.26	115.13	111.50
1	A	2293	C	C6-N1-C2	7.26	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2501	C	N3-C4-C5	7.26	124.80	121.90
1	A	2571	C	N1-C2-O2	-7.26	114.54	118.90
1	A	71	A	C8-N9-C4	-7.25	102.90	105.80
1	A	308	G	C8-N9-C4	-7.25	103.50	106.40
1	A	141	A	C4-C5-N7	7.24	114.32	110.70
1	A	1815	A	N1-C6-N6	-7.24	114.26	118.60
1	A	271(J)	C	C6-N1-C2	7.24	123.19	120.30
1	A	1391	U	N1-C2-O2	7.23	127.86	122.80
1	A	2144	U	C5-C6-N1	7.23	126.32	122.70
1	A	265	A	N7-C8-N9	7.23	117.42	113.80
1	A	1654	A	N1-C6-N6	-7.23	114.26	118.60
1	A	657	U	C5-C6-N1	-7.23	119.09	122.70
1	A	1779	U	N3-C4-C5	7.23	118.94	114.60
1	A	2277	G	C4-C5-N7	-7.23	107.91	110.80
1	A	760	G	C4-C5-N7	7.22	113.69	110.80
1	A	265	A	C8-N9-C4	-7.22	102.91	105.80
1	A	2821	A	N9-C4-C5	-7.21	102.92	105.80
1	A	1698	A	C2-N3-C4	-7.20	107.00	110.60
1	A	2878	U	N1-C2-O2	7.19	127.83	122.80
1	A	1142(A)	A	N3-C4-N9	-7.19	121.65	127.40
1	A	912	C	C6-N1-C2	-7.19	117.43	120.30
1	A	2598	A	N1-C6-N6	7.19	122.91	118.60
1	A	1790	C	N1-C2-O2	-7.18	114.59	118.90
1	A	1049	C	C2-N1-C1'	7.18	126.70	118.80
1	A	2318	G	C8-N9-C4	-7.18	103.53	106.40
1	A	583	G	N1-C6-O6	7.18	124.21	119.90
1	A	1698	A	C6-C5-N7	-7.17	127.28	132.30
1	A	735	A	N7-C8-N9	-7.17	110.22	113.80
1	A	2803	C	C5-C6-N1	7.17	124.58	121.00
1	A	2162	G	C2-N3-C4	7.16	115.48	111.90
1	A	280	C	C6-N1-C2	-7.14	117.44	120.30
1	A	679	C	N1-C2-O2	-7.14	114.62	118.90
1	A	751	A	N7-C8-N9	-7.12	110.24	113.80
1	A	123	G	N7-C8-N9	-7.12	109.54	113.10
1	A	1807	G	C5-C6-O6	-7.12	124.33	128.60
1	A	1558	A	C2-N3-C4	-7.11	107.04	110.60
1	A	2315	G	C8-N9-C4	7.11	109.24	106.40
1	A	530	G	C5-C6-N1	7.11	115.05	111.50
14	S	96	GLY	N-CA-C	-7.10	95.35	113.10
1	A	94	C	C2-N1-C1'	7.08	126.59	118.80
1	A	2312	U	C6-N1-C2	-7.08	116.75	121.00
1	A	676	A	N3-C4-N9	-7.08	121.74	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2791	C	C2-N1-C1'	7.08	126.58	118.80
1	A	535	C	N1-C2-O2	-7.07	114.66	118.90
1	A	729	G	N3-C2-N2	-7.07	114.95	119.90
1	A	2251	G	C8-N9-C4	-7.07	103.57	106.40
1	A	2361	A	N1-C6-N6	7.07	122.84	118.60
1	A	330	A	C4-C5-N7	7.06	114.23	110.70
1	A	1325	G	C5-C6-O6	-7.06	124.36	128.60
1	A	2437	U	C5-C4-O4	7.06	130.13	125.90
2	B	6	C	C6-N1-C2	7.05	123.12	120.30
1	A	774	A	C8-N9-C4	-7.05	102.98	105.80
1	A	728	G	N9-C4-C5	-7.05	102.58	105.40
1	A	791	C	C5-C6-N1	-7.04	117.48	121.00
1	A	893	C	N1-C2-O2	7.04	123.12	118.90
1	A	1566	A	N1-C6-N6	7.03	122.82	118.60
1	A	1372	U	N3-C2-O2	-7.02	117.29	122.20
1	A	587	C	N3-C4-C5	-7.02	119.09	121.90
1	A	1762	A	C2-N3-C4	7.00	114.10	110.60
1	A	2324	C	C6-N1-C2	7.00	123.10	120.30
1	A	41	C	C5-C6-N1	-7.00	117.50	121.00
1	A	154(A)	C	N3-C4-N4	-7.00	113.10	118.00
1	A	2182	G	C8-N9-C1'	7.00	136.10	127.00
1	A	1653	G	N3-C4-C5	-7.00	125.10	128.60
1	A	2353	G	C8-N9-C4	6.99	109.20	106.40
1	A	1612	C	C6-N1-C2	6.99	123.10	120.30
1	A	1142(A)	A	C5-N7-C8	-6.98	100.41	103.90
1	A	2250	G	C5-C6-O6	6.98	132.79	128.60
1	A	2360	A	C8-N9-C4	6.97	108.59	105.80
1	A	2087	G	N9-C4-C5	-6.97	102.61	105.40
1	A	2525	G	N9-C4-C5	-6.96	102.61	105.40
1	A	102	G	C4-N9-C1'	6.96	135.55	126.50
1	A	2182	G	C6-C5-N7	6.96	134.57	130.40
1	A	2420	C	C5-C4-N4	-6.96	115.33	120.20
1	A	1989	G	N1-C6-O6	6.95	124.07	119.90
1	A	2087	G	N1-C6-O6	6.95	124.07	119.90
1	A	750	A	N1-C2-N3	6.94	132.77	129.30
1	A	2146	C	N1-C2-O2	6.93	123.06	118.90
1	A	731	C	C6-N1-C2	6.92	123.07	120.30
1	A	2476	A	C8-N9-C4	-6.92	103.03	105.80
1	A	1755	A	N1-C6-N6	-6.92	114.45	118.60
1	A	2277	G	C6-C5-N7	6.92	134.55	130.40
1	A	2221	G	N1-C6-O6	6.92	124.05	119.90
1	A	652(T)	C	C2-N3-C4	6.91	123.35	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1372	U	N1-C2-O2	6.91	127.63	122.80
1	A	2680	C	C5-C6-N1	-6.91	117.55	121.00
1	A	122	G	C6-C5-N7	-6.90	126.26	130.40
1	A	1490	A	N1-C2-N3	-6.90	125.85	129.30
1	A	679	C	C6-N1-C2	6.90	123.06	120.30
1	A	198	C	C2-N3-C4	-6.90	116.45	119.90
2	B	61	G	N1-C6-O6	6.88	124.03	119.90
1	A	679	C	N3-C4-C5	6.88	124.65	121.90
1	A	1800	C	C2-N3-C4	-6.88	116.46	119.90
1	A	2323	G	C8-N9-C4	6.88	109.15	106.40
1	A	2724	C	C6-N1-C2	6.88	123.05	120.30
1	A	2782	G	N1-C6-O6	6.88	124.03	119.90
1	A	409	C	C6-N1-C2	6.88	123.05	120.30
1	A	1252	G	N7-C8-N9	-6.88	109.66	113.10
1	A	1123	C	C5-C6-N1	-6.88	117.56	121.00
1	A	1645	G	C4-C5-N7	-6.87	108.05	110.80
1	A	1698	A	N1-C2-N3	6.87	132.74	129.30
1	A	1795	C	N3-C4-C5	6.87	124.65	121.90
1	A	736	C	N3-C2-O2	6.87	126.71	121.90
1	A	769	G	N7-C8-N9	-6.87	109.67	113.10
1	A	2689	U	C5-C6-N1	-6.87	119.27	122.70
1	A	988	A	C5-C6-N6	-6.87	118.21	123.70
1	A	928	G	N7-C8-N9	6.86	116.53	113.10
1	A	2322	A	N1-C2-N3	6.86	132.73	129.30
1	A	2835	A	N1-C6-N6	-6.85	114.49	118.60
8	I	106	GLY	N-CA-C	6.84	130.21	113.10
1	A	271(J)	C	N3-C4-C5	6.84	124.64	121.90
1	A	1403	C	C2-N1-C1'	-6.84	111.28	118.80
1	A	2375	G	N3-C4-C5	6.83	132.02	128.60
1	A	2791	C	C5-C6-N1	6.83	124.42	121.00
1	A	1791	A	N1-C6-N6	6.83	122.70	118.60
1	A	2107	C	N3-C4-C5	-6.83	119.17	121.90
1	A	2497	A	N1-C6-N6	6.83	122.70	118.60
1	A	147	U	C5-C6-N1	-6.83	119.29	122.70
1	A	2744	G	N1-C6-O6	6.83	124.00	119.90
1	A	2286	A	N1-C2-N3	6.82	132.71	129.30
1	A	1829	A	C8-N9-C4	6.81	108.53	105.80
1	A	1949	G	C8-N9-C4	6.81	109.12	106.40
1	A	2321	G	C8-N9-C4	-6.81	103.68	106.40
1	A	2323	G	N3-C4-C5	6.80	132.00	128.60
1	A	2189	U	N1-C2-O2	6.80	127.56	122.80
1	A	645	C	C2-N1-C1'	6.80	126.28	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1827	C	N3-C4-N4	-6.79	113.24	118.00
1	A	2782	G	C4-C5-N7	6.79	113.52	110.80
1	A	253	C	N3-C4-C5	-6.79	119.18	121.90
1	A	2074	U	C5-C6-N1	6.79	126.09	122.70
1	A	2312	U	N3-C2-O2	-6.79	117.45	122.20
1	A	647	G	C8-N9-C4	-6.79	103.69	106.40
1	A	1304	C	C6-N1-C2	6.79	123.01	120.30
1	A	840	C	C6-N1-C2	6.78	123.01	120.30
1	A	389	G	C8-N9-C1'	-6.77	118.19	127.00
1	A	1567	A	C2-N3-C4	-6.77	107.21	110.60
1	A	1992	G	N1-C6-O6	-6.77	115.84	119.90
1	A	2179	C	N1-C2-O2	6.77	122.96	118.90
1	A	2289	G	C8-N9-C4	6.77	109.11	106.40
1	A	2699	C	C6-N1-C2	6.77	123.01	120.30
1	A	195	A	N1-C6-N6	6.77	122.66	118.60
1	A	2618	G	C4-C5-N7	-6.76	108.09	110.80
1	A	141	A	N1-C6-N6	6.76	122.65	118.60
1	A	205	G	C4-C5-N7	6.76	113.50	110.80
1	A	2031	A	N1-C6-N6	6.76	122.65	118.60
1	A	2238	G	N3-C4-C5	-6.76	125.22	128.60
1	A	132	G	N1-C6-O6	6.75	123.95	119.90
1	A	2725	A	C2-N3-C4	-6.75	107.22	110.60
1	A	2335	A	C8-N9-C4	6.75	108.50	105.80
1	A	1277	G	C2-N3-C4	-6.74	108.53	111.90
1	A	417	C	C6-N1-C2	6.73	122.99	120.30
1	A	2226	C	C6-N1-C2	6.73	122.99	120.30
1	A	197	A	C5-C6-N1	6.73	121.06	117.70
1	A	2411	A	C8-N9-C4	6.73	108.49	105.80
1	A	924	C	N3-C4-C5	6.73	124.59	121.90
1	A	426	C	C6-N1-C2	6.72	122.99	120.30
1	A	2515	C	C2-N3-C4	-6.72	116.54	119.90
1	A	680	G	C2-N3-C4	-6.72	108.54	111.90
1	A	2304	G	C8-N9-C1'	6.72	135.74	127.00
1	A	1612	C	C5-C4-N4	-6.71	115.50	120.20
1	A	1611	C	C6-N1-C2	6.71	122.98	120.30
1	A	2464	C	C6-N1-C1'	-6.71	112.74	120.80
1	A	2028	U	C4-C5-C6	-6.71	115.67	119.70
1	A	1256	G	N3-C2-N2	-6.71	115.20	119.90
1	A	588	U	C5-C4-O4	6.71	129.92	125.90
1	A	39	C	N3-C2-O2	-6.70	117.21	121.90
1	A	1021	A	N1-C2-N3	6.70	132.65	129.30
1	A	1531	C	C5-C6-N1	6.70	124.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1112	G	N3-C4-C5	6.70	131.95	128.60
1	A	2856	C	C6-N1-C2	-6.70	117.62	120.30
1	A	446	G	N3-C4-N9	6.70	130.02	126.00
1	A	1471	A	C8-N9-C4	-6.70	103.12	105.80
1	A	1616	A	C4-C5-N7	6.70	114.05	110.70
1	A	570	G	N9-C4-C5	-6.69	102.72	105.40
1	A	2321	G	N9-C4-C5	6.69	108.08	105.40
1	A	1304	C	C5-C6-N1	-6.69	117.66	121.00
1	A	12	U	C2-N1-C1'	6.68	125.72	117.70
1	A	994	C	C6-N1-C2	6.68	122.97	120.30
1	A	2371	G	C6-C5-N7	-6.68	126.39	130.40
1	A	71	A	N3-C4-C5	6.68	131.47	126.80
1	A	936	C	N3-C2-O2	6.68	126.57	121.90
1	A	2182	G	C5-C6-O6	6.68	132.61	128.60
1	A	465	G	N1-C6-O6	6.67	123.90	119.90
1	A	272(H)	C	C5-C4-N4	-6.67	115.53	120.20
1	A	669	G	C8-N9-C4	6.67	109.07	106.40
1	A	2070	G	N3-C4-N9	6.67	130.00	126.00
1	A	94	C	C6-N1-C2	-6.67	117.63	120.30
1	A	271(M)	G	N3-C4-C5	-6.67	125.27	128.60
1	A	2491	U	N3-C4-C5	6.67	118.60	114.60
1	A	2609	U	N1-C2-O2	-6.67	118.13	122.80
1	A	113	G	C5-C6-O6	-6.66	124.60	128.60
1	A	2632	A	C8-N9-C4	6.66	108.46	105.80
1	A	389	G	C8-N9-C4	6.66	109.06	106.40
1	A	895	U	C5-C6-N1	6.66	126.03	122.70
1	A	265	A	C6-C5-N7	-6.65	127.64	132.30
1	A	444	C	N3-C4-C5	6.65	124.56	121.90
1	A	607	U	C6-N1-C2	6.64	124.99	121.00
1	A	1925	C	N1-C2-O2	-6.64	114.91	118.90
1	A	682	G	C5-C6-O6	-6.64	124.61	128.60
1	A	1785	A	N1-C6-N6	6.64	122.59	118.60
1	A	2286	A	C5-C6-N1	-6.64	114.38	117.70
1	A	663	G	N3-C2-N2	-6.64	115.25	119.90
1	A	2464	C	N3-C4-C5	6.64	124.56	121.90
1	A	772	C	N3-C2-O2	6.63	126.54	121.90
1	A	1264	G	N1-C6-O6	6.63	123.88	119.90
2	B	64	C	C5-C6-N1	-6.63	117.69	121.00
1	A	335	C	N3-C4-C5	-6.62	119.25	121.90
1	A	2329	G	N7-C8-N9	-6.62	109.79	113.10
1	A	1374	G	C8-N9-C4	-6.62	103.75	106.40
1	A	2396	G	C8-N9-C4	-6.62	103.75	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1107	G	N3-C2-N2	6.61	124.53	119.90
1	A	2591	C	C6-N1-C2	-6.61	117.66	120.30
1	A	188	G	N1-C2-N2	-6.60	110.26	116.20
1	A	465	G	C6-C5-N7	-6.59	126.44	130.40
1	A	1604	C	N1-C2-O2	-6.59	114.94	118.90
1	A	2335	A	C4-C5-C6	-6.59	113.70	117.00
1	A	2487	G	N1-C6-O6	6.59	123.86	119.90
1	A	286	C	N1-C2-O2	6.58	122.85	118.90
1	A	2206	G	C8-N9-C1'	6.58	135.56	127.00
1	A	2552	U	C2-N3-C4	-6.58	123.05	127.00
1	A	2487	G	C6-C5-N7	-6.58	126.45	130.40
1	A	2689	U	C5-C4-O4	6.58	129.85	125.90
1	A	802	A	C5-C6-N1	6.58	120.99	117.70
1	A	1963	U	C2-N1-C1'	6.57	125.59	117.70
1	A	449	A	C5-N7-C8	-6.57	100.62	103.90
1	A	746	A	C6-N1-C2	-6.56	114.66	118.60
1	A	327	G	N1-C6-O6	6.56	123.83	119.90
1	A	1200	C	C6-N1-C2	6.56	122.92	120.30
1	A	2264	C	C5-C6-N1	-6.55	117.72	121.00
1	A	1459	G	C8-N9-C4	-6.55	103.78	106.40
1	A	2609	U	N3-C2-O2	6.55	126.78	122.20
2	B	81	G	C4-C5-N7	6.55	113.42	110.80
1	A	2849	U	C5-C6-N1	-6.55	119.43	122.70
1	A	978	G	N7-C8-N9	-6.55	109.83	113.10
1	A	1269	A	C8-N9-C4	6.55	108.42	105.80
1	A	1204	A	C2-N3-C4	-6.54	107.33	110.60
1	A	207	A	C2-N3-C4	-6.54	107.33	110.60
1	A	2329	G	N9-C4-C5	-6.54	102.78	105.40
1	A	2283	C	N1-C2-O2	-6.54	114.97	118.90
1	A	2525	G	C5-C6-O6	-6.54	124.67	128.60
1	A	2596	U	N1-C2-N3	6.54	118.83	114.90
1	A	2615	U	C5-C4-O4	6.54	129.82	125.90
1	A	114	U	C2-N1-C1'	6.54	125.55	117.70
1	A	185	U	C5-C6-N1	-6.54	119.43	122.70
1	A	154	G	N1-C6-O6	6.53	123.82	119.90
1	A	535	C	C2-N1-C1'	-6.53	111.61	118.80
1	A	96	G	C2-N3-C4	-6.53	108.64	111.90
1	A	1763	G	N3-C4-N9	-6.53	122.08	126.00
1	A	727	A	C6-C5-N7	-6.53	127.73	132.30
1	A	1613	G	N3-C2-N2	6.51	124.46	119.90
1	A	535	C	C6-N1-C2	6.51	122.90	120.30
1	A	2689	U	C2-N3-C4	-6.51	123.10	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652(B)	A	C2-N3-C4	6.50	113.85	110.60
1	A	1365	A	C8-N9-C4	-6.50	103.20	105.80
1	A	1045	A	C2-N3-C4	6.50	113.85	110.60
1	A	1677	A	C2-N3-C4	-6.50	107.35	110.60
1	A	1539	G	C6-C5-N7	-6.50	126.50	130.40
1	A	463	G	C5-C6-O6	6.49	132.50	128.60
1	A	1192	G	C8-N9-C4	6.48	108.99	106.40
1	A	746	A	C5-N7-C8	-6.48	100.66	103.90
1	A	2420	C	N3-C4-C5	6.48	124.49	121.90
1	A	2618	G	C6-N1-C2	-6.48	121.21	125.10
1	A	1258	C	C6-N1-C2	6.48	122.89	120.30
1	A	1788	C	N3-C4-C5	-6.48	119.31	121.90
1	A	2461	C	C5-C6-N1	-6.48	117.76	121.00
1	A	584	C	N1-C2-O2	-6.47	115.02	118.90
2	B	63	G	C8-N9-C4	6.47	108.99	106.40
1	A	2047	U	C5-C6-N1	-6.47	119.47	122.70
1	A	2182	G	C6-N1-C2	6.47	128.98	125.10
1	A	102	G	C8-N9-C1'	-6.46	118.60	127.00
1	A	2028	U	N1-C2-N3	-6.46	111.02	114.90
1	A	2312	U	C5-C6-N1	6.46	125.93	122.70
1	A	39	C	C2-N3-C4	-6.46	116.67	119.90
1	A	62	C	C2-N3-C4	-6.46	116.67	119.90
1	A	453	C	C5-C6-N1	-6.46	117.77	121.00
1	A	1368	G	N3-C2-N2	-6.46	115.38	119.90
1	A	1979	C	C5-C6-N1	6.46	124.23	121.00
1	A	287	C	C6-N1-C2	6.45	122.88	120.30
1	A	1021	A	N7-C8-N9	6.45	117.02	113.80
1	A	1141	U	N3-C4-O4	-6.45	114.89	119.40
1	A	1299	G	C8-N9-C4	-6.44	103.82	106.40
1	A	2680	C	C6-N1-C2	6.44	122.88	120.30
1	A	2335	A	O4'-C1'-N9	6.44	113.35	108.20
1	A	2048	G	C8-N9-C4	-6.43	103.83	106.40
1	A	1191	G	C8-N9-C4	6.43	108.97	106.40
1	A	2321	G	N3-C2-N2	-6.43	115.40	119.90
1	A	2393	A	N9-C4-C5	6.43	108.37	105.80
1	A	1239	G	N3-C2-N2	-6.43	115.40	119.90
1	A	265	A	C4-C5-C6	6.42	120.21	117.00
1	A	1315	C	C6-N1-C2	-6.42	117.73	120.30
1	A	2681	C	C2-N3-C4	-6.42	116.69	119.90
1	A	1955	U	C5-C6-N1	-6.41	119.49	122.70
2	B	76	G	N3-C4-C5	6.41	131.81	128.60
1	A	113	G	N1-C6-O6	6.41	123.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	C	C5-C6-N1	-6.41	117.80	121.00
1	A	297	C	N3-C4-C5	-6.41	119.34	121.90
1	A	2676	C	C6-N1-C2	6.41	122.86	120.30
1	A	664	C	C2-N3-C4	-6.40	116.70	119.90
1	A	673	C	N1-C2-O2	-6.40	115.06	118.90
1	A	1651	G	C5-C6-N1	6.40	114.70	111.50
1	A	2250	G	N9-C4-C5	6.40	107.96	105.40
1	A	2623	G	N3-C4-C5	-6.40	125.40	128.60
1	A	862	G	N9-C4-C5	6.40	107.96	105.40
1	A	1254	A	C6-N1-C2	-6.40	114.76	118.60
1	A	2421	G	N9-C4-C5	-6.40	102.84	105.40
1	A	2675	A	N1-C6-N6	6.40	122.44	118.60
1	A	2680	C	C2-N3-C4	-6.40	116.70	119.90
1	A	1308	A	C4-C5-C6	6.39	120.20	117.00
1	A	1950	G	C5-N7-C8	6.39	107.50	104.30
1	A	129	C	C2-N3-C4	-6.39	116.70	119.90
1	A	1942	C	N3-C4-N4	-6.39	113.53	118.00
1	A	2485	G	N9-C4-C5	-6.39	102.84	105.40
1	A	845	G	C6-C5-N7	-6.39	126.57	130.40
1	A	2356	C	N1-C2-O2	-6.39	115.07	118.90
1	A	389	G	N3-C2-N2	6.38	124.37	119.90
1	A	2030	A	C4-N9-C1'	-6.38	114.81	126.30
4	E	118	LYS	N-CA-C	-6.38	93.77	111.00
1	A	664	C	C6-N1-C2	6.38	122.85	120.30
1	A	1864	U	C5-C6-N1	-6.37	119.51	122.70
1	A	1359	A	C4-C5-C6	-6.37	113.82	117.00
1	A	1616	A	N9-C4-C5	-6.37	103.25	105.80
1	A	1930	G	C4-N9-C1'	-6.37	118.22	126.50
1	A	1216	G	N9-C4-C5	-6.36	102.85	105.40
1	A	2070	G	C6-N1-C2	-6.36	121.28	125.10
1	A	2285	C	C5-C4-N4	6.36	124.65	120.20
1	A	1942	C	C2-N1-C1'	-6.36	111.81	118.80
1	A	1284	A	C5-C6-N6	-6.36	118.61	123.70
2	B	76	G	C4-C5-N7	6.36	113.34	110.80
1	A	2755	C	C4-C5-C6	-6.35	114.22	117.40
1	A	179	G	C2-N3-C4	-6.35	108.73	111.90
1	A	1267	U	C4-C5-C6	-6.35	115.89	119.70
1	A	2030	A	C4-C5-C6	-6.35	113.83	117.00
1	A	2238	G	C2-N3-C4	6.35	115.07	111.90
1	A	745	G	C6-C5-N7	-6.34	126.59	130.40
1	A	80	G	C8-N9-C4	-6.34	103.87	106.40
1	A	1647	G	N1-C6-O6	6.34	123.70	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2030	A	C8-N9-C4	6.33	108.33	105.80
1	A	1248	G	N9-C4-C5	-6.33	102.87	105.40
1	A	122	G	N9-C4-C5	-6.33	102.87	105.40
1	A	458	G	C8-N9-C4	-6.33	103.87	106.40
1	A	2803	C	C2-N3-C4	6.33	123.06	119.90
1	A	1767	C	C2-N3-C4	-6.33	116.74	119.90
1	A	2396	G	N7-C8-N9	6.33	116.26	113.10
1	A	2607	G	C8-N9-C1'	-6.33	118.78	127.00
1	A	58	G	C8-N9-C4	-6.32	103.87	106.40
1	A	933	A	C4-C5-N7	6.32	113.86	110.70
1	A	2572	A	N9-C4-C5	-6.32	103.27	105.80
1	A	2332	U	N1-C2-O2	6.32	127.23	122.80
1	A	2499	C	C5-C6-N1	6.32	124.16	121.00
1	A	760	G	N1-C6-O6	6.32	123.69	119.90
1	A	2496	C	N3-C4-C5	6.32	124.43	121.90
1	A	188	G	C2-N3-C4	-6.32	108.74	111.90
1	A	664	C	C5-C6-N1	-6.32	117.84	121.00
1	A	1781	C	N1-C2-O2	6.31	122.69	118.90
1	A	444	C	N3-C4-N4	-6.31	113.58	118.00
1	A	1950	G	N9-C4-C5	6.31	107.92	105.40
1	A	2394	C	C5-C6-N1	-6.31	117.85	121.00
1	A	2224	G	N1-C6-O6	6.31	123.69	119.90
1	A	98	G	C8-N9-C4	6.31	108.92	106.40
1	A	1781	C	N3-C2-O2	-6.31	117.49	121.90
29	7	47	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	449	A	C5-C6-N6	-6.30	118.66	123.70
1	A	1614	A	C8-N9-C4	6.30	108.32	105.80
1	A	2182	G	C4-N9-C1'	-6.30	118.31	126.50
2	B	113	G	N9-C4-C5	-6.30	102.88	105.40
1	A	2296	U	C1'-O4'-C4'	-6.29	104.86	109.90
1	A	1309	G	N7-C8-N9	-6.28	109.96	113.10
1	A	1314	C	C6-N1-C1'	-6.28	113.26	120.80
1	A	645	C	C5-C6-N1	6.28	124.14	121.00
1	A	2525	G	N1-C6-O6	6.28	123.67	119.90
1	A	82	G	C8-N9-C4	6.28	108.91	106.40
1	A	2100	G	N3-C4-C5	-6.27	125.46	128.60
1	A	2435	A	C5-N7-C8	-6.27	100.77	103.90
1	A	750	A	C4-C5-C6	6.27	120.13	117.00
1	A	2306	C	C2-N3-C4	6.26	123.03	119.90
1	A	2084	C	C6-N1-C2	6.26	122.80	120.30
1	A	2353	G	N9-C4-C5	-6.26	102.90	105.40
1	A	928	G	C4-C5-N7	6.25	113.30	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2322	A	C5-C6-N1	6.25	120.83	117.70
1	A	776	G	C8-N9-C4	-6.25	103.90	106.40
1	A	1603	A	N7-C8-N9	6.25	116.92	113.80
1	A	2023	G	C5-C6-O6	-6.25	124.85	128.60
1	A	530	G	C5-C6-O6	-6.24	124.85	128.60
1	A	2260	C	C4-C5-C6	6.24	120.52	117.40
1	A	1839	G	N1-C6-O6	-6.24	116.16	119.90
1	A	2570	G	C5-C6-N1	-6.24	108.38	111.50
1	A	1022	G	C8-N9-C1'	6.24	135.11	127.00
1	A	1792	G	N7-C8-N9	-6.24	109.98	113.10
1	A	2827	C	N3-C2-O2	6.24	126.27	121.90
1	A	2596	U	C2-N3-C4	-6.23	123.26	127.00
2	B	115	G	N9-C4-C5	-6.22	102.91	105.40
1	A	404	C	C6-N1-C2	6.22	122.79	120.30
1	A	2723	C	C4-C5-C6	6.22	120.51	117.40
1	A	271(G)	C	N1-C2-O2	6.21	122.63	118.90
1	A	1616	A	C6-C5-N7	-6.21	127.95	132.30
1	A	675	A	C2-N3-C4	-6.21	107.49	110.60
1	A	2728	U	C2-N3-C4	-6.21	123.27	127.00
2	B	75	G	C8-N9-C4	6.21	108.88	106.40
1	A	2379	G	N7-C8-N9	6.21	116.20	113.10
1	A	2028	U	C5-C6-N1	-6.21	119.60	122.70
1	A	977	G	C5-C6-N1	6.20	114.60	111.50
1	A	196	A	N1-C6-N6	6.20	122.32	118.60
1	A	2782	G	C6-C5-N7	-6.20	126.68	130.40
1	A	1755	A	C5-C6-N6	6.20	128.66	123.70
1	A	389	G	C4-C5-N7	6.20	113.28	110.80
1	A	673	C	N3-C4-C5	6.20	124.38	121.90
1	A	1314	C	C5-C4-N4	-6.20	115.86	120.20
1	A	1987	G	N1-C6-O6	6.20	123.62	119.90
1	A	910	A	N1-C6-N6	6.19	122.31	118.60
1	A	2031	A	C4-C5-C6	6.19	120.10	117.00
1	A	2038	G	C4-C5-N7	6.19	113.27	110.80
1	A	1298	C	N3-C2-O2	-6.18	117.57	121.90
1	A	766	C	C6-N1-C2	-6.18	117.83	120.30
1	A	1938	A	C4-C5-C6	6.18	120.09	117.00
1	A	330	A	N1-C2-N3	6.18	132.39	129.30
1	A	1977	A	N7-C8-N9	-6.18	110.71	113.80
3	D	229	VAL	CB-CA-C	-6.18	99.67	111.40
1	A	459	U	N3-C4-O4	-6.17	115.08	119.40
1	A	1391	U	C2-N1-C1'	6.17	125.10	117.70
1	A	535	C	N3-C2-O2	6.17	126.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	995	C	N1-C2-O2	-6.17	115.20	118.90
1	A	1802	A	N1-C2-N3	6.17	132.38	129.30
1	A	2364	C	C5-C6-N1	-6.17	117.92	121.00
1	A	1478	G	N3-C2-N2	6.16	124.22	119.90
1	A	1963	U	C5-C6-N1	6.16	125.78	122.70
1	A	2055	C	C2-N1-C1'	-6.16	112.02	118.80
1	A	2371	G	C8-N9-C4	6.16	108.86	106.40
1	A	775	G	N1-C2-N2	-6.16	110.66	116.20
1	A	1327	C	N1-C2-O2	-6.16	115.20	118.90
1	A	1653	G	C4-N9-C1'	6.16	134.50	126.50
1	A	397	G	N3-C4-C5	6.15	131.68	128.60
1	A	2103	C	C2-N3-C4	6.15	122.98	119.90
1	A	361	G	N1-C6-O6	6.15	123.59	119.90
1	A	1204	A	N3-C4-C5	6.15	131.11	126.80
1	A	2182	G	N9-C4-C5	6.15	107.86	105.40
1	A	2581	G	C5-C6-O6	6.15	132.29	128.60
1	A	2335	A	N9-C4-C5	-6.15	103.34	105.80
1	A	1264	G	C5-C6-O6	-6.14	124.91	128.60
1	A	71	A	N3-C4-N9	-6.14	122.49	127.40
1	A	1371	G	N1-C6-O6	6.14	123.58	119.90
1	A	201	C	C5-C6-N1	-6.14	117.93	121.00
1	A	1934	C	C6-N1-C2	6.14	122.75	120.30
1	A	1047	G	N3-C4-N9	6.13	129.68	126.00
1	A	1992	G	C8-N9-C4	-6.13	103.95	106.40
1	A	2323	G	N9-C4-C5	-6.13	102.95	105.40
1	A	1991	U	C5-C6-N1	-6.12	119.64	122.70
1	A	2751	G	C8-N9-C4	-6.12	103.95	106.40
1	A	154	G	C5-C6-O6	-6.12	124.93	128.60
1	A	2107	C	C5-C4-N4	6.12	124.48	120.20
1	A	1419	A	C8-N9-C4	6.12	108.25	105.80
1	A	2607	G	N3-C2-N2	6.12	124.18	119.90
1	A	691	C	C6-N1-C2	6.12	122.75	120.30
1	A	865	C	C6-N1-C2	6.12	122.75	120.30
1	A	2689	U	C2-N1-C1'	-6.12	110.36	117.70
1	A	2340	G	N9-C4-C5	-6.11	102.95	105.40
1	A	530	G	C4-C5-N7	6.11	113.25	110.80
1	A	205	G	N3-C2-N2	6.11	124.18	119.90
1	A	446	G	N9-C4-C5	-6.11	102.96	105.40
1	A	279	C	C5-C6-N1	6.11	124.05	121.00
1	A	1006	C	C2-N1-C1'	-6.10	112.09	118.80
1	A	1531	C	C6-N1-C2	-6.10	117.86	120.30
1	A	1617	C	C5-C6-N1	-6.10	117.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2421	G	C5-C6-O6	-6.10	124.94	128.60
1	A	278	A	N9-C4-C5	-6.10	103.36	105.80
1	A	2031	A	C6-C5-N7	-6.10	128.03	132.30
1	A	2731	G	C6-N1-C2	-6.10	121.44	125.10
1	A	847	U	N1-C2-O2	6.09	127.07	122.80
1	A	1755	A	N1-C2-N3	6.09	132.35	129.30
1	A	2335	A	C6-N1-C2	-6.09	114.94	118.60
1	A	2623	G	C2-N3-C4	6.09	114.95	111.90
1	A	893	C	C2-N1-C1'	6.09	125.50	118.80
1	A	2510	C	C5-C4-N4	6.09	124.46	120.20
1	A	747	U	N1-C2-O2	-6.08	118.54	122.80
1	A	2881	C	N3-C2-O2	6.08	126.16	121.90
1	A	1830	C	C6-N1-C2	6.08	122.73	120.30
1	A	2129	C	N1-C2-O2	6.08	122.55	118.90
1	A	2300	G	N3-C4-N9	6.08	129.65	126.00
1	A	693	C	C2-N3-C4	-6.08	116.86	119.90
1	A	2768	C	C6-N1-C2	-6.08	117.87	120.30
1	A	271(W)	G	C8-N9-C4	-6.08	103.97	106.40
1	A	739	G	N7-C8-N9	-6.08	110.06	113.10
1	A	2264	C	C2-N3-C4	-6.08	116.86	119.90
1	A	695	G	C5-C6-O6	6.07	132.24	128.60
1	A	1989	G	C5-C6-O6	-6.07	124.96	128.60
1	A	1121	C	C5-C6-N1	-6.07	117.97	121.00
1	A	2099	U	C6-N1-C2	-6.07	117.36	121.00
1	A	62	C	N3-C4-N4	-6.07	113.75	118.00
1	A	791	C	N3-C2-O2	-6.07	117.65	121.90
1	A	1316	U	N3-C2-O2	-6.07	117.95	122.20
1	A	1845	G	N1-C6-O6	-6.07	116.26	119.90
1	A	2100	G	C4-N9-C1'	6.07	134.38	126.50
1	A	391	G	N9-C4-C5	-6.06	102.97	105.40
1	A	2500	U	N3-C4-C5	6.06	118.23	114.60
1	A	1313	U	C6-N1-C2	-6.06	117.37	121.00
1	A	1784	A	N1-C6-N6	-6.05	114.97	118.60
1	A	300	A	C8-N9-C4	6.05	108.22	105.80
1	A	975	C	C6-N1-C2	-6.05	117.88	120.30
1	A	1216	G	N1-C6-O6	6.05	123.53	119.90
1	A	1653	G	C8-N9-C4	-6.04	103.98	106.40
1	A	845	G	C8-N9-C1'	-6.04	119.14	127.00
1	A	1575	C	C6-N1-C2	6.04	122.72	120.30
1	A	468	G	N9-C4-C5	-6.04	102.98	105.40
1	A	2354	G	C8-N9-C4	-6.04	103.98	106.40
1	A	2782	G	C5-C6-O6	-6.04	124.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	G	C4-C5-C6	6.04	122.42	118.80
1	A	1530	C	C6-N1-C1'	-6.04	113.55	120.80
1	A	1313	U	C2-N1-C1'	6.04	124.94	117.70
1	A	1351	C	C6-N1-C2	6.04	122.71	120.30
1	A	90	U	C5-C6-N1	6.03	125.72	122.70
1	A	403	U	N3-C2-O2	-6.03	117.98	122.20
1	A	2111	C	C6-N1-C2	-6.03	117.89	120.30
1	A	2521	C	C5-C6-N1	-6.03	117.98	121.00
1	A	529	A	C2-N3-C4	-6.03	107.59	110.60
1	A	103	A	N1-C6-N6	6.03	122.22	118.60
1	A	122	G	C8-N9-C4	6.03	108.81	106.40
1	A	528	A	C8-N9-C1'	6.03	138.55	127.70
1	A	2719	G	C8-N9-C4	6.03	108.81	106.40
1	A	783	A	C2-N3-C4	6.02	113.61	110.60
1	A	988	A	N9-C4-C5	-6.02	103.39	105.80
1	A	2387	U	C5-C6-N1	-6.02	119.69	122.70
1	A	2805	G	N1-C6-O6	-6.02	116.29	119.90
1	A	926	A	N1-C6-N6	6.02	122.21	118.60
1	A	445	C	C2-N3-C4	-6.02	116.89	119.90
1	A	825	C	N3-C4-N4	6.02	122.21	118.00
1	A	2790	A	C2-N3-C4	6.01	113.61	110.60
1	A	1210	A	C5-N7-C8	-6.01	100.89	103.90
1	A	2312	U	C2-N1-C1'	6.01	124.91	117.70
1	A	141	A	C6-C5-N7	-6.01	128.09	132.30
1	A	205	G	C5-C6-O6	-6.01	125.00	128.60
1	A	2708	G	N1-C6-O6	-6.01	116.30	119.90
1	A	132	G	C5-C6-N1	-6.00	108.50	111.50
1	A	1808	U	C2-N3-C4	6.00	130.60	127.00
1	A	2759	G	N1-C6-O6	-6.00	116.30	119.90
1	A	1337	G	N1-C6-O6	-6.00	116.30	119.90
1	A	465	G	C8-N9-C4	-6.00	104.00	106.40
1	A	1762	A	N3-C4-C5	-6.00	122.60	126.80
1	A	1760	A	C6-N1-C2	-5.99	115.00	118.60
21	Z	151	HIS	N-CA-C	5.99	127.18	111.00
1	A	1325	G	N9-C4-C5	-5.99	103.00	105.40
1	A	1577	C	C6-N1-C2	5.99	122.70	120.30
1	A	2523	G	C8-N9-C4	5.99	108.80	106.40
1	A	2844	G	N1-C6-O6	5.99	123.49	119.90
1	A	627	A	N7-C8-N9	-5.99	110.81	113.80
1	A	2787	C	N1-C2-O2	5.99	122.49	118.90
1	A	1992	G	C5-C6-O6	5.98	132.19	128.60
2	B	7	G	C8-N9-C4	5.98	108.79	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1316	U	N1-C2-O2	5.98	126.98	122.80
1	A	1350	C	N3-C4-C5	5.98	124.29	121.90
1	A	2364	C	C6-N1-C2	5.98	122.69	120.30
1	A	179	G	C8-N9-C4	5.97	108.79	106.40
1	A	583	G	C5-C6-O6	-5.97	125.02	128.60
1	A	2452	C	N3-C4-C5	-5.97	119.51	121.90
1	A	1777	U	N3-C2-O2	-5.97	118.02	122.20
1	A	2315	G	N7-C8-N9	-5.97	110.11	113.10
1	A	2580	U	C5-C6-N1	-5.97	119.72	122.70
1	A	2599	G	N1-C2-N3	5.97	127.48	123.90
1	A	1698	A	C4-C5-N7	5.97	113.68	110.70
1	A	389	G	N3-C4-N9	5.97	129.58	126.00
1	A	446	G	C8-N9-C1'	-5.97	119.24	127.00
1	A	70	G	C4-C5-N7	5.96	113.19	110.80
1	A	327	G	C5-C6-N1	-5.96	108.52	111.50
1	A	915	C	N1-C2-O2	5.96	122.48	118.90
1	A	1282	U	C5-C6-N1	-5.96	119.72	122.70
1	A	1377	G	N3-C4-N9	5.96	129.58	126.00
1	A	2351	G	N3-C4-C5	-5.96	125.62	128.60
1	A	566	U	C5-C6-N1	-5.96	119.72	122.70
1	A	208	C	C5-C4-N4	-5.96	116.03	120.20
1	A	587	C	N3-C2-O2	-5.96	117.73	121.90
1	A	924	C	N3-C4-N4	-5.96	113.83	118.00
1	A	1270	C	C5-C6-N1	-5.96	118.02	121.00
1	A	1980	G	N3-C2-N2	-5.96	115.73	119.90
1	A	2622	C	C6-N1-C2	5.96	122.68	120.30
1	A	781	A	C8-N9-C4	5.96	108.18	105.80
1	A	676	A	C6-C5-N7	-5.95	128.13	132.30
1	A	392	C	N3-C2-O2	5.95	126.06	121.90
1	A	862	G	N1-C6-O6	-5.95	116.33	119.90
1	A	1129	A	N9-C4-C5	5.95	108.18	105.80
1	A	2240	C	C4-C5-C6	-5.95	114.42	117.40
1	A	512	G	N1-C6-O6	-5.95	116.33	119.90
1	A	756	C	C5-C6-N1	-5.95	118.03	121.00
1	A	629	G	N3-C4-N9	-5.95	122.43	126.00
1	A	34	C	N1-C2-O2	5.95	122.47	118.90
1	A	1896	G	N1-C6-O6	5.95	123.47	119.90
1	A	196	A	N9-C4-C5	-5.94	103.42	105.80
1	A	572	A	C2-N3-C4	-5.94	107.63	110.60
1	A	1618	A	C5-C6-N6	5.94	128.45	123.70
1	A	508	G	C8-N9-C4	5.94	108.78	106.40
1	A	762	U	N1-C2-N3	-5.94	111.34	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1944	U	C5-C6-N1	-5.94	119.73	122.70
1	A	1992	G	P-O3'-C3'	5.94	126.82	119.70
1	A	2107	C	C6-N1-C2	-5.94	117.92	120.30
1	A	659	C	C6-N1-C2	5.94	122.67	120.30
1	A	1301	A	N1-C2-N3	5.93	132.27	129.30
1	A	1296	G	N1-C2-N2	-5.93	110.86	116.20
1	A	2612	C	C6-N1-C2	5.93	122.67	120.30
1	A	2200	C	C2-N1-C1'	5.93	125.32	118.80
1	A	2746	U	C5-C6-N1	-5.93	119.73	122.70
1	A	652(T)	C	N1-C2-O2	5.93	122.46	118.90
1	A	776	G	N7-C8-N9	5.93	116.06	113.10
1	A	1213	A	C8-N9-C4	5.93	108.17	105.80
1	A	1583	A	C8-N9-C4	5.93	108.17	105.80
1	A	645	C	C2-N3-C4	5.92	122.86	119.90
1	A	2105	C	C5-C6-N1	5.92	123.96	121.00
1	A	1427	A	C6-N1-C2	-5.92	115.05	118.60
1	A	2641	G	C4-N9-C1'	5.92	134.19	126.50
1	A	51	G	C5-C6-O6	5.92	132.15	128.60
1	A	777	A	N9-C4-C5	5.91	108.17	105.80
1	A	2304	G	C4-N9-C1'	-5.91	118.81	126.50
1	A	2304	G	N9-C4-C5	5.91	107.76	105.40
1	A	363(B)	G	N3-C4-N9	5.91	129.54	126.00
1	A	679	C	C5-C6-N1	-5.91	118.05	121.00
1	A	765	G	N1-C6-O6	5.91	123.44	119.90
1	A	1777	U	N1-C2-O2	5.91	126.93	122.80
1	A	2525	G	C8-N9-C4	5.91	108.76	106.40
1	A	673	C	C2-N3-C4	-5.90	116.95	119.90
1	A	645	C	C6-N1-C2	-5.90	117.94	120.30
1	A	652(E)	G	N3-C2-N2	5.90	124.03	119.90
1	A	1695	G	N7-C8-N9	5.90	116.05	113.10
1	A	1539	G	N1-C6-O6	5.90	123.44	119.90
1	A	2162	G	N3-C4-N9	5.89	129.54	126.00
1	A	1271	G	N1-C6-O6	5.89	123.44	119.90
1	A	984	A	C8-N9-C4	5.89	108.16	105.80
1	A	2455	G	C8-N9-C1'	-5.89	119.34	127.00
1	A	214	G	C5-C6-O6	-5.89	125.07	128.60
1	A	179	G	N9-C4-C5	-5.88	103.05	105.40
1	A	1653	G	N3-C4-N9	5.88	129.53	126.00
2	B	81	G	C5-N7-C8	-5.88	101.36	104.30
1	A	625	G	C2-N3-C4	-5.88	108.96	111.90
1	A	1617	C	C4-C5-C6	5.88	120.34	117.40
1	A	1863	G	C8-N9-C4	5.88	108.75	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1464	C	N3-C4-C5	-5.88	119.55	121.90
1	A	242	G	C4-N9-C1'	-5.88	118.86	126.50
1	A	1298	C	C2-N3-C4	-5.88	116.96	119.90
1	A	1141	U	C5-C4-O4	5.88	129.43	125.90
1	A	1281	G	N1-C6-O6	5.88	123.42	119.90
1	A	1623	G	C2-N3-C4	-5.88	108.96	111.90
1	A	1359	A	C5-C6-N1	5.87	120.64	117.70
1	A	2587	A	N1-C6-N6	5.87	122.12	118.60
1	A	448	U	C4-C5-C6	5.87	123.22	119.70
1	A	582	G	C2-N3-C4	-5.87	108.97	111.90
1	A	629	G	N3-C4-C5	5.87	131.53	128.60
1	A	1257	C	N3-C4-C5	-5.87	119.55	121.90
1	A	2351	G	C4-N9-C1'	5.86	134.12	126.50
1	A	1265	A	N1-C6-N6	5.86	122.12	118.60
1	A	2464	C	C4-C5-C6	-5.86	114.47	117.40
1	A	1276	A	N1-C6-N6	5.86	122.12	118.60
1	A	2510	C	C4-C5-C6	5.86	120.33	117.40
1	A	2626	C	N3-C4-C5	5.86	124.24	121.90
1	A	2805	G	C5-C6-O6	5.86	132.12	128.60
1	A	1619	G	C5-C6-N1	5.86	114.43	111.50
2	B	4	C	C6-N1-C2	5.86	122.64	120.30
1	A	571	A	N7-C8-N9	-5.85	110.88	113.80
1	A	1881	C	C6-N1-C2	-5.84	117.96	120.30
2	B	64	C	C6-N1-C2	5.84	122.64	120.30
1	A	1252	G	C8-N9-C4	5.84	108.74	106.40
1	A	1946	U	N3-C4-C5	5.84	118.11	114.60
1	A	1261	C	C6-N1-C2	5.84	122.64	120.30
1	A	1751	C	N1-C2-O2	-5.84	115.40	118.90
1	A	928	G	C5-N7-C8	-5.84	101.38	104.30
1	A	1654	A	N9-C4-C5	5.83	108.13	105.80
1	A	300	A	N9-C4-C5	-5.83	103.47	105.80
1	A	1231	G	N1-C6-O6	5.83	123.40	119.90
1	A	391	G	C5-C6-O6	-5.83	125.10	128.60
1	A	624	C	N3-C4-C5	5.83	124.23	121.90
1	A	1776	G	N3-C2-N2	5.83	123.98	119.90
1	A	2464	C	C2-N1-C1'	5.83	125.22	118.80
1	A	529	A	C5-N7-C8	-5.83	100.98	103.90
1	A	856	C	C5-C6-N1	5.83	123.92	121.00
1	A	1292	U	N3-C2-O2	5.83	126.28	122.20
1	A	1618	A	N1-C6-N6	-5.83	115.10	118.60
1	A	2499	C	C6-N1-C2	-5.83	117.97	120.30
1	A	2843	G	N3-C2-N2	-5.83	115.82	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1435	G	C5-C6-O6	-5.82	125.11	128.60
1	A	2425	A	C5-N7-C8	-5.82	100.99	103.90
1	A	2617	C	C6-N1-C2	5.82	122.63	120.30
1	A	1304	C	N3-C4-C5	5.82	124.23	121.90
1	A	1647	G	N3-C4-C5	5.82	131.51	128.60
1	A	2070	G	N1-C2-N2	-5.82	110.96	116.20
1	A	1478	G	N3-C4-N9	5.82	129.49	126.00
1	A	938	G	C8-N9-C4	5.81	108.73	106.40
1	A	60	G	C4-C5-N7	5.81	113.12	110.80
1	A	445	C	C5-C6-N1	-5.81	118.10	121.00
1	A	750	A	C5-C6-N1	-5.81	114.80	117.70
1	A	362	U	C5-C4-O4	-5.81	122.42	125.90
1	A	1298	C	N3-C4-C5	5.81	124.22	121.90
1	A	1539	G	C4-C5-N7	5.81	113.12	110.80
1	A	1801	G	C5-C6-O6	-5.81	125.12	128.60
1	A	304	G	C5-C6-N1	-5.80	108.60	111.50
1	A	1373	A	N7-C8-N9	-5.80	110.90	113.80
1	A	2038	G	C5-N7-C8	-5.80	101.40	104.30
1	A	1243	G	C8-N9-C4	5.80	108.72	106.40
1	A	2497	A	C5-C6-N6	-5.80	119.06	123.70
1	A	656	G	C8-N9-C4	5.80	108.72	106.40
1	A	2413	G	C2-N3-C4	-5.80	109.00	111.90
1	A	391	G	C4-C5-N7	5.80	113.12	110.80
1	A	1200	C	C5-C6-N1	-5.79	118.10	121.00
1	A	644	A	N1-C6-N6	-5.79	115.13	118.60
1	A	2077	A	C2-N3-C4	5.79	113.50	110.60
1	A	2672	G	N1-C6-O6	5.79	123.37	119.90
1	A	792	G	C8-N9-C1'	-5.79	119.48	127.00
1	A	2323	G	C4-C5-N7	5.79	113.11	110.80
1	A	2395	C	C6-N1-C2	5.79	122.61	120.30
1	A	179	G	N3-C4-C5	5.78	131.49	128.60
1	A	825	C	C5-C4-N4	-5.78	116.15	120.20
1	A	2221	G	C5-C6-O6	-5.78	125.13	128.60
1	A	129	C	C5-C6-N1	-5.78	118.11	121.00
1	A	774	A	N7-C8-N9	5.78	116.69	113.80
1	A	2745	C	N1-C2-O2	5.78	122.37	118.90
1	A	39	C	C4-C5-C6	5.78	120.29	117.40
1	A	1381	G	C4-C5-N7	-5.78	108.49	110.80
1	A	2288	A	C8-N9-C4	-5.77	103.49	105.80
1	A	2517	C	C2-N3-C4	-5.77	117.01	119.90
2	B	27	C	N1-C2-O2	5.77	122.36	118.90
1	A	1914	C	C6-N1-C1'	5.77	127.73	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1994	C	N3-C4-N4	-5.77	113.96	118.00
1	A	2224	G	C4-C5-N7	5.77	113.11	110.80
2	B	33	G	N9-C4-C5	-5.77	103.09	105.40
1	A	327	G	C6-C5-N7	-5.77	126.94	130.40
1	A	775	G	N1-C6-O6	-5.77	116.44	119.90
1	A	1544	A	C8-N9-C4	-5.77	103.49	105.80
1	A	1208	C	C5-C4-N4	-5.77	116.16	120.20
1	A	2254	C	C6-N1-C2	5.77	122.61	120.30
1	A	208	C	C6-N1-C2	5.76	122.61	120.30
1	A	794	G	N1-C2-N2	-5.76	111.01	116.20
1	A	1304	C	C2-N3-C4	-5.76	117.02	119.90
1	A	2705	A	C2-N3-C4	-5.76	107.72	110.60
1	A	2444	G	N1-C6-O6	-5.76	116.44	119.90
1	A	1038	C	N3-C2-O2	-5.76	117.87	121.90
1	A	1261	C	N3-C4-C5	5.75	124.20	121.90
1	A	1695	G	C6-C5-N7	-5.75	126.95	130.40
1	A	2490	G	N1-C6-O6	5.75	123.35	119.90
1	A	2306	C	N1-C2-O2	5.75	122.35	118.90
1	A	2587	A	C4-C5-C6	5.75	119.88	117.00
1	A	2171	A	N1-C6-N6	5.75	122.05	118.60
1	A	1760	A	N9-C4-C5	5.75	108.10	105.80
1	A	2597	G	C8-N9-C1'	-5.75	119.53	127.00
1	A	2616	C	N3-C2-O2	-5.75	117.88	121.90
1	A	2525	G	C4-C5-N7	5.75	113.10	110.80
1	A	243	U	N3-C2-O2	-5.75	118.18	122.20
1	A	1930	G	C8-N9-C4	5.74	108.70	106.40
1	A	265	A	C5-C6-N1	-5.74	114.83	117.70
1	A	2506	U	N3-C2-O2	-5.74	118.18	122.20
1	A	1996	C	C6-N1-C2	5.74	122.59	120.30
1	A	2306	C	C6-N1-C1'	-5.74	113.92	120.80
1	A	216	A	C8-N9-C4	5.74	108.09	105.80
1	A	1005	C	C5-C6-N1	-5.74	118.13	121.00
1	A	968	G	C8-N9-C4	5.73	108.69	106.40
1	A	1989	G	C6-C5-N7	-5.73	126.96	130.40
1	A	2376	A	N1-C6-N6	5.73	122.04	118.60
1	A	2517	C	N3-C4-C5	5.73	124.19	121.90
1	A	1320	C	N3-C4-N4	5.73	122.01	118.00
1	A	1428	C	C2-N3-C4	-5.73	117.03	119.90
1	A	1637	A	N1-C6-N6	-5.73	115.16	118.60
1	A	2310	A	N1-C6-N6	5.73	122.04	118.60
5	F	45	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	A	2146	C	N3-C2-O2	-5.73	117.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1313	U	N3-C4-C5	-5.72	111.17	114.60
1	A	1380	G	C2-N3-C4	-5.72	109.04	111.90
1	A	1471	A	N1-C2-N3	5.72	132.16	129.30
1	A	51	G	C4-C5-N7	-5.72	108.51	110.80
1	A	695	G	N1-C6-O6	-5.72	116.47	119.90
1	A	2096	U	C6-N1-C2	-5.72	117.57	121.00
1	A	1222	C	C6-N1-C2	5.72	122.59	120.30
1	A	2681	C	N3-C2-O2	-5.72	117.90	121.90
1	A	728	G	C5-N7-C8	5.72	107.16	104.30
1	A	1210	A	C6-C5-N7	-5.71	128.30	132.30
1	A	1891	G	C2-N3-C4	-5.71	109.04	111.90
1	A	2286	A	C5-N7-C8	-5.71	101.04	103.90
1	A	986	C	N3-C2-O2	-5.71	117.91	121.90
1	A	1999	C	C5-C6-N1	-5.71	118.15	121.00
1	A	2023	G	N1-C6-O6	5.71	123.32	119.90
1	A	988	A	C6-C5-N7	-5.70	128.31	132.30
1	A	1648	C	N3-C2-O2	-5.70	117.91	121.90
1	A	47	C	C5-C6-N1	-5.70	118.15	121.00
1	A	1898	U	C5-C4-O4	5.70	129.32	125.90
1	A	1284	A	C4-C5-N7	5.70	113.55	110.70
1	A	2421	G	C4-C5-N7	5.70	113.08	110.80
1	A	141	A	C2-N3-C4	-5.70	107.75	110.60
1	A	733	G	N3-C2-N2	5.70	123.89	119.90
1	A	1394	U	N3-C2-O2	-5.69	118.21	122.20
1	A	1843	C	C6-N1-C2	5.69	122.58	120.30
1	A	1319	G	C8-N9-C1'	-5.69	119.60	127.00
1	A	1926	U	N3-C2-O2	-5.69	118.22	122.20
1	A	2300	G	N3-C4-C5	-5.69	125.75	128.60
1	A	945	A	C1'-O4'-C4'	-5.69	105.35	109.90
1	A	1990	C	N1-C2-O2	-5.69	115.49	118.90
1	A	2708	G	C5-C6-O6	5.69	132.01	128.60
1	A	1554	A	N1-C6-N6	5.69	122.01	118.60
1	A	509	C	N3-C2-O2	-5.68	117.92	121.90
1	A	932	G	C4-N9-C1'	-5.68	119.11	126.50
1	A	961	C	C5-C4-N4	-5.68	116.22	120.20
1	A	1464	C	C6-N1-C2	-5.68	118.03	120.30
1	A	751	A	C5-N7-C8	5.68	106.74	103.90
1	A	1340	U	C6-N1-C2	5.68	124.41	121.00
1	A	1659	U	C2-N3-C4	-5.68	123.59	127.00
1	A	2444	G	C4-C5-N7	-5.68	108.53	110.80
2	B	9	G	C5-C6-O6	-5.68	125.19	128.60
1	A	2100	G	C6-C5-N7	-5.68	126.99	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2287	A	C2-N3-C4	-5.68	107.76	110.60
2	B	115	G	C2-N3-C4	-5.68	109.06	111.90
1	A	2596	U	N1-C2-O2	-5.68	118.83	122.80
1	A	208	C	N3-C2-O2	5.67	125.87	121.90
1	A	1565	C	C2-N1-C1'	-5.67	112.56	118.80
1	A	2181	G	N3-C4-N9	-5.67	122.59	126.00
1	A	2287	A	N9-C4-C5	-5.67	103.53	105.80
1	A	449	A	N7-C8-N9	5.67	116.64	113.80
1	A	2100	G	C8-N9-C1'	-5.67	119.63	127.00
1	A	2100	G	C5-C6-O6	-5.67	125.20	128.60
1	A	2826	A	N1-C6-N6	-5.66	115.20	118.60
1	A	1325	G	N3-C4-N9	5.66	129.40	126.00
1	A	1191	G	N9-C4-C5	-5.66	103.14	105.40
1	A	509	C	C2-N3-C4	-5.66	117.07	119.90
1	A	1635	G	C6-C5-N7	-5.66	127.00	130.40
1	A	2318	G	N7-C8-N9	5.66	115.93	113.10
1	A	1645	G	N1-C2-N3	5.66	127.29	123.90
1	A	645	C	N3-C2-O2	-5.66	117.94	121.90
1	A	926	A	C5-C6-N6	-5.66	119.18	123.70
1	A	1359	A	N9-C4-C5	5.66	108.06	105.80
1	A	2861	G	C8-N9-C4	-5.66	104.14	106.40
1	A	2052	G	N3-C2-N2	-5.65	115.94	119.90
1	A	60	G	N9-C4-C5	-5.65	103.14	105.40
1	A	2189	U	N3-C2-O2	-5.65	118.25	122.20
4	E	119	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	1685	C	C5-C4-N4	-5.65	116.25	120.20
1	A	53	A	C2-N3-C4	-5.64	107.78	110.60
1	A	692	C	N3-C4-C5	5.64	124.16	121.90
1	A	308	G	C4-N9-C1'	5.64	133.83	126.50
1	A	1315	C	N3-C2-O2	-5.64	117.95	121.90
1	A	141	A	C8-N9-C4	-5.64	103.55	105.80
1	A	271(S)	G	C6-C5-N7	-5.64	127.02	130.40
1	A	1374	G	N7-C8-N9	5.64	115.92	113.10
1	A	2516	G	N9-C4-C5	5.64	107.66	105.40
1	A	787	U	N3-C4-O4	-5.63	115.46	119.40
1	A	2581	G	N1-C6-O6	-5.63	116.52	119.90
1	A	195	A	C4-C5-C6	5.63	119.81	117.00
1	A	2049	G	N3-C4-N9	-5.63	122.62	126.00
1	A	122	G	C4-C5-N7	5.63	113.05	110.80
2	B	99	G	N1-C6-O6	5.63	123.28	119.90
1	A	2785	C	C6-N1-C2	-5.62	118.05	120.30
1	A	816	C	C5-C4-N4	-5.62	116.26	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	C	C6-N1-C2	5.62	122.55	120.30
1	A	2087	G	N3-C4-C5	5.62	131.41	128.60
1	A	2510	C	N3-C2-O2	-5.62	117.96	121.90
1	A	251	A	C5-C6-N1	-5.62	114.89	117.70
1	A	255	A	C5-N7-C8	-5.62	101.09	103.90
1	A	1823	G	N3-C4-C5	5.62	131.41	128.60
1	A	2297	C	C6-N1-C1'	5.62	127.54	120.80
1	A	250	G	N1-C6-O6	5.62	123.27	119.90
1	A	821	A	C4-C5-C6	5.62	119.81	117.00
1	A	2351	G	N3-C4-N9	5.62	129.37	126.00
1	A	188	G	C6-C5-N7	-5.62	127.03	130.40
1	A	940	G	C5-C6-O6	-5.62	125.23	128.60
1	A	2286	A	C4-C5-N7	5.61	113.51	110.70
1	A	936	C	N1-C2-O2	-5.61	115.53	118.90
1	A	2125	G	C8-N9-C4	-5.61	104.16	106.40
1	A	2707	G	C4-C5-N7	5.61	113.05	110.80
1	A	229	A	C8-N9-C4	-5.61	103.56	105.80
1	A	582	G	C8-N9-C4	5.61	108.64	106.40
1	A	739	G	C5-N7-C8	5.61	107.10	104.30
1	A	1619	G	C4-C5-C6	-5.61	115.44	118.80
1	A	194	G	N3-C2-N2	-5.61	115.97	119.90
1	A	786	C	N3-C4-N4	-5.61	114.08	118.00
1	A	1968	G	N3-C2-N2	-5.61	115.98	119.90
1	A	311	A	N1-C6-N6	5.60	121.96	118.60
1	A	1207	C	N3-C2-O2	5.60	125.82	121.90
1	A	2260	C	C5-C6-N1	-5.60	118.20	121.00
1	A	2709	G	C4-C5-N7	5.60	113.04	110.80
1	A	188	G	N9-C4-C5	-5.60	103.16	105.40
1	A	1261	C	C2-N3-C4	-5.60	117.10	119.90
1	A	526	A	N1-C6-N6	-5.60	115.24	118.60
1	A	2395	C	N3-C4-C5	5.59	124.14	121.90
1	A	2452	C	N3-C4-N4	5.59	121.92	118.00
1	A	2746	U	N3-C4-O4	-5.59	115.48	119.40
1	A	130	C	C5-C6-N1	-5.59	118.20	121.00
1	A	988	A	C4-C5-N7	5.59	113.50	110.70
1	A	2000	G	C2-N3-C4	-5.59	109.10	111.90
1	A	975	C	N3-C2-O2	-5.59	117.99	121.90
1	A	2296	U	C6-N1-C2	5.59	124.35	121.00
1	A	1808	U	N1-C2-N3	-5.59	111.55	114.90
1	A	2021	C	C5-C6-N1	-5.59	118.21	121.00
1	A	2828	C	C5-C6-N1	-5.59	118.21	121.00
1	A	205	G	N1-C6-O6	5.59	123.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1373	A	C5-N7-C8	5.59	106.69	103.90
1	A	1155	A	N1-C6-N6	5.58	121.95	118.60
1	A	2148	G	C6-C5-N7	5.58	133.75	130.40
1	A	403	U	C5-C6-N1	-5.58	119.91	122.70
1	A	961	C	N3-C4-N4	5.58	121.91	118.00
1	A	2075	U	N1-C2-O2	-5.58	118.89	122.80
1	A	777	A	C8-N9-C4	-5.58	103.57	105.80
1	A	1617	C	C6-N1-C2	5.58	122.53	120.30
1	A	2245	U	N1-C2-O2	-5.58	118.89	122.80
1	A	1539	G	N7-C8-N9	5.58	115.89	113.10
1	A	2026	C	N3-C2-O2	5.58	125.80	121.90
1	A	143	G	C4-N9-C1'	-5.57	119.26	126.50
1	A	2424	C	C4-C5-C6	5.57	120.19	117.40
1	A	2439	A	C5-C6-N1	-5.57	114.91	117.70
1	A	205	G	N3-C4-N9	5.57	129.34	126.00
1	A	1125	G	C4-N9-C1'	5.57	133.74	126.50
1	A	713	G	N1-C6-O6	5.57	123.24	119.90
1	A	1022	G	C6-C5-N7	5.57	133.74	130.40
1	A	1116	C	C6-N1-C2	5.57	122.53	120.30
1	A	1819	A	N1-C6-N6	-5.57	115.26	118.60
1	A	2129	C	C5-C4-N4	5.57	124.10	120.20
3	D	131	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	A	704	G	C5-C6-O6	-5.57	125.26	128.60
1	A	848	G	N3-C4-N9	5.57	129.34	126.00
1	A	733	G	N1-C2-N2	-5.57	111.19	116.20
1	A	1616	A	C5-C6-N6	-5.57	119.25	123.70
1	A	2607	G	N3-C4-N9	5.56	129.34	126.00
1	A	1137	G	N3-C2-N2	-5.56	116.01	119.90
1	A	1940	U	N3-C4-O4	5.56	123.29	119.40
1	A	2259	G	C5-C6-N1	-5.56	108.72	111.50
1	A	2505	G	N3-C4-C5	5.56	131.38	128.60
1	A	2070	G	N1-C6-O6	-5.56	116.56	119.90
1	A	440	G	C5-C6-O6	5.56	131.94	128.60
1	A	2034	U	C5-C6-N1	-5.56	119.92	122.70
1	A	2321	G	C5-C6-O6	5.56	131.93	128.60
1	A	2363	C	C5-C6-N1	-5.56	118.22	121.00
2	B	113	G	C8-N9-C4	5.56	108.62	106.40
1	A	1645	G	N9-C4-C5	5.55	107.62	105.40
1	A	1779	U	C2-N1-C1'	5.55	124.36	117.70
1	A	2447	G	N9-C4-C5	-5.55	103.18	105.40
1	A	171	G	C6-N1-C2	5.55	128.43	125.10
1	A	1001	A	N7-C8-N9	-5.55	111.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2872	G	N1-C6-O6	5.55	123.23	119.90
1	A	190	A	C2-N3-C4	-5.55	107.83	110.60
1	A	665	C	C4-C5-C6	-5.55	114.63	117.40
1	A	822	U	C5-C4-O4	5.55	129.23	125.90
1	A	1041	C	C6-N1-C2	-5.55	118.08	120.30
1	A	1965	C	N1-C2-O2	5.55	122.23	118.90
1	A	1988	C	C5-C4-N4	-5.54	116.32	120.20
1	A	530	G	C8-N9-C1'	5.54	134.20	127.00
1	A	1670	C	C5-C4-N4	5.54	124.08	120.20
1	A	1677	A	N1-C6-N6	5.54	121.92	118.60
1	A	2292	C	C6-N1-C2	5.54	122.52	120.30
1	A	41	C	C2-N3-C4	-5.54	117.13	119.90
1	A	956	G	C4-C5-N7	-5.54	108.58	110.80
1	A	1315	C	N1-C2-N3	5.54	123.08	119.20
1	A	2056	G	C6-C5-N7	-5.54	127.08	130.40
1	A	2504	U	C6-N1-C2	5.54	124.32	121.00
1	A	383	U	C4-C5-C6	5.54	123.02	119.70
1	A	693	C	N3-C4-C5	5.54	124.11	121.90
1	A	85	G	C8-N9-C4	5.54	108.61	106.40
1	A	756	C	C4-C5-C6	5.54	120.17	117.40
1	A	2048	G	N7-C8-N9	5.54	115.87	113.10
1	A	2287	A	C8-N9-C4	5.54	108.01	105.80
1	A	2819	G	C8-N9-C4	5.54	108.61	106.40
1	A	115	C	N1-C2-O2	-5.53	115.58	118.90
1	A	2304	G	C6-C5-N7	5.53	133.72	130.40
1	A	2615	U	C4-C5-C6	-5.53	116.38	119.70
1	A	1193	G	C8-N9-C4	5.53	108.61	106.40
1	A	570	G	N3-C2-N2	5.53	123.77	119.90
1	A	742	G	N1-C2-N2	-5.53	111.22	116.20
1	A	856	C	C3'-C2'-C1'	-5.53	97.08	101.50
1	A	2775	A	C6-N1-C2	5.53	121.92	118.60
1	A	2870	C	C2-N3-C4	-5.53	117.14	119.90
1	A	508	G	N9-C4-C5	-5.52	103.19	105.40
1	A	292	C	C6-N1-C2	5.52	122.51	120.30
1	A	803	U	C5-C6-N1	-5.52	119.94	122.70
1	A	1021	A	N3-C4-C5	5.52	130.66	126.80
1	A	2026	C	N3-C4-C5	-5.52	119.69	121.90
1	A	252	G	C8-N9-C4	5.52	108.61	106.40
1	A	2126	A	C2-N3-C4	-5.52	107.84	110.60
1	A	2293	C	N3-C4-C5	5.52	124.11	121.90
1	A	2510	C	C5-C6-N1	-5.52	118.24	121.00
1	A	441	U	C5-C4-O4	-5.52	122.59	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1125	G	C8-N9-C1'	-5.52	119.83	127.00
1	A	1918	A	C8-N9-C4	5.52	108.01	105.80
1	A	1328	G	N9-C4-C5	-5.52	103.19	105.40
1	A	775	G	N3-C2-N2	5.51	123.76	119.90
1	A	1452	A	C2-N3-C4	-5.51	107.84	110.60
1	A	308	G	N7-C8-N9	5.51	115.86	113.10
1	A	1890	A	C8-N9-C4	5.51	108.00	105.80
1	A	1896	G	C5-C6-O6	-5.51	125.29	128.60
19	X	57	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	1990	C	C2-N3-C4	-5.51	117.15	119.90
1	A	2162	G	N3-C4-C5	-5.51	125.85	128.60
1	A	2326	C	N3-C4-C5	-5.50	119.70	121.90
1	A	2522	U	C2-N1-C1'	5.50	124.31	117.70
1	A	1340	U	C5-C4-O4	-5.50	122.60	125.90
1	A	1790	C	N3-C2-O2	5.50	125.75	121.90
1	A	833	U	N3-C4-C5	-5.50	111.30	114.60
1	A	1821	A	C5-C6-N1	5.50	120.45	117.70
1	A	514	A	C6-N1-C2	-5.50	115.30	118.60
1	A	1459	G	N3-C4-C5	-5.50	125.85	128.60
1	A	2354	G	N7-C8-N9	5.50	115.85	113.10
1	A	2447	G	C8-N9-C4	5.50	108.60	106.40
1	A	2709	G	N1-C6-O6	5.50	123.20	119.90
28	6	13	CYS	CA-CB-SG	5.50	123.89	114.00
1	A	732	C	C6-N1-C2	5.49	122.50	120.30
1	A	1192	G	N7-C8-N9	-5.49	110.36	113.10
1	A	1219	G	N1-C6-O6	5.49	123.19	119.90
1	A	33	U	C2-N1-C1'	-5.49	111.11	117.70
1	A	2447	G	C4-C5-N7	5.49	113.00	110.80
1	A	1193	G	N1-C6-O6	5.49	123.19	119.90
1	A	529	A	C4-C5-N7	5.49	113.44	110.70
1	A	952	G	C5-C6-N1	5.49	114.24	111.50
1	A	1211	U	C6-N1-C2	5.49	124.29	121.00
1	A	2007	C	N3-C4-C5	-5.49	119.71	121.90
1	A	2443	C	N1-C2-O2	-5.49	115.61	118.90
1	A	1247	A	C8-N9-C4	5.48	107.99	105.80
1	A	205	G	C6-C5-N7	-5.48	127.11	130.40
1	A	932	G	C4-C5-N7	-5.48	108.61	110.80
1	A	1202	C	C5-C6-N1	-5.48	118.26	121.00
1	A	2485	G	C4-C5-N7	5.48	112.99	110.80
1	A	1038	C	N1-C2-O2	5.47	122.18	118.90
1	A	449	A	N1-C6-N6	5.47	121.88	118.60
1	A	2723	C	C6-N1-C2	5.47	122.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1403	C	C6-N1-C1'	5.47	127.36	120.80
1	A	2558	C	C5-C6-N1	-5.47	118.26	121.00
1	A	1006	C	C5-C4-N4	5.47	124.03	120.20
1	A	657	U	C5-C4-O4	5.47	129.18	125.90
1	A	1763	G	N3-C4-C5	5.47	131.33	128.60
1	A	2817	G	N1-C6-O6	5.46	123.18	119.90
1	A	2294	C	N3-C4-C5	5.46	124.08	121.90
1	A	2711	A	C8-N9-C4	5.46	107.98	105.80
1	A	945	A	C6-C5-N7	-5.46	128.48	132.30
1	A	2055	C	C6-N1-C2	5.46	122.48	120.30
1	A	127	A	C2-N3-C4	-5.46	107.87	110.60
1	A	413	C	N3-C2-O2	5.46	125.72	121.90
1	A	1807	G	C8-N9-C4	5.46	108.58	106.40
1	A	2857	G	N1-C6-O6	5.46	123.17	119.90
1	A	124	G	C2-N3-C4	-5.45	109.17	111.90
1	A	1983	C	C2-N3-C4	-5.45	117.17	119.90
1	A	512	G	O4'-C1'-N9	5.45	112.56	108.20
1	A	2641	G	C8-N9-C1'	-5.45	119.91	127.00
1	A	662	G	N3-C4-C5	-5.45	125.88	128.60
1	A	1199	U	N1-C2-N3	5.45	118.17	114.90
1	A	351	G	C8-N9-C4	5.45	108.58	106.40
1	A	1609	A	C8-N9-C4	5.45	107.98	105.80
1	A	2032	G	C5-C6-O6	-5.45	125.33	128.60
1	A	2587	A	C2-N3-C4	-5.45	107.88	110.60
1	A	512	G	C5-C6-O6	5.44	131.87	128.60
1	A	2435	A	C4-C5-N7	5.44	113.42	110.70
1	A	623	G	C5-C6-O6	-5.44	125.33	128.60
1	A	1276	A	N9-C4-C5	-5.44	103.62	105.80
1	A	308	G	C6-C5-N7	-5.44	127.14	130.40
1	A	676	A	N1-C6-N6	5.44	121.86	118.60
1	A	915	C	C2-N1-C1'	5.44	124.78	118.80
1	A	1428	C	C5-C6-N1	-5.44	118.28	121.00
1	A	1938	A	N1-C2-N3	5.44	132.02	129.30
1	A	2149	G	N1-C2-N2	5.44	121.09	116.20
1	A	1377	G	C2-N3-C4	5.44	114.62	111.90
1	A	53	A	N1-C2-N3	5.44	132.02	129.30
1	A	624	C	C6-N1-C2	5.43	122.47	120.30
1	A	1112	G	N3-C4-N9	-5.43	122.74	126.00
1	A	1123	C	C2-N1-C1'	-5.43	112.83	118.80
1	A	265	A	C4-N9-C1'	5.43	136.07	126.30
1	A	546	C	C2-N1-C1'	5.43	124.77	118.80
1	A	1371	G	C6-C5-N7	-5.43	127.14	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1432	C	C6-N1-C2	5.43	122.47	120.30
1	A	2434	A	C8-N9-C4	5.43	107.97	105.80
1	A	263	C	N3-C2-O2	-5.43	118.10	121.90
1	A	1021	A	C8-N9-C4	-5.43	103.63	105.80
1	A	2338	G	N9-C4-C5	-5.42	103.23	105.40
1	A	652(R)	C	C5-C6-N1	5.42	123.71	121.00
1	A	1566	A	C2-N3-C4	-5.42	107.89	110.60
1	A	1995	U	N1-C2-N3	5.42	118.15	114.90
1	A	2728	U	C5-C6-N1	-5.42	119.99	122.70
1	A	768	G	C6-C5-N7	-5.42	127.15	130.40
1	A	529	A	N3-C4-C5	5.42	130.59	126.80
1	A	1266	G	N3-C2-N2	5.42	123.69	119.90
1	A	2444	G	C5-C6-O6	5.42	131.85	128.60
1	A	1238	G	C8-N9-C4	5.41	108.56	106.40
1	A	2491	U	C6-N1-C2	5.41	124.25	121.00
1	A	1026	U	N3-C2-O2	-5.41	118.41	122.20
1	A	1996	C	N3-C4-N4	-5.41	114.21	118.00
2	B	70	C	C6-N1-C2	-5.41	118.14	120.30
1	A	505	A	C2-N3-C4	-5.41	107.90	110.60
1	A	614(B)	G	C6-C5-N7	5.41	133.65	130.40
1	A	2283	C	N3-C2-O2	5.41	125.69	121.90
1	A	1688	U	N1-C2-O2	-5.41	119.02	122.80
1	A	2375	G	C2-N3-C4	-5.41	109.20	111.90
1	A	2393	A	N7-C8-N9	5.40	116.50	113.80
1	A	2731	G	C5-C6-O6	-5.40	125.36	128.60
1	A	1022	G	C4-N9-C1'	-5.40	119.48	126.50
1	A	268	C	N3-C4-N4	5.40	121.78	118.00
1	A	446	G	N7-C8-N9	-5.40	110.40	113.10
1	A	40	C	C6-N1-C2	5.40	122.46	120.30
1	A	1006	C	C6-N1-C1'	5.40	127.28	120.80
1	A	1530	C	C5-C4-N4	-5.40	116.42	120.20
1	A	2151	G	N1-C2-N2	5.40	121.06	116.20
1	A	383	U	N3-C4-C5	-5.39	111.36	114.60
1	A	2515	C	C5-C4-N4	-5.39	116.42	120.20
2	B	55	U	C6-N1-C2	-5.39	117.76	121.00
1	A	1941	C	N1-C2-O2	-5.39	115.67	118.90
1	A	62	C	N3-C4-C5	5.39	124.06	121.90
1	A	826	U	C4-C5-C6	5.39	122.93	119.70
1	A	2547	U	C6-N1-C2	5.39	124.23	121.00
1	A	348	G	C8-N9-C4	5.39	108.56	106.40
1	A	2027	G	N1-C2-N3	5.39	127.13	123.90
1	A	2272	U	N3-C2-O2	-5.39	118.43	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	148	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	261	G	N1-C6-O6	5.39	123.13	119.90
1	A	565	C	C4-C5-C6	5.39	120.09	117.40
1	A	2330	G	C8-N9-C4	5.39	108.55	106.40
1	A	530	G	C5-N7-C8	-5.38	101.61	104.30
1	A	1031	G	C2-N3-C4	-5.38	109.21	111.90
1	A	2515	C	C6-N1-C2	5.38	122.45	120.30
1	A	2676	C	N3-C4-C5	5.38	124.05	121.90
1	A	446	G	C5-N7-C8	5.38	106.99	104.30
1	A	312	G	C5-C6-O6	-5.38	125.37	128.60
1	A	60	G	N1-C6-O6	5.38	123.13	119.90
1	A	1377	G	C6-N1-C2	-5.38	121.87	125.10
1	A	2027	G	C6-N1-C2	-5.38	121.87	125.10
1	A	585	G	C8-N9-C4	5.38	108.55	106.40
1	A	1653	G	P-O3'-C3'	5.38	126.15	119.70
1	A	1654	A	C5-C6-N6	5.38	128.00	123.70
1	A	1912	A	N7-C8-N9	5.38	116.49	113.80
1	A	2297	C	N1-C2-O2	-5.37	115.68	118.90
1	A	600	G	N1-C6-O6	5.37	123.12	119.90
1	A	1658	C	C5-C6-N1	5.37	123.69	121.00
1	A	682	G	N3-C4-N9	5.37	129.22	126.00
1	A	1785	A	C6-C5-N7	-5.37	128.54	132.30
1	A	1220	A	C8-N9-C4	5.37	107.95	105.80
1	A	2312	U	N1-C2-O2	5.37	126.56	122.80
1	A	743	G	C5-C6-N1	5.36	114.18	111.50
1	A	1381	G	C5-C6-O6	5.36	131.82	128.60
1	A	2296	U	C3'-C2'-C1'	-5.36	97.21	101.50
1	A	2455	G	C4-N9-C1'	5.36	133.47	126.50
1	A	94	C	N3-C2-O2	-5.36	118.15	121.90
1	A	791	C	C2-N3-C4	-5.36	117.22	119.90
1	A	2300	G	C5-C6-O6	-5.36	125.38	128.60
1	A	2878	U	N3-C2-O2	-5.36	118.45	122.20
1	A	2442	C	N1-C2-O2	-5.36	115.69	118.90
1	A	546	C	C5-C6-N1	5.36	123.68	121.00
1	A	1994	C	C5-C4-N4	5.36	123.95	120.20
1	A	236	C	C6-N1-C2	5.35	122.44	120.30
1	A	652(S)	C	C5-C6-N1	5.35	123.68	121.00
1	A	1299	G	N7-C8-N9	5.35	115.78	113.10
1	A	2056	G	C2-N3-C4	-5.35	109.22	111.90
1	A	2447	G	N3-C4-C5	5.35	131.28	128.60
1	A	339	U	C6-N1-C2	5.35	124.21	121.00
1	A	2681	C	N1-C2-N3	5.35	122.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2099	U	C2-N1-C1'	5.35	124.12	117.70
1	A	2505	G	C2-N3-C4	-5.35	109.23	111.90
1	A	1283	G	N3-C4-C5	-5.35	125.93	128.60
1	A	2266	A	C4-C5-N7	5.35	113.37	110.70
2	B	64	C	C2-N1-C1'	-5.35	112.92	118.80
1	A	2849	U	C2-N3-C4	-5.35	123.79	127.00
1	A	1899	G	N3-C2-N2	-5.34	116.16	119.90
1	A	2363	C	C2-N1-C1'	-5.34	112.92	118.80
1	A	2396	G	C5-N7-C8	-5.34	101.63	104.30
1	A	2689	U	N1-C2-N3	5.34	118.11	114.90
26	4	42	PHE	C-N-CA	5.34	135.06	121.70
1	A	574	C	N3-C4-N4	-5.34	114.26	118.00
1	A	1645	G	C5-C6-O6	5.34	131.81	128.60
1	A	252	G	N7-C8-N9	-5.34	110.43	113.10
1	A	1777	U	C6-N1-C2	5.34	124.20	121.00
1	A	1359	A	C5-C6-N6	5.34	127.97	123.70
1	A	924	C	C2-N3-C4	-5.33	117.23	119.90
1	A	60	G	C5-C6-O6	-5.33	125.40	128.60
1	A	558	G	C8-N9-C4	5.33	108.53	106.40
1	A	71	A	C6-C5-N7	-5.33	128.57	132.30
1	A	271(A)	A	C8-N9-C4	5.33	107.93	105.80
1	A	1129	A	N1-C6-N6	-5.33	115.40	118.60
1	A	2224	G	C2-N3-C4	-5.33	109.23	111.90
1	A	2638	G	C5-C6-N1	-5.33	108.83	111.50
1	A	956	G	C5-N7-C8	5.33	106.97	104.30
1	A	2708	G	N1-C2-N3	5.33	127.10	123.90
1	A	818	G	N7-C8-N9	-5.32	110.44	113.10
1	A	1142(A)	A	C6-C5-N7	-5.32	128.57	132.30
1	A	1639	U	N3-C2-O2	-5.32	118.47	122.20
1	A	2028	U	C5-C4-O4	-5.32	122.71	125.90
1	A	2157	G	N9-C4-C5	5.32	107.53	105.40
1	A	2379	G	C8-N9-C4	-5.32	104.27	106.40
1	A	1380	G	N3-C2-N2	-5.32	116.17	119.90
1	A	509	C	C5-C6-N1	-5.32	118.34	121.00
1	A	1265	A	C4-C5-C6	5.32	119.66	117.00
1	A	1380	G	N3-C4-C5	5.32	131.26	128.60
1	A	599	G	C2-N3-C4	-5.32	109.24	111.90
1	A	1829	A	N7-C8-N9	-5.32	111.14	113.80
1	A	2699	C	N3-C4-C5	5.32	124.03	121.90
1	A	2744	G	C2-N3-C4	-5.32	109.24	111.90
1	A	2237	G	C8-N9-C4	5.31	108.53	106.40
1	A	1284	A	C5-N7-C8	-5.31	101.24	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2015	A	C5-C6-N6	5.31	127.95	123.70
2	B	104	U	C2-N1-C1'	-5.31	111.33	117.70
1	A	1181	C	N1-C2-O2	5.31	122.08	118.90
1	A	2622	C	N3-C4-C5	5.31	124.02	121.90
1	A	464	U	C5-C4-O4	5.31	129.08	125.90
1	A	1612	C	N3-C4-N4	5.31	121.72	118.00
1	A	2615	U	N1-C2-O2	5.31	126.52	122.80
1	A	2761	G	C8-N9-C4	-5.31	104.28	106.40
1	A	2547	U	C5-C6-N1	-5.31	120.05	122.70
1	A	2675	A	C5-C6-N6	-5.31	119.46	123.70
1	A	614(B)	G	C4-N9-C1'	-5.30	119.60	126.50
1	A	2059	A	C2-N3-C4	-5.30	107.95	110.60
1	A	2787	C	N3-C2-O2	-5.30	118.19	121.90
1	A	2082	A	N1-C6-N6	5.30	121.78	118.60
1	A	463	G	N3-C4-N9	-5.30	122.82	126.00
1	A	796	C	C2-N3-C4	-5.30	117.25	119.90
1	A	1216	G	N3-C4-N9	5.30	129.18	126.00
1	A	1881	C	C5-C6-N1	5.30	123.65	121.00
1	A	1452	A	C8-N9-C4	5.30	107.92	105.80
1	A	2334	G	C8-N9-C4	5.30	108.52	106.40
1	A	448	U	N3-C4-C5	-5.29	111.42	114.60
1	A	723	G	N9-C4-C5	-5.29	103.28	105.40
1	A	564	C	C5-C6-N1	-5.29	118.36	121.00
4	E	119	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	530	G	C8-N9-C4	-5.29	104.28	106.40
1	A	1581	G	C4-N9-C1'	5.29	133.38	126.50
2	B	30	C	N3-C4-N4	5.29	121.70	118.00
1	A	401	A	N1-C2-N3	5.29	131.94	129.30
1	A	874	G	N3-C4-C5	5.29	131.24	128.60
23	1	40	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	1692	U	C5-C6-N1	-5.28	120.06	122.70
1	A	1826	G	N1-C6-O6	-5.28	116.73	119.90
1	A	2182	G	C4-C5-N7	-5.28	108.69	110.80
1	A	602	G	C8-N9-C4	5.28	108.51	106.40
1	A	171	G	N3-C2-N2	5.28	123.60	119.90
1	A	1612	C	N3-C2-O2	5.28	125.60	121.90
1	A	2822	G	N1-C6-O6	5.28	123.07	119.90
1	A	1124	C	N3-C4-C5	5.28	124.01	121.90
1	A	2359	C	C4-C5-C6	5.28	120.04	117.40
1	A	737	C	C5-C4-N4	-5.28	116.50	120.20
1	A	2235	G	C6-C5-N7	-5.28	127.23	130.40
1	A	2379	G	C5-N7-C8	-5.28	101.66	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	A	N1-C2-N3	5.28	131.94	129.30
1	A	204	A	C5-N7-C8	-5.28	101.26	103.90
1	A	1120	G	C5-C6-O6	5.28	131.76	128.60
1	A	1210	A	N7-C8-N9	5.28	116.44	113.80
1	A	1800	C	N3-C4-C5	5.28	124.01	121.90
1	A	2297	C	C2-N1-C1'	-5.28	113.00	118.80
1	A	652(T)	C	C5-C4-N4	5.27	123.89	120.20
1	A	932	G	N3-C4-C5	5.27	131.24	128.60
1	A	1993	U	N3-C2-O2	5.27	125.89	122.20
1	A	2346	A	N3-C4-C5	-5.27	123.11	126.80
2	B	93	G	C5-C6-O6	-5.27	125.44	128.60
1	A	208	C	N1-C2-O2	-5.27	115.74	118.90
1	A	195	A	C6-C5-N7	-5.27	128.61	132.30
1	A	333	G	C4-N9-C1'	5.27	133.35	126.50
1	A	2866	U	C4-C5-C6	5.27	122.86	119.70
1	A	570	G	N1-C2-N2	-5.27	111.46	116.20
1	A	2487	G	C4-C5-N7	5.26	112.91	110.80
1	A	727	A	C4-C5-C6	5.26	119.63	117.00
1	A	732	C	C5-C4-N4	-5.26	116.52	120.20
1	A	1256	G	C2-N3-C4	-5.26	109.27	111.90
9	N	20	GLY	N-CA-C	-5.26	99.94	113.10
1	A	1816	G	C8-N9-C1'	-5.26	120.16	127.00
1	A	1992	G	C5-N7-C8	5.26	106.93	104.30
1	A	2099	U	C5-C6-N1	5.26	125.33	122.70
1	A	2096	U	C5-C6-N1	5.26	125.33	122.70
1	A	2329	G	C2-N3-C4	-5.26	109.27	111.90
1	A	2518	A	C8-N9-C4	-5.26	103.70	105.80
1	A	2032	G	C6-C5-N7	-5.26	127.25	130.40
1	A	1267	U	N1-C2-O2	5.25	126.48	122.80
1	A	990	A	N1-C6-N6	5.25	121.75	118.60
1	A	1775	U	C5-C6-N1	-5.25	120.08	122.70
1	A	557	U	N1-C2-N3	5.25	118.05	114.90
2	B	76	G	N1-C6-O6	5.25	123.05	119.90
1	A	254	G	N3-C4-C5	5.25	131.22	128.60
1	A	1942	C	C6-N1-C1'	5.25	127.09	120.80
1	A	2723	C	C2-N1-C1'	-5.25	113.03	118.80
1	A	39	C	N1-C2-N3	5.25	122.87	119.20
1	A	933	A	N7-C8-N9	5.25	116.42	113.80
1	A	2202	C	C6-N1-C2	5.25	122.40	120.30
1	A	392	C	C4-C5-C6	-5.24	114.78	117.40
1	A	412	A	C8-N9-C4	5.24	107.90	105.80
1	A	2010	G	N3-C2-N2	-5.24	116.23	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271(S)	G	C5-C6-N1	-5.24	108.88	111.50
1	A	1677	A	C8-N9-C4	5.24	107.90	105.80
1	A	1985	G	C6-N1-C2	-5.24	121.96	125.10
1	A	2011	U	N1-C2-O2	-5.24	119.13	122.80
1	A	1539	G	C5-N7-C8	-5.24	101.68	104.30
1	A	2105	C	C6-N1-C2	-5.24	118.20	120.30
1	A	822	U	N3-C4-O4	-5.24	115.73	119.40
1	A	51	G	C5-N7-C8	5.24	106.92	104.30
1	A	827	U	N3-C2-O2	5.24	125.86	122.20
1	A	1655	A	N7-C8-N9	-5.24	111.18	113.80
1	A	1546	C	C2-N1-C1'	5.23	124.56	118.80
1	A	1021	A	N3-C4-N9	-5.23	123.21	127.40
1	A	1311	G	C6-C5-N7	-5.23	127.26	130.40
1	A	2084	C	C5-C6-N1	-5.23	118.38	121.00
1	A	71	A	N1-C2-N3	5.23	131.92	129.30
1	A	1988	C	N3-C4-C5	5.23	123.99	121.90
1	A	2055	C	N1-C2-O2	-5.23	115.76	118.90
1	A	448	U	N3-C2-O2	-5.23	118.54	122.20
1	A	1424	G	C8-N9-C4	5.23	108.49	106.40
1	A	54	G	C8-N9-C4	5.22	108.49	106.40
1	A	202	U	N1-C2-N3	-5.22	111.77	114.90
1	A	702	G	N3-C2-N2	-5.22	116.24	119.90
1	A	758	C	N1-C2-O2	-5.22	115.77	118.90
1	A	839	U	C5-C4-O4	5.22	129.03	125.90
1	A	841	A	N1-C2-N3	5.22	131.91	129.30
1	A	154	G	N9-C4-C5	-5.22	103.31	105.40
1	A	1021	A	N1-C6-N6	5.22	121.73	118.60
1	A	1381	G	N1-C6-O6	-5.22	116.77	119.90
1	A	583	G	C6-C5-N7	-5.22	127.27	130.40
1	A	821	A	N1-C2-N3	5.22	131.91	129.30
1	A	1930	G	N7-C8-N9	-5.22	110.49	113.10
1	A	893	C	C6-N1-C1'	-5.22	114.54	120.80
1	A	1613	G	N1-C2-N2	-5.22	111.51	116.20
1	A	2071	A	C2-N3-C4	5.22	113.21	110.60
1	A	2496	C	C4-C5-C6	-5.21	114.79	117.40
1	A	2822	G	C8-N9-C4	5.21	108.49	106.40
1	A	2338	G	C6-C5-N7	-5.21	127.27	130.40
1	A	1170	G	N3-C4-N9	5.21	129.13	126.00
1	A	2609	U	C4-C5-C6	5.21	122.83	119.70
1	A	130	C	N1-C2-O2	5.21	122.03	118.90
1	A	1261	C	N1-C2-O2	-5.21	115.77	118.90
1	A	188	G	C8-N9-C4	5.21	108.48	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	A	N1-C6-N6	5.21	121.72	118.60
1	A	1321	A	N1-C2-N3	5.21	131.91	129.30
1	A	1270	C	C4-C5-C6	5.21	120.00	117.40
1	A	1530	C	N3-C4-C5	5.21	123.98	121.90
1	A	2351	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	2362	G	N3-C4-C5	5.21	131.20	128.60
1	A	2672	G	C2-N3-C4	-5.21	109.30	111.90
13	R	114	VAL	CB-CA-C	-5.21	101.51	111.40
1	A	363(F)	A	C8-N9-C4	5.21	107.88	105.80
1	A	527	C	N3-C4-N4	-5.20	114.36	118.00
1	A	1816	G	C4-N9-C1'	5.20	133.27	126.50
5	F	62	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	303	U	N3-C4-C5	5.20	117.72	114.60
1	A	1216	G	C5-C6-O6	-5.20	125.48	128.60
1	A	921	G	C5-C6-O6	5.20	131.72	128.60
1	A	2575	C	N3-C4-C5	-5.20	119.82	121.90
2	B	87	G	N1-C6-O6	5.20	123.02	119.90
1	A	229	A	N7-C8-N9	5.20	116.40	113.80
1	A	320	A	C4-C5-C6	5.20	119.60	117.00
1	A	271(M)	G	C8-N9-C4	-5.20	104.32	106.40
1	A	697	C	C5-C4-N4	-5.20	116.56	120.20
1	A	952	G	C2-N3-C4	5.20	114.50	111.90
1	A	2383	G	C5-C6-O6	5.20	131.72	128.60
1	A	2574	G	C2-N3-C4	-5.20	109.30	111.90
2	B	28	C	N3-C4-N4	-5.20	114.36	118.00
1	A	1471	A	N7-C8-N9	5.19	116.40	113.80
1	A	2191	G	C5-C6-O6	-5.19	125.48	128.60
1	A	612	C	C6-N1-C2	5.19	122.38	120.30
1	A	752	A	C8-N9-C4	-5.19	103.72	105.80
1	A	1391	U	C6-N1-C1'	-5.19	113.93	121.20
1	A	1983	C	N3-C2-O2	5.19	125.53	121.90
1	A	321	G	C8-N9-C4	5.19	108.48	106.40
1	A	984	A	C5-C6-N1	5.19	120.30	117.70
1	A	995	C	C2-N1-C1'	-5.19	113.09	118.80
1	A	2725	A	C8-N9-C4	5.19	107.88	105.80
1	A	680	G	N1-C2-N3	5.19	127.01	123.90
2	B	7	G	N1-C6-O6	5.19	123.01	119.90
2	B	35	U	N3-C4-O4	-5.19	115.77	119.40
1	A	1321	A	C2-N3-C4	-5.19	108.01	110.60
1	A	1882	C	C5-C6-N1	5.19	123.59	121.00
1	A	189	G	C5-C6-O6	-5.18	125.49	128.60
1	A	287	C	C5-C6-N1	-5.18	118.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1967	C	N1-C2-O2	5.18	122.01	118.90
1	A	481	G	P-O3'-C3'	5.18	125.92	119.70
1	A	2699	C	C2-N3-C4	-5.18	117.31	119.90
1	A	58	G	C4-N9-C1'	5.18	133.24	126.50
1	A	2049	G	N3-C4-C5	5.18	131.19	128.60
1	A	1319	G	C8-N9-C4	5.18	108.47	106.40
1	A	2036	C	N1-C2-N3	5.18	122.83	119.20
1	A	2103	C	N3-C4-C5	-5.18	119.83	121.90
1	A	2259	G	C2-N3-C4	-5.18	109.31	111.90
1	A	2485	G	C2-N3-C4	-5.18	109.31	111.90
1	A	2689	U	N3-C4-C5	5.18	117.71	114.60
1	A	254	G	C2-N3-C4	-5.18	109.31	111.90
1	A	564	C	C4-C5-C6	5.18	119.99	117.40
1	A	972	G	C4-C5-N7	-5.18	108.73	110.80
1	A	2255	G	C6-C5-N7	5.17	133.50	130.40
1	A	124	G	C4-C5-N7	5.17	112.87	110.80
1	A	1313	U	C5-C6-N1	5.17	125.29	122.70
1	A	1779	U	N1-C2-O2	5.17	126.42	122.80
1	A	516	C	N3-C2-O2	-5.17	118.28	121.90
1	A	823	G	C2-N3-C4	-5.17	109.32	111.90
1	A	1113	U	C5-C4-O4	5.17	129.00	125.90
1	A	1302	A	N9-C4-C5	5.17	107.87	105.80
1	A	2672	G	C6-C5-N7	-5.17	127.30	130.40
1	A	2682	U	C5-C6-N1	-5.17	120.12	122.70
2	B	9	G	N1-C2-N2	5.17	120.85	116.20
1	A	1779	U	C2-N3-C4	-5.17	123.90	127.00
1	A	2487	G	C8-N9-C1'	-5.17	120.28	127.00
1	A	2766	G	C4-C5-N7	5.17	112.87	110.80
1	A	71	A	P-O3'-C3'	5.16	125.90	119.70
1	A	845	G	C4-N9-C1'	5.16	133.21	126.50
1	A	1180	C	C6-N1-C2	5.16	122.36	120.30
1	A	1428	C	C4-C5-C6	5.16	119.98	117.40
1	A	196	A	C5-C6-N6	-5.16	119.57	123.70
1	A	792	G	N3-C2-N2	5.16	123.51	119.90
1	A	1142(A)	A	N1-C2-N3	5.16	131.88	129.30
1	A	1541	G	N3-C4-C5	-5.16	126.02	128.60
1	A	2013	A	N9-C4-C5	-5.16	103.74	105.80
1	A	2157	G	C4-C5-N7	-5.16	108.74	110.80
1	A	2157	G	N3-C4-N9	-5.16	122.90	126.00
1	A	254	G	C5-C6-N1	-5.16	108.92	111.50
1	A	736	C	N3-C4-C5	5.16	123.96	121.90
1	A	2070	G	N3-C4-C5	-5.16	126.02	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2277	G	C5-N7-C8	5.16	106.88	104.30
1	A	2296	U	C4-C5-C6	5.16	122.79	119.70
1	A	268	C	N3-C4-C5	-5.15	119.84	121.90
1	A	1772	G	N3-C4-C5	5.15	131.18	128.60
1	A	2627	G	C5-C6-O6	5.15	131.69	128.60
1	A	70	G	N9-C4-C5	-5.15	103.34	105.40
1	A	665	C	N1-C2-N3	-5.15	115.59	119.20
1	A	1039	G	N9-C4-C5	-5.15	103.34	105.40
1	A	1950	G	N3-C4-C5	-5.15	126.02	128.60
1	A	271(M)	G	N1-C6-O6	-5.15	116.81	119.90
1	A	692	C	N1-C2-O2	-5.15	115.81	118.90
1	A	2760	C	C6-N1-C2	5.15	122.36	120.30
1	A	607	U	C2-N1-C1'	-5.15	111.52	117.70
1	A	1300	U	P-O3'-C3'	5.15	125.88	119.70
1	A	1949	G	N9-C4-C5	-5.15	103.34	105.40
1	A	196	A	C4-C5-N7	5.15	113.27	110.70
1	A	2591	C	N1-C2-N3	5.15	122.80	119.20
1	A	260	G	N1-C6-O6	-5.15	116.81	119.90
1	A	2020	A	C6-N1-C2	-5.15	115.51	118.60
1	A	2116	G	P-O3'-C3'	5.15	125.88	119.70
1	A	2181	G	C6-C5-N7	5.15	133.49	130.40
1	A	2421	G	N1-C6-O6	5.15	122.99	119.90
1	A	843	G	N3-C4-N9	-5.14	122.91	126.00
1	A	1799	G	P-O3'-C3'	5.14	125.87	119.70
1	A	652(E)	G	C4-C5-N7	5.14	112.86	110.80
1	A	1477	A	C2-N3-C4	-5.14	108.03	110.60
1	A	2232	U	C5-C6-N1	-5.14	120.13	122.70
1	A	2550	G	C8-N9-C4	-5.14	104.34	106.40
1	A	1570	A	C6-N1-C2	-5.14	115.52	118.60
1	A	2039	C	C6-N1-C2	-5.14	118.24	120.30
1	A	2567	G	N1-C6-O6	5.14	122.98	119.90
1	A	1309	G	C8-N9-C4	5.14	108.45	106.40
1	A	272(G)	C	N1-C2-O2	5.13	121.98	118.90
1	A	715	G	C8-N9-C4	-5.13	104.35	106.40
1	A	755	C	N3-C4-N4	5.13	121.59	118.00
1	A	845	G	N9-C4-C5	-5.13	103.35	105.40
1	A	846	C	N1-C2-O2	-5.13	115.82	118.90
1	A	1845	G	N3-C4-C5	-5.13	126.03	128.60
1	A	1975	G	N1-C6-O6	5.13	122.98	119.90
1	A	188	G	N3-C4-N9	5.13	129.08	126.00
1	A	1368	G	N9-C4-C5	5.13	107.45	105.40
1	A	2107	C	C5-C6-N1	5.13	123.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2314	C	C2-N1-C1'	-5.13	113.16	118.80
1	A	1021	A	C4-C5-N7	5.13	113.26	110.70
1	A	955	C	C6-N1-C2	5.12	122.35	120.30
1	A	2233	U	C6-N1-C2	5.12	124.08	121.00
1	A	62	C	C2-N1-C1'	-5.12	113.16	118.80
1	A	528	A	C4-C5-C6	-5.12	114.44	117.00
1	A	790	C	C6-N1-C2	5.12	122.35	120.30
1	A	1372	U	C5-C4-O4	5.12	128.97	125.90
1	A	1577	C	C5-C6-N1	-5.12	118.44	121.00
1	A	1366	A	N9-C4-C5	-5.12	103.75	105.80
1	A	2550	G	N7-C8-N9	5.12	115.66	113.10
1	A	13	A	C5-C6-N6	5.12	127.80	123.70
1	A	748	G	C5-N7-C8	5.12	106.86	104.30
1	A	2336	A	C2-N3-C4	5.12	113.16	110.60
1	A	2861	G	N7-C8-N9	5.12	115.66	113.10
2	B	33	G	C4-C5-N7	5.12	112.85	110.80
1	A	526	A	C2-N3-C4	5.11	113.16	110.60
1	A	657	U	C4-C5-C6	5.11	122.77	119.70
1	A	1021	A	C6-C5-N7	-5.11	128.72	132.30
1	A	1337	G	C5-C6-N1	5.11	114.06	111.50
1	A	2070	G	N1-C2-N3	5.11	126.97	123.90
10	O	8	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	1394	U	C5-C4-O4	5.11	128.97	125.90
1	A	982	C	C6-N1-C2	-5.11	118.26	120.30
1	A	1543	C	N1-C2-O2	5.11	121.96	118.90
1	A	2844	G	C5-C6-O6	-5.11	125.54	128.60
1	A	125	G	C8-N9-C4	5.10	108.44	106.40
1	A	761	A	C5-N7-C8	5.10	106.45	103.90
1	A	930	U	N3-C2-O2	5.10	125.77	122.20
1	A	2288	A	N7-C8-N9	5.10	116.35	113.80
1	A	2061	G	C8-N9-C4	5.10	108.44	106.40
1	A	583	G	C4-C5-N7	5.10	112.84	110.80
1	A	928	G	C4-C5-C6	5.10	121.86	118.80
1	A	2610	C	P-O3'-C3'	5.10	125.81	119.70
1	A	453	C	N1-C2-O2	5.09	121.95	118.90
1	A	1047	G	N3-C4-C5	-5.09	126.06	128.60
1	A	1107	G	C2-N3-C4	5.09	114.44	111.90
1	A	1697	G	N3-C2-N2	-5.09	116.34	119.90
1	A	2319	G	C8-N9-C4	-5.09	104.36	106.40
1	A	2581	G	C8-N9-C1'	-5.09	120.38	127.00
1	A	325	G	C8-N9-C4	5.09	108.44	106.40
1	A	466	A	N1-C2-N3	5.09	131.84	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	C	C2-N1-C1'	5.09	124.40	118.80
1	A	329	G	C5-C6-N1	5.09	114.04	111.50
1	A	1280	G	N1-C6-O6	5.09	122.95	119.90
1	A	1553	A	C8-N9-C4	-5.09	103.77	105.80
1	A	1566	A	C5-C6-N1	-5.09	115.16	117.70
1	A	1604	C	C2-N3-C4	-5.09	117.36	119.90
2	B	74	U	N3-C2-O2	-5.09	118.64	122.20
1	A	1614	A	C2-N3-C4	-5.08	108.06	110.60
1	A	2036	C	C6-N1-C2	-5.08	118.27	120.30
1	A	951	C	N3-C4-C5	5.08	123.93	121.90
1	A	2723	C	C2-N3-C4	-5.08	117.36	119.90
1	A	1653	G	N3-C2-N2	5.08	123.45	119.90
1	A	2559	C	C6-N1-C2	5.08	122.33	120.30
1	A	2832	U	C6-N1-C1'	-5.08	114.09	121.20
1	A	2338	G	C5-C6-O6	-5.08	125.56	128.60
1	A	1914	C	C2-N1-C1'	-5.07	113.22	118.80
1	A	2265	U	C5-C6-N1	5.07	125.24	122.70
1	A	2292	C	N3-C4-N4	-5.07	114.45	118.00
1	A	1858	G	C4-N9-C1'	5.07	133.09	126.50
1	A	2191	G	C4-C5-N7	5.07	112.83	110.80
1	A	2607	G	C4-N9-C1'	5.07	133.09	126.50
1	A	94	C	N1-C2-O2	5.07	121.94	118.90
2	B	89	G	C4-C5-N7	5.07	112.83	110.80
1	A	2594	C	C2-N3-C4	-5.07	117.37	119.90
1	A	2644	G	C2-N3-C4	-5.07	109.37	111.90
1	A	1415	U	C2-N1-C1'	-5.07	111.62	117.70
1	A	1790	C	C4-C5-C6	5.07	119.93	117.40
1	A	1864	U	C6-N1-C2	5.07	124.04	121.00
1	A	1921	G	C4-C5-N7	5.07	112.83	110.80
1	A	2579	C	C4-C5-C6	5.07	119.93	117.40
1	A	1290	C	N3-C2-O2	-5.06	118.36	121.90
1	A	171	G	N9-C4-C5	-5.06	103.38	105.40
1	A	770	G	C5-C6-N1	5.06	114.03	111.50
1	A	1802	A	C2-N3-C4	-5.06	108.07	110.60
1	A	2241	A	N1-C2-N3	5.06	131.83	129.30
1	A	2304	G	C4-C5-N7	-5.06	108.78	110.80
1	A	2876	G	C5-C6-N1	5.06	114.03	111.50
1	A	532	A	C4-C5-N7	5.06	113.23	110.70
1	A	1193	G	N9-C4-C5	-5.06	103.38	105.40
1	A	2647	U	C5-C6-N1	-5.06	120.17	122.70
1	A	362	U	N3-C4-O4	5.06	122.94	119.40
1	A	662	G	N1-C6-O6	-5.06	116.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2447	G	C6-C5-N7	-5.06	127.37	130.40
1	A	1261	C	C5-C6-N1	-5.05	118.47	121.00
1	A	1635	G	N1-C6-O6	5.05	122.93	119.90
1	A	2030	A	N3-C4-C5	5.05	130.34	126.80
2	B	15	A	C8-N9-C4	5.05	107.82	105.80
1	A	235	U	C5-C6-N1	-5.05	120.17	122.70
1	A	104	U	C6-N1-C2	5.05	124.03	121.00
1	A	1205	U	C5-C6-N1	-5.05	120.17	122.70
1	A	2359	C	N3-C4-C5	-5.05	119.88	121.90
1	A	1526	G	C8-N9-C4	5.05	108.42	106.40
18	W	17	VAL	CB-CA-C	-5.05	101.81	111.40
1	A	1481	U	C5-C4-O4	5.05	128.93	125.90
1	A	1315	C	C4-C5-C6	5.05	119.92	117.40
1	A	1926	U	C5-C4-O4	5.05	128.93	125.90
1	A	2548	G	N7-C8-N9	-5.05	110.58	113.10
1	A	2013	A	C2-N3-C4	-5.04	108.08	110.60
1	A	2292	C	C2-N3-C4	-5.04	117.38	119.90
1	A	2477	C	C5-C6-N1	-5.04	118.48	121.00
1	A	2275	C	N1-C2-O2	5.04	121.93	118.90
1	A	2711	A	C4-C5-C6	-5.04	114.48	117.00
1	A	2744	G	N3-C2-N2	-5.04	116.37	119.90
1	A	181	A	N9-C4-C5	5.04	107.82	105.80
1	A	728	G	C8-N9-C1'	-5.04	120.45	127.00
1	A	1802	A	C6-N1-C2	-5.04	115.58	118.60
1	A	2429	G	C8-N9-C4	-5.04	104.38	106.40
1	A	1238	G	N7-C8-N9	-5.04	110.58	113.10
1	A	1257	C	C5-C6-N1	-5.04	118.48	121.00
1	A	2439	A	C2-N3-C4	-5.04	108.08	110.60
1	A	531	C	C5-C6-N1	-5.03	118.48	121.00
1	A	608	A	C5-N7-C8	-5.03	101.38	103.90
1	A	1596	A	N1-C6-N6	-5.03	115.58	118.60
1	A	18	C	C6-N1-C2	-5.03	118.29	120.30
1	A	45	C	C4-C5-C6	5.03	119.92	117.40
1	A	682	G	C8-N9-C1'	-5.03	120.46	127.00
1	A	819	A	C5-N7-C8	-5.03	101.38	103.90
1	A	1121	C	C4-C5-C6	5.03	119.92	117.40
1	A	1677	A	N9-C4-C5	-5.03	103.79	105.80
1	A	154	G	C4-C5-N7	5.03	112.81	110.80
1	A	363(B)	G	N9-C4-C5	-5.03	103.39	105.40
1	A	1016	G	N1-C6-O6	5.03	122.92	119.90
1	A	1546	C	C6-N1-C1'	-5.03	114.77	120.80
1	A	1695	G	N1-C6-O6	5.03	122.92	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2417	C	C4-C5-C6	5.03	119.91	117.40
1	A	2487	G	C5-C6-O6	-5.03	125.58	128.60
1	A	2445	G	N1-C6-O6	-5.03	116.89	119.90
1	A	2602	A	P-O3'-C3'	5.03	125.73	119.70
2	B	7	G	N9-C4-C5	-5.03	103.39	105.40
1	A	1231	G	C2-N3-C4	-5.02	109.39	111.90
1	A	2444	G	N1-C2-N3	5.02	126.91	123.90
1	A	760	G	N9-C4-C5	-5.02	103.39	105.40
1	A	1325	G	C5-N7-C8	-5.02	101.79	104.30
1	A	1526	G	N9-C4-C5	-5.02	103.39	105.40
1	A	2373	G	N1-C6-O6	5.02	122.91	119.90
1	A	2568	C	N1-C2-O2	-5.02	115.89	118.90
1	A	85	G	N3-C4-C5	5.01	131.11	128.60
1	A	1688	U	N1-C2-N3	5.01	117.91	114.90
1	A	2023	G	C8-N9-C4	-5.01	104.39	106.40
1	A	2502	G	C5-N7-C8	-5.01	101.79	104.30
1	A	2669	G	C5-C6-O6	-5.01	125.59	128.60
1	A	476	G	N1-C6-O6	5.01	122.91	119.90
1	A	691	C	C2-N1-C1'	-5.01	113.28	118.80
1	A	727	A	C5-C6-N6	-5.01	119.69	123.70
1	A	932	G	C8-N9-C1'	5.01	133.52	127.00
1	A	1049	C	N1-C2-O2	5.01	121.91	118.90
1	A	1368	G	C4-C5-N7	-5.01	108.80	110.80
1	A	1772	G	C4-N9-C1'	-5.01	119.99	126.50
1	A	2417	C	N1-C2-N3	5.01	122.71	119.20
1	A	1236	G	C2-N3-C4	-5.01	109.40	111.90
1	A	1256	G	C4-N9-C1'	5.01	133.01	126.50
1	A	2379	G	C6-C5-N7	-5.01	127.39	130.40
1	A	2395	C	N3-C2-O2	5.01	125.41	121.90
1	A	2056	G	N9-C4-C5	-5.01	103.40	105.40
1	A	272(H)	C	C2-N1-C1'	5.01	124.31	118.80
1	A	452	G	N7-C8-N9	5.01	115.60	113.10
1	A	2607	G	C5-N7-C8	5.01	106.80	104.30
1	A	1943	U	C4-C5-C6	5.00	122.70	119.70
1	A	1036	G	N1-C2-N3	5.00	126.90	123.90
1	A	1050	A	C8-N9-C4	-5.00	103.80	105.80
1	A	1372	U	N3-C4-O4	-5.00	115.90	119.40
1	A	678	C	C5-C6-N1	-5.00	118.50	121.00
1	A	819	A	N7-C8-N9	5.00	116.30	113.80
1	A	1639	U	C5-C6-N1	-5.00	120.20	122.70
1	A	2020	A	C4-C5-C6	5.00	119.50	117.00

There are no chirality outliers.



All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	1	83	GLU	Peptide
26	4	43	TYR	Peptide
1	A	2335	A	Sidechain
4	E	72	VAL	Peptide
5	F	85	GLY	Peptide
8	I	86	THR	Peptide
12	Q	18	LYS	Peptide
14	S	82	ILE	Peptide
19	X	93	GLU	Peptide
21	Z	191	VAL	Peptide

## 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60621	0	30566	1216	0
2	B	2573	0	1306	55	0
3	D	2136	0	2218	77	0
4	E	1555	0	1607	56	0
5	F	1580	0	1621	63	0
6	G	1368	0	1324	86	0
7	H	1317	0	1376	36	0
8	I	953	0	858	38	0
9	N	1112	0	1180	44	0
10	O	923	0	981	26	0
11	P	1131	0	1201	55	0
12	Q	1122	0	1179	49	0
13	R	968	0	1033	36	0
14	S	865	0	905	50	0
15	T	1063	0	1103	39	0
16	U	959	0	1019	35	0
17	V	771	0	830	25	0
18	W	881	0	935	31	0
19	X	742	0	799	26	0
20	Y	785	0	828	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Z	1522	0	1511	65	0
22	0	594	0	604	17	0
23	1	745	0	804	24	0
24	2	588	0	643	19	0
25	3	458	0	503	12	0
26	4	349	0	336	28	0
27	5	455	0	472	14	0
28	6	449	0	462	15	0
29	7	418	0	467	18	0
30	8	509	0	565	22	0
31	9	297	0	316	9	0
32	0	2	0	0	0	0
32	8	2	0	0	0	0
32	A	595	0	0	0	0
32	B	8	0	0	0	0
32	D	2	0	0	0	0
32	E	4	0	0	0	0
32	F	1	0	0	0	0
32	O	1	0	0	0	0
32	P	1	0	0	0	0
32	Q	2	0	0	0	0
32	R	3	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	6	1	0	0	0	0
33	9	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	1	0	0	0	0
34	1	4	0	0	0	0
34	3	1	0	0	0	0
34	7	3	0	0	0	0
34	8	1	0	0	0	0
34	A	1166	0	0	170	0
34	B	19	0	0	0	0
34	D	8	0	0	0	0
34	E	10	0	0	2	0
34	F	6	0	0	1	0
34	N	1	0	0	0	0
34	P	9	0	0	1	0
34	Q	3	0	0	0	0
34	R	2	0	0	1	0
34	T	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	U	4	0	0	0	0
34	V	2	0	0	1	0
34	W	2	0	0	0	0
34	X	2	0	0	1	0
34	Y	1	0	0	0	0
All	All	91682	0	59552	2077	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (2077) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2296:U:O4	1:A:2335:A:N6	1.77	1.15
1:A:2820:A:OP2	13:R:2:ARG:NH2	1.88	1.06
1:A:2711:A:OP2	34:A:3982:HOH:O	1.73	1.04
1:A:847:U:O4	1:A:933:A:N6	1.92	1.02
1:A:1439:A:OP1	34:A:4117:HOH:O	1.79	1.01
1:A:527:C:OP1	34:A:4525:HOH:O	1.77	1.00
1:A:1671:U:OP2	34:A:3797:HOH:O	1.78	0.99
26:4:42:PHE:HB3	26:4:43:TYR:HB2	1.45	0.96
1:A:563:G:OP2	34:A:4616:HOH:O	1.83	0.96
1:A:2122:U:H3	1:A:2176:A:N6	1.64	0.94
1:A:2227:A:OP2	34:A:4136:HOH:O	1.85	0.94
15:T:16:ARG:NH2	15:T:83:ILE:O	2.02	0.93
1:A:271(I):G:H1	1:A:271(O):C:H42	0.94	0.92
1:A:271(I):G:H1	1:A:271(O):C:N4	1.68	0.92
1:A:1970:A:OP1	34:A:4201:HOH:O	1.88	0.91
1:A:2036:C:OP1	34:A:4422:HOH:O	1.88	0.91
1:A:631:A:OP1	11:P:65:ARG:NH1	2.03	0.90
1:A:2304:G:H1	1:A:2312:U:H3	1.19	0.90
1:A:330:A:H2	1:A:1210:A:H2'	1.36	0.89
1:A:407:G:OP2	34:A:4597:HOH:O	1.89	0.89
1:A:1359:A:N6	1:A:1372:U:O4	2.06	0.89
1:A:2036:C:H6	1:A:2036:C:H5'	1.37	0.89
1:A:2122:U:H3	1:A:2176:A:H61	0.91	0.88
6:G:41:GLN:HB3	6:G:43:LEU:HD13	1.52	0.88
1:A:1376:C:OP2	34:A:3924:HOH:O	1.90	0.88
11:P:39:LYS:HB2	11:P:45:LEU:HG	1.55	0.88
1:A:2228:G:OP1	3:D:261:LYS:NZ	2.05	0.88
1:A:785:G:OP2	34:A:4104:HOH:O	1.92	0.87
1:A:1019:U:H3	1:A:1142(A):A:H62	1.21	0.87
1:A:2322:A:H61	1:A:2335:A:N6	1.72	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:927:G:N7	34:A:4224:HOH:O	2.08	0.87
1:A:1865:G:N7	34:A:4463:HOH:O	2.06	0.87
1:A:1689:A:H62	1:A:1698:A:H2	1.19	0.86
1:A:1352:U:OP2	34:A:3925:HOH:O	1.94	0.86
1:A:1345:C:OP2	34:A:3933:HOH:O	1.92	0.86
1:A:1204:A:H2	1:A:1241:A:H62	1.23	0.86
1:A:2287:A:N6	1:A:2344:U:H3	1.73	0.86
23:1:82:LEU:HA	23:1:85:LEU:HD23	1.58	0.86
6:G:63:ILE:HA	6:G:143:GLU:HG3	1.58	0.85
6:G:15:VAL:HG13	6:G:175:LEU:HB3	1.57	0.85
1:A:1641:A:OP2	34:A:4167:HOH:O	1.94	0.85
1:A:2526:G:O6	34:A:4278:HOH:O	1.95	0.84
1:A:833:U:O2	11:P:55:ARG:NH2	2.09	0.84
1:A:1980:G:O2'	1:A:1982:C:OP2	1.95	0.84
1:A:2808:U:O2	1:A:2892:A:N6	2.10	0.84
1:A:1530:C:O2'	1:A:1531:C:O5'	1.96	0.84
1:A:1271:G:OP2	34:A:3838:HOH:O	1.96	0.84
1:A:2161:C:OP2	1:A:2161:C:C5	2.30	0.83
1:A:2298:A:H62	1:A:2318:G:H8	1.24	0.83
1:A:2385:C:OP1	34:A:4150:HOH:O	1.95	0.83
1:A:2161:C:C6	1:A:2161:C:OP2	2.31	0.83
8:I:3:VAL:HG12	8:I:38:LEU:HA	1.60	0.82
1:A:2074:U:OP1	34:A:4292:HOH:O	1.97	0.82
11:P:126:VAL:HG12	11:P:148:LEU:HD22	1.61	0.82
1:A:2694:G:N7	34:A:4765:HOH:O	2.12	0.82
1:A:2194:G:N7	34:A:4543:HOH:O	2.13	0.82
1:A:810:U:OP1	34:A:4442:HOH:O	1.96	0.82
9:N:130:HIS:HB3	9:N:133:GLN:HE21	1.43	0.82
1:A:2317:C:H2'	1:A:2318:G:H5'	1.62	0.81
1:A:676:A:H8	1:A:2069:G:H21	1.25	0.81
1:A:1303:G:OP1	34:A:4517:HOH:O	1.97	0.81
1:A:2134:A:O2'	1:A:2159:G:N2	2.15	0.80
1:A:271(A):A:N7	1:A:271(W):G:N2	2.30	0.80
1:A:1022:G:H22	1:A:1142(A):A:H2	1.29	0.80
1:A:71:A:C2	19:X:31:HIS:HE1	1.99	0.80
30:8:33:ASN:HA	30:8:36:LYS:HD2	1.63	0.79
1:A:1403:C:H5''	1:A:1471:A:H1'	1.65	0.79
5:F:178:PRO:HB2	5:F:201:VAL:HG11	1.64	0.79
1:A:2472:G:H5'	1:A:2473:U:H5''	1.65	0.79
1:A:80:G:N7	34:A:4040:HOH:O	2.15	0.79
18:W:25:ARG:NH2	18:W:74:ALA:O	2.16	0.79
1:A:1604:C:OP1	34:A:3780:HOH:O	2.01	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:T:95:ARG:HG2	15:T:95:ARG:HH11	1.47	0.78
6:G:138:GLN:HG3	6:G:144:ILE:HG21	1.64	0.78
1:A:1670:C:OP1	34:A:3797:HOH:O	2.01	0.78
1:A:1022:G:O2'	34:A:3677:HOH:O	2.01	0.78
1:A:1416:G:O6	34:A:4481:HOH:O	2.02	0.77
5:F:101:LEU:O	5:F:106:ARG:NH1	2.18	0.77
1:A:411:G:OP1	34:A:4055:HOH:O	2.02	0.77
1:A:1639:U:OP1	34:A:3975:HOH:O	2.02	0.77
1:A:574:C:OP1	34:A:3893:HOH:O	2.03	0.77
1:A:945:A:N7	34:A:3673:HOH:O	2.17	0.77
1:A:2206:G:H5'	1:A:2207:G:N7	1.99	0.77
1:A:1971:A:OP1	34:A:4201:HOH:O	2.02	0.77
1:A:452:G:OP2	34:A:4024:HOH:O	2.01	0.76
1:A:1639:U:H2'	1:A:1640:C:H5''	1.66	0.76
2:B:66:A:H61	2:B:109:C:H5'	1.49	0.76
9:N:20:GLY:HA2	9:N:61:ARG:HG3	1.66	0.76
1:A:2296:U:O4	1:A:2335:A:C6	2.38	0.76
1:A:2136:C:H42	1:A:2155:G:H1	1.33	0.76
1:A:1236:G:OP1	34:A:4242:HOH:O	2.04	0.75
1:A:1607:C:N4	1:A:1622:G:OP2	2.19	0.75
1:A:2407:G:OP1	34:A:4058:HOH:O	2.04	0.75
1:A:386:G:O3'	34:A:4066:HOH:O	2.03	0.75
1:A:2005:A:OP1	34:A:3792:HOH:O	2.03	0.75
1:A:1226:A:OP1	17:V:84:LYS:NZ	2.18	0.75
1:A:1268:A:OP1	34:A:3870:HOH:O	2.04	0.75
1:A:399:G:OP2	34:A:4072:HOH:O	2.04	0.75
1:A:853:G:O6	34:A:4217:HOH:O	2.04	0.75
1:A:1376:C:OP2	34:A:3923:HOH:O	2.05	0.75
1:A:2296:U:OP2	14:S:9:ARG:NH2	2.18	0.75
1:A:1817:G:OP1	3:D:88:ARG:NH2	2.19	0.74
9:N:47:ALA:HB2	9:N:112:LEU:HD11	1.68	0.74
8:I:87:LYS:H	8:I:122:GLU:HA	1.52	0.74
1:A:2147:G:H2'	1:A:2148:G:O4'	1.87	0.74
1:A:2712:U:O2'	1:A:2712(A):A:OP2	2.06	0.74
6:G:76:SER:HA	6:G:83:ARG:HA	1.69	0.74
1:A:528:A:O2'	34:A:4762:HOH:O	2.04	0.74
3:D:118:VAL:H	3:D:129:ASN:HD22	1.36	0.74
1:A:1637:A:OP2	34:A:3950:HOH:O	2.06	0.74
1:A:1913:A:H3'	1:A:1913:A:OP2	1.86	0.74
26:4:18:CYS:SG	26:4:39:CYS:HB3	2.28	0.74
1:A:71:A:H2	19:X:31:HIS:HE1	1.36	0.73
1:A:346:A:OP2	34:A:4499:HOH:O	2.05	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:10:ARG:NH2	21:Z:26:GLY:O	2.20	0.73
1:A:1377:G:OP2	34:A:3919:HOH:O	2.06	0.73
1:A:607:U:OP1	5:F:102:PRO:HA	1.88	0.73
27:5:16:ARG:HH11	27:5:16:ARG:HG2	1.52	0.73
1:A:271(F):C:H2'	1:A:271(G):C:H6	1.51	0.73
1:A:278:A:O2'	1:A:279:C:OP1	2.06	0.73
1:A:141:A:H8	1:A:1408:C:HO2'	1.32	0.73
1:A:154(A):C:N4	1:A:171:G:H1	1.85	0.73
1:A:29:U:H2'	1:A:30:G:C8	2.22	0.73
8:I:40:THR:O	8:I:44:LEU:N	2.17	0.73
1:A:1250:G:N7	11:P:18:ARG:NH2	2.37	0.73
15:T:118:ARG:HA	15:T:118:ARG:CZ	2.19	0.73
1:A:768:G:N7	34:A:3968:HOH:O	2.21	0.72
1:A:2526:G:H21	31:9:2:LYS:HG2	1.54	0.72
1:A:1721:G:H8	1:A:1741:A:H62	1.37	0.72
1:A:1019:U:HO2'	1:A:1021:A:H2	1.37	0.72
14:S:11:LYS:HG3	14:S:91:PRO:HD3	1.72	0.72
1:A:1237:A:OP1	34:A:4008:HOH:O	2.06	0.72
12:Q:58:PHE:HB3	12:Q:61:GLY:HA3	1.72	0.72
1:A:411:G:H5''	34:A:4055:HOH:O	1.90	0.72
1:A:404:C:OP1	34:A:4241:HOH:O	2.06	0.72
15:T:64:ARG:NH1	15:T:103:ARG:HA	2.05	0.72
3:D:17:THR:O	3:D:211:ARG:NH2	2.21	0.72
1:A:1394:U:OP1	34:A:3780:HOH:O	2.08	0.72
1:A:1507:A:O2'	1:A:1508:A:H8	1.72	0.72
1:A:2287:A:H62	1:A:2344:U:H3	1.37	0.71
1:A:2126:A:N6	1:A:2163:C:H5'	2.05	0.71
1:A:1332:G:OP1	34:A:3773:HOH:O	2.08	0.71
6:G:105:LYS:NZ	26:4:25:TYR:O	2.22	0.71
1:A:2109:U:H3	1:A:2180:U:H3	1.38	0.71
1:A:2268:A:OP1	34:A:4326:HOH:O	2.08	0.71
17:V:62:LEU:HD11	17:V:95:LEU:HB2	1.72	0.71
1:A:1495:A:OP2	34:A:4265:HOH:O	2.07	0.71
1:A:2226:C:OP2	34:A:4137:HOH:O	2.07	0.71
1:A:2646:C:OP2	1:A:2732:G:O2'	2.07	0.71
21:Z:110:GLY:HA3	21:Z:174:VAL:HG11	1.71	0.71
1:A:1560:G:OP1	34:A:4332:HOH:O	2.08	0.71
17:V:56:SER:H	17:V:100:ARG:HB2	1.53	0.71
28:6:3:SER:OG	28:6:4:GLU:N	2.24	0.71
1:A:392:C:OP1	34:A:4588:HOH:O	2.07	0.71
6:G:56:ALA:HB2	6:G:153:ARG:HE	1.56	0.71
1:A:2042:A:OP1	34:A:3604:HOH:O	2.09	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1313:U:OP1	34:A:3765:HOH:O	2.09	0.71
1:A:1047:G:H2'	1:A:1110:G:H22	1.54	0.71
1:A:2747:G:N7	34:A:4471:HOH:O	2.24	0.70
7:H:56:SER:OG	7:H:61:HIS:ND1	2.24	0.70
1:A:1914:C:H2'	1:A:1915:U:C6	2.26	0.70
1:A:1210:A:C8	1:A:1210:A:H5''	2.26	0.70
1:A:370:G:OP2	34:A:4069:HOH:O	2.08	0.70
4:E:175:VAL:HG23	4:E:177:PRO:HD3	1.73	0.70
1:A:882:G:H1	1:A:894:C:H42	1.38	0.70
8:I:83:ALA:HA	8:I:89:TYR:CE2	2.27	0.70
1:A:1186:G:OP1	34:A:4631:HOH:O	2.09	0.70
1:A:2781:A:H5''	1:A:2782:G:H5'	1.71	0.70
1:A:2115:G:H4'	1:A:2167:U:H4'	1.74	0.70
1:A:531:C:OP1	1:A:561:G:N2	2.24	0.70
2:B:31:C:O2'	2:B:53:A:N6	2.24	0.70
1:A:2285:C:OP2	28:6:6:ARG:NH1	2.24	0.70
21:Z:82:ARG:HB3	21:Z:82:ARG:HH21	1.56	0.70
1:A:2130:U:HO2'	1:A:2133:G:HO2'	1.38	0.70
17:V:72:VAL:HG13	17:V:85:LYS:HB3	1.73	0.70
19:X:56:THR:O	34:X:102:HOH:O	2.09	0.70
6:G:16:ARG:HE	6:G:31:VAL:HG21	1.57	0.69
1:A:1364:G:OP2	23:1:3:LYS:HG2	1.92	0.69
14:S:10:ARG:HH21	14:S:91:PRO:HB2	1.57	0.69
1:A:89:G:H3'	1:A:90:U:H5''	1.74	0.69
1:A:1778:U:OP2	34:A:4132:HOH:O	2.10	0.69
1:A:842:G:N7	34:A:4651:HOH:O	2.24	0.69
1:A:2887:U:H2'	1:A:2888:C:C6	2.27	0.69
1:A:15:G:OP2	34:A:4612:HOH:O	2.09	0.69
1:A:1266:G:O5'	18:W:15:ARG:NH2	2.24	0.69
1:A:1380:G:OP2	34:A:4629:HOH:O	2.09	0.69
16:U:92:ARG:HA	16:U:95:LEU:HB2	1.75	0.69
21:Z:45:ASP:OD2	21:Z:49:ARG:NH1	2.25	0.69
1:A:1026:U:O2'	1:A:1027:A:O5'	2.10	0.69
1:A:2117:A:H61	1:A:2166:G:H22	1.37	0.69
6:G:124:SER:HB2	6:G:131:TYR:CE1	2.28	0.69
8:I:126:TYR:HB2	8:I:142:VAL:HG23	1.75	0.69
1:A:1434:A:H61	1:A:1558:A:N6	1.90	0.69
1:A:2002:G:O6	34:A:3863:HOH:O	2.11	0.69
1:A:1828:G:OP2	34:A:3763:HOH:O	2.10	0.69
1:A:587:C:OP2	11:P:21:ARG:NH2	2.26	0.69
5:F:53:THR:HG23	5:F:55:GLY:H	1.57	0.69
4:E:28:ALA:HB3	4:E:93:VAL:HG12	1.74	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2322:A:N6	1:A:2335:A:H61	1.91	0.69
1:A:1495:A:OP2	34:A:4262:HOH:O	2.11	0.69
11:P:59:LEU:HD11	30:8:10:ALA:HB2	1.75	0.68
21:Z:33:LEU:HD23	21:Z:90:VAL:HG21	1.75	0.68
6:G:106:LEU:HD12	6:G:110:ALA:HB3	1.75	0.68
18:W:84:ARG:HG3	18:W:98:LYS:HD2	1.76	0.68
1:A:2134:A:C2	1:A:2159:G:H1'	2.28	0.68
1:A:2760:C:H2'	1:A:2761:G:H5''	1.74	0.68
1:A:2773:C:H5''	4:E:164:ARG:HG2	1.75	0.68
1:A:248:G:OP1	34:A:4067:HOH:O	2.10	0.68
2:B:48:A:H4'	14:S:95:HIS:HD2	1.58	0.68
5:F:7:TYR:H	5:F:22:ALA:HB3	1.59	0.68
18:W:18:ARG:HG3	18:W:76:VAL:HB	1.75	0.68
25:3:23:LEU:HD13	25:3:50:VAL:HG11	1.75	0.68
5:F:185:ASP:HA	5:F:188:ARG:HD3	1.75	0.68
1:A:1120:G:O6	34:A:4635:HOH:O	2.08	0.68
1:A:1355:G:O6	34:A:4111:HOH:O	2.10	0.68
1:A:1763:G:OP1	1:A:1763:G:H4'	1.94	0.68
17:V:35:LEU:HB2	17:V:57:VAL:HG13	1.74	0.67
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.29	0.67
1:A:1670:C:H5''	34:A:3797:HOH:O	1.95	0.67
1:A:2206:G:H5'	1:A:2207:G:C5	2.29	0.67
1:A:1529:G:C6	1:A:1530:C:N4	2.61	0.67
1:A:1045:A:N3	1:A:1045:A:H2'	2.08	0.67
1:A:2322:A:H61	1:A:2335:A:H61	1.43	0.67
13:R:11:ASN:ND2	34:R:302:HOH:O	2.27	0.67
1:A:27:G:O2'	1:A:28:A:OP2	2.09	0.67
1:A:2519:U:OP2	34:A:4283:HOH:O	2.13	0.67
1:A:2431:U:O4	34:A:3988:HOH:O	2.10	0.67
1:A:1014:U:H2'	1:A:1015:G:H8	1.60	0.67
26:4:42:PHE:CB	26:4:43:TYR:HB2	2.25	0.67
1:A:2427:C:OP2	34:A:4438:HOH:O	2.12	0.67
1:A:1351:C:OP2	34:A:3920:HOH:O	2.12	0.67
23:1:50:ARG:HG2	23:1:59:THR:HG22	1.76	0.67
3:D:71:ASP:HB3	3:D:103:ARG:HH22	1.60	0.67
1:A:2199:A:H3'	1:A:2200:C:H6	1.58	0.67
1:A:365:C:OP2	34:A:4238:HOH:O	2.12	0.67
22:0:53:MET:HG3	22:0:59:LEU:HD23	1.77	0.66
1:A:856:C:H5'	22:0:27:GLU:OE2	1.94	0.66
1:A:1132:A:OP2	34:A:3679:HOH:O	2.13	0.66
1:A:2022:U:OP1	34:A:3874:HOH:O	2.13	0.66
20:Y:9:LYS:NZ	20:Y:28:LYS:O	2.28	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:47:VAL:HG11	4:E:86:PRO:HD2	1.77	0.66
1:A:512:G:N7	34:A:3826:HOH:O	2.29	0.66
1:A:674:G:H1'	5:F:74:ARG:HD3	1.78	0.66
1:A:2130:U:O2'	1:A:2133:G:O2'	2.10	0.66
9:N:15:LEU:HB2	9:N:135:PRO:HB2	1.77	0.66
1:A:1970:A:H4'	34:A:4201:HOH:O	1.95	0.66
1:A:2786:U:O2'	4:E:62:PRO:O	2.07	0.66
1:A:1315:C:OP2	34:A:3773:HOH:O	2.14	0.66
7:H:86:GLU:OE2	7:H:132:ARG:NH1	2.29	0.66
1:A:123:G:OP1	34:A:3611:HOH:O	2.13	0.66
1:A:1405:U:H2'	1:A:1406:U:C6	2.30	0.65
1:A:910:A:C5	12:Q:13:GLN:HG3	2.31	0.65
1:A:552:G:O6	34:A:4475:HOH:O	2.13	0.65
15:T:56:GLY:O	15:T:59:THR:HG22	1.95	0.65
1:A:688:U:O4	34:A:3964:HOH:O	2.11	0.65
1:A:154(A):C:N4	1:A:171:G:N1	2.45	0.65
1:A:1838:C:O2'	34:A:4301:HOH:O	2.13	0.65
6:G:11:TYR:CE2	6:G:16:ARG:HD3	2.31	0.65
4:E:11:MET:HG2	4:E:24:THR:HB	1.79	0.65
1:A:1423:G:H2'	1:A:1424:G:H8	1.62	0.65
3:D:118:VAL:H	3:D:129:ASN:ND2	1.94	0.65
1:A:1352:U:OP2	34:A:3922:HOH:O	2.14	0.65
1:A:71:A:H2	19:X:31:HIS:CE1	2.15	0.65
10:O:25:LEU:HD21	10:O:40:VAL:HG23	1.79	0.65
1:A:301:G:OP2	20:Y:84:ARG:NH2	2.29	0.65
29:7:24:THR:HG23	29:7:27:GLY:H	1.61	0.65
1:A:2319:G:N2	14:S:3:ARG:HD2	2.11	0.65
1:A:1379:A:H4'	1:A:1380:G:OP2	1.95	0.65
1:A:1914:C:H2'	1:A:1915:U:H6	1.61	0.65
6:G:122:PRO:HG3	6:G:180:PHE:HB3	1.79	0.65
1:A:2322:A:N6	1:A:2335:A:N6	2.44	0.65
1:A:252:G:OP2	11:P:50:ARG:NH1	2.30	0.65
1:A:484:C:H2'	1:A:485:C:C6	2.32	0.65
1:A:1359:A:N6	1:A:1372:U:C4	2.63	0.65
8:I:120:ILE:HG21	8:I:126:TYR:CE1	2.31	0.65
1:A:639:U:H2'	1:A:640:C:C6	2.32	0.65
1:A:2122:U:H2'	1:A:2123:G:C8	2.32	0.64
1:A:250:G:OP2	30:8:13:ARG:NH2	2.29	0.64
1:A:2305:A:H5''	6:G:134:GLY:HA3	1.79	0.64
18:W:4:LYS:HB2	18:W:106:ILE:HG12	1.79	0.64
4:E:112:GLY:O	4:E:159:HIS:HA	1.97	0.64
27:5:16:ARG:NH1	27:5:17:ASP:OD1	2.31	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:129:PHE:CD2	5:F:163:VAL:HG21	2.32	0.64
19:X:27:THR:HG23	19:X:80:ILE:HG13	1.79	0.64
1:A:96:G:H4'	24:2:48:HIS:CD2	2.31	0.64
13:R:117:VAL:HG12	13:R:118:GLU:H	1.62	0.64
12:Q:111:GLU:OE1	12:Q:133:ARG:NH2	2.30	0.64
1:A:1778:U:H2'	1:A:1784:A:N6	2.12	0.64
16:U:76:TYR:HH	16:U:92:ARG:HH11	1.43	0.64
1:A:816:C:OP2	34:A:4431:HOH:O	2.14	0.64
14:S:14:VAL:O	14:S:18:ILE:HG12	1.97	0.64
8:I:83:ALA:HB2	8:I:88:ILE:HA	1.77	0.64
1:A:910:A:H62	12:Q:12:GLN:HA	1.61	0.64
11:P:50:ARG:HD3	30:8:7:HIS:CD2	2.32	0.64
1:A:1429:G:H2'	1:A:1430:C:C6	2.32	0.64
1:A:2637:U:H5''	4:E:82:ARG:HH21	1.62	0.64
5:F:116:ASP:OD1	5:F:119:ARG:NH2	2.31	0.64
1:A:526:A:OP1	34:A:4525:HOH:O	2.15	0.64
1:A:1210:A:H5''	1:A:1210:A:H8	1.62	0.64
6:G:101:ILE:HD13	26:4:25:TYR:HB2	1.80	0.64
1:A:188:G:H1	1:A:208:C:H42	1.44	0.64
1:A:8:A:OP1	9:N:121:LYS:NZ	2.30	0.64
1:A:2833:G:H3'	1:A:2834:G:H5'	1.79	0.64
1:A:1786:A:H1'	1:A:1938:A:N6	2.13	0.64
1:A:1650:G:O6	34:A:4749:HOH:O	2.11	0.64
1:A:467:G:OP1	29:7:33:ARG:NH1	2.31	0.64
23:1:3:LYS:HB2	23:1:61:ARG:HH11	1.63	0.64
1:A:2206:G:O2'	1:A:2207:G:OP1	2.15	0.64
1:A:553:G:O6	34:A:4475:HOH:O	2.14	0.64
1:A:271(J):C:O2'	1:A:271(K):U:H5'	1.97	0.63
5:F:68:LYS:HB3	5:F:69:HIS:ND1	2.13	0.63
7:H:70:THR:HA	7:H:73:ALA:HB3	1.80	0.63
1:A:2602:A:H4'	1:A:2603:G:OP1	1.98	0.63
3:D:5:LYS:HA	3:D:17:THR:HG22	1.81	0.63
1:A:90:U:H2'	1:A:92:A:C8	2.33	0.63
1:A:1784:A:OP1	34:A:4598:HOH:O	2.15	0.63
1:A:2306:C:H3'	1:A:2307:G:C8	2.33	0.63
1:A:1011:G:OP2	16:U:66:ASN:ND2	2.28	0.63
1:A:83:G:OP1	20:Y:95:LYS:NZ	2.31	0.63
1:A:2336:A:H61	22:0:43:THR:HG22	1.64	0.63
16:U:28:ARG:NH1	16:U:38:THR:OG1	2.31	0.63
11:P:38:GLN:HA	11:P:41:ARG:HG2	1.80	0.63
1:A:668:G:H5''	1:A:669:G:OP2	1.97	0.63
3:D:108:PRO:HG2	3:D:111:LEU:HG	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2592:G:OP1	34:A:3758:HOH:O	2.15	0.63
4:E:9:VAL:HG22	4:E:25:VAL:HB	1.81	0.63
1:A:68:G:O6	34:A:4036:HOH:O	2.15	0.63
1:A:95:G:O2'	24:2:46:GLN:HA	1.99	0.63
1:A:546:C:H2'	1:A:547:A:H5'	1.80	0.63
8:I:1:MET:N	8:I:21:VAL:O	2.31	0.63
1:A:2243:U:H2'	1:A:2244:U:C6	2.34	0.63
1:A:1140:C:O3'	9:N:25:ARG:NH1	2.31	0.62
1:A:1485:G:H1	1:A:1504:C:H42	1.47	0.62
1:A:993:G:OP1	16:U:50:ARG:NH2	2.31	0.62
18:W:13:SER:HB3	18:W:16:LYS:HD2	1.80	0.62
1:A:459:U:H5''	29:7:40:TRP:CD2	2.33	0.62
14:S:58:LEU:HB2	14:S:59:LYS:HB2	1.80	0.62
1:A:2394:C:OP1	30:8:30:ARG:NH1	2.32	0.62
1:A:956:G:OP2	12:Q:14:ARG:NH2	2.33	0.62
1:A:644:A:H4'	1:A:645:C:C5	2.34	0.62
1:A:2119:A:C2	1:A:2170:A:H2'	2.35	0.62
1:A:2318:G:N2	14:S:3:ARG:HD3	2.14	0.62
1:A:2306:C:H5'	1:A:2307:G:H2'	1.80	0.62
4:E:135:HIS:CD2	4:E:135:HIS:H	2.18	0.62
5:F:185:ASP:HA	5:F:188:ARG:CD	2.30	0.62
3:D:148:GLU:OE1	3:D:151:LYS:NZ	2.22	0.62
14:S:96:GLY:HA2	14:S:97:ARG:C	2.20	0.62
1:A:184:C:H2'	1:A:185:U:C6	2.35	0.62
1:A:271(I):G:N2	1:A:271(O):C:N3	2.43	0.62
1:A:1495:A:H2'	1:A:1496:A:C8	2.35	0.62
19:X:36:LYS:HG2	19:X:54:VAL:HB	1.81	0.62
1:A:203:C:H3'	1:A:204:A:H5''	1.81	0.62
1:A:1494:A:H2'	1:A:1495:A:C8	2.35	0.61
1:A:2377:A:H2'	1:A:2378:A:C8	2.34	0.61
1:A:2161:C:H2'	1:A:2162:G:C8	2.35	0.61
10:O:64:ARG:HG2	10:O:79:PHE:CG	2.35	0.61
1:A:2302:G:O2'	6:G:126:ASP:O	2.16	0.61
1:A:2036:C:C6	1:A:2036:C:H5'	2.29	0.61
1:A:1351:C:H3'	34:A:3925:HOH:O	1.99	0.61
1:A:2127:G:H21	1:A:2173:A:H1'	1.64	0.61
16:U:58:ARG:HA	16:U:61:TRP:CE3	2.36	0.61
1:A:559:G:H22	16:U:49:HIS:CD2	2.19	0.61
1:A:2591:C:OP2	3:D:239:ARG:HB3	1.99	0.61
1:A:2162:G:H1'	1:A:2173:A:H1'	1.81	0.61
1:A:2318:G:O2'	1:A:2319:G:OP1	2.15	0.61
1:A:15:G:H5''	34:A:4613:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1815:A:OP2	3:D:54:ARG:NH2	2.33	0.61
1:A:1048:A:H4'	1:A:1049:C:OP1	2.01	0.61
1:A:143(A):C:H2'	1:A:144:C:H6	1.65	0.61
1:A:1327:C:OP2	34:A:4443:HOH:O	2.16	0.61
1:A:1584:C:H2'	1:A:1586:A:H5'	1.83	0.61
16:U:76:TYR:CE2	16:U:80:ILE:HG13	2.35	0.61
5:F:126:VAL:HG21	5:F:129:PHE:CE1	2.36	0.61
6:G:145:THR:OG1	6:G:146:TYR:N	2.34	0.61
1:A:2567:G:H2'	1:A:2568:C:C6	2.36	0.61
1:A:1278:A:OP1	13:R:36:THR:HG23	2.01	0.61
1:A:606:U:H4'	1:A:658:C:H4'	1.83	0.61
1:A:492:A:H2'	1:A:493:G:O4'	2.01	0.61
3:D:206:LEU:HD22	3:D:211:ARG:HG2	1.83	0.60
1:A:2327:A:H2'	1:A:2328:A:C8	2.35	0.60
1:A:1816:G:OP2	34:A:3694:HOH:O	2.16	0.60
1:A:1014:U:H2'	1:A:1015:G:C8	2.35	0.60
29:7:23:ARG:HH11	29:7:23:ARG:HB3	1.65	0.60
8:I:102:SER:HA	8:I:106:GLY:HA3	1.83	0.60
19:X:32:PRO:HA	19:X:77:LYS:HB2	1.84	0.60
1:A:143:G:H2'	1:A:143(A):C:C6	2.36	0.60
2:B:110:G:H2'	2:B:111:G:H8	1.66	0.60
1:A:2835:A:N3	34:A:4311:HOH:O	2.30	0.60
20:Y:102:CYS:O	20:Y:104:GLY:N	2.34	0.60
1:A:1047:G:H21	1:A:1111:A:N6	1.99	0.60
1:A:1153:C:OP1	16:U:92:ARG:NH1	2.33	0.60
2:B:110:G:H2'	2:B:111:G:C8	2.35	0.60
5:F:46:ARG:HG2	5:F:46:ARG:HH11	1.66	0.60
1:A:528:A:N1	1:A:2042:A:H2'	2.17	0.60
27:5:20:ARG:HG2	27:5:23:HIS:CD2	2.36	0.60
1:A:2228:G:O6	34:A:4139:HOH:O	2.11	0.60
6:G:11:TYR:CZ	6:G:16:ARG:HD3	2.36	0.60
1:A:1587:A:H2'	1:A:1588:C:C6	2.36	0.60
1:A:1470:G:N7	34:A:4114:HOH:O	2.32	0.60
1:A:1165:U:H2'	1:A:1166:C:C6	2.37	0.60
1:A:2572:A:N7	4:E:145:LYS:HB2	2.16	0.60
1:A:760:G:OP1	34:A:3624:HOH:O	2.17	0.60
11:P:127:ALA:O	11:P:148:LEU:HD23	2.02	0.60
21:Z:48:PHE:HE2	21:Z:71:VAL:HG11	1.66	0.60
1:A:1430:C:H2'	1:A:1431:U:C6	2.36	0.60
2:B:14:U:O3'	2:B:108:U:O2'	2.19	0.60
1:A:620:G:H5''	1:A:620:G:N3	2.16	0.60
1:A:1021:A:H62	1:A:1141:U:H3	1.48	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:S:10:ARG:NH2	14:S:91:PRO:HB2	2.16	0.60
2:B:49:C:OP1	14:S:97:ARG:N	2.33	0.60
3:D:108:PRO:HB3	3:D:143:HIS:HE1	1.66	0.60
1:A:226:G:H21	1:A:228:A:H62	1.49	0.60
4:E:32:PRO:HA	4:E:90:THR:HG22	1.84	0.60
18:W:80:PRO:O	18:W:100:THR:HB	2.01	0.60
29:7:34:ARG:NH1	29:7:41:ARG:O	2.34	0.60
1:A:2335:A:N7	1:A:2337:G:C5	2.70	0.60
2:B:52:A:N6	14:S:33:LYS:HG2	2.16	0.60
1:A:2199:A:H3'	1:A:2200:C:C6	2.37	0.60
12:Q:122:GLY:HA2	12:Q:125:LEU:HD12	1.83	0.60
1:A:2712(A):A:H5''	1:A:2713:A:OP2	2.01	0.60
1:A:1721:G:H2'	1:A:1740:G:O6	2.01	0.60
16:U:76:TYR:OH	16:U:92:ARG:NH1	2.35	0.60
26:4:14:ILE:HG22	26:4:33:VAL:HG23	1.84	0.60
1:A:2808:U:H5'	1:A:2891:G:O6	2.02	0.59
22:0:53:MET:HG3	22:0:59:LEU:CD2	2.32	0.59
3:D:33:LEU:O	3:D:64:ILE:HG13	2.02	0.59
1:A:994:C:H3'	16:U:54:LYS:HE3	1.83	0.59
1:A:94:C:H5'	1:A:94(A):G:OP2	2.01	0.59
1:A:1796:U:H2'	1:A:1797:C:C6	2.37	0.59
1:A:2104:G:N7	1:A:2186:G:N2	2.49	0.59
1:A:580:C:H2'	1:A:581:C:H6	1.66	0.59
1:A:330:A:C2	1:A:1210:A:H2'	2.27	0.59
1:A:192:C:OP1	34:A:3815:HOH:O	2.16	0.59
4:E:128:SER:OG	4:E:129:HIS:N	2.35	0.59
1:A:1639:U:C2'	1:A:1640:C:H5''	2.33	0.59
1:A:1049:C:H4'	1:A:1050:A:OP1	2.02	0.59
1:A:2294:C:P	14:S:89:ARG:HH22	2.26	0.59
1:A:873:G:N2	1:A:905:U:O2	2.36	0.59
16:U:76:TYR:HH	16:U:92:ARG:NH1	2.00	0.59
18:W:79:GLY:HA3	18:W:100:THR:HG22	1.85	0.59
1:A:911:A:OP1	34:A:4336:HOH:O	2.17	0.59
14:S:67:ARG:HG2	14:S:71:ARG:NH2	2.18	0.59
1:A:928:G:N1	34:A:4221:HOH:O	2.32	0.59
20:Y:23:ARG:HG2	20:Y:42:VAL:HG22	1.83	0.59
1:A:1050:A:H2'	1:A:1051:G:H8	1.68	0.59
1:A:1509(A):A:H3'	1:A:1509(B):A:H8	1.67	0.59
1:A:2321:G:N3	1:A:2321:G:H2'	2.17	0.58
19:X:8:ILE:O	24:2:36:ARG:NH2	2.36	0.58
1:A:1156:A:C8	16:U:51:LYS:HD2	2.38	0.58
1:A:2150:U:H2'	1:A:2151:G:H8	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:60:LEU:HD23	6:G:63:ILE:HD12	1.85	0.58
1:A:908:C:OP1	12:Q:22:LYS:HB3	2.03	0.58
1:A:1882:C:H5'	1:A:1883:G:OP2	2.02	0.58
1:A:1997:G:OP2	34:A:4349:HOH:O	2.17	0.58
1:A:2406:U:C2	11:P:72:PRO:HG2	2.38	0.58
2:B:43:C:H5''	26:4:1:MET:HG2	1.86	0.58
3:D:142:VAL:HG23	3:D:193:VAL:HA	1.85	0.58
1:A:1833:U:H2'	1:A:1834:U:H6	1.68	0.58
1:A:2612:C:O5'	27:5:2:ALA:HB3	2.03	0.58
6:G:72:ARG:HH12	6:G:87:PRO:HG3	1.68	0.58
1:A:1899:G:N3	1:A:1899:G:H2'	2.17	0.58
1:A:2298:A:N6	1:A:2318:G:H8	1.98	0.58
7:H:124:GLU:HB2	7:H:132:ARG:HB3	1.85	0.58
1:A:314:A:C2'	1:A:315:G:H5'	2.32	0.58
11:P:39:LYS:CB	11:P:45:LEU:HG	2.32	0.58
1:A:2023:G:H5'	1:A:2617:C:H4'	1.85	0.58
6:G:56:ALA:HA	6:G:153:ARG:HH21	1.67	0.58
1:A:1045:A:H4'	1:A:1047:G:C4	2.38	0.58
1:A:2406:U:H2'	1:A:2406:U:OP2	2.04	0.58
1:A:1991:U:H2'	1:A:1992:G:H5''	1.86	0.58
23:1:23:LYS:HB3	23:1:29:GLY:HA3	1.85	0.58
1:A:2115:G:C2	1:A:2117:A:N7	2.71	0.58
7:H:46:GLU:HB2	7:H:49:VAL:HG12	1.83	0.58
15:T:11:GLU:OE1	15:T:57:PHE:HB3	2.03	0.58
29:7:47:ARG:HH11	29:7:47:ARG:HG3	1.69	0.58
1:A:1047:G:H2'	1:A:1110:G:H1	1.67	0.58
8:I:104:GLN:HG2	8:I:105:HIS:CD2	2.38	0.58
12:Q:43:THR:OG1	12:Q:45:GLN:HG2	2.04	0.58
1:A:546:C:H6	1:A:547:A:H5'	1.68	0.58
1:A:19:C:H2'	1:A:20:C:H6	1.69	0.58
1:A:548:A:N6	17:V:19:LYS:H	2.02	0.58
1:A:1188:U:H4'	17:V:79:VAL:HG22	1.84	0.58
1:A:2235:G:O6	34:A:4459:HOH:O	2.17	0.58
1:A:2136:C:N4	1:A:2155:G:H1	1.98	0.58
1:A:1602:U:O4	34:A:3931:HOH:O	2.14	0.58
1:A:536:A:H2'	1:A:537:C:C6	2.39	0.58
1:A:543:C:H3'	1:A:545:G:O4'	2.04	0.58
1:A:661:C:O3'	34:A:4429:HOH:O	2.17	0.58
1:A:1047:G:H2'	1:A:1110:G:N2	2.19	0.58
1:A:1628:G:H2'	1:A:1629:U:C6	2.39	0.58
1:A:298:G:H5''	1:A:299:A:OP1	2.04	0.58
6:G:77:ILE:N	6:G:82:LEU:O	2.37	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:101:LEU:HD12	5:F:102:PRO:HD2	1.85	0.57
1:A:2562:U:H1'	10:O:23:ARG:HH11	1.69	0.57
28:6:9:LEU:HD13	28:6:51:GLU:HG3	1.85	0.57
20:Y:92:ASN:N	20:Y:93:GLY:HA2	2.19	0.57
1:A:271(M):G:O2'	1:A:271(N):U:OP1	2.18	0.57
1:A:1406:U:H2'	1:A:1407:C:C6	2.39	0.57
7:H:3:ARG:CZ	7:H:4:ILE:H	2.17	0.57
1:A:1935:G:H1'	1:A:1964:G:N2	2.19	0.57
11:P:46:LYS:HE3	11:P:51:PHE:CD1	2.40	0.57
3:D:274:ARG:HA	3:D:275:LYS:HB3	1.85	0.57
13:R:36:THR:HG22	13:R:37:THR:H	1.70	0.57
12:Q:37:LEU:HD21	12:Q:130:LYS:HB2	1.87	0.57
1:A:2853:C:H2'	1:A:2854:G:H8	1.67	0.57
6:G:19:LEU:HD22	6:G:23:PHE:HE1	1.70	0.57
1:A:1963:U:H4'	1:A:1964:G:OP1	2.05	0.57
1:A:1627:G:OP2	34:A:3944:HOH:O	2.17	0.57
6:G:32:PRO:HB2	6:G:172:LEU:HD22	1.87	0.57
27:5:45:VAL:HG11	27:5:58:LEU:HD13	1.87	0.57
1:A:1434:A:H61	1:A:1558:A:H62	1.52	0.57
1:A:1049:C:H2'	1:A:1050:A:H8	1.70	0.57
27:5:45:VAL:HA	27:5:52:TYR:HB2	1.87	0.57
3:D:2:ALA:HB3	3:D:20:ASP:HB3	1.86	0.57
1:A:1329:U:H5''	1:A:1330:C:H5	1.69	0.57
1:A:971:C:OP2	34:A:4245:HOH:O	2.18	0.57
20:Y:76:CYS:HB3	20:Y:79:CYS:HB2	1.87	0.57
28:6:16:CYS:HB3	28:6:43:CYS:SG	2.44	0.57
21:Z:108:PRO:HB2	21:Z:111:VAL:HG23	1.85	0.57
8:I:123:LEU:HD23	8:I:123:LEU:H	1.69	0.57
1:A:2184:G:H2'	1:A:2185:C:O4'	2.05	0.57
1:A:642:G:O6	34:A:3704:HOH:O	2.16	0.57
1:A:1657:C:H2'	1:A:1658:C:C6	2.39	0.57
1:A:821:A:H2'	1:A:946:G:H5''	1.87	0.57
1:A:848:G:OP1	34:A:4226:HOH:O	2.18	0.56
5:F:184:TYR:O	5:F:188:ARG:HG3	2.05	0.56
31:9:10:ILE:N	31:9:14:CYS:SG	2.77	0.56
1:A:495:G:H21	18:W:61:ASN:HD21	1.53	0.56
11:P:52:GLU:OE2	30:8:57:ARG:NH1	2.37	0.56
1:A:2591:C:OP1	3:D:239:ARG:HG2	2.05	0.56
1:A:580:C:H2'	1:A:581:C:C6	2.40	0.56
1:A:422:A:OP2	34:A:4071:HOH:O	2.18	0.56
1:A:1030:G:OP2	12:Q:128:LYS:NZ	2.35	0.56
15:T:93:ARG:HH11	15:T:93:ARG:HG2	1.69	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1403:C:C5'	1:A:1471:A:H1'	2.35	0.56
1:A:1607:C:H4'	1:A:1608:A:O5'	2.04	0.56
1:A:271(E):U:H2'	1:A:271(F):C:C6	2.39	0.56
14:S:96:GLY:N	14:S:99:LYS:H	2.03	0.56
21:Z:82:ARG:HB3	21:Z:82:ARG:NH2	2.19	0.56
18:W:18:ARG:NH1	18:W:76:VAL:O	2.38	0.56
1:A:1050:A:C4	1:A:1051:G:C8	2.93	0.56
1:A:2273:A:H2'	1:A:2274:A:C8	2.40	0.56
24:2:50:ILE:C	24:2:52:ASP:H	2.07	0.56
18:W:60:ASN:HD22	18:W:60:ASN:N	2.02	0.56
1:A:747:U:O2	1:A:2014:A:H1'	2.04	0.56
9:N:24:GLY:HA2	9:N:27:ALA:HB3	1.85	0.56
1:A:2110:G:OP2	1:A:2110:G:H8	1.88	0.56
1:A:2661:G:H2'	1:A:2662:A:C8	2.41	0.56
1:A:2322:A:H2'	1:A:2323:G:O4'	2.05	0.56
1:A:1131:G:H21	9:N:73:THR:HG21	1.71	0.56
1:A:1858:G:H1'	1:A:1884:A:N6	2.21	0.56
1:A:1812:A:O2'	3:D:45:ASN:N	2.38	0.56
4:E:201:THR:OG1	4:E:202:LYS:N	2.38	0.56
15:T:24:PRO:HA	15:T:49:VAL:HG22	1.87	0.56
15:T:60:THR:HG22	15:T:77:PRO:HA	1.87	0.56
1:A:631:A:OP2	30:8:47:LYS:NZ	2.25	0.56
13:R:20:LEU:HD21	13:R:40:LYS:HD3	1.87	0.56
16:U:36:ARG:HD2	16:U:40:PHE:CZ	2.41	0.56
6:G:86:MET:O	6:G:88:ILE:HG13	2.06	0.56
26:4:35:VAL:HA	26:4:39:CYS:SG	2.44	0.56
1:A:2835:A:N7	34:A:4341:HOH:O	2.33	0.56
1:A:1762:A:H8	1:A:1762:A:O5'	1.87	0.56
6:G:5:VAL:HG12	26:4:25:TYR:CE1	2.41	0.56
12:Q:24:GLY:O	12:Q:102:VAL:HG23	2.05	0.56
1:A:2477:C:O2	31:9:4:ARG:NH2	2.35	0.56
1:A:2335:A:O2'	1:A:2336:A:OP2	2.21	0.56
1:A:1375:C:H3'	34:A:3924:HOH:O	2.05	0.56
1:A:1601:G:N7	34:A:3931:HOH:O	2.33	0.56
21:Z:158:PRO:O	21:Z:161:VAL:HB	2.06	0.56
1:A:1449:A:H5'	1:A:1450:G:OP2	2.05	0.56
1:A:1865:G:H5'	1:A:1866:C:OP2	2.06	0.56
14:S:15:ARG:O	14:S:19:LYS:HG2	2.06	0.56
14:S:99:LYS:HE2	14:S:103:GLU:OE2	2.06	0.56
7:H:144:VAL:O	7:H:148:ILE:HG12	2.05	0.56
1:A:2492:U:H2'	1:A:2493:U:C6	2.40	0.56
1:A:751:A:H5'	18:W:90:ARG:HA	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:174:ASP:OD2	4:E:175:VAL:N	2.37	0.56
21:Z:151:HIS:HD2	21:Z:168:GLU:O	1.89	0.56
24:2:13:ALA:HA	24:2:16:LEU:HD12	1.88	0.56
1:A:1635:G:OP1	34:A:3949:HOH:O	2.18	0.56
1:A:275:G:C2'	1:A:276:A:H5'	2.36	0.56
10:O:73:ASP:OD1	15:T:32:TYR:OH	2.07	0.55
2:B:66:A:N6	2:B:109:C:H5'	2.19	0.55
1:A:1364:G:C8	23:1:3:LYS:HD3	2.41	0.55
21:Z:52:SER:OG	21:Z:53:ILE:N	2.39	0.55
4:E:52:LEU:HB3	4:E:76:ARG:HG2	1.89	0.55
1:A:2845:G:O2'	1:A:2846:G:H5'	2.06	0.55
1:A:1019:U:H3	1:A:1142(A):A:N6	1.99	0.55
1:A:1366:A:OP1	23:1:3:LYS:NZ	2.38	0.55
1:A:364:C:OP2	34:A:4238:HOH:O	2.18	0.55
1:A:2014:A:OP1	34:A:3646:HOH:O	2.18	0.55
1:A:1632:A:N6	34:A:3936:HOH:O	2.40	0.55
1:A:27:G:HO2'	1:A:28:A:P	2.27	0.55
1:A:1833:U:H2'	1:A:1834:U:C6	2.41	0.55
1:A:652(S):C:H2'	1:A:652(T):C:O4'	2.05	0.55
6:G:59:GLU:O	6:G:63:ILE:N	2.40	0.55
26:4:14:ILE:HD11	26:4:24:THR:OG1	2.06	0.55
1:A:1509(B):A:H3'	1:A:1510:G:H8	1.72	0.55
1:A:922:U:O4	34:A:4215:HOH:O	2.16	0.55
2:B:52:A:O2'	2:B:53:A:H5''	2.06	0.55
9:N:99:LEU:HD22	9:N:103:VAL:HG23	1.89	0.55
12:Q:42:ILE:HD13	12:Q:97:VAL:HG21	1.89	0.55
1:A:2463:C:C2'	1:A:2464:C:H5'	2.37	0.55
15:T:23:ARG:HG3	15:T:120:ARG:NH1	2.22	0.55
1:A:2319:G:H22	14:S:3:ARG:HD2	1.71	0.55
1:A:196:A:O4'	11:P:46:LYS:HE2	2.07	0.55
13:R:12:ARG:HG2	13:R:16:HIS:CG	2.42	0.55
11:P:112:LEU:HD22	11:P:113:LYS:N	2.22	0.55
5:F:65:TRP:HH2	5:F:72:ARG:HH21	1.55	0.55
16:U:59:ARG:O	16:U:63:VAL:HG23	2.07	0.55
5:F:123:LEU:HD13	5:F:192:LEU:HD13	1.88	0.55
2:B:55:U:O3'	6:G:27:ASN:ND2	2.40	0.55
3:D:175:LEU:HD12	3:D:185:VAL:HG21	1.89	0.55
1:A:1419:A:O2'	1:A:1421:G:N7	2.29	0.55
20:Y:43:ASN:OD1	20:Y:65:ALA:HB3	2.07	0.55
15:T:109:GLU:O	15:T:113:LYS:N	2.35	0.55
1:A:517:C:OP1	27:5:16:ARG:NH2	2.40	0.55
1:A:1494:A:H2'	1:A:1495:A:H8	1.70	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2463:C:O2'	1:A:2464:C:H5'	2.07	0.55
1:A:2699:C:H2'	1:A:2700:C:O4'	2.06	0.55
1:A:1300:U:H4'	1:A:1301:A:C5'	2.36	0.55
1:A:1019:U:O2'	1:A:1021:A:H2	1.90	0.54
1:A:271(D):G:H2'	1:A:271(E):U:O4'	2.07	0.54
1:A:530:G:N3	1:A:530:G:O4'	2.40	0.54
1:A:2867:G:OP2	15:T:119:LYS:NZ	2.35	0.54
1:A:1912:A:O2'	1:A:1913:A:OP2	2.25	0.54
6:G:178:PHE:HB3	6:G:180:PHE:CE1	2.43	0.54
5:F:28:ILE:HD13	5:F:119:ARG:HE	1.71	0.54
15:T:53:ARG:HH11	15:T:53:ARG:HB3	1.71	0.54
6:G:38:VAL:HG22	6:G:93:THR:HG23	1.89	0.54
8:I:12:LEU:HD22	8:I:19:VAL:HG21	1.89	0.54
1:A:652(B):A:H2'	1:A:652(B):A:N3	2.22	0.54
11:P:38:GLN:O	11:P:40:SER:N	2.40	0.54
19:X:5:TYR:CZ	24:2:30:ARG:HB2	2.42	0.54
1:A:2753:A:N3	31:9:15:LYS:NZ	2.55	0.54
6:G:37:VAL:HG23	6:G:99:MET:HG3	1.88	0.54
1:A:2884:U:O2	27:5:53:ALA:HB2	2.08	0.54
1:A:2526:G:H5'	1:A:2742:C:O2'	2.08	0.54
1:A:997:G:OP1	16:U:92:ARG:HG2	2.07	0.54
1:A:2836:U:C4	1:A:2883:A:N6	2.76	0.54
4:E:72:VAL:HA	4:E:73:GLU:OE2	2.08	0.54
1:A:185:U:H4'	1:A:218:A:H4'	1.90	0.54
1:A:446:G:OP2	34:A:4018:HOH:O	2.19	0.54
9:N:56:ASN:H	9:N:125:GLY:HA3	1.72	0.54
1:A:1028:A:N6	1:A:1125:G:H2'	2.22	0.54
22:0:27:GLU:HG3	22:0:68:GLU:HA	1.90	0.54
1:A:315:G:H2'	1:A:316:C:C6	2.43	0.54
1:A:2357:U:O2	34:A:4154:HOH:O	2.18	0.54
1:A:2850:A:C2	1:A:2851:A:C4	2.96	0.54
2:B:61:G:C6	2:B:62:C:C4	2.95	0.54
25:3:18:ASP:OD1	25:3:18:ASP:N	2.35	0.54
1:A:1507:A:O2'	1:A:1508:A:O5'	2.17	0.54
7:H:69:ARG:HG3	7:H:70:THR:N	2.23	0.54
2:B:105:A:OP1	21:Z:72:ARG:NH1	2.38	0.54
1:A:2116:G:H4'	1:A:2117:A:OP1	2.08	0.54
5:F:11:VAL:O	5:F:17:ARG:HA	2.08	0.54
1:A:903:C:H2'	1:A:904:C:C6	2.43	0.54
1:A:2849:U:H4'	1:A:2868:A:C2	2.43	0.54
23:1:2:SER:HB3	23:1:46:LEU:HD11	1.90	0.54
29:7:9:ARG:HH21	29:7:47:ARG:HD3	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2562:U:H1'	10:O:23:ARG:HD3	1.90	0.54
1:A:1321:A:H2'	1:A:1322:A:O4'	2.08	0.54
1:A:603:A:H4'	1:A:604:G:H5'	1.89	0.54
17:V:78:LYS:O	34:V:202:HOH:O	2.18	0.54
1:A:878:A:H2'	1:A:879:G:H5'	1.90	0.54
1:A:307:G:N2	1:A:309:G:H3'	2.23	0.54
1:A:2461:C:H2'	1:A:2462:U:C6	2.43	0.54
1:A:828:U:H4'	1:A:831:G:N1	2.23	0.54
6:G:124:SER:HB2	6:G:131:TYR:CZ	2.43	0.53
1:A:911:A:H2'	12:Q:9:TYR:OH	2.08	0.53
3:D:148:GLU:HB2	3:D:151:LYS:HD2	1.90	0.53
13:R:36:THR:HG22	13:R:37:THR:N	2.23	0.53
8:I:101:LEU:HD21	8:I:107:VAL:HG12	1.90	0.53
1:A:9:U:H3	1:A:2629:A:H2	1.52	0.53
9:N:120:LEU:HD22	9:N:122:VAL:HG23	1.90	0.53
1:A:1140:C:OP1	9:N:23:LEU:O	2.25	0.53
14:S:99:LYS:O	14:S:103:GLU:HG3	2.08	0.53
1:A:674:G:C1'	5:F:74:ARG:HD3	2.38	0.53
1:A:19:C:H2'	1:A:20:C:C6	2.43	0.53
10:O:73:ASP:OD2	10:O:73:ASP:N	2.39	0.53
8:I:5:LEU:HD11	8:I:19:VAL:HG22	1.90	0.53
10:O:10:VAL:HG13	10:O:17:ARG:O	2.09	0.53
1:A:649:G:H2'	1:A:650:C:C6	2.43	0.53
1:A:330:A:HO2'	1:A:331:A:H8	1.55	0.53
1:A:2741:A:H2'	1:A:2742:C:O4'	2.08	0.53
1:A:71:A:H5'	1:A:71:A:C8	2.44	0.53
15:T:64:ARG:HB2	15:T:73:GLU:HG2	1.89	0.53
1:A:2732:G:H3'	1:A:2733:A:O4'	2.07	0.53
1:A:769:G:H5'	1:A:1379:A:N6	2.23	0.53
1:A:1026:U:O2	1:A:1026:U:H5''	2.09	0.53
1:A:2602:A:H1'	1:A:2603:G:C5'	2.39	0.53
4:E:9:VAL:HG13	4:E:25:VAL:O	2.09	0.53
1:A:1279:G:H4'	13:R:31:HIS:CD2	2.43	0.53
1:A:1252:G:C2	1:A:1253:A:C2	2.96	0.53
11:P:84:ASN:HB2	11:P:86:LYS:HD3	1.90	0.53
1:A:729:G:OP2	3:D:13:ARG:NH1	2.40	0.53
9:N:36:GLY:HA2	9:N:38:HIS:CE1	2.43	0.53
1:A:1138:G:O2'	9:N:105:GLY:HA3	2.08	0.53
1:A:413:C:H6	1:A:413:C:O5'	1.92	0.53
1:A:1352:U:P	34:A:3922:HOH:O	2.67	0.53
1:A:2318:G:H22	14:S:3:ARG:HH11	1.56	0.53
20:Y:79:CYS:HB3	20:Y:81:LYS:H	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2097:C:H2'	1:A:2098:U:O4'	2.08	0.53
2:B:2:C:H2'	2:B:3:C:C6	2.42	0.53
1:A:2133:G:H21	1:A:2158:A:H62	1.55	0.53
1:A:2638:G:P	4:E:82:ARG:HH22	2.31	0.53
1:A:2513:G:N2	4:E:143:ASN:HD21	2.07	0.53
19:X:35:THR:O	19:X:39:ILE:HG13	2.08	0.53
3:D:131:LEU:HD22	3:D:136:ILE:HG12	1.91	0.53
27:5:41:PRO:O	27:5:44:THR:OG1	2.27	0.53
1:A:71:A:OP2	1:A:71:A:H3'	2.09	0.53
6:G:105:LYS:NZ	26:4:26:SER:HB2	2.24	0.53
1:A:1587:A:H2'	1:A:1588:C:H6	1.74	0.53
1:A:1858:G:H1'	1:A:1884:A:H61	1.72	0.53
21:Z:152:ALA:HA	21:Z:155:LEU:HD13	1.89	0.53
13:R:55:ALA:HB2	13:R:79:LEU:HD13	1.90	0.53
1:A:566:U:H5''	11:P:29:LYS:HE3	1.89	0.53
12:Q:27:VAL:N	12:Q:138:ASP:OD1	2.41	0.53
1:A:1288:U:C2	1:A:1327:C:O2	2.61	0.53
18:W:71:VAL:HA	18:W:107:LEU:HD12	1.91	0.53
25:3:7:LYS:HG3	25:3:34:GLU:HG2	1.91	0.53
1:A:826:U:OP1	1:A:2428:G:H3'	2.09	0.53
15:T:53:ARG:NH1	15:T:53:ARG:HB3	2.24	0.53
1:A:2629:A:O2'	1:A:2630:G:OP2	2.21	0.53
1:A:2324:C:H5''	1:A:2325:G:H5'	1.90	0.53
26:4:40:HIS:CE1	26:4:42:PHE:HB2	2.44	0.53
1:A:2312:U:O2'	6:G:40:ASN:ND2	2.37	0.53
1:A:2126:A:H4'	1:A:2127:G:O5'	2.09	0.53
6:G:111:LEU:HB2	6:G:112:PRO:HD3	1.91	0.53
20:Y:23:ARG:HH11	20:Y:23:ARG:HB2	1.74	0.53
1:A:896:A:N1	12:Q:60:ARG:NH2	2.56	0.53
28:6:13:CYS:SG	28:6:47:THR:HG21	2.49	0.53
1:A:917:A:H5'	1:A:918:A:OP2	2.08	0.53
1:A:61:G:H1	1:A:94:C:H42	1.58	0.52
1:A:2364:C:H2'	1:A:2365:G:O4'	2.09	0.52
4:E:195:LEU:HG	4:E:196:VAL:N	2.24	0.52
8:I:135:GLU:C	8:I:137:PRO:HD3	2.30	0.52
28:6:14:THR:HB	28:6:48:VAL:O	2.09	0.52
1:A:243:U:OP1	30:8:6:THR:OG1	2.14	0.52
1:A:2173:A:OP2	1:A:2174:C:H5	1.93	0.52
3:D:85:ASP:OD2	3:D:88:ARG:NH1	2.40	0.52
1:A:819:A:C4	1:A:1189:A:C2	2.97	0.52
1:A:2282:G:H4'	1:A:2389:G:O2'	2.08	0.52
6:G:150:ASP:CG	6:G:151:ALA:H	2.11	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2180:U:H2'	1:A:2181:G:C8	2.44	0.52
1:A:485:C:H2'	1:A:486:C:H6	1.74	0.52
1:A:1628:G:H2'	1:A:1629:U:H6	1.74	0.52
24:2:51:ARG:O	24:2:55:ARG:HB2	2.09	0.52
3:D:130:ALA:HB2	3:D:192:THR:HB	1.91	0.52
1:A:443:A:N7	5:F:45:ARG:HG2	2.24	0.52
1:A:853:G:H1	1:A:924:C:H42	1.56	0.52
1:A:528:A:C2	1:A:2042:A:H2'	2.44	0.52
14:S:11:LYS:O	14:S:15:ARG:HG3	2.10	0.52
1:A:1914:C:OP2	1:A:1914:C:H6	1.91	0.52
1:A:7:G:H2'	1:A:8:A:C8	2.44	0.52
5:F:164:ARG:HD2	5:F:175:THR:HG23	1.90	0.52
1:A:1049:C:O2'	1:A:1050:A:O5'	2.25	0.52
12:Q:26:TYR:CE1	12:Q:28:ALA:HB2	2.44	0.52
1:A:1546:C:H5'	1:A:1547:C:H5'	1.92	0.52
21:Z:182:LYS:O	21:Z:186:GLU:HG2	2.09	0.52
2:B:20:C:C2'	2:B:21:G:H5'	2.39	0.52
1:A:2200:C:H5'	1:A:2201:C:OP2	2.07	0.52
1:A:1790:C:H5''	1:A:1791:A:OP1	2.09	0.52
1:A:602:G:O2'	1:A:655:A:N6	2.43	0.52
1:A:863:A:H2'	1:A:864:G:C8	2.44	0.52
1:A:652(O):C:H2'	1:A:652(P):G:C8	2.45	0.52
1:A:2690:C:OP2	13:R:14:SER:HB3	2.10	0.52
20:Y:28:LYS:HG3	20:Y:40:GLU:HG2	1.92	0.52
1:A:143(A):C:H2'	1:A:144:C:C6	2.44	0.52
9:N:96:GLU:H	9:N:96:GLU:CD	2.13	0.52
1:A:2096:U:H3	1:A:2193:G:H1	1.57	0.52
1:A:1669:A:H5''	1:A:2550:G:OP1	2.10	0.52
14:S:26:LEU:HD22	14:S:87:PHE:CD1	2.45	0.52
1:A:71:A:H5'	1:A:71:A:H8	1.75	0.52
1:A:2308:G:H4'	1:A:2309:A:OP2	2.08	0.52
13:R:37:THR:OG1	13:R:40:LYS:HG3	2.09	0.52
1:A:1819:A:H4'	1:A:1820:U:O5'	2.10	0.52
1:A:944:G:O3'	34:A:3783:HOH:O	2.19	0.52
15:T:95:ARG:HG2	15:T:95:ARG:NH1	2.19	0.52
1:A:2537:U:H2'	1:A:2538:C:C6	2.45	0.52
16:U:44:ASN:ND2	17:V:75:PHE:O	2.36	0.52
1:A:1810:A:H2'	1:A:1811:G:O4'	2.09	0.52
7:H:7:LEU:HD12	7:H:8:PRO:HD2	1.92	0.52
1:A:2109:U:H1'	1:A:2181:G:N2	2.25	0.51
1:A:1688:U:H1'	1:A:1701:A:C6	2.45	0.51
1:A:2564:A:C2	1:A:2647:U:H4'	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:706:A:H2'	1:A:707:G:O4'	2.10	0.51
1:A:764:A:OP1	3:D:208:LYS:HE2	2.10	0.51
2:B:13:A:N1	2:B:69:G:O2'	2.38	0.51
6:G:116:ASP:H	6:G:136:ARG:HH22	1.57	0.51
1:A:2880:C:O3'	13:R:90:ARG:NH1	2.43	0.51
1:A:229:A:H3'	1:A:229:A:C8	2.45	0.51
1:A:581:C:H2'	1:A:582:G:C8	2.46	0.51
1:A:2790:A:H3'	1:A:2790:A:N3	2.25	0.51
1:A:2441:C:OP2	1:A:2586:C:O2'	2.27	0.51
4:E:111:ARG:HD3	4:E:160:TYR:CE1	2.45	0.51
1:A:588:U:H2'	1:A:589:C:C6	2.45	0.51
26:4:40:HIS:O	26:4:42:PHE:N	2.41	0.51
6:G:41:GLN:HG3	6:G:60:LEU:HD11	1.93	0.51
1:A:2319:G:C2	14:S:3:ARG:HA	2.46	0.51
1:A:83:G:N2	1:A:102:G:H2'	2.25	0.51
1:A:228:A:H2'	1:A:230:U:O4'	2.11	0.51
1:A:2853:C:H2'	1:A:2854:G:C8	2.46	0.51
1:A:1427:A:H4'	1:A:1428:C:O5'	2.11	0.51
5:F:183:VAL:O	5:F:187:VAL:HG23	2.11	0.51
7:H:154:PRO:HB3	7:H:163:TYR:CZ	2.44	0.51
28:6:11:LEU:HB2	28:6:21:TYR:HB2	1.90	0.51
1:A:2208:A:H1'	1:A:2219:G:C5	2.46	0.51
1:A:1530:C:O2'	1:A:1531:C:P	2.68	0.51
1:A:573:G:O2'	1:A:574:C:H3'	2.11	0.51
5:F:129:PHE:O	5:F:132:VAL:HG13	2.10	0.51
1:A:188:G:H1	1:A:208:C:N4	2.09	0.51
1:A:1113:U:H2'	1:A:1114:G:C8	2.46	0.51
8:I:134:PRO:C	8:I:136:VAL:H	2.14	0.51
6:G:3:LEU:HD11	6:G:97:ASP:HB3	1.92	0.51
1:A:187:G:N3	1:A:1365:A:H2	2.08	0.51
7:H:40:GLU:OE2	7:H:60:ARG:NH1	2.43	0.51
10:O:31:LYS:HB3	10:O:32:TYR:CE2	2.45	0.51
1:A:2144:U:H2'	1:A:2146:C:N4	2.26	0.51
30:8:23:VAL:HG12	30:8:47:LYS:HB3	1.92	0.51
1:A:2134:A:N6	1:A:2157:G:H1'	2.26	0.51
2:B:7:G:H5''	2:B:7:G:H8	1.76	0.51
3:D:67:PHE:HB3	3:D:153:ALA:H	1.76	0.51
6:G:6:ALA:O	6:G:10:LYS:N	2.38	0.51
30:8:61:LEU:C	30:8:63:PRO:HD3	2.31	0.51
11:P:95:VAL:HG22	11:P:125:VAL:HB	1.93	0.51
1:A:2199:A:H5''	1:A:2200:C:OP2	2.10	0.51
1:A:396:G:O3'	23:1:44:PRO:HA	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2318:G:N2	14:S:3:ARG:HH11	2.09	0.51
14:S:14:VAL:HG11	14:S:90:GLY:O	2.10	0.51
6:G:133:LEU:HG	6:G:157:ILE:HB	1.92	0.51
21:Z:151:HIS:N	21:Z:154:ASP:OD1	2.42	0.51
9:N:55:VAL:HG22	9:N:125:GLY:HA3	1.92	0.51
1:A:627:A:H62	11:P:84:ASN:HD21	1.59	0.51
4:E:111:ARG:HD3	4:E:160:TYR:CD1	2.45	0.51
4:E:37:ARG:HB2	4:E:46:ALA:N	2.26	0.51
1:A:340:A:H2'	1:A:341:G:O4'	2.10	0.51
1:A:784:A:C5	3:D:229:VAL:HG21	2.46	0.51
1:A:1018:C:O2'	1:A:1019:U:H5'	2.10	0.51
1:A:1510:G:H2'	1:A:1511:C:C6	2.46	0.51
21:Z:160:GLY:HA2	21:Z:161:VAL:HB	1.92	0.51
21:Z:101:PRO:O	21:Z:102:LEU:HD12	2.11	0.51
18:W:35:ILE:HG23	27:5:28:PRO:HD2	1.93	0.51
1:A:1336:A:H2'	1:A:1337:G:C8	2.46	0.51
23:1:86:SER:HB3	23:1:89:GLU:OE2	2.10	0.51
1:A:265:A:H1'	1:A:266:G:O4'	2.11	0.51
5:F:181:LEU:HD11	5:F:186:ILE:HD11	1.93	0.51
1:A:2320:A:N3	1:A:2320:A:H2'	2.25	0.51
1:A:271(F):C:H2'	1:A:271(G):C:C6	2.38	0.51
1:A:1796:U:H2'	1:A:1797:C:H6	1.74	0.51
1:A:1342:A:OP2	34:A:3929:HOH:O	2.19	0.51
1:A:1297:C:OP1	1:A:2710:C:H4'	2.11	0.51
1:A:229:A:H8	1:A:229:A:H3'	1.76	0.51
1:A:2839:G:H5'	13:R:46:GLY:HA2	1.92	0.51
13:R:72:ASP:O	13:R:76:VAL:HG23	2.11	0.51
1:A:2610:C:H4'	1:A:2611:U:OP2	2.11	0.51
2:B:37:C:C5	2:B:38:C:C5	2.99	0.50
1:A:2672:G:H5''	1:A:2672:G:H8	1.76	0.50
1:A:1693:U:O2'	3:D:14:ARG:NH2	2.44	0.50
7:H:80:SER:OG	7:H:81:GLU:N	2.44	0.50
1:A:796:C:H2'	1:A:797:C:C6	2.47	0.50
21:Z:39:VAL:HG21	21:Z:44:PHE:HB2	1.93	0.50
19:X:21:PHE:CZ	19:X:92:LEU:HD12	2.46	0.50
1:A:459:U:H4'	29:7:40:TRP:CZ3	2.46	0.50
1:A:2590:A:OP2	3:D:238:GLY:HA2	2.12	0.50
1:A:1586:A:O5'	1:A:1586:A:H8	1.93	0.50
1:A:2350:C:H2'	1:A:2351:G:O4'	2.12	0.50
1:A:2632:A:O2'	1:A:2811:G:O2'	2.23	0.50
15:T:106:SER:O	15:T:110:ILE:HG12	2.11	0.50
1:A:662:G:OP1	34:A:4430:HOH:O	2.19	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:89:GLY:C	6:G:90:LEU:HD23	2.31	0.50
6:G:11:TYR:HA	6:G:15:VAL:HB	1.92	0.50
1:A:1641:A:H2'	1:A:1642:G:O4'	2.11	0.50
1:A:207:A:H2'	1:A:208:C:O4'	2.11	0.50
1:A:2150:U:H2'	1:A:2151:G:C8	2.47	0.50
1:A:863:A:N7	34:A:4338:HOH:O	2.35	0.50
1:A:1799:G:H5'	1:A:1819:A:H61	1.76	0.50
8:I:56:LYS:O	8:I:60:GLU:HG2	2.11	0.50
26:4:12:ALA:HA	26:4:29:PRO:HA	1.93	0.50
1:A:1925:C:O2'	1:A:1926:U:H5'	2.11	0.50
1:A:2114:A:O2'	1:A:2168:G:H5'	2.11	0.50
1:A:2173:A:H2'	1:A:2174:C:H5'	1.92	0.50
1:A:1364:G:OP1	23:1:2:SER:HA	2.12	0.50
1:A:2104:G:O6	1:A:2185:C:N3	2.44	0.50
1:A:2465:C:O2	1:A:2486:G:C2	2.64	0.50
1:A:1638:C:O2	1:A:2698:U:O2'	2.25	0.50
1:A:1794:U:H2'	1:A:1795:C:C6	2.47	0.50
1:A:979:G:H3'	1:A:980:A:C5'	2.41	0.50
7:H:24:VAL:HG13	7:H:37:VAL:HG21	1.92	0.50
1:A:375:C:H5''	34:A:4590:HOH:O	2.10	0.50
2:B:90:A:N7	2:B:91:C:H1'	2.27	0.50
1:A:2272:U:H5''	1:A:2273:A:OP1	2.11	0.50
4:E:37:ARG:HB2	4:E:46:ALA:H	1.77	0.50
1:A:1766:U:H2'	1:A:1767:C:H6	1.76	0.50
4:E:38:THR:O	4:E:42:ASP:N	2.43	0.50
14:S:49:VAL:HG13	14:S:76:LYS:HD2	1.92	0.50
19:X:31:HIS:CD2	19:X:33:LYS:H	2.29	0.50
5:F:22:ALA:HB1	5:F:24:LEU:HD22	1.92	0.50
1:A:1430:C:H2'	1:A:1431:U:H6	1.77	0.50
1:A:1328:G:O5'	1:A:1328:G:H8	1.94	0.50
9:N:34:LEU:O	9:N:49:GLY:HA3	2.11	0.50
2:B:77:U:H4'	21:Z:84:GLU:OE1	2.12	0.50
5:F:71:GLY:N	34:F:401:HOH:O	2.21	0.50
1:A:2296:U:N3	1:A:2333:A:N3	2.60	0.50
28:6:4:GLU:HG3	28:6:5:VAL:N	2.27	0.50
12:Q:27:VAL:HG11	12:Q:134:ARG:HG2	1.94	0.50
1:A:2345:G:O6	34:A:4158:HOH:O	2.19	0.50
23:1:51:VAL:HG11	23:1:74:VAL:HG21	1.92	0.50
9:N:67:LEU:HA	9:N:87:LEU:HD12	1.93	0.50
15:T:51:ARG:HG3	15:T:98:LYS:HE3	1.94	0.50
6:G:81:LYS:CB	6:G:82:LEU:HD12	2.41	0.50
1:A:2126:A:H1'	1:A:2127:G:OP2	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:996:A:C2	1:A:997:G:C8	3.00	0.50
1:A:2773:C:O2'	1:A:2774:C:H5'	2.12	0.50
1:A:69:C:N4	34:A:4036:HOH:O	2.45	0.50
28:6:14:THR:HG21	28:6:48:VAL:HG13	1.93	0.50
1:A:2755:C:HO2'	1:A:2756:U:H6	1.60	0.50
21:Z:180:VAL:O	21:Z:183:LEU:HB2	2.12	0.50
6:G:44:GLY:HA2	6:G:88:ILE:HG22	1.94	0.50
1:A:784:A:H5'	1:A:785:G:OP1	2.11	0.50
1:A:2125:G:N2	1:A:2126:A:H62	2.10	0.50
3:D:101:GLU:OE1	3:D:103:ARG:HD3	2.12	0.50
2:B:111:G:H2'	2:B:112:U:H6	1.77	0.50
8:I:76:THR:O	8:I:105:HIS:HE1	1.94	0.50
3:D:254:THR:O	3:D:254:THR:OG1	2.28	0.50
1:A:1689:A:N6	1:A:1698:A:H2	1.98	0.49
23:1:82:LEU:O	23:1:83:GLU:HG3	2.11	0.49
1:A:2472:G:H5'	1:A:2473:U:C5'	2.39	0.49
1:A:1328:G:H2'	1:A:1330:C:C5	2.47	0.49
2:B:17:C:H2'	2:B:18:G:O4'	2.12	0.49
29:7:8:ASN:OD1	29:7:8:ASN:C	2.50	0.49
1:A:1506:C:H2'	1:A:1507:A:H5'	1.95	0.49
1:A:184:C:H2'	1:A:185:U:H6	1.77	0.49
21:Z:179:ASP:HB2	21:Z:182:LYS:HD3	1.94	0.49
1:A:2496:C:OP1	12:Q:82:ARG:HB3	2.12	0.49
11:P:38:GLN:C	11:P:40:SER:H	2.13	0.49
1:A:1513:C:H2'	1:A:1514:U:H6	1.77	0.49
1:A:102:G:HO2'	1:A:103:A:P	2.34	0.49
3:D:238:GLY:O	3:D:239:ARG:HB3	2.13	0.49
19:X:9:LEU:HA	24:2:36:ARG:HH21	1.77	0.49
7:H:171:LEU:H	7:H:171:LEU:HD23	1.77	0.49
21:Z:138:GLU:HG2	21:Z:156:LYS:NZ	2.28	0.49
1:A:2010:G:O6	34:A:4663:HOH:O	2.19	0.49
1:A:1268:A:H2'	1:A:1269:A:O4'	2.12	0.49
1:A:1512:U:H2'	1:A:1513:C:C6	2.46	0.49
20:Y:40:GLU:O	20:Y:42:VAL:HG23	2.11	0.49
1:A:443:A:H1'	1:A:1201:C:O4'	2.12	0.49
1:A:1889:A:H2'	1:A:1890:A:C8	2.47	0.49
1:A:557:U:H2'	1:A:558:G:H8	1.77	0.49
1:A:2250:G:C5	12:Q:83:MET:HB2	2.47	0.49
1:A:105:C:H2'	1:A:106:C:C6	2.47	0.49
1:A:1489:U:H3'	1:A:1489:U:H6	1.78	0.49
25:3:46:ASN:O	25:3:50:VAL:HG22	2.13	0.49
2:B:15:A:H1'	2:B:110:G:C5	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1774:C:H6	1:A:1774:C:O5'	1.94	0.49
31:9:10:ILE:HD12	31:9:32:HIS:HA	1.93	0.49
21:Z:125:LEU:HG	21:Z:164:ALA:HB3	1.94	0.49
1:A:2711:A:OP1	1:A:2712(A):A:OP1	2.31	0.49
2:B:90:A:C5	2:B:91:C:H1'	2.48	0.49
10:O:115:VAL:HG13	10:O:121:VAL:HG21	1.94	0.49
1:A:1031:G:H1	1:A:1123:C:H42	1.59	0.49
1:A:1405:U:H2'	1:A:1406:U:H6	1.74	0.49
1:A:2307:G:H5'	1:A:2308:G:N2	2.28	0.49
1:A:143:G:H2'	1:A:143(A):C:H6	1.77	0.49
1:A:1156:A:OP2	34:A:4254:HOH:O	2.20	0.49
8:I:58:LEU:HG	8:I:59:ALA:N	2.28	0.49
1:A:2125:G:N2	1:A:2126:A:N6	2.61	0.49
1:A:2158:A:H1'	1:A:2159:G:C8	2.48	0.49
1:A:947:G:N2	1:A:971:C:C2	2.81	0.49
1:A:271(E):U:H3	1:A:271(S):G:H1	1.60	0.49
11:P:64:LYS:HA	30:8:13:ARG:HB3	1.94	0.49
1:A:2854:G:H2'	1:A:2855:C:C6	2.47	0.49
11:P:83:VAL:CG1	11:P:112:LEU:HD21	2.43	0.49
1:A:2462:U:H1'	1:A:2491:U:O4	2.13	0.49
1:A:704:G:H1'	1:A:726:G:N2	2.27	0.49
1:A:1593:G:H2'	1:A:1594:G:C8	2.48	0.49
1:A:774:A:N3	1:A:774:A:H2'	2.28	0.49
1:A:848:G:H2'	1:A:849:A:C8	2.48	0.48
9:N:132:ALA:HB3	9:N:133:GLN:NE2	2.28	0.48
1:A:2293:C:H2'	1:A:2294:C:C6	2.48	0.48
20:Y:6:HIS:CD2	20:Y:6:HIS:H	2.31	0.48
1:A:955:C:OP1	12:Q:87:LYS:HE2	2.13	0.48
1:A:2154:G:H2'	1:A:2155:G:C8	2.48	0.48
1:A:870:A:C2	1:A:908:C:C2	3.01	0.48
1:A:2648:C:H2'	1:A:2649:U:C6	2.48	0.48
19:X:11:PRO:HG2	19:X:13:LEU:HD21	1.95	0.48
9:N:62:VAL:CG1	9:N:66:LYS:HB2	2.44	0.48
1:A:1654:A:OP1	13:R:1:MET:HA	2.13	0.48
10:O:35:VAL:HG21	10:O:103:ALA:HB3	1.95	0.48
1:A:171:G:H2'	1:A:172:C:O4'	2.14	0.48
1:A:1505:C:H2'	1:A:1506:C:H6	1.78	0.48
1:A:102:G:O2'	1:A:103:A:O5'	2.26	0.48
26:4:22:ILE:HG22	26:4:24:THR:HG23	1.95	0.48
1:A:1316:U:H2'	1:A:1317:A:C8	2.49	0.48
1:A:975:C:H5	34:A:4446:HOH:O	1.95	0.48
1:A:333:G:H5''	1:A:334:C:OP2	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:444:C:H4'	5:F:49:ALA:HB2	1.94	0.48
21:Z:150:LEU:O	21:Z:171:ILE:HG13	2.13	0.48
13:R:103:ARG:HH12	13:R:110:PRO:HD3	1.77	0.48
1:A:2713:A:N3	1:A:2713:A:H2'	2.29	0.48
1:A:2165:G:H2'	1:A:2166:G:C8	2.48	0.48
1:A:2318:G:N3	1:A:2318:G:H2'	2.29	0.48
20:Y:15:VAL:HG21	20:Y:42:VAL:HG11	1.94	0.48
1:A:968:G:H2'	1:A:969:U:O4'	2.13	0.48
10:O:77:ILE:HG13	15:T:74:ARG:HG2	1.95	0.48
1:A:223:A:O2'	1:A:420:C:O2	2.32	0.48
15:T:28:VAL:HG13	15:T:86:ILE:HG23	1.95	0.48
5:F:50:SER:OG	5:F:51:THR:N	2.45	0.48
1:A:659:C:H4'	5:F:100:THR:O	2.12	0.48
1:A:2275:C:H5'	1:A:2275:C:H6	1.78	0.48
1:A:2748:A:H5'	7:H:4:ILE:HD12	1.94	0.48
1:A:493:G:H2'	1:A:494:G:O4'	2.14	0.48
9:N:30:ILE:HG22	9:N:34:LEU:HD22	1.94	0.48
1:A:335:C:H2'	1:A:336:C:H6	1.79	0.48
1:A:2469:A:H5'	1:A:2470:G:OP2	2.13	0.48
9:N:39:ARG:NH2	9:N:41:ASP:OD2	2.46	0.48
17:V:60:GLU:HB2	17:V:97:LYS:HE2	1.95	0.48
14:S:96:GLY:H	14:S:99:LYS:H	1.60	0.48
1:A:910:A:C6	1:A:911:A:C6	3.01	0.48
1:A:485:C:H2'	1:A:486:C:C6	2.48	0.48
1:A:1040:C:H2'	1:A:1041:C:H1'	1.95	0.48
7:H:67:LEU:O	7:H:71:LEU:HB2	2.14	0.48
1:A:1999:C:H5''	1:A:2723:C:O2'	2.14	0.48
6:G:104:GLU:O	6:G:108:ASN:ND2	2.47	0.48
10:O:4:PRO:O	10:O:5:GLN:HB2	2.13	0.48
6:G:59:GLU:O	6:G:63:ILE:HG13	2.14	0.48
1:A:2001:A:H2'	1:A:2002:G:C8	2.49	0.48
1:A:300:A:P	20:Y:86:ARG:HH22	2.36	0.48
1:A:2464:C:H1'	34:A:3655:HOH:O	2.13	0.48
9:N:67:LEU:HA	9:N:67:LEU:HD22	1.71	0.48
1:A:1488:G:N2	1:A:1502:C:C2	2.82	0.48
5:F:39:TRP:O	5:F:43:LYS:HG2	2.13	0.48
1:A:709:U:H2'	1:A:710:G:C8	2.49	0.48
15:T:26:ASP:OD2	15:T:91:ARG:NH1	2.47	0.48
12:Q:38:GLU:HB2	12:Q:127:ILE:HG22	1.95	0.48
1:A:1001:A:H2'	1:A:1002:G:O4'	2.13	0.48
1:A:1651:G:N2	1:A:2007:C:C2	2.82	0.48
7:H:117:PRO:HB3	7:H:123:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:498:G:O2'	1:A:499:U:H5'	2.14	0.48
4:E:175:VAL:CG2	4:E:177:PRO:HD3	2.43	0.48
14:S:62:LYS:HB3	14:S:97:ARG:HD2	1.96	0.48
1:A:1159:U:H2'	1:A:1160:G:H8	1.79	0.48
1:A:645:C:H2'	1:A:645:C:O2	2.13	0.48
2:B:110:G:C2	2:B:111:G:C5	3.01	0.48
8:I:5:LEU:HD12	8:I:5:LEU:H	1.79	0.48
1:A:1652:A:OP1	13:R:8:ARG:NH1	2.44	0.48
8:I:79:ILE:HA	8:I:80:PRO:HD2	1.66	0.48
5:F:34:TRP:HE3	5:F:35:GLU:HG2	1.79	0.48
1:A:1464:C:H2'	1:A:1465:G:C8	2.48	0.48
4:E:120:TRP:CE3	4:E:155:LYS:HD3	2.49	0.48
21:Z:43:GLU:O	21:Z:47:VAL:HG23	2.14	0.48
2:B:33:G:C6	2:B:34:U:N3	2.82	0.48
8:I:29:TYR:O	8:I:32:PRO:HD2	2.14	0.48
1:A:2722:G:H5'	13:R:4:LEU:HD12	1.96	0.48
1:A:784:A:O4'	3:D:227:ASN:ND2	2.46	0.48
26:4:14:ILE:HG23	26:4:31:ILE:HB	1.95	0.48
21:Z:98:MET:HE3	21:Z:100:VAL:HG22	1.95	0.48
1:A:2196:C:OP2	34:A:4142:HOH:O	2.20	0.48
23:1:94:LEU:O	23:1:97:LEU:HB2	2.13	0.48
22:0:40:GLN:OE1	22:0:44:ARG:N	2.37	0.48
17:V:82:ARG:HD2	17:V:82:ARG:N	2.29	0.48
1:A:2319:G:N2	14:S:3:ARG:HA	2.29	0.48
18:W:82:LEU:HD22	18:W:84:ARG:NH2	2.28	0.48
1:A:973:A:O4'	1:A:1188:U:C6	2.66	0.48
1:A:1188:U:C4'	17:V:79:VAL:HG22	2.44	0.48
1:A:1467:C:C5	1:A:1546:C:H2'	2.49	0.48
1:A:1996:C:O3'	34:A:4350:HOH:O	2.20	0.48
1:A:2665:A:OP2	34:A:3735:HOH:O	2.20	0.48
13:R:50:HIS:CE1	13:R:54:LEU:HD21	2.48	0.48
7:H:20:ALA:HB3	7:H:23:ARG:HB2	1.96	0.48
1:A:1564:C:H2'	1:A:1565:C:C6	2.48	0.48
3:D:71:ASP:HB3	3:D:103:ARG:NH2	2.27	0.47
14:S:56:LEU:C	14:S:58:LEU:HD22	2.34	0.47
21:Z:98:MET:CE	21:Z:100:VAL:HG22	2.43	0.47
1:A:1388:G:H4'	1:A:1525:G:O2'	2.13	0.47
22:0:14:ARG:HH11	22:0:14:ARG:HG3	1.78	0.47
14:S:35:ILE:HG12	14:S:101:LEU:HD12	1.96	0.47
3:D:158:ALA:O	3:D:161:THR:OG1	2.25	0.47
1:A:1047:G:H2'	1:A:1110:G:N1	2.29	0.47
5:F:64:ILE:HD11	5:F:75:HIS:HB2	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:Q:39:PRO:HA	12:Q:97:VAL:O	2.14	0.47
5:F:117:ARG:HD3	5:F:117:ARG:HA	1.57	0.47
12:Q:2:LEU:HB3	12:Q:70:PRO:HG3	1.96	0.47
1:A:1268:A:P	34:A:3870:HOH:O	2.70	0.47
1:A:557:U:O2	9:N:45:ASN:HB2	2.15	0.47
1:A:445:C:OP1	16:U:2:PRO:HA	2.14	0.47
1:A:1540:U:H2'	1:A:1541:G:O4'	2.15	0.47
3:D:118:VAL:N	3:D:129:ASN:ND2	2.60	0.47
21:Z:126:VAL:HG21	21:Z:161:VAL:HG13	1.96	0.47
1:A:652(T):C:H2'	1:A:652(U):G:C8	2.49	0.47
5:F:158:THR:O	5:F:164:ARG:NH1	2.44	0.47
1:A:868:U:H2'	1:A:869:G:O4'	2.14	0.47
1:A:322:A:OP1	5:F:168:ARG:NH1	2.48	0.47
1:A:141:A:C8	1:A:1408:C:O2'	2.55	0.47
2:B:31:C:N4	14:S:32:LEU:HD13	2.30	0.47
1:A:530:G:C6	1:A:2022:U:H5''	2.50	0.47
1:A:1488:G:N1	1:A:1489:U:O2	2.47	0.47
1:A:1339:G:H5''	19:X:16:LYS:HD3	1.97	0.47
1:A:212:G:O2'	1:A:213:A:H5'	2.15	0.47
1:A:684:G:OP1	29:7:16:HIS:ND1	2.46	0.47
1:A:2336:A:H61	22:0:43:THR:CG2	2.28	0.47
1:A:2127:G:N2	1:A:2173:A:H1'	2.29	0.47
1:A:2117:A:N6	1:A:2166:G:H22	2.11	0.47
1:A:218:A:C2	1:A:235:U:H4'	2.49	0.47
1:A:226:G:H21	1:A:228:A:N6	2.13	0.47
1:A:192:C:O2'	1:A:802:A:N3	2.42	0.47
1:A:543:C:H42	1:A:549:G:H1	1.62	0.47
15:T:93:ARG:NH1	15:T:93:ARG:HG2	2.30	0.47
1:A:2698:U:H2'	1:A:2699:C:C6	2.50	0.47
1:A:879:G:H2'	1:A:880:G:O4'	2.14	0.47
1:A:1545:A:H2'	1:A:1546:C:O4'	2.14	0.47
1:A:396:G:H1'	23:1:42:GLN:HB3	1.97	0.47
7:H:37:VAL:HG12	7:H:38:SER:O	2.14	0.47
1:A:2011:U:OP1	18:W:42:ARG:NH1	2.48	0.47
1:A:1578:U:H2'	1:A:1579:A:H5'	1.97	0.47
1:A:2881:C:H2'	1:A:2882:A:O4'	2.15	0.47
10:O:98:VAL:HG13	10:O:117:LEU:HB3	1.96	0.47
17:V:65:GLY:HA3	17:V:91:TYR:CZ	2.50	0.47
11:P:138:LEU:HD23	11:P:145:PRO:HG3	1.97	0.47
16:U:14:HIS:HA	16:U:32:PHE:CE2	2.50	0.47
1:A:1849:G:H2'	1:A:1850:G:H8	1.79	0.47
1:A:86:C:H4'	1:A:104:U:H1'	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1204:A:N1	1:A:1241:A:N7	2.63	0.47
1:A:1429:G:H2'	1:A:1430:C:H6	1.77	0.47
1:A:2262:U:H4'	1:A:2328:A:C2	2.50	0.47
13:R:50:HIS:O	13:R:54:LEU:HD22	2.15	0.47
1:A:614(C):A:C4	5:F:180:GLY:HA2	2.50	0.47
25:3:44:ARG:O	25:3:48:GLU:HG3	2.15	0.47
1:A:1039:G:H1'	1:A:1117:G:N2	2.30	0.47
21:Z:40:ASP:OD1	21:Z:42:VAL:HG13	2.15	0.47
1:A:2807:G:N1	1:A:2808:U:C2	2.83	0.47
6:G:5:VAL:HG11	6:G:101:ILE:HG12	1.96	0.47
16:U:76:TYR:CZ	16:U:80:ILE:HG13	2.49	0.47
4:E:67:PHE:HD1	4:E:72:VAL:HG12	1.80	0.47
9:N:30:ILE:HG23	9:N:52:VAL:HG11	1.97	0.47
3:D:172:TYR:CD1	3:D:186:HIS:HA	2.50	0.47
8:I:110:ASP:N	8:I:130:TYR:OH	2.45	0.47
8:I:124:GLY:H	8:I:144:VAL:HG13	1.80	0.47
1:A:2777:G:H5''	1:A:2778:A:H5'	1.97	0.47
1:A:2820:A:O2'	1:A:2821:A:OP1	2.29	0.47
1:A:2311:A:O2'	1:A:2312:U:O4'	2.33	0.47
1:A:2317:C:N4	1:A:2318:G:C6	2.83	0.47
1:A:2319:G:H1'	1:A:2320:A:H5''	1.97	0.47
6:G:66:GLN:HG2	26:4:1:MET:HE3	1.97	0.47
1:A:2846:G:H2'	1:A:2847:U:O4'	2.15	0.47
11:P:84:ASN:ND2	11:P:117:GLU:HB2	2.29	0.47
21:Z:102:LEU:HD13	21:Z:123:ASP:HA	1.97	0.47
1:A:1695:G:H2'	1:A:1696:G:O4'	2.15	0.47
1:A:272:G:N7	1:A:421:U:H2'	2.30	0.47
2:B:24:G:H4'	2:B:25:A:C8	2.49	0.47
10:O:107:ARG:CZ	15:T:36:GLU:HG3	2.44	0.47
28:6:25:LYS:HE3	28:6:30:THR:O	2.13	0.47
1:A:652(Q):G:H2'	1:A:652(R):C:C6	2.50	0.47
4:E:92:THR:O	4:E:95:ILE:HG23	2.14	0.47
31:9:17:ILE:HA	31:9:17:ILE:HD13	1.61	0.47
1:A:1891:G:H8	1:A:1891:G:O5'	1.97	0.47
1:A:1021:A:H3'	1:A:1021:A:C8	2.50	0.46
6:G:11:TYR:HB2	6:G:176:LEU:HD21	1.97	0.46
1:A:1530:C:H1'	1:A:1531:C:OP1	2.14	0.46
1:A:2206:G:HO2'	1:A:2207:G:P	2.38	0.46
20:Y:86:ARG:HD2	20:Y:100:ALA:HA	1.97	0.46
12:Q:133:ARG:HG2	12:Q:134:ARG:N	2.29	0.46
1:A:2536:G:C6	1:A:2537:U:C4	3.03	0.46
21:Z:121:HIS:HB3	21:Z:123:ASP:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:132:ASN:OD1	6:G:158:ALA:HA	2.15	0.46
3:D:132:PRO:HD3	3:D:190:TYR:CZ	2.50	0.46
21:Z:19:ARG:HA	21:Z:23:LYS:O	2.15	0.46
20:Y:7:VAL:HG21	20:Y:72:VAL:HG12	1.96	0.46
1:A:527:C:C4	1:A:2779:U:H2'	2.49	0.46
1:A:2169:A:H3'	1:A:2170:A:H8	1.81	0.46
1:A:2298:A:H2'	1:A:2299:G:O4'	2.15	0.46
1:A:910:A:N7	12:Q:13:GLN:HG3	2.29	0.46
1:A:1049:C:H1'	1:A:1113:U:H4'	1.97	0.46
5:F:110:LEU:HD21	5:F:181:LEU:HG	1.96	0.46
25:3:10:LYS:NZ	25:3:15:TYR:OH	2.47	0.46
11:P:65:ARG:HD3	11:P:66:GLY:N	2.30	0.46
6:G:19:LEU:HG	6:G:175:LEU:HD22	1.97	0.46
3:D:118:VAL:N	3:D:129:ASN:HD22	2.09	0.46
15:T:118:ARG:HG3	15:T:118:ARG:HH11	1.80	0.46
1:A:2544:G:H1'	1:A:2646:C:H4'	1.97	0.46
1:A:512:G:C8	34:A:3826:HOH:O	2.68	0.46
1:A:582:G:H2'	1:A:583:G:C8	2.50	0.46
7:H:149:ARG:HG3	7:H:162:ILE:O	2.15	0.46
7:H:149:ARG:NH1	7:H:167:GLU:OE1	2.49	0.46
1:A:2870:C:H2'	1:A:2871:C:O4'	2.16	0.46
1:A:1106:G:O2'	1:A:1107:G:OP1	2.29	0.46
1:A:1945:G:H2'	1:A:1946:U:C6	2.51	0.46
1:A:2175:C:H2'	1:A:2176:A:O4'	2.16	0.46
17:V:95:LEU:HD13	17:V:97:LYS:HD3	1.98	0.46
1:A:2002:G:OP2	13:R:9:LYS:NZ	2.48	0.46
12:Q:103:MET:CE	12:Q:125:LEU:HD13	2.45	0.46
29:7:9:ARG:HB3	29:7:46:VAL:HG23	1.97	0.46
1:A:2110:G:O2'	1:A:2120:G:H5'	2.15	0.46
1:A:1040:C:H2'	1:A:1041:C:C1'	2.44	0.46
25:3:10:LYS:HB3	25:3:53:LEU:HA	1.97	0.46
3:D:112:GLN:HB2	3:D:115:GLN:OE1	2.16	0.46
3:D:77:ALA:HA	3:D:97:TYR:HA	1.97	0.46
1:A:634:C:H2'	1:A:635:C:C6	2.51	0.46
1:A:775:G:C4	1:A:794:G:C8	3.03	0.46
1:A:1282:U:H2'	1:A:1283:G:O4'	2.15	0.46
1:A:39:C:H2'	1:A:40:C:H6	1.78	0.46
1:A:2133:G:C2'	1:A:2158:A:H61	2.28	0.46
5:F:185:ASP:OD1	5:F:188:ARG:NH1	2.45	0.46
10:O:23:ARG:HG3	10:O:24:VAL:N	2.30	0.46
12:Q:2:LEU:HB3	12:Q:70:PRO:CG	2.45	0.46
1:A:1025:G:C4	1:A:1135:C:H1'	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2818:G:O2'	1:A:2819:G:H5'	2.16	0.46
10:O:87:ILE:HG22	10:O:93:PRO:HA	1.97	0.46
1:A:448:U:H1'	5:F:84:VAL:HG11	1.97	0.46
15:T:18:ASP:N	15:T:18:ASP:OD1	2.28	0.46
1:A:1866:C:H2'	1:A:1876:A:O4'	2.16	0.46
1:A:2130:U:OP2	1:A:2132:U:H5	1.98	0.46
1:A:247:G:H4'	1:A:386:G:C5	2.51	0.46
12:Q:134:ARG:O	12:Q:138:ASP:HB2	2.15	0.46
1:A:1797:C:C2'	1:A:1798:U:H5'	2.46	0.46
12:Q:26:TYR:HE1	12:Q:28:ALA:HB2	1.80	0.46
6:G:10:LYS:O	6:G:14:GLU:HB3	2.16	0.46
1:A:2839:G:C5'	13:R:46:GLY:HA2	2.46	0.46
1:A:2279:G:O6	22:O:14:ARG:HD2	2.16	0.46
2:B:8:U:H5'	2:B:9:G:OP2	2.16	0.46
1:A:787:U:OP1	34:A:4081:HOH:O	2.20	0.46
30:8:31:HIS:O	30:8:32:LEU:HB2	2.16	0.46
25:3:40:THR:HG23	25:3:43:ILE:HD12	1.98	0.46
1:A:1910:G:O2'	1:A:1911:U:H5'	2.15	0.46
1:A:2054:A:H5''	1:A:2055:C:O5'	2.16	0.46
11:P:6:LEU:HD23	11:P:6:LEU:HA	1.60	0.46
1:A:848:G:N3	1:A:933:A:H1'	2.30	0.46
1:A:1003:G:N2	1:A:1153:C:C2	2.84	0.46
6:G:106:LEU:HD12	6:G:110:ALA:CB	2.43	0.46
23:1:50:ARG:HG2	23:1:59:THR:CG2	2.45	0.46
1:A:1485:G:H1	1:A:1504:C:N4	2.13	0.46
15:T:105:LEU:HB3	15:T:109:GLU:HB2	1.98	0.46
1:A:319:C:H2'	1:A:320:A:O4'	2.16	0.46
6:G:129:GLY:HA2	6:G:166:ASP:HA	1.98	0.46
4:E:2:LYS:HG3	4:E:200:GLU:HB2	1.97	0.46
1:A:1529:G:O2'	1:A:1530:C:H5'	2.15	0.46
18:W:9:TYR:H	18:W:102:HIS:CE1	2.34	0.46
12:Q:43:THR:N	12:Q:46:GLN:OE1	2.42	0.46
21:Z:75:ASN:HB2	21:Z:85:HIS:HB3	1.98	0.46
1:A:2440:C:H5'	34:A:4286:HOH:O	2.14	0.46
8:I:46:ALA:HA	8:I:49:ALA:HB3	1.97	0.46
1:A:1646:C:H3'	34:A:3840:HOH:O	2.15	0.46
1:A:2172:U:H4'	1:A:2173:A:OP2	2.15	0.46
2:B:66:A:H61	2:B:109:C:C5'	2.24	0.46
1:A:1026:U:HO2'	1:A:1027:A:P	2.38	0.46
1:A:760:G:H2'	1:A:761:A:O4'	2.15	0.46
1:A:2208:A:H1'	1:A:2219:G:C4	2.51	0.46
1:A:2190:G:H2'	1:A:2191:G:O4'	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:2:22:GLU:HG2	24:2:64:LEU:HD11	1.97	0.46
22:0:55:ARG:CZ	22:0:55:ARG:HB3	2.46	0.46
23:1:54:ALA:HB1	23:1:83:GLU:HB3	1.97	0.46
11:P:52:GLU:HG3	30:8:57:ARG:HH22	1.81	0.46
6:G:76:SER:CA	6:G:83:ARG:HA	2.44	0.46
26:4:34:GLU:CD	26:4:35:VAL:H	2.20	0.46
1:A:1423:G:H2'	1:A:1424:G:C8	2.46	0.46
30:8:61:LEU:O	30:8:63:PRO:HD3	2.16	0.46
5:F:34:TRP:CE3	5:F:35:GLU:HG2	2.51	0.46
5:F:168:ARG:HH11	5:F:168:ARG:CB	2.29	0.46
1:A:213:A:H2'	1:A:214:G:O4'	2.16	0.46
1:A:1699:G:N2	34:A:4396:HOH:O	2.34	0.46
18:W:40:ASN:O	18:W:41:LYS:HG2	2.16	0.46
1:A:77:C:OP1	24:2:59:ARG:HD3	2.16	0.46
1:A:363(D):G:O2'	1:A:363(E):U:H5'	2.16	0.46
3:D:146:GLU:HB2	3:D:189:CYS:HB3	1.96	0.46
14:S:74:ALA:HB2	14:S:105:ALA:HA	1.97	0.46
3:D:154:LYS:C	3:D:155:LEU:HD12	2.36	0.46
1:A:833:U:O2'	11:P:52:GLU:HG2	2.15	0.45
1:A:29:U:H2'	1:A:30:G:H8	1.77	0.45
1:A:1434:A:O2'	1:A:1435:G:H5'	2.16	0.45
6:G:110:ALA:HA	6:G:140:ILE:O	2.16	0.45
9:N:13:TRP:O	9:N:135:PRO:HA	2.15	0.45
1:A:2592:G:H2'	1:A:2593:U:O4'	2.16	0.45
11:P:84:ASN:CG	11:P:117:GLU:HB2	2.35	0.45
25:3:7:LYS:HE2	25:3:32:GLN:O	2.16	0.45
1:A:2784:C:H1'	4:E:37:ARG:HH12	1.80	0.45
10:O:117:LEU:HD23	10:O:117:LEU:HA	1.74	0.45
1:A:414:C:H2'	1:A:415:A:C8	2.50	0.45
1:A:2657:A:O3'	7:H:160:LYS:NZ	2.49	0.45
34:A:4209:HOH:O	29:7:48:LYS:NZ	2.47	0.45
1:A:2335:A:N6	1:A:2337:G:H1'	2.31	0.45
1:A:997:G:O2'	1:A:998:C:H5'	2.16	0.45
1:A:535:C:O3'	16:U:53:ARG:NH1	2.48	0.45
1:A:725:G:C6	1:A:726:G:N1	2.84	0.45
1:A:1178:C:H2'	1:A:1179:C:C6	2.51	0.45
8:I:45:LYS:HD2	8:I:45:LYS:HA	1.73	0.45
1:A:2815:C:H5'	27:5:29:THR:HG21	1.97	0.45
1:A:288:C:H2'	1:A:289:A:H8	1.81	0.45
1:A:2296:U:H4'	1:A:2297:C:OP1	2.15	0.45
1:A:1352:U:O2	1:A:1570:A:H2	1.99	0.45
1:A:2318:G:O2'	1:A:2319:G:H5''	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:W:4:LYS:HE2	18:W:6:ILE:HD11	1.98	0.45
1:A:1050:A:H2'	1:A:1051:G:C8	2.50	0.45
1:A:314:A:O2'	1:A:315:G:H5'	2.15	0.45
1:A:878:A:C6	1:A:900:A:C8	3.03	0.45
1:A:1205:U:H4'	1:A:1206:G:OP2	2.16	0.45
17:V:52:VAL:CG2	17:V:55:ALA:HB3	2.45	0.45
4:E:181:LEU:HA	4:E:181:LEU:HD13	1.66	0.45
1:A:1425:G:H2'	1:A:1426:G:C8	2.51	0.45
20:Y:44:ILE:HA	20:Y:63:LYS:O	2.17	0.45
2:B:28:C:H2'	2:B:29:A:C8	2.50	0.45
1:A:2872:G:O2'	1:A:2873:A:H5'	2.16	0.45
1:A:2505:G:O6	1:A:2576:G:H2'	2.16	0.45
1:A:586:A:N1	1:A:809:G:O2'	2.34	0.45
1:A:614(A):U:H6	1:A:614(A):U:O5'	2.00	0.45
1:A:2117:A:H61	1:A:2166:G:N2	2.10	0.45
1:A:2173:A:C2'	1:A:2174:C:H5'	2.47	0.45
1:A:945:A:H2	34:A:3910:HOH:O	2.00	0.45
14:S:32:LEU:O	14:S:62:LYS:HE2	2.15	0.45
1:A:2887:U:H2'	1:A:2888:C:H6	1.80	0.45
1:A:1266:G:O2'	1:A:2012:G:O6	2.28	0.45
1:A:1154:G:H8	1:A:1154:G:O5'	1.99	0.45
21:Z:69:THR:HG22	21:Z:90:VAL:HA	1.98	0.45
1:A:2271:G:C6	1:A:2272:U:C4	3.05	0.45
5:F:64:ILE:HG13	5:F:65:TRP:N	2.31	0.45
1:A:863:A:H2'	1:A:864:G:H8	1.80	0.45
1:A:1794:U:H2'	1:A:1795:C:H6	1.80	0.45
21:Z:144:LEU:HD12	21:Z:144:LEU:HA	1.77	0.45
5:F:51:THR:HG23	5:F:92:PRO:HG2	1.97	0.45
21:Z:61:LEU:HD13	21:Z:61:LEU:HA	1.72	0.45
1:A:1441:G:H2'	1:A:1442:G:C8	2.50	0.45
1:A:2290:G:C2	1:A:2343:C:O2	2.69	0.45
22:O:51:VAL:N	22:O:62:LEU:HD12	2.31	0.45
1:A:2408:U:OP2	34:A:4062:HOH:O	2.21	0.45
1:A:1394:U:C4	1:A:1395:A:C5	3.04	0.45
1:A:102:G:O2'	1:A:103:A:P	2.75	0.45
1:A:581:C:H2'	1:A:582:G:H8	1.80	0.45
2:B:21:G:H2'	2:B:22:U:O4'	2.16	0.45
1:A:979:G:H3'	1:A:980:A:H5''	1.98	0.45
1:A:2275:C:H5'	1:A:2275:C:C6	2.51	0.45
1:A:2505:G:H2'	1:A:2576:G:O6	2.17	0.45
4:E:178:GLU:CD	4:E:178:GLU:H	2.19	0.45
1:A:850:C:O3'	25:3:49:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2137:C:H42	1:A:2154:G:H1	1.64	0.45
1:A:528:A:C2'	1:A:529:A:H5'	2.47	0.45
19:X:36:LYS:HG3	19:X:56:THR:HG23	1.99	0.45
21:Z:48:PHE:O	21:Z:52:SER:N	2.47	0.45
1:A:242:G:O4'	30:8:3:LYS:HE3	2.17	0.45
11:P:63:PRO:HG2	30:8:25:MET:HB2	1.98	0.45
14:S:66:ALA:HA	14:S:69:VAL:CG1	2.47	0.45
1:A:2615:U:C2	27:5:7:PRO:HA	2.52	0.45
1:A:2133:G:H2'	1:A:2158:A:H61	1.81	0.45
1:A:2309:A:N6	1:A:2310:A:N1	2.64	0.45
1:A:534:U:O2'	16:U:49:HIS:CD2	2.70	0.45
11:P:71:VAL:HG23	11:P:72:PRO:HA	1.98	0.45
1:A:1028:A:H61	1:A:1125:G:H2'	1.82	0.45
2:B:2:C:H2'	2:B:3:C:H6	1.82	0.45
3:D:130:ALA:C	3:D:131:LEU:HD12	2.37	0.45
1:A:2062:A:P	34:A:4031:HOH:O	2.74	0.45
5:F:88:VAL:HG21	5:F:91:GLY:HA3	1.98	0.45
1:A:2820:A:OP1	13:R:4:LEU:HD23	2.17	0.45
1:A:2319:G:H22	14:S:3:ARG:CD	2.29	0.45
6:G:106:LEU:HA	6:G:110:ALA:HB3	1.99	0.45
1:A:2601:C:H3'	1:A:2602:A:C8	2.52	0.45
1:A:652(E):G:O6	1:A:652(T):C:N3	2.50	0.45
5:F:64:ILE:HD12	5:F:65:TRP:CE3	2.51	0.45
1:A:1845:G:OP1	3:D:258:LYS:NZ	2.39	0.45
21:Z:54:HIS:ND1	21:Z:101:PRO:HG3	2.31	0.45
1:A:1651:G:H2'	1:A:1652:A:O4'	2.17	0.45
4:E:179:GLU:HB3	4:E:181:LEU:HD23	1.99	0.45
6:G:33:ARG:HD3	6:G:162:THR:OG1	2.17	0.45
1:A:2203:U:O2	1:A:2221:G:C2	2.70	0.45
2:B:106:G:H5'	21:Z:31:ARG:HG2	1.99	0.45
16:U:74:LEU:H	16:U:74:LEU:HD12	1.82	0.45
1:A:1903:G:OP1	3:D:241:PRO:HB2	2.16	0.45
19:X:31:HIS:HA	19:X:32:PRO:HD3	1.83	0.45
26:4:36:CYS:N	26:4:39:CYS:SG	2.89	0.45
23:1:3:LYS:HB2	23:1:61:ARG:NH1	2.29	0.45
9:N:137:LYS:O	9:N:138:LEU:HD23	2.17	0.45
18:W:4:LYS:CB	18:W:106:ILE:HG12	2.47	0.45
18:W:9:TYR:HA	18:W:100:THR:HG23	1.99	0.45
9:N:73:THR:CG2	9:N:82:LEU:HD11	2.47	0.45
1:A:1419:A:O2'	1:A:1420:U:H5''	2.17	0.45
1:A:2290:G:H2'	1:A:2291:U:O4'	2.16	0.45
1:A:2251:G:C6	1:A:2252:G:C5	3.05	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2563:U:O2	1:A:2565:A:H8	2.00	0.45
1:A:1448:G:H5''	1:A:1542:A:OP1	2.17	0.45
1:A:2581:G:H4'	1:A:2582:G:C8	2.51	0.45
1:A:116:C:H2'	1:A:117:G:O4'	2.17	0.45
1:A:673:C:H5''	5:F:81:PRO:HD2	1.99	0.45
15:T:13:ARG:HG2	15:T:13:ARG:H	1.29	0.45
1:A:1357:U:H2'	1:A:1358:G:O4'	2.17	0.45
1:A:2741:A:H61	1:A:2763:G:H1'	1.81	0.45
8:I:87:LYS:N	8:I:122:GLU:HA	2.27	0.45
1:A:1814:G:H2'	1:A:1815:A:C8	2.52	0.45
1:A:2186:G:H2'	1:A:2186:G:N3	2.32	0.45
3:D:147:LEU:HD13	3:D:155:LEU:HD11	1.99	0.45
14:S:27:SER:HA	14:S:88:ASP:HB3	1.98	0.45
1:A:2674:G:H2'	1:A:2675:A:C8	2.52	0.45
1:A:576:U:H5	34:A:3895:HOH:O	2.00	0.45
1:A:529:A:H5''	34:A:4757:HOH:O	2.17	0.44
5:F:7:TYR:N	5:F:22:ALA:HB3	2.29	0.44
1:A:530:G:O6	1:A:2023:G:OP1	2.35	0.44
7:H:5:GLY:HA2	7:H:69:ARG:HB3	1.99	0.44
1:A:986:C:C2'	1:A:987:G:H5'	2.47	0.44
1:A:186:G:H2'	1:A:187:G:H8	1.82	0.44
1:A:1782:C:H2'	1:A:2608:G:O2'	2.17	0.44
4:E:171:GLU:O	4:E:184:VAL:HG23	2.16	0.44
11:P:101:VAL:HA	11:P:106:LEU:O	2.17	0.44
1:A:257:A:H2'	1:A:258:G:O4'	2.16	0.44
1:A:272(H):C:H5''	1:A:272(H):C:H6	1.81	0.44
1:A:34:C:H41	1:A:447:A:H61	1.65	0.44
21:Z:28:MET:HG3	21:Z:35:ARG:HB2	1.99	0.44
5:F:20:LEU:HD23	5:F:20:LEU:HA	1.82	0.44
1:A:2228:G:C5	1:A:2229:C:C4	3.05	0.44
6:G:22:ARG:HH21	6:G:175:LEU:HD11	1.81	0.44
1:A:1566:A:OP1	3:D:211:ARG:NH1	2.50	0.44
1:A:300:A:H3'	20:Y:84:ARG:NH2	2.33	0.44
14:S:36:TYR:N	14:S:36:TYR:CD1	2.85	0.44
16:U:112:ARG:NH2	17:V:47:VAL:HB	2.32	0.44
4:E:33:VAL:HG12	4:E:89:ASP:O	2.16	0.44
24:2:65:ASN:O	24:2:69:ARG:NH1	2.50	0.44
28:6:8:LYS:HD3	30:8:34:TRP:CD2	2.52	0.44
14:S:53:SER:O	14:S:57:LYS:N	2.50	0.44
1:A:2356:C:O3'	22:0:20:ARG:HD3	2.17	0.44
1:A:2130:U:H2'	1:A:2131:G:N7	2.31	0.44
6:G:133:LEU:HD12	6:G:134:GLY:N	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1509(A):A:H3'	1:A:1509(B):A:C8	2.50	0.44
21:Z:111:VAL:C	21:Z:113:ALA:H	2.21	0.44
18:W:60:ASN:HD22	18:W:60:ASN:H	1.63	0.44
2:B:104:U:O3'	21:Z:72:ARG:NH1	2.50	0.44
1:A:649:G:H2'	1:A:650:C:H6	1.82	0.44
12:Q:59:ARG:HB3	12:Q:60:ARG:H	1.69	0.44
10:O:3:GLN:HB2	10:O:4:PRO:HD2	2.00	0.44
1:A:1108:U:O2	1:A:1108:U:H2'	2.17	0.44
1:A:500:G:N1	1:A:503:A:OP2	2.50	0.44
1:A:2751:G:C4	7:H:2:SER:N	2.86	0.44
1:A:646:A:H2'	1:A:647:G:O4'	2.17	0.44
1:A:2226:C:H3'	34:A:4136:HOH:O	2.18	0.44
1:A:2125:G:H21	1:A:2126:A:N6	2.15	0.44
6:G:56:ALA:CA	6:G:153:ARG:HH21	2.31	0.44
1:A:528:A:O2'	1:A:529:A:H5'	2.17	0.44
14:S:10:ARG:O	14:S:14:VAL:HG12	2.17	0.44
1:A:627:A:C6	1:A:637:A:C8	3.05	0.44
1:A:729:G:H2'	1:A:1775:U:H1'	2.00	0.44
2:B:20:C:H2'	2:B:21:G:H5'	2.00	0.44
19:X:60:ARG:HB3	19:X:60:ARG:HE	1.45	0.44
1:A:389:G:H8	1:A:389:G:O5'	2.01	0.44
1:A:1804:C:H2'	1:A:1805:U:H6	1.83	0.44
1:A:1007:C:OP1	9:N:35:ARG:NH1	2.50	0.44
1:A:2695:C:H2'	1:A:2696:U:C6	2.53	0.44
13:R:85:PRO:O	13:R:87:TYR:N	2.50	0.44
9:N:128:HIS:CD2	9:N:128:HIS:H	2.36	0.44
3:D:148:GLU:CB	3:D:151:LYS:HD2	2.47	0.44
5:F:123:LEU:HD11	5:F:194:MET:HE2	2.00	0.44
1:A:864:G:C6	1:A:865:C:N4	2.86	0.44
4:E:119:ARG:HG2	4:E:160:TYR:HB2	2.00	0.44
7:H:38:SER:HB2	7:H:64:LEU:HD22	1.99	0.44
13:R:103:ARG:NH1	13:R:103:ARG:HG2	2.33	0.44
1:A:1827:C:OP2	3:D:222:ARG:HD2	2.17	0.44
7:H:137:ASP:HB3	7:H:140:LYS:HE2	2.00	0.44
1:A:1717:G:C2	1:A:1718:G:C8	3.05	0.44
5:F:79:GLY:HA2	5:F:86:GLY:HA2	1.99	0.44
8:I:33:ARG:HB2	8:I:35:LEU:HD12	1.98	0.44
1:A:848:G:N9	1:A:933:A:H8	2.15	0.44
6:G:16:ARG:HB2	6:G:17:PRO:HD3	2.00	0.44
6:G:178:PHE:HB3	6:G:180:PHE:HE1	1.82	0.44
1:A:83:G:H22	1:A:102:G:H2'	1.81	0.44
1:A:579:G:H2'	1:A:580:C:C6	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:921:G:C5	1:A:922:U:C4	3.05	0.44
7:H:27:LYS:HE2	7:H:27:LYS:HB3	1.77	0.44
1:A:311:A:C8	1:A:332:A:N7	2.86	0.44
20:Y:68:HIS:ND1	20:Y:70:SER:HB3	2.32	0.44
1:A:975(A):G:H1'	1:A:990:A:C2	2.53	0.44
30:8:39:LYS:HA	30:8:42:ARG:NH1	2.33	0.44
1:A:1161:C:O2'	17:V:8:GLY:HA2	2.17	0.44
11:P:77:ARG:HB2	11:P:78:PRO:HD2	1.99	0.44
13:R:95:THR:HG22	13:R:116:LEU:HD23	1.99	0.44
1:A:297:C:H3'	34:A:3750:HOH:O	2.18	0.44
18:W:19:LEU:HA	18:W:19:LEU:HD12	1.70	0.44
1:A:2117:A:N6	1:A:2171:A:C6	2.86	0.44
1:A:1557:C:H5''	1:A:1558:A:OP2	2.18	0.44
1:A:1547:C:H2'	1:A:1548:C:C6	2.53	0.44
21:Z:98:MET:O	21:Z:125:LEU:HD12	2.17	0.44
1:A:1426:G:N7	3:D:31:LYS:NZ	2.58	0.44
1:A:2291:U:O2'	1:A:2374:C:O2	2.35	0.44
2:B:96:U:H2'	2:B:97:G:C8	2.53	0.44
3:D:68:LYS:HD2	3:D:70:TRP:CZ2	2.52	0.44
22:0:24:LYS:O	22:0:25:ARG:HD3	2.17	0.44
1:A:857:C:H4'	22:0:23:VAL:HG21	1.99	0.44
1:A:1126:A:OP1	1:A:1126:A:H8	2.01	0.44
1:A:511:U:C5	1:A:512:G:C5	3.05	0.44
1:A:2748:A:C6	1:A:2749:A:C5	3.06	0.44
1:A:2378:A:H4'	14:S:23:ARG:HH11	1.83	0.44
1:A:548:A:H61	17:V:19:LYS:H	1.65	0.44
21:Z:111:VAL:O	21:Z:112:ARG:HB2	2.18	0.44
1:A:2884:U:H1'	27:5:53:ALA:HB2	2.00	0.44
11:P:2:LYS:HG2	11:P:4:SER:H	1.83	0.44
1:A:303:U:H2'	1:A:304:G:C8	2.53	0.44
6:G:169:ALA:O	6:G:173:LEU:HG	2.17	0.44
1:A:2064:C:H2'	1:A:2065:C:C6	2.53	0.44
12:Q:57:HIS:CD2	12:Q:117:ALA:HB2	2.53	0.44
1:A:733:G:N7	34:A:3789:HOH:O	2.36	0.44
6:G:47:LYS:HG3	6:G:48:GLU:H	1.82	0.44
1:A:815:C:C2	1:A:1193:G:C2	3.06	0.44
1:A:2687:U:H2'	1:A:2688:U:O4'	2.18	0.44
1:A:2119:A:OP1	1:A:2119:A:H2'	2.18	0.44
1:A:2133:G:N2	1:A:2158:A:H62	2.16	0.44
1:A:30:G:H2'	1:A:31:C:C6	2.53	0.44
1:A:1153:C:H2'	1:A:1154:G:O4'	2.17	0.44
1:A:1478:G:HO2'	1:A:1558:A:H2	1.63	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:484:C:H2'	1:A:485:C:H6	1.80	0.44
6:G:72:ARG:HD3	6:G:85:GLY:HA2	1.99	0.44
1:A:830:G:H4'	1:A:831:G:OP2	2.18	0.44
1:A:1766:U:H2'	1:A:1767:C:C6	2.53	0.44
1:A:272(H):C:H5'	1:A:272(I):U:OP2	2.17	0.44
2:B:38:C:O2	2:B:48:A:H1'	2.17	0.43
1:A:2305:A:C5'	6:G:134:GLY:HA3	2.47	0.43
1:A:980:A:N3	1:A:2037:G:O2'	2.40	0.43
1:A:1316:U:H2'	1:A:1317:A:H8	1.83	0.43
1:A:51:G:O2'	1:A:119:A:N1	2.39	0.43
1:A:1804:C:H6	1:A:1804:C:O5'	1.99	0.43
17:V:76:LYS:HD2	17:V:81:TYR:CD1	2.53	0.43
1:A:2677:G:H2'	1:A:2678:C:C6	2.53	0.43
1:A:55:G:N3	1:A:127:A:H2	2.15	0.43
2:B:40:U:H1'	2:B:45:A:N6	2.33	0.43
2:B:46:A:C5	2:B:47:C:C5	3.06	0.43
1:A:2238:G:N7	34:A:4642:HOH:O	2.36	0.43
1:A:2176:A:H5'	1:A:2177:C:OP2	2.18	0.43
1:A:1210:A:C5'	1:A:1210:A:H8	2.30	0.43
1:A:1340:U:H4'	1:A:1394:U:O2'	2.18	0.43
1:A:1364:G:P	23:1:3:LYS:HG2	2.57	0.43
12:Q:60:ARG:NH1	21:Z:177:PRO:HG3	2.33	0.43
3:D:77:ALA:HB2	3:D:97:TYR:CD2	2.53	0.43
14:S:74:ALA:CB	14:S:108:GLY:HA3	2.48	0.43
1:A:2343:C:HO2'	1:A:2373:G:HO2'	1.64	0.43
21:Z:35:ARG:HA	21:Z:35:ARG:HD2	1.64	0.43
1:A:54:G:O2'	29:7:35:ARG:HD3	2.18	0.43
17:V:18:LEU:HA	17:V:18:LEU:HD23	1.84	0.43
1:A:354:G:H2'	1:A:355:G:O4'	2.18	0.43
1:A:824:A:H1'	1:A:2358:G:N7	2.34	0.43
3:D:96:HIS:HD2	3:D:102:LYS:HG2	1.82	0.43
1:A:2685:G:H2'	1:A:2686:G:H5''	2.00	0.43
1:A:675:A:N6	1:A:676:A:N6	2.66	0.43
5:F:197:ASP:O	5:F:201:VAL:HG12	2.18	0.43
1:A:768:G:C5	34:A:3968:HOH:O	2.67	0.43
14:S:30:ARG:HG3	14:S:97:ARG:CZ	2.48	0.43
21:Z:45:ASP:O	21:Z:48:PHE:N	2.50	0.43
1:A:1513:C:H2'	1:A:1514:U:C6	2.53	0.43
1:A:322:A:OP2	5:F:169:ASN:HB2	2.17	0.43
15:T:36:GLU:HB3	15:T:37:GLY:H	1.72	0.43
1:A:34:C:H5''	1:A:35:G:OP2	2.18	0.43
23:1:98:LEU:HD23	23:1:98:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:166:SER:HA	21:Z:167:PRO:HD3	1.93	0.43
1:A:2223:G:H2'	1:A:2224:G:H5'	2.00	0.43
1:A:2704:C:H2'	1:A:2705:A:O4'	2.18	0.43
1:A:2793:G:N2	1:A:2804:C:H1'	2.32	0.43
6:G:43:LEU:HB3	6:G:44:GLY:H	1.64	0.43
1:A:842:G:H2'	1:A:843:G:O4'	2.17	0.43
1:A:2774:C:H2'	1:A:2775:A:O4'	2.19	0.43
1:A:272(E):G:C2	1:A:364:C:N3	2.87	0.43
4:E:52:LEU:O	4:E:76:ARG:HG2	2.18	0.43
13:R:103:ARG:HH11	13:R:103:ARG:CG	2.32	0.43
13:R:103:ARG:HH11	13:R:103:ARG:HG2	1.83	0.43
1:A:2387:U:OP1	22:0:55:ARG:NH2	2.51	0.43
3:D:145:VAL:HG12	3:D:146:GLU:O	2.18	0.43
1:A:2494:G:C4	1:A:2495:G:C8	3.06	0.43
24:2:10:LEU:HD23	24:2:10:LEU:HA	1.75	0.43
22:0:56:ASP:OD2	22:0:56:ASP:N	2.48	0.43
1:A:1358:G:O2'	1:A:1359:A:H5'	2.18	0.43
1:A:1722:A:C5	1:A:1740:G:C6	3.07	0.43
1:A:1740:G:H2'	1:A:1741:A:H8	1.83	0.43
11:P:59:LEU:HD11	30:8:10:ALA:CB	2.45	0.43
1:A:234:C:H2'	1:A:235:U:C6	2.54	0.43
1:A:2850:A:OP2	1:A:2866:U:H5	2.01	0.43
1:A:2470:G:C2	1:A:2471:C:C6	3.07	0.43
16:U:39:LEU:HA	16:U:39:LEU:HD23	1.85	0.43
1:A:2070:G:C2	1:A:2442:C:C2	3.07	0.43
1:A:2556:C:H2'	1:A:2557:G:O4'	2.19	0.43
19:X:50:LYS:HB3	19:X:84:ALA:HB2	1.99	0.43
18:W:14:PRO:HG2	18:W:78:GLU:HG2	1.99	0.43
11:P:27:HIS:O	11:P:31:ALA:HA	2.19	0.43
1:A:475:U:C4	1:A:481:G:O6	2.71	0.43
1:A:2287:A:C5	1:A:2289:G:C5	3.06	0.43
6:G:19:LEU:HD22	6:G:23:PHE:CE1	2.51	0.43
8:I:83:ALA:HA	8:I:89:TYR:CD2	2.54	0.43
1:A:2760:C:C2'	1:A:2761:G:H5''	2.45	0.43
1:A:819:A:OP2	1:A:1187:G:N2	2.35	0.43
1:A:2273:A:O2'	1:A:2274:A:H5'	2.19	0.43
19:X:5:TYR:HB3	24:2:33:MET:HB2	2.00	0.43
1:A:2850:A:OP2	1:A:2866:U:C5	2.72	0.43
1:A:2259:G:C2	1:A:2282:G:N1	2.87	0.43
1:A:39:C:H2'	1:A:40:C:C6	2.53	0.43
11:P:101:VAL:HG23	11:P:106:LEU:HB3	2.00	0.43
1:A:2695:C:H2'	1:A:2696:U:H6	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:83:TYR:O	7:H:134:SER:HA	2.19	0.43
13:R:38:VAL:HB	13:R:39:PRO:HD3	1.99	0.43
12:Q:66:ILE:HG12	12:Q:104:PHE:CD2	2.53	0.43
1:A:363(A):A:H2'	1:A:363(B):G:H8	1.82	0.43
13:R:29:LEU:HB3	13:R:75:LEU:HD21	1.99	0.43
1:A:2315:G:H2'	1:A:2316:C:C6	2.53	0.43
1:A:271(H):G:O2'	1:A:271(I):G:P	2.76	0.43
1:A:2286:A:OP1	28:6:29:ASN:ND2	2.52	0.43
1:A:2301:C:H2'	1:A:2302:G:C8	2.54	0.43
1:A:1287:A:C5	1:A:1288:U:C4	3.07	0.43
21:Z:151:HIS:C	21:Z:153:SER:H	2.21	0.43
1:A:1419:A:C8	1:A:1421:G:C6	3.06	0.43
3:D:10:THR:OG1	3:D:13:ARG:HB2	2.19	0.43
1:A:566:U:H2'	1:A:567:A:O4'	2.19	0.43
1:A:2647:U:H2'	1:A:2648:C:C6	2.54	0.43
9:N:58:ASP:N	9:N:58:ASP:OD1	2.51	0.43
23:1:52:ARG:HA	23:1:56:GLN:O	2.18	0.43
21:Z:93:ASP:HA	21:Z:130:PRO:HG2	2.00	0.43
1:A:1893:C:C5	1:A:1894:C:C5	3.06	0.43
1:A:428:A:H8	1:A:428:A:OP2	2.02	0.43
1:A:1204:A:H2	1:A:1241:A:N6	2.04	0.43
29:7:24:THR:O	29:7:28:ARG:HG3	2.19	0.43
1:A:188:G:N2	1:A:208:C:N3	2.46	0.43
1:A:221:A:N1	1:A:265:A:O2'	2.47	0.43
21:Z:44:PHE:CE2	21:Z:86:VAL:HG11	2.54	0.43
13:R:103:ARG:NH1	13:R:108:GLY:O	2.52	0.43
21:Z:28:MET:HG2	21:Z:37:VAL:HG11	2.00	0.43
8:I:108:THR:OG1	8:I:109:ILE:N	2.51	0.43
30:8:54:GLU:O	30:8:58:ILE:HG12	2.19	0.43
4:E:5:LEU:HD21	4:E:79:ARG:HB2	2.01	0.43
1:A:533:G:H5'	16:U:24:TYR:CD2	2.53	0.43
1:A:1169:G:N2	1:A:1181:C:C2	2.87	0.43
10:O:106:LEU:HD23	10:O:106:LEU:HA	1.75	0.43
6:G:98:ARG:NH1	6:G:98:ARG:HB2	2.33	0.43
1:A:2119:A:N6	1:A:2168:G:H1'	2.34	0.43
1:A:1503:U:H2'	1:A:1504:C:C6	2.53	0.43
1:A:1647:G:H3'	1:A:1647:G:P	2.59	0.43
4:E:52:LEU:HA	4:E:53:PRO:HD2	1.82	0.43
21:Z:137:ILE:HG23	21:Z:156:LYS:HD2	2.01	0.43
1:A:1946:U:H2'	1:A:1947:C:C6	2.54	0.43
1:A:328:U:H4'	20:Y:68:HIS:CD2	2.54	0.43
13:R:28:LEU:HD12	13:R:48:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:8:62:LEU:HB3	30:8:65:GLU:HG2	1.99	0.43
1:A:2031:A:C6	1:A:2498:C:H1'	2.54	0.43
1:A:1356:G:C6	1:A:1357:U:C4	3.07	0.43
1:A:2171:A:H4'	1:A:2172:U:O5'	2.18	0.43
14:S:96:GLY:N	14:S:99:LYS:HB3	2.34	0.43
1:A:1035:U:O4	34:A:4635:HOH:O	2.22	0.43
3:D:101:GLU:OE1	3:D:103:ARG:NH1	2.46	0.43
1:A:2593:U:H2'	1:A:2594:C:C6	2.54	0.43
1:A:1586:A:H2'	1:A:1587:A:H5'	2.00	0.43
24:2:50:ILE:O	24:2:52:ASP:N	2.45	0.43
15:T:37:GLY:HA2	15:T:38:ASN:HA	1.52	0.43
7:H:90:LYS:O	7:H:160:LYS:HA	2.19	0.43
1:A:1042:G:C6	1:A:1043:C:C4	3.07	0.43
1:A:2360:A:H2'	1:A:2361:A:O4'	2.18	0.43
11:P:107:LYS:O	11:P:110:TYR:HB2	2.19	0.43
1:A:64:A:O3'	19:X:71:GLY:HA3	2.19	0.43
18:W:36:LEU:HA	18:W:36:LEU:HD23	1.77	0.43
24:2:61:LEU:HA	24:2:61:LEU:HD23	1.84	0.43
1:A:1359:A:N6	1:A:1372:U:C5	2.87	0.42
1:A:1352:U:P	34:A:3925:HOH:O	2.71	0.42
6:G:5:VAL:HG12	26:4:25:TYR:HE1	1.81	0.42
1:A:2544:G:H2'	1:A:2545:G:O4'	2.19	0.42
12:Q:137:TYR:HE2	21:Z:49:ARG:NH1	2.17	0.42
8:I:92:VAL:CG1	8:I:120:ILE:HB	2.49	0.42
9:N:36:GLY:HA3	9:N:49:GLY:HA2	2.01	0.42
1:A:1488:G:C2	1:A:1489:U:O2	2.72	0.42
2:B:28:C:H2'	2:B:29:A:O4'	2.19	0.42
1:A:2252:G:H2'	1:A:2253:G:O4'	2.18	0.42
1:A:2678:C:H2'	1:A:2679:A:O4'	2.19	0.42
2:B:78:A:C2	2:B:100:A:C4	3.07	0.42
26:4:16:CYS:HB3	26:4:20:ASN:HB3	2.00	0.42
1:A:2474:C:H5''	1:A:2475:C:OP2	2.18	0.42
12:Q:63:LYS:HD2	12:Q:65:PHE:CZ	2.53	0.42
5:F:41:LEU:O	5:F:44:ARG:HG2	2.19	0.42
1:A:12:U:H2'	1:A:12:U:O2	2.19	0.42
1:A:330:A:H2	1:A:1210:A:C2'	2.20	0.42
1:A:807:U:OP2	11:P:41:ARG:NH2	2.52	0.42
11:P:38:GLN:O	11:P:39:LYS:HB3	2.19	0.42
1:A:1022:G:C5	1:A:1140:C:C4	3.08	0.42
1:A:2169:A:H3'	1:A:2170:A:C8	2.54	0.42
1:A:1046:A:O2'	1:A:1047:G:OP2	2.31	0.42
9:N:15:LEU:HD12	9:N:137:LYS:HG2	1.99	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1823:G:OP1	3:D:54:ARG:NH1	2.53	0.42
1:A:1649:G:N1	1:A:2009:G:C6	2.87	0.42
1:A:588:U:O4	1:A:670:A:H1'	2.20	0.42
1:A:190:A:O5'	1:A:205:G:N2	2.51	0.42
1:A:2580:U:C5	1:A:2581:G:C6	3.07	0.42
21:Z:27:VAL:HA	21:Z:35:ARG:O	2.19	0.42
1:A:2684:U:C4	1:A:2685:G:N7	2.87	0.42
1:A:236:C:H2'	1:A:237:C:C6	2.54	0.42
1:A:866:A:C6	1:A:914:C:C5	3.07	0.42
1:A:2706:G:O2'	13:R:64:ARG:HD3	2.19	0.42
1:A:817:C:O2'	1:A:839:U:H5''	2.20	0.42
1:A:839:U:H2'	1:A:840:C:C6	2.54	0.42
1:A:479:A:H4'	1:A:480:A:OP1	2.17	0.42
4:E:21:VAL:HA	4:E:22:PRO:HD2	1.94	0.42
6:G:138:GLN:HE21	6:G:144:ILE:HD13	1.83	0.42
1:A:248:G:H5'	1:A:250:G:N7	2.35	0.42
26:4:1:MET:HB3	26:4:6:HIS:CD2	2.53	0.42
3:D:180:GLY:HA3	3:D:275:LYS:CG	2.49	0.42
3:D:180:GLY:HA3	3:D:275:LYS:HG2	2.00	0.42
21:Z:128:VAL:HG23	21:Z:161:VAL:HG22	2.01	0.42
15:T:19:LEU:HA	15:T:20:PRO:HD3	1.79	0.42
17:V:52:VAL:HG21	17:V:55:ALA:HB3	2.01	0.42
1:A:311:A:C6	1:A:328:U:C4	3.07	0.42
12:Q:66:ILE:HG12	12:Q:104:PHE:HD2	1.84	0.42
24:2:9:GLN:HE22	24:2:56:GLN:HG2	1.84	0.42
1:A:623:G:H2'	1:A:624:C:C6	2.54	0.42
1:A:362:U:O2'	1:A:363:G:H5''	2.20	0.42
10:O:11:ALA:O	10:O:99:PHE:N	2.40	0.42
1:A:2683:C:O2	10:O:70:LYS:NZ	2.29	0.42
1:A:744:G:OP1	4:E:132:HIS:ND1	2.50	0.42
1:A:1292:U:H2'	1:A:1293:C:C6	2.54	0.42
23:1:32:LYS:HB3	23:1:32:LYS:HE2	1.90	0.42
6:G:143:GLU:H	6:G:143:GLU:HG2	1.51	0.42
11:P:52:GLU:CD	30:8:57:ARG:HH12	2.22	0.42
1:A:279:C:H42	1:A:361:G:H1	1.66	0.42
14:S:95:HIS:C	14:S:99:LYS:HB3	2.39	0.42
4:E:93:VAL:HG13	34:E:401:HOH:O	2.19	0.42
1:A:2235:G:H2'	1:A:2236:C:C6	2.54	0.42
9:N:34:LEU:HD12	9:N:34:LEU:HA	1.76	0.42
2:B:7:G:C8	2:B:7:G:H5''	2.54	0.42
1:A:2202:C:H2'	1:A:2203:U:O4'	2.19	0.42
1:A:576:U:H2'	1:A:577:G:C8	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:U:83:LEU:HD12	16:U:113:ALA:HB2	2.01	0.42
4:E:35:GLN:HG3	4:E:36:ARG:N	2.35	0.42
25:3:8:LEU:HD13	25:3:31:LEU:HD23	2.02	0.42
18:W:65:LEU:HA	18:W:65:LEU:HD23	1.86	0.42
6:G:43:LEU:HD22	6:G:90:LEU:HG	2.01	0.42
9:N:23:LEU:HB2	9:N:60:ILE:HG12	2.00	0.42
1:A:2114:A:H3'	1:A:2115:G:C8	2.55	0.42
1:A:1913:A:H3'	1:A:1913:A:P	2.59	0.42
1:A:2309:A:C6	1:A:2310:A:C2	3.08	0.42
14:S:56:LEU:O	14:S:58:LEU:HD22	2.20	0.42
1:A:1288:U:O2'	1:A:1647:G:N2	2.52	0.42
1:A:2273:A:H2'	1:A:2274:A:H8	1.83	0.42
1:A:1638:C:H4'	1:A:2710:C:O2	2.19	0.42
1:A:566:U:OP1	11:P:29:LYS:HD2	2.19	0.42
1:A:916:G:H5'	1:A:917:A:OP1	2.20	0.42
1:A:1799:G:H5'	1:A:1819:A:N6	2.33	0.42
1:A:2755:C:C4	31:9:19:ARG:NH1	2.87	0.42
1:A:1489:U:H3'	1:A:1489:U:C6	2.53	0.42
19:X:11:PRO:HD3	24:2:37:PHE:CE2	2.55	0.42
1:A:2664:G:H3'	34:A:3735:HOH:O	2.18	0.42
1:A:323:G:OP1	1:A:338:G:N2	2.48	0.42
1:A:2290:G:O2'	1:A:2381:C:H1'	2.20	0.42
16:U:82:GLY:HA3	16:U:113:ALA:HB1	2.00	0.42
3:D:39:LYS:NZ	3:D:57:GLY:O	2.53	0.42
15:T:27:THR:HB	15:T:89:VAL:HG23	2.02	0.42
1:A:2018:G:H2'	1:A:2019:A:O4'	2.19	0.42
1:A:719:C:H2'	1:A:720:C:C6	2.54	0.42
1:A:656:G:H2'	1:A:657:U:O4'	2.19	0.42
1:A:271(S):G:C6	1:A:271(T):C:C4	3.07	0.42
15:T:118:ARG:HA	15:T:118:ARG:NE	2.34	0.42
4:E:29:GLY:HA3	34:E:401:HOH:O	2.20	0.42
11:P:59:LEU:HA	11:P:59:LEU:HD23	1.70	0.42
1:A:674:G:H1'	5:F:74:ARG:CD	2.49	0.42
2:B:91:C:C2'	2:B:92:C:H5'	2.49	0.42
1:A:2309:A:C6	1:A:2310:A:N1	2.88	0.42
1:A:1287:A:H5''	1:A:1288:U:OP2	2.19	0.42
31:9:32:HIS:O	31:9:34:GLN:HG3	2.19	0.42
1:A:922:U:H2'	1:A:923:C:C6	2.55	0.42
11:P:82:GLY:HA2	11:P:113:LYS:O	2.20	0.42
1:A:2836:U:H2'	1:A:2837:G:C8	2.55	0.42
1:A:229:A:OP1	1:A:229:A:C8	2.73	0.42
1:A:1849:G:H2'	1:A:1850:G:C8	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:112:MET:HB2	5:F:112:MET:HE2	1.86	0.42
1:A:1927:A:H2'	1:A:1928:A:C8	2.54	0.42
1:A:663:G:C6	1:A:664:C:C4	3.08	0.42
1:A:2420:C:O5'	1:A:2420:C:H6	2.02	0.42
11:P:55:ARG:HA	34:P:308:HOH:O	2.20	0.42
1:A:2005:A:H5''	1:A:2006:C:OP2	2.20	0.42
1:A:860:U:C2	1:A:2268:A:C8	3.08	0.42
1:A:2561:A:H2'	1:A:2562:U:O4'	2.19	0.42
5:F:64:ILE:HG13	5:F:65:TRP:H	1.85	0.42
1:A:1300:U:H4'	1:A:1301:A:H5'	2.02	0.42
8:I:9:LEU:HB3	8:I:12:LEU:HB2	2.01	0.42
10:O:17:ARG:HD2	10:O:47:ILE:HG23	2.02	0.42
21:Z:152:ALA:HA	21:Z:155:LEU:HB2	2.00	0.42
1:A:335:C:H2'	1:A:336:C:C6	2.55	0.42
12:Q:70:PRO:HA	12:Q:94:VAL:O	2.19	0.42
2:B:96:U:H2'	2:B:97:G:H8	1.85	0.42
2:B:40:U:H1'	2:B:45:A:H61	1.83	0.42
1:A:696:G:O2'	1:A:697:C:H5'	2.20	0.42
16:U:43:GLY:HA3	17:V:73:SER:OG	2.18	0.42
12:Q:78:PRO:O	12:Q:81:VAL:HG13	2.20	0.42
1:A:2862:G:H2'	1:A:2863:C:H6	1.85	0.42
1:A:1932:A:H2'	1:A:1933:G:O4'	2.19	0.42
1:A:1844:C:OP1	3:D:257:LEU:HD23	2.19	0.42
1:A:1577:C:OP2	34:A:4256:HOH:O	2.21	0.42
1:A:1022:G:C6	1:A:1140:C:C4	3.08	0.42
1:A:2114:A:C6	1:A:2115:G:C2	3.07	0.42
1:A:71:A:H5''	1:A:73:A:C8	2.54	0.42
1:A:2833:G:C3'	1:A:2834:G:H5'	2.48	0.42
1:A:1833:U:O2'	1:A:1969:A:N1	2.34	0.42
20:Y:90:LEU:C	20:Y:92:ASN:H	2.21	0.42
24:2:50:ILE:C	24:2:52:ASP:N	2.72	0.42
1:A:1525:G:H2'	1:A:1526:G:O4'	2.19	0.42
1:A:117:G:C6	1:A:119:A:C6	3.08	0.42
1:A:2019:A:H4'	16:U:34:LYS:HD2	2.01	0.42
29:7:1:MET:O	29:7:2:LYS:C	2.57	0.42
1:A:1163:G:O2'	1:A:1164:G:H5'	2.20	0.42
1:A:907:U:O2'	12:Q:101:ARG:NH2	2.43	0.42
1:A:271(I):G:H2'	1:A:271(J):C:C6	2.55	0.42
6:G:105:LYS:HZ1	26:4:26:SER:HB2	1.84	0.42
1:A:2022:U:O2'	1:A:2617:C:H5'	2.20	0.42
1:A:7:G:H4'	9:N:13:TRP:CH2	2.55	0.42
1:A:652(E):G:C2	1:A:652(U):G:C2	3.08	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1179:C:H2'	1:A:1180:C:C6	2.55	0.42
14:S:34:HIS:ND1	14:S:53:SER:OG	2.52	0.42
16:U:106:PHE:O	16:U:110:VAL:HG23	2.20	0.42
1:A:2525:G:C2	1:A:2539:C:C2	3.08	0.42
1:A:2304:G:O6	1:A:2312:U:O4	2.38	0.42
1:A:1319:G:C6	1:A:1320:C:N4	2.87	0.42
15:T:110:ILE:HG12	15:T:110:ILE:H	1.58	0.42
26:4:13:ARG:N	26:4:29:PRO:O	2.37	0.42
10:O:70:LYS:HB3	10:O:70:LYS:HE2	1.76	0.42
28:6:19:ARG:H	28:6:19:ARG:HD2	1.85	0.42
21:Z:6:LYS:HE2	21:Z:6:LYS:HB3	1.88	0.42
1:A:2516:G:C6	1:A:2517:C:C4	3.08	0.42
1:A:1518:U:H2'	1:A:1519:G:O4'	2.20	0.42
1:A:21:A:O2'	1:A:22:C:H5'	2.20	0.42
2:B:32:C:C2	2:B:51:G:N2	2.88	0.42
1:A:675:A:C8	1:A:804:A:C6	3.08	0.41
1:A:816:C:P	34:A:4431:HOH:O	2.77	0.41
1:A:2748:A:N6	1:A:2749:A:C6	2.88	0.41
1:A:2293:C:H2'	1:A:2294:C:H6	1.83	0.41
1:A:2464:C:O2'	1:A:2465:C:P	2.78	0.41
1:A:565:C:H2'	1:A:566:U:O4'	2.20	0.41
14:S:66:ALA:O	14:S:69:VAL:N	2.53	0.41
19:X:72:LYS:HB3	19:X:72:LYS:HE3	1.92	0.41
7:H:13:LYS:HA	7:H:14:GLY:HA2	1.59	0.41
12:Q:11:LYS:HE2	12:Q:88:GLY:O	2.20	0.41
19:X:61:GLY:HA3	19:X:73:ARG:O	2.20	0.41
16:U:5:LYS:HB2	16:U:5:LYS:HE3	1.83	0.41
1:A:1530:C:O2'	1:A:1531:C:H6	2.03	0.41
5:F:101:LEU:HB3	5:F:106:ARG:HD3	2.01	0.41
1:A:1912:A:HO2'	1:A:1913:A:P	2.43	0.41
8:I:44:LEU:HA	8:I:44:LEU:HD12	1.74	0.41
1:A:1740:G:H2'	1:A:1741:A:C8	2.55	0.41
26:4:1:MET:HB3	26:4:6:HIS:NE2	2.35	0.41
24:2:50:ILE:O	24:2:51:ARG:HB3	2.20	0.41
9:N:24:GLY:HA2	9:N:27:ALA:CB	2.50	0.41
34:A:4430:HOH:O	11:P:16:ARG:HG3	2.20	0.41
1:A:323:G:H1'	1:A:1205:U:O2	2.19	0.41
2:B:28:C:H2'	2:B:29:A:H8	1.85	0.41
18:W:10:VAL:HG21	18:W:103:ILE:HD12	2.02	0.41
1:A:44:G:H5"	1:A:45:C:OP1	2.20	0.41
7:H:87:LEU:HD23	7:H:87:LEU:HA	1.87	0.41
2:B:89:G:H8	2:B:89:G:OP2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2821:A:H2'	1:A:2822:G:O4'	2.19	0.41
1:A:849:A:H5''	1:A:850:C:OP2	2.19	0.41
1:A:945:A:C4	1:A:2448:A:C2	3.07	0.41
1:A:860:U:H1'	1:A:2268:A:H5'	2.02	0.41
3:D:107:ALA:HA	3:D:108:PRO:HD2	1.94	0.41
20:Y:23:ARG:HB2	20:Y:23:ARG:NH1	2.35	0.41
1:A:2321:G:C2'	1:A:2321:G:N3	2.81	0.41
15:T:53:ARG:NH1	15:T:60:THR:OG1	2.53	0.41
1:A:2464:C:O2'	1:A:2465:C:OP2	2.34	0.41
1:A:900:A:H2'	1:A:901:A:H8	1.85	0.41
1:A:1925:C:C2'	1:A:1926:U:H5'	2.50	0.41
21:Z:100:VAL:HG11	21:Z:134:PRO:HG2	2.03	0.41
16:U:106:PHE:O	16:U:109:LEU:HB2	2.20	0.41
19:X:24:GLY:O	19:X:83:VAL:HG22	2.20	0.41
1:A:2554:U:H2'	1:A:2555:U:C6	2.55	0.41
28:6:10:LEU:HG	28:6:54:ILE:HD12	2.03	0.41
6:G:125:PHE:CZ	6:G:170:ARG:HA	2.55	0.41
1:A:2016:U:H2'	1:A:2017:U:C6	2.55	0.41
8:I:25:TYR:CD1	8:I:30:LEU:HD11	2.55	0.41
1:A:2742:C:OP1	31:9:35:ARG:HD3	2.20	0.41
1:A:1530:C:H42	1:A:1539:G:H1	1.68	0.41
1:A:2173:A:C3'	1:A:2174:C:H5'	2.50	0.41
1:A:2153:G:H2'	1:A:2154:G:O4'	2.21	0.41
4:E:47:VAL:CG1	4:E:86:PRO:HD2	2.47	0.41
1:A:2261:C:O2'	1:A:2262:U:H5'	2.21	0.41
1:A:1783:A:C2	1:A:2587:A:C5	3.09	0.41
3:D:210:GLY:O	3:D:213:ARG:N	2.53	0.41
18:W:97:LYS:HE3	18:W:99:ARG:NH2	2.35	0.41
1:A:2299:G:N1	1:A:2318:G:C8	2.89	0.41
7:H:3:ARG:NH2	7:H:5:GLY:H	2.19	0.41
1:A:1051:G:N3	1:A:1051:G:H2'	2.36	0.41
17:V:76:LYS:HB2	17:V:81:TYR:HB3	2.03	0.41
1:A:286:C:H42	1:A:355:G:H1	1.68	0.41
1:A:478:A:C6	1:A:480:A:C6	3.08	0.41
1:A:2812:G:C2	1:A:2813:A:C4	3.08	0.41
10:O:7:TYR:OH	10:O:44:LYS:HG3	2.20	0.41
1:A:2092:U:H4'	1:A:2093:G:O5'	2.21	0.41
1:A:909:A:C6	1:A:912:C:C2	3.08	0.41
7:H:35:VAL:HA	7:H:36:PRO:HD2	1.77	0.41
4:E:137:HIS:HB3	4:E:138:PRO:HD2	2.02	0.41
21:Z:106:GLY:HA3	21:Z:142:SER:OG	2.21	0.41
1:A:2239:G:H5'	3:D:251:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:O:9:GLU:HB2	10:O:83:ALA:HB2	2.03	0.41
12:Q:54:MET:HE2	12:Q:54:MET:HB2	1.86	0.41
8:I:139:GLN:HA	8:I:139:GLN:HE21	1.85	0.41
1:A:2127:G:H1'	1:A:2173:A:C2	2.56	0.41
1:A:2130:U:O3'	1:A:2133:G:H4'	2.20	0.41
6:G:138:GLN:HE22	6:G:153:ARG:NH2	2.19	0.41
15:T:55:ASN:H	15:T:59:THR:HB	1.84	0.41
6:G:66:GLN:HG2	26:4:1:MET:CE	2.51	0.41
2:B:73:A:C4	2:B:105:A:C2	3.08	0.41
1:A:1253:A:C5	34:A:4441:HOH:O	2.72	0.41
5:F:158:THR:HG1	5:F:160:ASN:H	1.59	0.41
15:T:20:PRO:HG2	15:T:86:ILE:O	2.20	0.41
12:Q:72:LYS:HB3	12:Q:94:VAL:HG23	2.03	0.41
1:A:2528:U:H2'	1:A:2530:A:O5'	2.21	0.41
1:A:2178:C:H2'	1:A:2179:C:O4'	2.20	0.41
18:W:64:MET:HE3	18:W:109:GLU:HG3	2.02	0.41
4:E:51:PHE:O	4:E:75:VAL:HG13	2.21	0.41
4:E:7:VAL:HG12	4:E:51:PHE:CE1	2.55	0.41
6:G:8:LYS:O	6:G:12:TYR:HD1	2.03	0.41
1:A:2233:U:H2'	1:A:2234:G:C8	2.56	0.41
1:A:2791:C:H2'	1:A:2792:G:C8	2.55	0.41
9:N:102:ALA:O	9:N:106:MET:HG3	2.21	0.41
6:G:82:LEU:HD22	6:G:86:MET:CB	2.51	0.41
1:A:826:U:C4'	11:P:55:ARG:HB2	2.51	0.41
1:A:2165:G:H2'	1:A:2166:G:H8	1.84	0.41
1:A:528:A:C2	1:A:2043:C:H4'	2.55	0.41
6:G:106:LEU:O	6:G:111:LEU:HG	2.21	0.41
6:G:174:GLU:HG2	6:G:180:PHE:CD1	2.56	0.41
7:H:3:ARG:HG2	7:H:6:ARG:CZ	2.49	0.41
1:A:1814:G:H4'	3:D:51:VAL:HG21	2.03	0.41
8:I:106:GLY:HA2	8:I:107:VAL:HB	2.03	0.41
1:A:928:G:O5'	1:A:928:G:H8	2.04	0.41
6:G:72:ARG:NH1	6:G:87:PRO:HG3	2.34	0.41
1:A:1648:C:H2'	1:A:1649:G:O5'	2.20	0.41
9:N:96:GLU:HB2	9:N:122:VAL:HG12	2.03	0.41
1:A:725:G:O5'	1:A:725:G:H8	2.04	0.41
1:A:647:G:H2'	1:A:648:G:O4'	2.21	0.41
1:A:401:A:H2'	1:A:402:A:O4'	2.21	0.41
1:A:2091:U:O2'	23:1:47:GLN:HG3	2.21	0.41
1:A:224:G:H2'	1:A:225:A:O4'	2.21	0.41
1:A:1709:U:H2'	1:A:1710:C:C6	2.56	0.41
12:Q:34:LEU:HA	12:Q:34:LEU:HD12	1.77	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:S:11:LYS:HD3	14:S:15:ARG:NH2	2.36	0.41
1:A:272(E):G:C2	1:A:364:C:C2	3.08	0.41
6:G:39:ILE:HG23	6:G:157:ILE:HD13	2.02	0.41
1:A:534:U:H5'	16:U:42:ALA:HB1	2.03	0.41
1:A:1188:U:O2'	1:A:1189:A:H5'	2.20	0.41
1:A:1131:G:H21	9:N:73:THR:CG2	2.34	0.41
1:A:2463:C:H2'	1:A:2464:C:H5'	2.03	0.41
21:Z:72:ARG:HA	21:Z:72:ARG:HD3	1.61	0.41
1:A:918:A:C5	1:A:919:G:H1'	2.56	0.41
21:Z:39:VAL:CG2	21:Z:44:PHE:HB2	2.51	0.41
1:A:1441:G:H2'	1:A:1442:G:H8	1.85	0.41
4:E:4:ILE:HG12	4:E:5:LEU:O	2.20	0.41
17:V:2:PHE:CZ	17:V:41:GLY:HA3	2.56	0.41
3:D:26:LYS:HE2	3:D:28:GLU:O	2.21	0.41
1:A:563:G:H5'	1:A:572:A:H4'	2.02	0.41
1:A:1376:C:N4	1:A:1377:G:C6	2.89	0.41
11:P:38:GLN:HG3	11:P:45:LEU:HD23	2.02	0.41
23:1:82:LEU:CA	23:1:85:LEU:HD23	2.40	0.41
1:A:1185:C:H5''	1:A:1186:G:OP1	2.21	0.41
1:A:2305:A:H2'	1:A:2306:C:O4'	2.20	0.41
1:A:2572:A:N7	4:E:144:ARG:HD2	2.35	0.41
26:4:14:ILE:HD12	26:4:22:ILE:HB	2.03	0.41
1:A:928:G:O6	34:A:3675:HOH:O	2.22	0.41
8:I:12:LEU:HD23	8:I:12:LEU:HA	1.88	0.41
3:D:136:ILE:HA	3:D:137:PRO:HD3	1.95	0.41
7:H:22:GLY:HA2	7:H:37:VAL:O	2.20	0.41
1:A:1668:A:OP1	10:O:5:GLN:HG3	2.21	0.41
1:A:708:C:H5'	1:A:709:U:OP2	2.21	0.41
1:A:794:G:H2'	1:A:795:C:C6	2.55	0.41
1:A:1171:G:OP2	1:A:1171:G:H8	2.03	0.41
1:A:2203:U:O2'	1:A:2205:C:H5'	2.20	0.41
1:A:2607:G:H2'	1:A:2608:G:O4'	2.21	0.41
1:A:127:A:H5''	1:A:128:C:C6	2.54	0.41
2:B:46:A:C5	2:B:47:C:C4	3.09	0.41
1:A:285:C:H2'	1:A:286:C:H6	1.86	0.41
1:A:2498:C:O2'	1:A:2499:C:H5'	2.21	0.41
4:E:14:ILE:HG13	4:E:21:VAL:HG13	2.03	0.41
1:A:271(Y):U:H6	1:A:271(Y):U:H2'	1.69	0.41
1:A:458:G:O2'	29:7:39:ARG:HD3	2.20	0.41
7:H:143:GLN:HG3	7:H:147:ASN:ND2	2.36	0.41
1:A:1742:G:H2'	1:A:1743:C:O4'	2.20	0.41
28:6:40:CYS:SG	28:6:42:TRP:N	2.92	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:S:77:ALA:O	14:S:80:LEU:N	2.48	0.41
5:F:167:ALA:HB1	5:F:173:VAL:HG11	2.02	0.41
19:X:25:LYS:HG3	19:X:82:GLN:OE1	2.21	0.41
1:A:1712:C:H2'	1:A:1713:U:C6	2.55	0.41
21:Z:124:ILE:HD11	21:Z:165:VAL:HG11	2.03	0.41
3:D:221:VAL:HG22	3:D:226:MET:CE	2.51	0.41
15:T:35:LYS:HA	15:T:40:THR:HG22	2.03	0.41
9:N:12:ARG:HG3	9:N:14:VAL:HG23	2.03	0.41
1:A:2115:G:H4'	1:A:2167:U:C4'	2.45	0.41
1:A:1507:A:O2'	1:A:1508:A:C8	2.63	0.41
1:A:198:C:H5'	1:A:2244:U:OP1	2.21	0.41
18:W:79:GLY:CA	18:W:100:THR:HG22	2.49	0.41
1:A:322:A:H4'	1:A:323:G:OP2	2.21	0.41
1:A:189:G:H2'	1:A:205:G:N2	2.36	0.41
1:A:481:G:H1'	1:A:507:A:N1	2.36	0.41
2:B:113:G:H2'	2:B:114:C:O4'	2.21	0.41
1:A:410:G:C2	1:A:418:G:C2	3.09	0.41
1:A:2338:G:O2'	1:A:2339:G:H5'	2.21	0.41
25:3:36:VAL:O	25:3:37:LEU:HD23	2.20	0.41
12:Q:110:THR:HG23	12:Q:113:GLN:HB2	2.02	0.41
1:A:1957:C:H2'	1:A:1958:C:C6	2.56	0.41
1:A:862:G:OP2	34:A:4340:HOH:O	2.21	0.41
1:A:1971:A:H5''	34:A:4200:HOH:O	2.19	0.40
11:P:38:GLN:C	11:P:40:SER:N	2.74	0.40
1:A:26:G:H1'	1:A:515:A:H61	1.86	0.40
1:A:2110:G:C6	1:A:2120:G:C8	3.09	0.40
1:A:2464:C:N3	1:A:2487:G:C2	2.89	0.40
1:A:652(B):A:O2'	1:A:652(C):G:H5'	2.21	0.40
1:A:1790:C:H2'	1:A:1791:A:C5	2.56	0.40
3:D:146:GLU:HG2	3:D:152:GLY:C	2.41	0.40
1:A:2791:C:H3'	1:A:2791:C:OP2	2.21	0.40
11:P:147:LEU:HA	11:P:147:LEU:HD22	1.87	0.40
12:Q:30:GLY:HA2	12:Q:107:ALA:HB2	2.03	0.40
1:A:1417:C:H2'	1:A:1418:G:O4'	2.21	0.40
13:R:62:ALA:O	13:R:66:VAL:HG23	2.21	0.40
1:A:686:G:N2	1:A:788:A:H61	2.20	0.40
1:A:1655:A:H3'	1:A:1656:C:H6	1.86	0.40
1:A:1971:A:C4	3:D:241:PRO:HD3	2.56	0.40
1:A:28:A:C5	1:A:29:U:C5	3.09	0.40
1:A:31:C:C4	1:A:32:C:C5	3.10	0.40
1:A:1512:U:H2'	1:A:1513:C:H6	1.87	0.40
3:D:275:LYS:O	3:D:275:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2492:U:H2'	1:A:2493:U:H6	1.83	0.40
11:P:86:LYS:HB3	11:P:117:GLU:O	2.22	0.40
8:I:45:LYS:O	8:I:48:GLU:N	2.54	0.40
1:A:610:G:N2	1:A:619:G:H1'	2.35	0.40
1:A:2360:A:H8	1:A:2360:A:O5'	2.05	0.40
1:A:478:A:N6	1:A:502:A:N6	2.69	0.40
1:A:719:C:H2'	1:A:720:C:H6	1.87	0.40
9:N:12:ARG:HD3	9:N:50:ASP:OD2	2.21	0.40
1:A:2714:G:O2'	1:A:2715:C:H5'	2.20	0.40
1:A:2100:G:C6	1:A:2101:G:C5	3.09	0.40
1:A:2584:U:H2'	1:A:2585:U:H2'	2.02	0.40
5:F:202:PHE:O	5:F:205:ARG:HB3	2.21	0.40
5:F:93:LYS:HD3	5:F:93:LYS:HA	1.85	0.40
1:A:895:U:H5''	1:A:895:U:H6	1.86	0.40
1:A:2286:A:H4'	1:A:2287:A:O4'	2.22	0.40
6:G:97:ASP:O	6:G:101:ILE:HG13	2.22	0.40
1:A:996:A:N6	1:A:1160:G:C6	2.90	0.40
1:A:1558:A:N3	1:A:1558:A:O4'	2.52	0.40
1:A:123:G:H2'	1:A:124:G:O4'	2.21	0.40
18:W:59:VAL:HG12	18:W:60:ASN:HD22	1.86	0.40
1:A:275:G:H2'	1:A:276:A:H5'	2.04	0.40
2:B:60:C:C2	2:B:61:G:C8	3.09	0.40
9:N:67:LEU:O	9:N:88:GLU:HG3	2.21	0.40
1:A:414:C:O2'	1:A:415:A:H5'	2.22	0.40
11:P:106:LEU:HD23	11:P:106:LEU:HA	1.88	0.40
1:A:303:U:H2'	1:A:304:G:H8	1.86	0.40
13:R:67:LEU:HD13	13:R:67:LEU:HA	1.72	0.40
21:Z:92:SER:HB2	21:Z:94:GLU:HG2	2.03	0.40
5:F:170:LEU:HA	5:F:171:PRO:HD3	1.90	0.40
1:A:1864:U:H5''	1:A:2410:G:O2'	2.22	0.40
4:E:203:LYS:CB	4:E:204:ALA:HA	2.51	0.40
27:5:36:CYS:O	27:5:37:LYS:HD3	2.22	0.40
1:A:2287:A:N6	1:A:2344:U:N3	2.56	0.40
6:G:16:ARG:NE	6:G:31:VAL:HG21	2.33	0.40
1:A:2427:C:H5''	1:A:2428:G:OP1	2.22	0.40
1:A:1606:G:H5''	1:A:1607:C:OP1	2.21	0.40
9:N:47:ALA:HB2	9:N:112:LEU:CD1	2.45	0.40
1:A:1722:A:C2	1:A:1740:G:C8	3.09	0.40
26:4:9:LEU:HD22	26:4:26:SER:HA	2.02	0.40
4:E:9:VAL:HB	15:T:3:ARG:HG2	2.02	0.40
1:A:994:C:OP1	16:U:53:ARG:NH2	2.53	0.40
1:A:315:G:H2'	1:A:316:C:H6	1.87	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1602:U:O4	34:A:3929:HOH:O	2.21	0.40
12:Q:42:ILE:CG2	12:Q:47:ILE:HG13	2.51	0.40
22:0:14:ARG:HG3	22:0:14:ARG:NH1	2.36	0.40
1:A:1579:A:H2'	1:A:1580:A:C8	2.56	0.40
1:A:2099:U:H3	1:A:2190:G:H1	1.68	0.40
4:E:179:GLU:HB3	4:E:181:LEU:CD2	2.51	0.40
12:Q:35:VAL:HG23	12:Q:101:ARG:O	2.20	0.40
1:A:1756:G:H4'	1:A:1758:G:O4'	2.22	0.40
17:V:24:LYS:HA	17:V:92:THR:OG1	2.22	0.40
1:A:1918:A:O2'	1:A:1920:C:N4	2.54	0.40
12:Q:7:MET:HB2	12:Q:7:MET:HE3	1.66	0.40
1:A:1204:A:N6	1:A:1240:U:H2'	2.37	0.40
1:A:26:G:C6	1:A:27:G:N1	2.89	0.40
1:A:94:C:O2	1:A:94:C:H2'	2.20	0.40
1:A:2406:U:H6	1:A:2406:U:OP2	2.04	0.40
29:7:47:ARG:HH11	29:7:47:ARG:CG	2.33	0.40
2:B:23:G:H1	2:B:60:C:H42	1.69	0.40
21:Z:144:LEU:HD21	21:Z:150:LEU:HG	2.03	0.40
3:D:154:LYS:HB2	3:D:155:LEU:HD12	2.03	0.40
29:7:48:LYS:HB2	29:7:48:LYS:HE2	1.88	0.40
1:A:2576:G:O2'	1:A:2579:C:OP2	2.29	0.40
1:A:2070:G:H2'	1:A:2071:A:C8	2.57	0.40
1:A:2729:G:H2'	1:A:2730:C:C6	2.56	0.40
1:A:705:A:C2	1:A:727:A:H1'	2.57	0.40
1:A:65:C:O2'	1:A:456:C:O2	2.39	0.40
1:A:2028:U:H2'	1:A:2029:G:O4'	2.22	0.40
1:A:194:G:H2'	1:A:195:A:O4'	2.21	0.40
1:A:2139:C:H2'	1:A:2140:C:O4'	2.22	0.40
1:A:1676:A:C8	34:A:4359:HOH:O	2.72	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	
3	D	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	43	84
4	E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	22	68
5	F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	38	81
6	G	179/182 (98%)	150 (84%)	29 (16%)	0	100	100
7	H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	33	78
8	I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	16	58
9	N	138/140 (99%)	128 (93%)	7 (5%)	3 (2%)	10	46
10	O	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
11	P	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
12	Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	30	76
13	R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	T	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
16	U	114/118 (97%)	114 (100%)	0	0	100	100
17	V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
18	W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	22	68
21	Z	196/206 (95%)	180 (92%)	14 (7%)	2 (1%)	22	68
22	0	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
23	1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	65
24	2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
27	5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	10	46
30	8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	9	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	3373/3526 (96%)	3156 (94%)	201 (6%)	16 (0%)	38	81

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	18	ALA
12	Q	135	ASP
9	N	4	TYR
9	N	5	VAL
21	Z	192	ALA
23	1	3	LYS
29	7	46	VAL
7	H	170	ARG
8	I	10	GLU
5	F	130	ALA
8	I	107	VAL
4	E	52	LEU
4	E	72	VAL
3	D	3	VAL
20	Y	3	VAL
21	Z	161	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	
3	D	215/218 (99%)	183 (85%)	32 (15%)	4	17
4	E	163/166 (98%)	137 (84%)	26 (16%)	3	13
5	F	159/166 (96%)	134 (84%)	25 (16%)	4	14
6	G	128/156 (82%)	109 (85%)	19 (15%)	4	17
7	H	141/148 (95%)	123 (87%)	18 (13%)	6	24
8	I	74/124 (60%)	60 (81%)	14 (19%)	2	9
9	N	117/119 (98%)	98 (84%)	19 (16%)	3	13
10	O	98/100 (98%)	83 (85%)	15 (15%)	4	15
11	P	114/116 (98%)	99 (87%)	15 (13%)	6	23
12	Q	111/111 (100%)	96 (86%)	15 (14%)	6	22
13	R	101/101 (100%)	77 (76%)	24 (24%)	1	4
14	S	84/88 (96%)	68 (81%)	16 (19%)	2	9
15	T	110/127 (87%)	95 (86%)	15 (14%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	93/94 (99%)	83 (89%)	10 (11%)	9	34
17	V	80/82 (98%)	63 (79%)	17 (21%)	1	7
18	W	89/92 (97%)	78 (88%)	11 (12%)	7	25
19	X	75/78 (96%)	70 (93%)	5 (7%)	23	63
20	Y	80/91 (88%)	63 (79%)	17 (21%)	1	7
21	Z	159/179 (89%)	139 (87%)	20 (13%)	7	24
22	0	59/67 (88%)	50 (85%)	9 (15%)	4	15
23	1	78/83 (94%)	66 (85%)	12 (15%)	4	15
24	2	65/67 (97%)	55 (85%)	10 (15%)	4	15
25	3	49/52 (94%)	44 (90%)	5 (10%)	11	37
26	4	39/63 (62%)	33 (85%)	6 (15%)	4	15
27	5	50/52 (96%)	41 (82%)	9 (18%)	2	10
28	6	50/52 (96%)	40 (80%)	10 (20%)	2	8
29	7	41/42 (98%)	34 (83%)	7 (17%)	3	11
30	8	52/55 (94%)	42 (81%)	10 (19%)	2	9
31	9	32/34 (94%)	28 (88%)	4 (12%)	7	25
All	All	2706/2923 (93%)	2291 (85%)	415 (15%)	4	15

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	12	SER
3	D	13	ARG
3	D	18	VAL
3	D	24	ILE
3	D	54	ARG
3	D	83	GLU
3	D	94	LEU
3	D	103	ARG
3	D	106	ILE
3	D	111	LEU
3	D	126	GLN
3	D	131	LEU
3	D	138	VAL
3	D	141	VAL
3	D	150	LYS

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Mol	Chain	Res	Type
3	D	154	LYS
3	D	173	VAL
3	D	192	THR
3	D	200	ASP
3	D	211	ARG
3	D	212	SER
3	D	217	ARG
3	D	218	ARG
3	D	221	VAL
3	D	229	VAL
3	D	254	THR
3	D	257	LEU
3	D	259	THR
3	D	260	ARG
3	D	271	ILE
3	D	273	ARG
3	D	274	ARG
4	E	7	VAL
4	E	12	THR
4	E	21	VAL
4	E	24	THR
4	E	33	VAL
4	E	40	GLU
4	E	49	LEU
4	E	52	LEU
4	E	61	ARG
4	E	69	LYS
4	E	72	VAL
4	E	75	VAL
4	E	77	ILE
4	E	82	ARG
4	E	92	THR
4	E	111	ARG
4	E	116	VAL
4	E	119	ARG
4	E	128	SER
4	E	144	ARG
4	E	154	LYS
4	E	167	VAL
4	E	170	LEU
4	E	179	GLU
4	E	181	LEU

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Mol	Chain	Res	Type
4	E	195	LEU
5	F	12	LEU
5	F	18	ARG
5	F	20	LEU
5	F	24	LEU
5	F	33	LEU
5	F	41	LEU
5	F	50	SER
5	F	57	VAL
5	F	69	HIS
5	F	77	ASP
5	F	88	VAL
5	F	96	ASP
5	F	106	ARG
5	F	110	LEU
5	F	112	MET
5	F	132	VAL
5	F	137	LYS
5	F	140	LEU
5	F	158	THR
5	F	161	GLU
5	F	168	ARG
5	F	170	LEU
5	F	175	THR
5	F	188	ARG
5	F	192	LEU
6	G	3	LEU
6	G	5	VAL
6	G	7	LEU
6	G	21	ARG
6	G	28	VAL
6	G	35	GLU
6	G	47	LYS
6	G	98	ARG
6	G	128	ARG
6	G	136	ARG
6	G	139	LEU
6	G	140	ILE
6	G	143	GLU
6	G	146	TYR
6	G	149	VAL
6	G	155	MET

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Mol	Chain	Res	Type
6	G	161	THR
6	G	170	ARG
6	G	175	LEU
7	H	3	ARG
7	H	6	ARG
7	H	7	LEU
7	H	15	VAL
7	H	24	VAL
7	H	41	MET
7	H	44	VAL
7	H	49	VAL
7	H	51	ARG
7	H	58	GLU
7	H	68	THR
7	H	69	ARG
7	H	88	LEU
7	H	98	LEU
7	H	113	VAL
7	H	122	THR
7	H	134	SER
7	H	139	GLN
8	I	1	MET
8	I	42	SER
8	I	44	LEU
8	I	45	LYS
8	I	47	LEU
8	I	81	VAL
8	I	101	LEU
8	I	120	ILE
8	I	123	LEU
8	I	129	THR
8	I	130	TYR
8	I	139	GLN
8	I	142	VAL
8	I	145	VAL
9	N	1	MET
9	N	5	VAL
9	N	12	ARG
9	N	28	THR
9	N	33	LEU
9	N	34	LEU
9	N	38	HIS

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Mol	Chain	Res	Type
9	N	46	VAL
9	N	48	MET
9	N	62	VAL
9	N	67	LEU
9	N	68	GLU
9	N	85	ILE
9	N	99	LEU
9	N	112	LEU
9	N	120	LEU
9	N	130	HIS
9	N	133	GLN
9	N	140	VAL
10	O	8	LEU
10	O	10	VAL
10	O	17	ARG
10	O	24	VAL
10	O	25	LEU
10	O	26	LYS
10	O	29	ASN
10	O	32	TYR
10	O	52	VAL
10	O	53	LYS
10	O	58	VAL
10	O	94	ARG
10	O	98	VAL
10	O	104	ARG
10	O	113	LYS
11	P	21	ARG
11	P	32	THR
11	P	40	SER
11	P	42	SER
11	P	45	LEU
11	P	55	ARG
11	P	59	LEU
11	P	65	ARG
11	P	71	VAL
11	P	83	VAL
11	P	86	LYS
11	P	95	VAL
11	P	106	LEU
11	P	112	LEU
11	P	125	VAL

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Mol	Chain	Res	Type
12	Q	1	MET
12	Q	5	ARG
12	Q	7	MET
12	Q	16	ARG
12	Q	45	GLN
12	Q	55	VAL
12	Q	56	ARG
12	Q	59	ARG
12	Q	63	LYS
12	Q	75	THR
12	Q	81	VAL
12	Q	109	VAL
12	Q	110	THR
12	Q	134	ARG
12	Q	138	ASP
13	R	1	MET
13	R	2	ARG
13	R	6	SER
13	R	9	LYS
13	R	15	SER
13	R	18	LEU
13	R	24	GLN
13	R	28	LEU
13	R	29	LEU
13	R	33	ARG
13	R	44	LEU
13	R	54	LEU
13	R	57	ARG
13	R	60	LEU
13	R	63	ARG
13	R	65	LEU
13	R	67	LEU
13	R	79	LEU
13	R	86	ARG
13	R	100	LEU
13	R	103	ARG
13	R	111	LEU
13	R	113	LEU
13	R	117	VAL
14	S	3	ARG
14	S	8	GLU
14	S	12	PHE

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Mol	Chain	Res	Type
14	S	13	ARG
14	S	20	ARG
14	S	30	ARG
14	S	36	TYR
14	S	50	SER
14	S	57	LYS
14	S	58	LEU
14	S	69	VAL
14	S	75	GLU
14	S	78	LEU
14	S	84	GLN
14	S	85	VAL
14	S	95	HIS
15	T	6	LEU
15	T	13	ARG
15	T	16	ARG
15	T	17	THR
15	T	36	GLU
15	T	39	ARG
15	T	49	VAL
15	T	64	ARG
15	T	74	ARG
15	T	82	LEU
15	T	95	ARG
15	T	96	ARG
15	T	107	ASP
15	T	111	ARG
15	T	118	ARG
16	U	8	VAL
16	U	30	LYS
16	U	31	SER
16	U	36	ARG
16	U	59	ARG
16	U	60	LEU
16	U	74	LEU
16	U	101	ARG
16	U	104	GLN
16	U	108	GLU
17	V	7	THR
17	V	12	TYR
17	V	13	ARG
17	V	18	LEU

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Mol	Chain	Res	Type
17	V	21	ARG
17	V	28	GLU
17	V	32	THR
17	V	33	VAL
17	V	57	VAL
17	V	61	VAL
17	V	62	LEU
17	V	72	VAL
17	V	73	SER
17	V	79	VAL
17	V	85	LYS
17	V	95	LEU
17	V	100	ARG
18	W	11	ARG
18	W	15	ARG
18	W	19	LEU
18	W	23	LEU
18	W	27	LYS
18	W	41	LYS
18	W	51	LEU
18	W	60	ASN
18	W	77	ASP
18	W	100	THR
18	W	107	LEU
19	X	15	GLU
19	X	25	LYS
19	X	57	LEU
19	X	65	ARG
19	X	76	ARG
20	Y	2	ARG
20	Y	3	VAL
20	Y	6	HIS
20	Y	9	LYS
20	Y	23	ARG
20	Y	45	VAL
20	Y	49	VAL
20	Y	55	TYR
20	Y	61	ILE
20	Y	72	VAL
20	Y	90	LEU
20	Y	91	GLU
20	Y	92	ASN

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Mol	Chain	Res	Type
20	Y	97	ARG
20	Y	101	LYS
20	Y	102	CYS
20	Y	107	ASP
21	Z	5	LEU
21	Z	10	ARG
21	Z	11	GLU
21	Z	19	ARG
21	Z	24	LEU
21	Z	42	VAL
21	Z	52	SER
21	Z	56	VAL
21	Z	66	SER
21	Z	76	LEU
21	Z	82	ARG
21	Z	97	GLU
21	Z	98	MET
21	Z	118	GLN
21	Z	126	VAL
21	Z	155	LEU
21	Z	156	LYS
21	Z	165	VAL
21	Z	179	ASP
21	Z	185	GLU
22	0	10	THR
22	0	19	LYS
22	0	20	ARG
22	0	38	VAL
22	0	49	LYS
22	0	55	ARG
22	0	74	ARG
22	0	77	ARG
22	0	83	PRO
23	1	4	VAL
23	1	5	CYS
23	1	14	VAL
23	1	21	ARG
23	1	40	ARG
23	1	46	LEU
23	1	51	VAL
23	1	58	ILE
23	1	82	LEU

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Mol	Chain	Res	Type
23	1	83	GLU
23	1	86	SER
23	1	95	LEU
24	2	17	SER
24	2	32	LEU
24	2	34	GLU
24	2	43	GLN
24	2	44	LEU
24	2	47	ASN
24	2	53	LEU
24	2	55	ARG
24	2	68	ARG
24	2	70	GLN
25	3	8	LEU
25	3	18	ASP
25	3	23	LEU
25	3	31	LEU
25	3	40	THR
26	4	14	ILE
26	4	16	CYS
26	4	27	THR
26	4	34	GLU
26	4	43	TYR
26	4	46	GLN
27	5	6	VAL
27	5	8	LYS
27	5	9	LYS
27	5	23	HIS
27	5	29	THR
27	5	37	LYS
27	5	40	LYS
27	5	46	CYS
27	5	58	LEU
28	6	4	GLU
28	6	6	ARG
28	6	13	CYS
28	6	14	THR
28	6	28	ARG
28	6	30	THR
28	6	34	LEU
28	6	38	LYS
28	6	40	CYS

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Mol	Chain	Res	Type
28	6	44	ARG
29	7	1	MET
29	7	4	THR
29	7	8	ASN
29	7	9	ARG
29	7	23	ARG
29	7	32	LYS
29	7	47	ARG
30	8	6	THR
30	8	11	LYS
30	8	14	VAL
30	8	23	VAL
30	8	31	HIS
30	8	32	LEU
30	8	34	TRP
30	8	35	GLN
30	8	41	ILE
30	8	49	VAL
31	9	6	SER
31	9	7	VAL
31	9	17	ILE
31	9	26	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	112	GLN
3	D	129	ASN
3	D	143	HIS
6	G	40	ASN
6	G	66	GLN
6	G	108	ASN
6	G	138	GLN
7	H	74	ASN
7	H	147	ASN
8	I	105	HIS
8	I	139	GLN
9	N	128	HIS
9	N	133	GLN
10	O	3	GLN
11	P	84	ASN
14	S	68	GLN

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Mol	Chain	Res	Type
15	T	58	ASN
16	U	49	HIS
18	W	61	ASN
19	X	31	HIS
21	Z	151	HIS
24	2	9	GLN
26	4	46	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2807/2913 (96%)	600 (21%)	56 (1%)
2	B	119/122 (97%)	26 (21%)	0
All	All	2926/3035 (96%)	626 (21%)	56 (1%)

All (626) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	12	U
1	A	14	A
1	A	15	G
1	A	34	C
1	A	36	G
1	A	45	C
1	A	55	G
1	A	69	C
1	A	71	A
1	A	72	U
1	A	74	A
1	A	75	G
1	A	82	G
1	A	84	A
1	A	90	U
1	A	94	C
1	A	95	G
1	A	96	G
1	A	100	G
1	A	102	G
1	A	103	A
1	A	118	A

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Mol	Chain	Res	Type
1	A	119	A
1	A	120	U
1	A	131	G
1	A	141	A
1	A	154	G
1	A	154(A)	C
1	A	157	U
1	A	181	A
1	A	182	A
1	A	188	G
1	A	196	A
1	A	199	A
1	A	200	U
1	A	201	C
1	A	204	A
1	A	205	G
1	A	214	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	225	A
1	A	229	A
1	A	233	A
1	A	248	G
1	A	250	G
1	A	269	U
1	A	271(I)	G
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	271(N)	U
1	A	271(Y)	U
1	A	272(B)	G
1	A	272(H)	C
1	A	272(I)	U
1	A	272(J)	C
1	A	275	G
1	A	276	A
1	A	277	C
1	A	278	A
1	A	279	C

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Mol	Chain	Res	Type
1	A	280	C
1	A	286	C
1	A	311	A
1	A	315	G
1	A	316	C
1	A	324	A
1	A	329	G
1	A	330	A
1	A	331	A
1	A	332	A
1	A	333	G
1	A	335	C
1	A	338	G
1	A	342	G
1	A	352	G
1	A	353	G
1	A	363	G
1	A	363(C)	G
1	A	363(F)	A
1	A	386	G
1	A	404	C
1	A	405	U
1	A	407	G
1	A	411	G
1	A	412	A
1	A	428	A
1	A	444	C
1	A	448	U
1	A	455	C
1	A	457	A
1	A	459	U
1	A	460	A
1	A	470	A
1	A	471	A
1	A	481	G
1	A	482	A
1	A	505	A
1	A	509	C
1	A	512	G
1	A	529	A
1	A	530	G
1	A	531	C

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Mol	Chain	Res	Type
1	A	532	A
1	A	533	G
1	A	543	C
1	A	545	G
1	A	546	C
1	A	547	A
1	A	548	A
1	A	563	G
1	A	573	G
1	A	575	A
1	A	587	C
1	A	588	U
1	A	602	G
1	A	603	A
1	A	604	G
1	A	607	U
1	A	614(A)	U
1	A	614(B)	G
1	A	614(C)	A
1	A	615	G
1	A	620	G
1	A	627	A
1	A	632	A
1	A	637	A
1	A	645	C
1	A	646	A
1	A	647	G
1	A	652(B)	A
1	A	652(C)	G
1	A	652(E)	G
1	A	652(F)	G
1	A	652(J)	G
1	A	652(Q)	G
1	A	652(R)	C
1	A	652(T)	C
1	A	652(U)	G
1	A	668	G
1	A	669	G
1	A	686	G
1	A	701	G
1	A	702	G
1	A	707	G

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Mol	Chain	Res	Type
1	A	708	C
1	A	709	U
1	A	715	G
1	A	717	G
1	A	730	C
1	A	752	A
1	A	753	C
1	A	762	U
1	A	764	A
1	A	765	G
1	A	771	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	A
1	A	785	G
1	A	790	C
1	A	792	G
1	A	805	G
1	A	810	U
1	A	811	U
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	857	C
1	A	859	G
1	A	879	G
1	A	882	G
1	A	895	U
1	A	896	A
1	A	897	C
1	A	900	A
1	A	901	A
1	A	908	C
1	A	910	A
1	A	914	C
1	A	917	A
1	A	932	G
1	A	938	G
1	A	941	A

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Mol	Chain	Res	Type
1	A	945	A
1	A	946	G
1	A	953	A
1	A	958	U
1	A	959	A
1	A	961	C
1	A	965	C
1	A	974	G
1	A	975	C
1	A	975(A)	G
1	A	983	A
1	A	990	A
1	A	991	C
1	A	996	A
1	A	1005	C
1	A	1012	U
1	A	1013	C
1	A	1020	A
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	U
1	A	1027	A
1	A	1033	U
1	A	1038	C
1	A	1039	G
1	A	1040	C
1	A	1041	C
1	A	1042	G
1	A	1043	C
1	A	1045	A
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1049	C
1	A	1050	A
1	A	1052	C
1	A	1107	G
1	A	1109	C
1	A	1110	G
1	A	1112	G
1	A	1115	G

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Mol	Chain	Res	Type
1	A	1128	A
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1141	U
1	A	1155	A
1	A	1170	G
1	A	1171	G
1	A	1188	U
1	A	1210	A
1	A	1211	U
1	A	1224	C
1	A	1244	G
1	A	1250	G
1	A	1252	G
1	A	1253	A
1	A	1256	G
1	A	1267	U
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1300	U
1	A	1301	A
1	A	1305	C
1	A	1314	C
1	A	1320	C
1	A	1321	A
1	A	1329	U
1	A	1345	C
1	A	1352	U
1	A	1359	A
1	A	1360	A
1	A	1365	A
1	A	1368	G
1	A	1370	C
1	A	1373	A
1	A	1374	G
1	A	1378	A
1	A	1379	A
1	A	1383	C

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Mol	Chain	Res	Type
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1395	A
1	A	1405	U
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	U
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1437	C
1	A	1445	A
1	A	1449	A
1	A	1455	G
1	A	1459	G
1	A	1467	C
1	A	1471	A
1	A	1472	A
1	A	1482	G
1	A	1488	G
1	A	1490	A
1	A	1493	C
1	A	1497	U
1	A	1507	A
1	A	1508	A
1	A	1509	C
1	A	1509(A)	A
1	A	1510	G
1	A	1520	G
1	A	1531	C
1	A	1539	G
1	A	1542	A
1	A	1543	C
1	A	1545	A
1	A	1548	C
1	A	1554	A
1	A	1558	A
1	A	1559	G
1	A	1560	G
1	A	1566	A

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Mol	Chain	Res	Type
1	A	1569	A
1	A	1578	U
1	A	1579	A
1	A	1580	A
1	A	1581	G
1	A	1584	C
1	A	1586	A
1	A	1598	C
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1617	C
1	A	1640	C
1	A	1647	G
1	A	1648	C
1	A	1652	A
1	A	1654	A
1	A	1655	A
1	A	1674	G
1	A	1675	C
1	A	1696	G
1	A	1698	A
1	A	1700	A
1	A	1701	A
1	A	1703	G
1	A	1721	G
1	A	1722	A
1	A	1746	G
1	A	1750	G
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1777	U
1	A	1780	A
1	A	1782	C
1	A	1791	A
1	A	1799	G
1	A	1800	C
1	A	1801	G
1	A	1812	A
1	A	1816	G
1	A	1819	A

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Mol	Chain	Res	Type
1	A	1820	U
1	A	1829	A
1	A	1835	G
1	A	1838	C
1	A	1840	G
1	A	1847	A
1	A	1848	A
1	A	1858	G
1	A	1865	G
1	A	1866	C
1	A	1877	A
1	A	1878	G
1	A	1881	C
1	A	1882	C
1	A	1896	G
1	A	1900	A
1	A	1905	C
1	A	1906	G
1	A	1912	A
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	U
1	A	1952	A
1	A	1955	U
1	A	1963	U
1	A	1964	G
1	A	1966	A
1	A	1967	C
1	A	1969	A
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1982	C
1	A	1991	U
1	A	1993	U
1	A	1997	G

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Mol	Chain	Res	Type
1	A	2005	A
1	A	2018	G
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2036	C
1	A	2043	C
1	A	2049	G
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2069	G
1	A	2099	U
1	A	2100	G
1	A	2103	C
1	A	2104	G
1	A	2108	C
1	A	2110	G
1	A	2111	C
1	A	2112	G
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2119	A
1	A	2123	G
1	A	2126	A
1	A	2127	G
1	A	2128	C
1	A	2131	G
1	A	2133	G
1	A	2134	A
1	A	2135	A
1	A	2136	C
1	A	2146	C
1	A	2147	G
1	A	2150	U
1	A	2159	G
1	A	2160	G

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Mol	Chain	Res	Type
1	A	2161	C
1	A	2162	G
1	A	2164	C
1	A	2169	A
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2174	C
1	A	2176	A
1	A	2179	C
1	A	2180	U
1	A	2183	C
1	A	2185	C
1	A	2186	G
1	A	2187	G
1	A	2188	C
1	A	2191	G
1	A	2192	G
1	A	2193	G
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2225	A
1	A	2234	G
1	A	2238	G
1	A	2239	G
1	A	2248	C
1	A	2252	G
1	A	2268	A
1	A	2273	A
1	A	2275	C
1	A	2278	A
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2289	G
1	A	2291	U
1	A	2294	C
1	A	2305	A

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Mol	Chain	Res	Type
1	A	2306	C
1	A	2307	G
1	A	2308	G
1	A	2309	A
1	A	2311	A
1	A	2316	C
1	A	2319	G
1	A	2320	A
1	A	2321	G
1	A	2325	G
1	A	2327	A
1	A	2334	G
1	A	2336	A
1	A	2343	C
1	A	2347	C
1	A	2350	C
1	A	2354	G
1	A	2379	G
1	A	2383	G
1	A	2385	C
1	A	2388	A
1	A	2391	G
1	A	2400	G
1	A	2406	U
1	A	2407	G
1	A	2410	G
1	A	2414	G
1	A	2418	A
1	A	2422	A
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2439	A
1	A	2440	C
1	A	2441	C
1	A	2448	A
1	A	2465	C
1	A	2469	A
1	A	2470	G
1	A	2472	G
1	A	2474	C

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Mol	Chain	Res	Type
1	A	2476	A
1	A	2477	C
1	A	2486	G
1	A	2487	G
1	A	2502	G
1	A	2504	U
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2520	C
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2554	U
1	A	2564	A
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2582	G
1	A	2585	U
1	A	2586	C
1	A	2602	A
1	A	2603	G
1	A	2604	U
1	A	2608	G
1	A	2609	U
1	A	2610	C
1	A	2611	U
1	A	2612	C
1	A	2615	U
1	A	2628	C
1	A	2629	A
1	A	2630	G
1	A	2654	A
1	A	2663	G
1	A	2672	G
1	A	2674	G
1	A	2686	G
1	A	2690	C
1	A	2691	C
1	A	2702	U
1	A	2703	C

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Mol	Chain	Res	Type
1	A	2707	G
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2718	G
1	A	2726	U
1	A	2733	A
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2758	A
1	A	2761	G
1	A	2765	A
1	A	2766	G
1	A	2775	A
1	A	2778	A
1	A	2790	A
1	A	2791	C
1	A	2802	G
1	A	2803	C
1	A	2808	U
1	A	2820	A
1	A	2821	A
1	A	2833	G
1	A	2834	G
1	A	2835	A
1	A	2847	U
1	A	2872	G
1	A	2873	A
1	A	2880	C
1	A	2892	A
2	B	2	C
2	B	8	U
2	B	9	G
2	B	12	C
2	B	13	A
2	B	15	A
2	B	19	G
2	B	21	G
2	B	24	G
2	B	25	A
2	B	26	A

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Mol	Chain	Res	Type
2	B	28	C
2	B	33	G
2	B	34	U
2	B	40	U
2	B	53	A
2	B	54	G
2	B	56	G
2	B	73	A
2	B	74	U
2	B	75	G
2	B	85	G
2	B	88	C
2	B	89	G
2	B	106	G
2	B	110	G

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	71	A
1	A	102	G
1	A	196	A
1	A	249	C
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	278	A
1	A	363(E)	U
1	A	481	G
1	A	542	C
1	A	547	A
1	A	587	C
1	A	669	G
1	A	685	A
1	A	752	A
1	A	764	A
1	A	827	U
1	A	856	C
1	A	900	A
1	A	945	A
1	A	1026	U
1	A	1047	G

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Mol	Chain	Res	Type
1	A	1049	C
1	A	1106	G
1	A	1108	U
1	A	1110	G
1	A	1155	A
1	A	1210	A
1	A	1300	U
1	A	1301	A
1	A	1378	A
1	A	1396	U
1	A	1419	A
1	A	1427	A
1	A	1507	A
1	A	1530	C
1	A	1538	G
1	A	1558	A
1	A	1608	A
1	A	1653	G
1	A	1799	G
1	A	1819	A
1	A	1992	G
1	A	2116	G
1	A	2126	A
1	A	2172	U
1	A	2308	G
1	A	2318	G
1	A	2406	U
1	A	2439	A
1	A	2602	A
1	A	2610	C
1	A	2689	U
1	A	2778	A
1	A	2802	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 626 ligands modelled in this entry, 626 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2814/2913 (96%)	-0.04	59 (2%) 60 11	28, 50, 133, 176	0
2	B	120/122 (98%)	0.14	1 (0%) 83 28	48, 81, 106, 117	0
3	D	275/276 (99%)	0.29	4 (1%) 70 16	30, 47, 66, 116	0
4	E	204/206 (99%)	0.42	7 (3%) 43 6	29, 50, 76, 95	0
5	F	203/210 (96%)	0.41	9 (4%) 33 5	31, 59, 90, 112	0
6	G	181/182 (99%)	1.42	54 (29%) 1 0	86, 117, 138, 148	0
7	H	174/180 (96%)	0.89	23 (13%) 4 1	65, 82, 101, 119	0
8	I	146/148 (98%)	0.47	10 (6%) 17 3	56, 89, 108, 120	0
9	N	140/140 (100%)	0.57	8 (5%) 23 3	40, 54, 82, 96	0
10	O	122/122 (100%)	0.15	3 (2%) 54 9	36, 52, 69, 77	0
11	P	149/150 (99%)	0.81	17 (11%) 6 1	31, 62, 92, 112	0
12	Q	141/141 (100%)	0.32	10 (7%) 16 3	41, 58, 77, 88	0
13	R	118/118 (100%)	0.55	8 (6%) 17 3	36, 47, 62, 78	0
14	S	110/112 (98%)	1.57	35 (31%) 1 0	55, 74, 94, 102	0
15	T	131/146 (89%)	0.38	7 (5%) 25 4	46, 57, 93, 128	0
16	U	116/118 (98%)	0.43	5 (4%) 34 5	34, 48, 66, 73	0
17	V	101/101 (100%)	0.27	4 (3%) 36 5	32, 62, 85, 103	0
18	W	112/113 (99%)	0.69	6 (5%) 25 4	35, 42, 67, 105	0
19	X	95/96 (98%)	0.44	2 (2%) 60 11	41, 52, 77, 90	0
20	Y	107/110 (97%)	1.26	30 (28%) 1 0	52, 65, 89, 113	0
21	Z	198/206 (96%)	0.60	15 (7%) 14 2	62, 81, 102, 121	0
22	0	76/85 (89%)	0.80	10 (13%) 4 1	43, 52, 66, 92	0
23	1	97/98 (98%)	0.88	13 (13%) 4 1	36, 51, 83, 98	0
24	2	70/72 (97%)	0.18	3 (4%) 34 5	50, 64, 81, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	3	59/60 (98%)	0.85	11 (18%) 2 0	41, 53, 93, 102	0
26	4	46/71 (64%)	0.92	11 (23%) 1 0	113, 133, 144, 152	0
27	5	59/60 (98%)	0.01	2 (3%) 43 6	32, 47, 68, 81	0
28	6	53/54 (98%)	0.79	5 (9%) 9 2	43, 54, 72, 82	0
29	7	48/49 (97%)	1.39	14 (29%) 1 0	32, 35, 58, 84	0
30	8	64/65 (98%)	0.75	6 (9%) 9 2	40, 45, 55, 70	0
31	9	36/37 (97%)	1.27	8 (22%) 1 0	47, 59, 68, 75	0
All	All	6365/6561 (97%)	0.33	400 (6%) 22 3	28, 55, 118, 176	0

All (400) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1052	C	7.2
6	G	138	GLN	7.2
20	Y	1	MET	7.1
20	Y	2	ARG	7.0
26	4	11	PRO	6.9
11	P	1	MET	6.6
7	H	171	LEU	6.4
1	A	652(B)	A	6.4
6	G	30	GLU	5.9
3	D	276	LYS	5.8
20	Y	94	LYS	5.6
20	Y	3	VAL	5.6
26	4	23	GLU	5.4
14	S	59	LYS	5.2
1	A	2165	G	5.2
20	Y	55	TYR	5.0
29	7	46	VAL	4.7
14	S	64	GLU	4.7
29	7	47	ARG	4.7
26	4	29	PRO	4.6
1	A	1532	C	4.6
1	A	2169	A	4.6
6	G	81	LYS	4.5
6	G	25	TYR	4.5
6	G	164	GLU	4.5
6	G	63	ILE	4.4
1	A	2174	C	4.4
7	H	159	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
15	T	112	ARG	4.3
6	G	32	PRO	4.3
26	4	10	VAL	4.3
1	A	2132	U	4.3
6	G	35	GLU	4.2
16	U	89	GLU	4.2
11	P	74	GLU	4.2
6	G	33	ARG	4.2
1	A	1509	C	4.1
1	A	2129	C	4.1
6	G	162	THR	4.1
1	A	2146	C	4.1
3	D	275	LYS	4.0
6	G	26	GLN	4.0
6	G	152	LEU	4.0
7	H	173	PRO	3.9
21	Z	134	PRO	3.9
6	G	27	ASN	3.9
1	A	652(A)	A	3.9
20	Y	29	GLU	3.9
11	P	2	LYS	3.9
20	Y	57	GLN	3.8
25	3	36	VAL	3.8
21	Z	162	GLU	3.8
23	1	72	GLU	3.8
8	I	20	ASP	3.8
14	S	58	LEU	3.8
25	3	19	GLN	3.8
20	Y	4	LYS	3.8
31	9	36	GLN	3.8
14	S	80	LEU	3.8
6	G	20	ILE	3.7
7	H	172	LYS	3.7
15	T	113	LYS	3.7
4	E	204	ALA	3.7
14	S	56	LEU	3.7
20	Y	91	GLU	3.7
14	S	65	VAL	3.7
25	3	60	GLU	3.7
22	0	71	ASP	3.7
6	G	21	ARG	3.7
26	4	13	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1051	G	3.6
1	A	6	A	3.6
1	A	2164	C	3.6
4	E	168	MET	3.6
1	A	2191	G	3.6
6	G	182	LYS	3.6
26	4	30	GLU	3.6
5	F	188	ARG	3.5
22	0	70	GLN	3.5
6	G	29	TRP	3.5
22	0	74	ARG	3.4
14	S	62	LYS	3.4
31	9	22	ARG	3.4
21	Z	164	ALA	3.4
11	P	94	GLU	3.4
1	A	362	U	3.4
7	H	101	ARG	3.4
23	1	6	GLU	3.4
7	H	108	GLY	3.4
1	A	2789	C	3.4
9	N	1	MET	3.4
14	S	84	GLN	3.3
6	G	54	GLU	3.3
23	1	71	TYR	3.3
24	2	8	LYS	3.3
11	P	109	GLY	3.3
23	1	70	VAL	3.3
1	A	2166	G	3.3
24	2	7	ARG	3.3
8	I	126	TYR	3.3
11	P	76	LYS	3.3
29	7	48	LYS	3.3
23	1	5	CYS	3.3
25	3	2	PRO	3.3
15	T	36	GLU	3.3
1	A	283	A	3.2
14	S	61	ASN	3.2
14	S	72	ALA	3.2
31	9	17	ILE	3.2
6	G	34	LEU	3.2
8	I	127	VAL	3.2
14	S	8	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	2124	G	3.1
6	G	82	LEU	3.1
15	T	95	ARG	3.1
20	Y	93	GLY	3.1
14	S	43	GLU	3.1
31	9	8	LYS	3.1
6	G	74	LYS	3.1
31	9	37	GLY	3.1
9	N	10	GLU	3.1
20	Y	32	PRO	3.1
22	0	23	VAL	3.1
7	H	166	GLY	3.1
6	G	64	THR	3.1
13	R	79	LEU	3.0
1	A	2125	G	3.0
20	Y	90	LEU	3.0
20	Y	35	TYR	3.0
8	I	1	MET	3.0
14	S	44	LYS	3.0
12	Q	112	GLU	3.0
18	W	31	GLU	3.0
13	R	63	ARG	3.0
1	A	1886	C	3.0
6	G	19	LEU	2.9
20	Y	41	GLY	2.9
6	G	17	PRO	2.9
14	S	76	LYS	2.9
20	Y	63	LYS	2.9
9	N	7	LYS	2.9
1	A	2442	C	2.9
9	N	9	VAL	2.9
20	Y	89	PHE	2.9
25	3	35	ARG	2.9
6	G	84	LYS	2.9
20	Y	22	GLY	2.9
14	S	110	LEU	2.8
7	H	42	ARG	2.8
14	S	20	ARG	2.8
6	G	39	ILE	2.8
1	A	1046	A	2.8
7	H	43	VAL	2.8
25	3	38	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
29	7	45	ALA	2.8
6	G	28	VAL	2.8
21	Z	56	VAL	2.8
6	G	136	ARG	2.8
1	A	2062	A	2.8
14	S	102	ALA	2.8
1	A	2116	G	2.8
7	H	58	GLU	2.8
6	G	94	LEU	2.8
11	P	3	LEU	2.8
29	7	44	PRO	2.8
31	9	24	TYR	2.8
12	Q	20	ALA	2.8
2	B	12	C	2.7
18	W	111	HIS	2.7
7	H	105	LEU	2.7
14	S	66	ALA	2.7
21	Z	190	GLU	2.7
6	G	62	LEU	2.7
14	S	4	LEU	2.7
28	6	11	LEU	2.7
28	6	54	ILE	2.7
21	Z	80	ARG	2.7
31	9	18	ARG	2.7
11	P	149	GLU	2.7
7	H	169	VAL	2.7
10	O	105	GLU	2.7
8	I	2	LYS	2.7
5	F	35	GLU	2.7
11	P	59	LEU	2.7
14	S	73	LEU	2.7
12	Q	1	MET	2.6
22	0	76	GLY	2.6
20	Y	23	ARG	2.6
6	G	31	VAL	2.6
4	E	1	MET	2.6
1	A	2602	A	2.6
6	G	120	LEU	2.6
14	S	68	GLN	2.6
5	F	131	GLY	2.6
20	Y	87	LYS	2.6
12	Q	59	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
20	Y	40	GLU	2.6
6	G	24	GLY	2.6
1	A	9	U	2.6
1	A	2176	A	2.6
18	W	86	LEU	2.6
1	A	2147	G	2.6
8	I	84	GLY	2.6
5	F	208	GLY	2.6
12	Q	19	GLY	2.6
21	Z	191	VAL	2.6
22	O	25	ARG	2.6
14	S	69	VAL	2.6
20	Y	5	MET	2.6
26	4	27	THR	2.6
17	V	3	ALA	2.6
13	R	74	LYS	2.5
1	A	405	U	2.5
18	W	84	ARG	2.5
1	A	2334	G	2.5
14	S	60	GLY	2.5
12	Q	22	LYS	2.5
5	F	113	ALA	2.5
14	S	7	TYR	2.5
1	A	2109	U	2.5
14	S	54	LEU	2.5
22	O	75	LEU	2.5
6	G	93	THR	2.5
17	V	38	LEU	2.5
23	1	66	HIS	2.5
27	5	25	LEU	2.5
13	R	80	PHE	2.5
8	I	83	ALA	2.5
23	1	37	ILE	2.5
17	V	72	VAL	2.5
1	A	1642	G	2.5
14	S	75	GLU	2.4
9	N	118	LYS	2.4
21	Z	158	PRO	2.4
23	1	73	LEU	2.4
14	S	97	ARG	2.4
5	F	183	VAL	2.4
28	6	50	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
29	7	23	ARG	2.4
6	G	168	GLU	2.4
26	4	28	LYS	2.4
30	8	54	GLU	2.4
1	A	361	G	2.4
6	G	153	ARG	2.4
5	F	189	THR	2.4
1	A	1383	C	2.4
17	V	71	LEU	2.4
20	Y	67	LEU	2.4
7	H	158	HIS	2.4
20	Y	66	PRO	2.4
25	3	50	VAL	2.4
11	P	110	TYR	2.4
29	7	24	THR	2.4
4	E	26	ILE	2.4
23	1	7	ILE	2.4
11	P	46	LYS	2.4
1	A	758	C	2.4
13	R	77	ARG	2.4
20	Y	34	LYS	2.4
14	S	101	LEU	2.4
29	7	9	ARG	2.4
3	D	262	ARG	2.3
6	G	2	PRO	2.3
1	A	652(J)	G	2.3
23	1	68	PRO	2.3
6	G	83	ARG	2.3
21	Z	133	ILE	2.3
7	H	98	LEU	2.3
29	7	39	ARG	2.3
23	1	69	LYS	2.3
31	9	23	VAL	2.3
1	A	352	G	2.3
1	A	2168	G	2.3
8	I	21	VAL	2.3
1	A	1913	A	2.3
15	T	78	LEU	2.3
15	T	111	ARG	2.3
14	S	39	ILE	2.3
30	8	15	LYS	2.3
1	A	2173	A	2.3

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Mol	Chain	Res	Type	RSRZ
6	G	16	ARG	2.3
7	H	100	GLY	2.3
29	7	10	ARG	2.3
7	H	103	LEU	2.3
10	O	73	ASP	2.3
6	G	53	LEU	2.3
12	Q	16	ARG	2.3
10	O	74	GLY	2.3
9	N	70	LYS	2.2
7	H	93	GLY	2.2
13	R	67	LEU	2.2
25	3	59	VAL	2.2
12	Q	60	ARG	2.2
29	7	41	ARG	2.2
1	A	1627	G	2.2
6	G	68	PRO	2.2
20	Y	44	ILE	2.2
6	G	155	MET	2.2
11	P	68	GLN	2.2
19	X	1	MET	2.2
6	G	3	LEU	2.2
6	G	163	ALA	2.2
21	Z	75	ASN	2.2
4	E	170	LEU	2.2
16	U	36	ARG	2.2
6	G	145	THR	2.2
20	Y	56	PRO	2.2
16	U	112	ARG	2.2
14	S	92	TYR	2.2
6	G	61	ALA	2.2
11	P	79	ARG	2.2
20	Y	73	ARG	2.2
26	4	9	LEU	2.2
12	Q	18	LYS	2.2
21	Z	156	LYS	2.2
25	3	37	LEU	2.2
28	6	10	LEU	2.2
22	0	26	TYR	2.2
15	T	109	GLU	2.2
1	A	900	A	2.2
6	G	171	ALA	2.2
11	P	4	SER	2.2

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Mol	Chain	Res	Type	RSRZ
6	G	118	ARG	2.2
7	H	60	ARG	2.2
1	A	272(A)	U	2.2
30	8	58	ILE	2.2
30	8	11	LYS	2.2
1	A	614(B)	G	2.2
1	A	2790	A	2.2
14	S	49	VAL	2.2
16	U	90	VAL	2.2
26	4	26	SER	2.2
6	G	157	ILE	2.2
1	A	2150	U	2.2
18	W	43	GLY	2.2
30	8	14	VAL	2.1
4	E	27	LEU	2.1
22	0	24	LYS	2.1
21	Z	97	GLU	2.1
8	I	23	PRO	2.1
1	A	1641	A	2.1
29	7	32	LYS	2.1
1	A	2175	C	2.1
13	R	72	ASP	2.1
18	W	24	ILE	2.1
22	0	38	VAL	2.1
1	A	1885	A	2.1
13	R	100	LEU	2.1
11	P	108	LYS	2.1
19	X	43	VAL	2.1
6	G	52	ILE	2.1
5	F	28	ILE	2.1
1	A	901	A	2.1
1	A	953	A	2.1
7	H	109	PHE	2.1
11	P	135	LEU	2.1
27	5	58	LEU	2.1
1	A	1113	U	2.1
14	S	111	GLU	2.1
7	H	160	LYS	2.1
14	S	83	LYS	2.1
5	F	186	ILE	2.1
1	A	268	C	2.1
6	G	65	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
6	G	137	GLU	2.1
20	Y	69	ALA	2.1
26	4	25	TYR	2.1
24	2	12	GLU	2.1
9	N	69	GLN	2.1
7	H	19	VAL	2.1
9	N	140	VAL	2.1
25	3	26	LEU	2.1
30	8	10	ALA	2.1
29	7	11	LYS	2.0
23	1	2	SER	2.0
1	A	1643	G	2.0
20	Y	62	GLU	2.0
16	U	5	LYS	2.0
7	H	97	ARG	2.0
25	3	3	ARG	2.0
1	A	756	C	2.0
4	E	7	VAL	2.0
14	S	3	ARG	2.0
20	Y	14	LEU	2.0
21	Z	157	LEU	2.0
28	6	19	ARG	2.0
1	A	2694	G	2.0
12	Q	74	TYR	2.0
3	D	261	LYS	2.0
6	G	56	ALA	2.0
23	1	67	ILE	2.0
29	7	37	LYS	2.0
11	P	118	GLY	2.0
21	Z	59	LEU	2.0
8	I	22	LYS	2.0
14	S	12	PHE	2.0
7	H	41	MET	2.0
1	A	2274	A	2.0
6	G	45	GLU	2.0
21	Z	70	LEU	2.0

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3336	1/1	0.07	-	44,44,44,44	0
32	MG	A	3343	1/1	0.07	-	35,35,35,35	0
32	MG	A	3426	1/1	0.33	-	56,56,56,56	0
32	MG	A	3545	1/1	0.53	-	89,89,89,89	0
32	MG	A	3366	1/1	0.27	-	50,50,50,50	0
32	MG	A	3496	1/1	0.11	-	67,67,67,67	0
32	MG	A	3507	1/1	0.14	-	74,74,74,74	0
32	MG	A	3232	1/1	0.19	-	47,47,47,47	0
32	MG	A	3359	1/1	0.09	-	26,26,26,26	0
32	MG	A	3139	1/1	0.48	-	42,42,42,42	0
32	MG	A	3271	1/1	0.42	-	61,61,61,61	0
32	MG	A	3416	1/1	0.21	-	44,44,44,44	0
32	MG	A	3114	1/1	0.23	-	48,48,48,48	0
32	MG	A	3018	1/1	0.26	-	43,43,43,43	0
32	MG	A	3273	1/1	0.76	-	60,60,60,60	0
32	MG	A	3116	1/1	0.71	-	34,34,34,34	0
32	MG	A	3414	1/1	0.16	-	31,31,31,31	0
32	MG	A	3516	1/1	0.35	-	52,52,52,52	0
32	MG	A	3259	1/1	0.35	-	40,40,40,40	0
32	MG	A	3036	1/1	0.46	-	36,36,36,36	0
32	MG	A	3197	1/1	0.44	-	49,49,49,49	0
32	MG	A	3481	1/1	0.15	-	64,64,64,64	0
32	MG	A	3595	1/1	0.41	-	76,76,76,76	0
32	MG	A	3354	1/1	0.12	-	36,36,36,36	0
32	MG	A	3247	1/1	0.34	-	40,40,40,40	0
32	MG	A	3560	1/1	0.25	-	70,70,70,70	0
32	MG	R	201	1/1	0.74	-	40,40,40,40	0
32	MG	A	3483	1/1	0.25	-	64,64,64,64	0
32	MG	A	3469	1/1	0.22	-	50,50,50,50	0
32	MG	A	3511	1/1	0.21	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3337	1/1	0.17	-	45,45,45,45	0
32	MG	A	3590	1/1	0.11	-	83,83,83,83	0
32	MG	A	3379	1/1	0.15	-	53,53,53,53	0
32	MG	A	3087	1/1	0.43	-	41,41,41,41	0
32	MG	A	3281	1/1	0.41	-	55,55,55,55	0
32	MG	A	3403	1/1	0.19	-	58,58,58,58	0
32	MG	A	3056	1/1	0.43	-	32,32,32,32	0
32	MG	A	3571	1/1	0.14	-	41,41,41,41	0
32	MG	A	3125	1/1	0.52	-	47,47,47,47	0
32	MG	A	3428	1/1	0.10	-	59,59,59,59	0
32	MG	A	3543	1/1	0.11	-	64,64,64,64	0
32	MG	A	3296	1/1	0.39	-	65,65,65,65	0
32	MG	A	3214	1/1	0.76	-	62,62,62,62	0
32	MG	A	3395	1/1	0.47	-	88,88,88,88	0
32	MG	A	3262	1/1	0.33	-	47,47,47,47	0
32	MG	A	3327	1/1	0.36	-	37,37,37,37	0
32	MG	A	3446	1/1	0.35	-	42,42,42,42	0
32	MG	A	3124	1/1	0.14	-	61,61,61,61	0
32	MG	A	3084	1/1	0.15	-	52,52,52,52	0
32	MG	A	3144	1/1	0.68	-	53,53,53,53	0
32	MG	B	208	1/1	0.10	-	104,104,104,104	0
32	MG	A	3457	1/1	0.24	-	65,65,65,65	0
32	MG	A	3234	1/1	0.39	-	56,56,56,56	0
32	MG	A	3325	1/1	0.41	-	57,57,57,57	0
32	MG	A	3042	1/1	0.68	-	38,38,38,38	0
32	MG	A	3444	1/1	0.14	-	74,74,74,74	0
32	MG	A	3510	1/1	0.13	-	34,34,34,34	0
32	MG	A	3061	1/1	0.27	-	62,62,62,62	0
32	MG	A	3570	1/1	0.08	-	31,31,31,31	0
32	MG	A	3233	1/1	0.44	-	62,62,62,62	0
32	MG	A	3565	1/1	0.12	-	78,78,78,78	0
32	MG	A	3227	1/1	0.31	-	36,36,36,36	0
32	MG	A	3538	1/1	0.32	-	130,130,130,130	0
32	MG	A	3208	1/1	0.95	-	75,75,75,75	0
32	MG	A	3520	1/1	0.19	-	74,74,74,74	0
32	MG	A	3221	1/1	0.52	-	51,51,51,51	0
32	MG	A	3519	1/1	0.24	-	61,61,61,61	0
32	MG	A	3419	1/1	0.39	-	43,43,43,43	0
32	MG	A	3009	1/1	0.17	-	31,31,31,31	0
32	MG	A	3132	1/1	0.47	-	38,38,38,38	0
32	MG	A	3319	1/1	0.46	-	49,49,49,49	0
32	MG	A	3107	1/1	0.34	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	8	101	1/1	0.46	-	48,48,48,48	0
32	MG	A	3397	1/1	0.40	-	66,66,66,66	0
32	MG	A	3075	1/1	0.13	-	44,44,44,44	0
32	MG	A	3489	1/1	0.15	-	56,56,56,56	0
32	MG	A	3317	1/1	0.20	-	38,38,38,38	0
32	MG	A	3026	1/1	0.35	-	53,53,53,53	0
32	MG	A	3357	1/1	0.20	-	37,37,37,37	0
32	MG	A	3017	1/1	0.17	-	34,34,34,34	0
32	MG	A	3287	1/1	0.74	-	58,58,58,58	0
32	MG	A	3537	1/1	0.17	-	53,53,53,53	0
32	MG	A	3252	1/1	0.35	-	52,52,52,52	0
32	MG	A	3437	1/1	0.38	-	42,42,42,42	0
32	MG	A	3062	1/1	0.25	-	49,49,49,49	0
32	MG	A	3200	1/1	0.34	-	43,43,43,43	0
32	MG	A	3280	1/1	0.43	-	61,61,61,61	0
32	MG	A	3330	1/1	0.11	-	37,37,37,37	0
32	MG	A	3344	1/1	0.11	-	35,35,35,35	0
32	MG	A	3412	1/1	0.20	-	43,43,43,43	0
32	MG	A	3189	1/1	0.75	-	40,40,40,40	0
32	MG	A	3541	1/1	0.24	-	72,72,72,72	0
32	MG	A	3098	1/1	0.88	-	54,54,54,54	0
32	MG	A	3320	1/1	0.29	-	40,40,40,40	0
32	MG	A	3071	1/1	0.26	-	42,42,42,42	0
32	MG	A	3047	1/1	0.28	-	52,52,52,52	0
32	MG	A	3082	1/1	0.30	-	54,54,54,54	0
32	MG	A	3007	1/1	0.20	-	30,30,30,30	0
32	MG	A	3127	1/1	0.40	-	49,49,49,49	0
32	MG	A	3306	1/1	0.25	-	28,28,28,28	0
32	MG	A	3215	1/1	0.19	-	38,38,38,38	0
32	MG	A	3167	1/1	0.47	-	61,61,61,61	0
32	MG	A	3015	1/1	0.24	-	56,56,56,56	0
32	MG	A	3152	1/1	0.24	-	35,35,35,35	0
32	MG	A	3099	1/1	0.14	-	34,34,34,34	0
32	MG	A	3393	1/1	0.16	-	52,52,52,52	0
32	MG	A	3090	1/1	0.23	-	53,53,53,53	0
32	MG	A	3532	1/1	0.16	-	64,64,64,64	0
32	MG	A	3059	1/1	0.27	-	48,48,48,48	0
32	MG	A	3369	1/1	0.14	-	41,41,41,41	0
32	MG	A	3401	1/1	0.10	-	36,36,36,36	0
32	MG	A	3459	1/1	0.29	-	51,51,51,51	0
32	MG	A	3223	1/1	0.56	-	52,52,52,52	0
32	MG	A	3522	1/1	0.31	-	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3450	1/1	0.10	-	79,79,79,79	0
32	MG	A	3513	1/1	0.28	-	32,32,32,32	0
32	MG	A	3594	1/1	0.06	-	93,93,93,93	0
32	MG	A	3312	1/1	0.25	-	31,31,31,31	0
32	MG	A	3524	1/1	0.16	-	91,91,91,91	0
32	MG	A	3269	1/1	0.29	-	30,30,30,30	0
32	MG	A	3563	1/1	0.15	-	54,54,54,54	0
32	MG	A	3340	1/1	0.09	-	37,37,37,37	0
32	MG	A	3408	1/1	0.15	-	49,49,49,49	0
32	MG	A	3282	1/1	0.10	-	64,64,64,64	0
32	MG	A	3019	1/1	0.28	-	47,47,47,47	0
32	MG	A	3346	1/1	0.07	-	35,35,35,35	0
32	MG	A	3315	1/1	0.26	-	58,58,58,58	0
32	MG	A	3169	1/1	0.57	-	52,52,52,52	0
32	MG	A	3039	1/1	0.38	-	46,46,46,46	0
32	MG	A	3240	1/1	0.45	-	33,33,33,33	0
32	MG	A	3392	1/1	0.18	-	39,39,39,39	0
32	MG	A	3445	1/1	0.07	-	42,42,42,42	0
32	MG	A	3297	1/1	1.08	-	41,41,41,41	0
32	MG	A	3035	1/1	0.24	-	48,48,48,48	0
32	MG	A	3142	1/1	0.37	-	54,54,54,54	0
32	MG	A	3347	1/1	0.10	-	47,47,47,47	0
32	MG	A	3328	1/1	0.93	-	71,71,71,71	0
32	MG	A	3407	1/1	0.22	-	86,86,86,86	0
32	MG	A	3149	1/1	0.20	-	26,26,26,26	0
32	MG	B	205	1/1	0.19	-	55,55,55,55	0
32	MG	A	3303	1/1	0.23	-	29,29,29,29	0
32	MG	A	3554	1/1	0.34	-	103,103,103,103	0
32	MG	F	301	1/1	0.16	-	50,50,50,50	0
32	MG	A	3400	1/1	0.10	-	34,34,34,34	0
32	MG	A	3455	1/1	0.14	-	62,62,62,62	0
32	MG	A	3556	1/1	0.51	-	79,79,79,79	0
32	MG	A	3368	1/1	0.15	-	43,43,43,43	0
32	MG	A	3161	1/1	0.72	-	60,60,60,60	0
32	MG	A	3583	1/1	0.42	-	49,49,49,49	0
32	MG	A	3383	1/1	0.17	-	39,39,39,39	0
32	MG	A	3355	1/1	0.19	-	39,39,39,39	0
32	MG	A	3371	1/1	0.15	-	37,37,37,37	0
32	MG	A	3568	1/1	0.19	-	55,55,55,55	0
32	MG	A	3540	1/1	0.12	-	53,53,53,53	0
33	ZN	9	101	1/1	0.09	-	65,65,65,65	0
32	MG	A	3119	1/1	0.34	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3338	1/1	0.15	-	43,43,43,43	0
32	MG	A	3151	1/1	0.20	-	52,52,52,52	0
32	MG	A	3112	1/1	0.29	-	47,47,47,47	0
32	MG	A	3194	1/1	1.06	-	57,57,57,57	0
32	MG	A	3146	1/1	0.21	-	43,43,43,43	0
32	MG	A	3183	1/1	0.17	-	71,71,71,71	0
32	MG	A	3558	1/1	0.18	-	71,71,71,71	0
32	MG	A	3329	1/1	0.45	-	53,53,53,53	0
32	MG	A	3057	1/1	0.34	-	49,49,49,49	0
32	MG	A	3020	1/1	0.64	-	49,49,49,49	0
32	MG	A	3314	1/1	0.38	-	47,47,47,47	0
32	MG	A	3141	1/1	0.41	-	44,44,44,44	0
32	MG	A	3360	1/1	0.09	-	26,26,26,26	0
32	MG	A	3438	1/1	0.20	-	48,48,48,48	0
32	MG	A	3525	1/1	0.25	-	124,124,124,124	0
32	MG	A	3191	1/1	0.90	-	48,48,48,48	0
32	MG	A	3002	1/1	0.18	-	48,48,48,48	0
32	MG	A	3573	1/1	0.30	-	48,48,48,48	0
32	MG	A	3298	1/1	0.21	-	50,50,50,50	0
32	MG	A	3012	1/1	0.39	-	50,50,50,50	0
32	MG	A	3492	1/1	0.14	-	83,83,83,83	0
32	MG	A	3305	1/1	0.24	-	33,33,33,33	0
32	MG	A	3292	1/1	0.28	-	59,59,59,59	0
32	MG	A	3569	1/1	0.14	-	71,71,71,71	0
32	MG	A	3539	1/1	0.16	-	83,83,83,83	0
32	MG	A	3222	1/1	0.22	-	55,55,55,55	0
32	MG	A	3582	1/1	0.18	-	33,33,33,33	0
32	MG	A	3349	1/1	0.10	-	33,33,33,33	0
32	MG	A	3473	1/1	0.14	-	66,66,66,66	0
32	MG	A	3097	1/1	0.54	-	40,40,40,40	0
32	MG	A	3467	1/1	0.13	-	47,47,47,47	0
32	MG	A	3509	1/1	0.12	-	42,42,42,42	0
32	MG	A	3382	1/1	0.11	-	49,49,49,49	0
32	MG	A	3301	1/1	0.28	-	29,29,29,29	0
32	MG	A	3275	1/1	0.09	-	83,83,83,83	0
32	MG	A	3154	1/1	0.50	-	46,46,46,46	0
32	MG	A	3552	1/1	0.32	-	56,56,56,56	0
32	MG	A	3526	1/1	0.06	-	56,56,56,56	0
32	MG	A	3121	1/1	0.42	-	63,63,63,63	0
32	MG	A	3555	1/1	0.13	-	36,36,36,36	0
32	MG	A	3122	1/1	0.48	-	56,56,56,56	0
32	MG	A	3201	1/1	0.14	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3055	1/1	0.24	-	41,41,41,41	0
32	MG	A	3512	1/1	0.50	-	37,37,37,37	0
33	ZN	6	101	1/1	0.05	-	63,63,63,63	0
32	MG	A	3137	1/1	0.18	-	37,37,37,37	0
32	MG	A	3372	1/1	0.10	-	31,31,31,31	0
32	MG	A	3410	1/1	0.13	-	56,56,56,56	0
32	MG	A	3206	1/1	0.38	-	53,53,53,53	0
32	MG	A	3577	1/1	0.29	-	52,52,52,52	0
32	MG	A	3487	1/1	0.35	-	33,33,33,33	0
32	MG	A	3079	1/1	0.16	-	37,37,37,37	0
32	MG	A	3321	1/1	0.26	-	51,51,51,51	0
32	MG	A	3478	1/1	0.35	-	61,61,61,61	0
32	MG	A	3452	1/1	0.28	-	68,68,68,68	0
32	MG	A	3358	1/1	0.10	-	30,30,30,30	0
32	MG	A	3052	1/1	0.15	-	35,35,35,35	0
32	MG	A	3202	1/1	0.78	-	52,52,52,52	0
32	MG	A	3063	1/1	0.26	-	33,33,33,33	0
32	MG	A	3249	1/1	0.28	-	50,50,50,50	0
32	MG	A	3034	1/1	0.23	-	28,28,28,28	0
32	MG	A	3022	1/1	0.85	-	56,56,56,56	0
32	MG	A	3166	1/1	0.59	-	56,56,56,56	0
32	MG	A	3076	1/1	1.09	-	58,58,58,58	0
32	MG	A	3439	1/1	0.27	-	82,82,82,82	0
32	MG	0	101	1/1	0.30	-	41,41,41,41	0
32	MG	D	302	1/1	0.25	-	38,38,38,38	0
32	MG	A	3421	1/1	0.10	-	52,52,52,52	0
32	MG	A	3041	1/1	0.49	-	42,42,42,42	0
32	MG	D	301	1/1	0.73	-	47,47,47,47	0
32	MG	A	3442	1/1	0.18	-	42,42,42,42	0
32	MG	A	3217	1/1	0.32	-	51,51,51,51	0
32	MG	A	3527	1/1	0.07	-	132,132,132,132	0
32	MG	A	3427	1/1	0.15	-	30,30,30,30	0
32	MG	A	3550	1/1	0.09	-	54,54,54,54	0
32	MG	A	3562	1/1	0.19	-	34,34,34,34	0
32	MG	A	3480	1/1	0.12	-	59,59,59,59	0
32	MG	A	3493	1/1	0.16	-	66,66,66,66	0
32	MG	A	3415	1/1	0.18	-	31,31,31,31	0
32	MG	A	3592	1/1	0.10	-	58,58,58,58	0
32	MG	A	3334	1/1	0.28	-	30,30,30,30	0
32	MG	A	3237	1/1	0.21	-	35,35,35,35	0
32	MG	A	3261	1/1	0.36	-	44,44,44,44	0
32	MG	A	3341	1/1	0.12	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3032	1/1	0.14	-	43,43,43,43	0
32	MG	A	3348	1/1	0.09	-	40,40,40,40	0
32	MG	A	3430	1/1	0.38	-	47,47,47,47	0
32	MG	A	3284	1/1	0.24	-	57,57,57,57	0
32	MG	E	301	1/1	0.50	-	41,41,41,41	0
32	MG	A	3466	1/1	0.16	-	56,56,56,56	0
32	MG	A	3103	1/1	0.47	-	42,42,42,42	0
32	MG	A	3053	1/1	0.57	-	58,58,58,58	0
32	MG	A	3204	1/1	0.29	-	53,53,53,53	0
32	MG	A	3126	1/1	0.36	-	56,56,56,56	0
32	MG	A	3474	1/1	0.18	-	53,53,53,53	0
32	MG	A	3038	1/1	0.28	-	54,54,54,54	0
32	MG	A	3085	1/1	0.24	-	53,53,53,53	0
32	MG	Q	202	1/1	0.17	-	33,33,33,33	0
32	MG	A	3528	1/1	0.09	-	91,91,91,91	0
32	MG	A	3175	1/1	0.41	-	68,68,68,68	0
32	MG	A	3536	1/1	0.38	-	67,67,67,67	0
32	MG	A	3394	1/1	0.12	-	34,34,34,34	0
32	MG	A	3503	1/1	0.33	-	96,96,96,96	0
32	MG	A	3225	1/1	0.15	-	44,44,44,44	0
32	MG	A	3212	1/1	0.34	-	51,51,51,51	0
32	MG	A	3066	1/1	0.26	-	44,44,44,44	0
32	MG	P	201	1/1	0.22	-	54,54,54,54	0
32	MG	O	102	1/1	0.23	-	72,72,72,72	0
32	MG	A	3501	1/1	0.12	-	63,63,63,63	0
32	MG	A	3155	1/1	0.33	-	45,45,45,45	0
32	MG	A	3453	1/1	0.08	-	42,42,42,42	0
32	MG	A	3188	1/1	0.61	-	50,50,50,50	0
32	MG	A	3447	1/1	0.37	-	67,67,67,67	0
32	MG	A	3092	1/1	0.28	-	23,23,23,23	0
32	MG	A	3490	1/1	0.12	-	63,63,63,63	0
32	MG	E	303	1/1	0.18	-	45,45,45,45	0
32	MG	A	3291	1/1	0.10	-	42,42,42,42	0
32	MG	A	3385	1/1	0.21	-	43,43,43,43	0
32	MG	A	3318	1/1	0.58	-	51,51,51,51	0
32	MG	A	3373	1/1	0.11	-	30,30,30,30	0
32	MG	A	3054	1/1	0.29	-	45,45,45,45	0
32	MG	A	3544	1/1	0.15	-	29,29,29,29	0
32	MG	A	3236	1/1	0.24	-	53,53,53,53	0
32	MG	A	3302	1/1	0.20	-	35,35,35,35	0
32	MG	A	3211	1/1	0.25	-	49,49,49,49	0
32	MG	A	3135	1/1	0.39	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3425	1/1	0.09	-	68,68,68,68	0
32	MG	R	203	1/1	0.42	-	51,51,51,51	0
32	MG	A	3156	1/1	0.18	-	42,42,42,42	0
32	MG	A	3251	1/1	0.28	-	58,58,58,58	0
32	MG	A	3031	1/1	0.45	-	44,44,44,44	0
32	MG	A	3168	1/1	0.48	-	64,64,64,64	0
32	MG	A	3238	1/1	0.34	-	34,34,34,34	0
32	MG	A	3089	1/1	0.49	-	56,56,56,56	0
32	MG	A	3514	1/1	0.35	-	66,66,66,66	0
32	MG	A	3591	1/1	0.06	-	58,58,58,58	0
32	MG	A	3460	1/1	0.26	-	69,69,69,69	0
32	MG	A	3043	1/1	0.28	-	40,40,40,40	0
32	MG	A	3088	1/1	0.23	-	56,56,56,56	0
32	MG	A	3258	1/1	0.72	-	53,53,53,53	0
32	MG	A	3316	1/1	0.21	-	57,57,57,57	0
32	MG	A	3581	1/1	0.85	-	48,48,48,48	0
32	MG	A	3140	1/1	0.33	-	61,61,61,61	0
32	MG	A	3398	1/1	0.90	-	108,108,108,108	0
32	MG	A	3362	1/1	0.21	-	40,40,40,40	0
32	MG	A	3067	1/1	0.52	-	50,50,50,50	0
32	MG	A	3205	1/1	0.29	-	51,51,51,51	0
32	MG	A	3080	1/1	0.27	-	43,43,43,43	0
32	MG	A	3578	1/1	0.17	-	52,52,52,52	0
32	MG	A	3029	1/1	0.24	-	32,32,32,32	0
32	MG	B	203	1/1	0.42	-	58,58,58,58	0
32	MG	A	3133	1/1	0.14	-	41,41,41,41	0
32	MG	A	3387	1/1	0.13	-	47,47,47,47	0
32	MG	A	3502	1/1	0.17	-	91,91,91,91	0
32	MG	A	3307	1/1	0.38	-	28,28,28,28	0
32	MG	A	3244	1/1	0.09	-	42,42,42,42	0
32	MG	A	3134	1/1	0.15	-	59,59,59,59	0
32	MG	A	3016	1/1	0.44	-	51,51,51,51	0
32	MG	A	3173	1/1	0.28	-	88,88,88,88	0
32	MG	A	3207	1/1	0.25	-	48,48,48,48	0
32	MG	A	3210	1/1	0.17	-	37,37,37,37	0
32	MG	A	3045	1/1	0.33	-	34,34,34,34	0
32	MG	A	3288	1/1	0.34	-	53,53,53,53	0
32	MG	A	3576	1/1	0.08	-	57,57,57,57	0
32	MG	A	3209	1/1	0.40	-	48,48,48,48	0
32	MG	A	3265	1/1	0.24	-	54,54,54,54	0
32	MG	A	3476	1/1	0.28	-	62,62,62,62	0
32	MG	A	3027	1/1	0.20	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3404	1/1	0.20	-	70,70,70,70	0
32	MG	A	3431	1/1	0.18	-	60,60,60,60	0
32	MG	A	3409	1/1	0.21	-	58,58,58,58	0
32	MG	A	3308	1/1	0.14	-	26,26,26,26	0
32	MG	A	3458	1/1	0.18	-	41,41,41,41	0
32	MG	A	3218	1/1	1.57	-	68,68,68,68	0
32	MG	A	3069	1/1	0.21	-	54,54,54,54	0
32	MG	A	3203	1/1	0.55	-	54,54,54,54	0
32	MG	A	3008	1/1	0.13	-	37,37,37,37	0
32	MG	A	3147	1/1	0.27	-	61,61,61,61	0
32	MG	A	3228	1/1	0.28	-	57,57,57,57	0
32	MG	A	3049	1/1	0.25	-	46,46,46,46	0
32	MG	A	3226	1/1	0.58	-	45,45,45,45	0
32	MG	A	3465	1/1	0.19	-	53,53,53,53	0
32	MG	E	304	1/1	0.39	-	42,42,42,42	0
32	MG	A	3587	1/1	0.64	-	82,82,82,82	0
32	MG	A	3145	1/1	0.20	-	42,42,42,42	0
32	MG	A	3224	1/1	0.42	-	40,40,40,40	0
32	MG	A	3322	1/1	0.80	-	38,38,38,38	0
32	MG	A	3361	1/1	0.13	-	32,32,32,32	0
32	MG	A	3549	1/1	0.18	-	35,35,35,35	0
32	MG	A	3559	1/1	0.25	-	58,58,58,58	0
32	MG	A	3241	1/1	1.11	-	57,57,57,57	0
32	MG	A	3040	1/1	0.13	-	38,38,38,38	0
32	MG	A	3096	1/1	0.29	-	39,39,39,39	0
32	MG	A	3424	1/1	0.12	-	59,59,59,59	0
32	MG	A	3231	1/1	0.25	-	54,54,54,54	0
32	MG	A	3030	1/1	0.18	-	60,60,60,60	0
32	MG	A	3159	1/1	0.26	-	30,30,30,30	0
32	MG	A	3199	1/1	0.34	-	33,33,33,33	0
32	MG	A	3279	1/1	0.35	-	64,64,64,64	0
32	MG	A	3014	1/1	0.36	-	40,40,40,40	0
32	MG	A	3405	1/1	0.48	-	51,51,51,51	0
32	MG	A	3485	1/1	0.30	-	58,58,58,58	0
32	MG	A	3499	1/1	0.20	-	37,37,37,37	0
32	MG	A	3580	1/1	0.50	-	65,65,65,65	0
32	MG	A	3177	1/1	0.54	-	49,49,49,49	0
32	MG	A	3331	1/1	0.15	-	52,52,52,52	0
32	MG	A	3257	1/1	0.12	-	44,44,44,44	0
32	MG	A	3118	1/1	0.31	-	53,53,53,53	0
32	MG	A	3164	1/1	0.21	-	42,42,42,42	0
32	MG	A	3083	1/1	0.42	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3463	1/1	0.13	-	68,68,68,68	0
32	MG	A	3051	1/1	0.19	-	43,43,43,43	0
32	MG	A	3150	1/1	0.24	-	64,64,64,64	0
32	MG	A	3411	1/1	0.10	-	51,51,51,51	0
32	MG	A	3448	1/1	0.18	-	103,103,103,103	0
32	MG	A	3374	1/1	0.10	-	33,33,33,33	0
32	MG	A	3256	1/1	0.71	-	41,41,41,41	0
32	MG	A	3272	1/1	0.35	-	47,47,47,47	0
32	MG	A	3561	1/1	0.26	-	61,61,61,61	0
32	MG	B	202	1/1	0.47	-	50,50,50,50	0
32	MG	A	3413	1/1	0.21	-	66,66,66,66	0
32	MG	A	3593	1/1	0.14	-	125,125,125,125	0
32	MG	A	3300	1/1	0.31	-	34,34,34,34	0
32	MG	A	3376	1/1	0.10	-	59,59,59,59	0
32	MG	A	3533	1/1	0.11	-	51,51,51,51	0
32	MG	A	3115	1/1	0.46	-	43,43,43,43	0
32	MG	A	3353	1/1	0.24	-	60,60,60,60	0
32	MG	A	3451	1/1	0.25	-	64,64,64,64	0
32	MG	A	3113	1/1	0.30	-	43,43,43,43	0
32	MG	A	3046	1/1	0.33	-	38,38,38,38	0
32	MG	A	3290	1/1	0.15	-	33,33,33,33	0
32	MG	A	3239	1/1	0.20	-	28,28,28,28	0
32	MG	B	204	1/1	0.71	-	74,74,74,74	0
32	MG	A	3230	1/1	0.25	-	41,41,41,41	0
32	MG	A	3104	1/1	0.17	-	59,59,59,59	0
32	MG	A	3461	1/1	0.16	-	89,89,89,89	0
32	MG	A	3003	1/1	0.61	-	58,58,58,58	0
32	MG	A	3523	1/1	0.23	-	98,98,98,98	0
32	MG	A	3574	1/1	0.12	-	57,57,57,57	0
32	MG	A	3505	1/1	0.16	-	60,60,60,60	0
32	MG	A	3171	1/1	0.20	-	44,44,44,44	0
32	MG	A	3091	1/1	0.55	-	59,59,59,59	0
32	MG	A	3065	1/1	0.26	-	57,57,57,57	0
32	MG	A	3120	1/1	0.23	-	50,50,50,50	0
32	MG	A	3184	1/1	0.14	-	69,69,69,69	0
32	MG	A	3310	1/1	0.19	-	29,29,29,29	0
32	MG	A	3180	1/1	0.25	-	46,46,46,46	0
32	MG	A	3345	1/1	0.13	-	41,41,41,41	0
32	MG	A	3530	1/1	0.14	-	89,89,89,89	0
32	MG	A	3176	1/1	0.53	-	49,49,49,49	0
32	MG	A	3484	1/1	0.31	-	48,48,48,48	0
32	MG	A	3402	1/1	0.12	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3094	1/1	0.18	-	36,36,36,36	0
32	MG	A	3005	1/1	0.33	-	42,42,42,42	0
32	MG	A	3436	1/1	0.19	-	57,57,57,57	0
32	MG	A	3324	1/1	0.44	-	52,52,52,52	0
32	MG	A	3518	1/1	0.31	-	86,86,86,86	0
32	MG	A	3546	1/1	0.12	-	45,45,45,45	0
32	MG	A	3423	1/1	0.22	-	81,81,81,81	0
32	MG	A	3454	1/1	0.32	-	64,64,64,64	0
32	MG	A	3418	1/1	0.18	-	93,93,93,93	0
32	MG	A	3255	1/1	0.28	-	43,43,43,43	0
32	MG	A	3388	1/1	0.08	-	37,37,37,37	0
32	MG	A	3585	1/1	0.21	-	34,34,34,34	0
32	MG	A	3295	1/1	0.26	-	49,49,49,49	0
32	MG	A	3193	1/1	0.28	-	49,49,49,49	0
32	MG	A	3468	1/1	0.14	-	31,31,31,31	0
32	MG	A	3260	1/1	0.50	-	61,61,61,61	0
32	MG	A	3060	1/1	0.24	-	53,53,53,53	0
32	MG	A	3399	1/1	0.17	-	44,44,44,44	0
32	MG	A	3333	1/1	0.16	-	41,41,41,41	0
32	MG	A	3367	1/1	0.23	-	32,32,32,32	0
32	MG	A	3111	1/1	0.23	-	43,43,43,43	0
32	MG	A	3074	1/1	0.35	-	47,47,47,47	0
32	MG	A	3364	1/1	0.15	-	30,30,30,30	0
32	MG	A	3564	1/1	0.31	-	46,46,46,46	0
32	MG	A	3185	1/1	0.22	-	84,84,84,84	0
32	MG	A	3072	1/1	0.86	-	49,49,49,49	0
32	MG	B	207	1/1	0.09	-	57,57,57,57	0
32	MG	A	3432	1/1	0.34	-	57,57,57,57	0
32	MG	A	3495	1/1	0.09	-	28,28,28,28	0
32	MG	A	3174	1/1	0.24	-	32,32,32,32	0
32	MG	A	3464	1/1	0.18	-	43,43,43,43	0
32	MG	A	3434	1/1	0.11	-	85,85,85,85	0
32	MG	A	3497	1/1	0.12	-	74,74,74,74	0
32	MG	A	3229	1/1	0.33	-	38,38,38,38	0
32	MG	A	3162	1/1	0.57	-	45,45,45,45	0
32	MG	A	3567	1/1	0.10	-	28,28,28,28	0
32	MG	A	3037	1/1	0.83	-	33,33,33,33	0
32	MG	A	3377	1/1	0.08	-	42,42,42,42	0
32	MG	A	3093	1/1	0.22	-	37,37,37,37	0
32	MG	A	3299	1/1	0.46	-	21,21,21,21	0
32	MG	A	3165	1/1	0.40	-	45,45,45,45	0
32	MG	A	3242	1/1	0.54	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3352	1/1	0.14	-	49,49,49,49	0
32	MG	A	3274	1/1	0.19	-	77,77,77,77	0
32	MG	A	3435	1/1	0.20	-	90,90,90,90	0
32	MG	A	3335	1/1	0.17	-	42,42,42,42	0
32	MG	A	3081	1/1	0.46	-	48,48,48,48	0
33	ZN	4	101	1/1	0.08	-	214,214,214,214	0
32	MG	A	3482	1/1	0.34	-	58,58,58,58	0
32	MG	A	3506	1/1	0.35	-	37,37,37,37	0
32	MG	A	3588	1/1	0.16	-	66,66,66,66	0
32	MG	A	3129	1/1	0.33	-	62,62,62,62	0
32	MG	A	3332	1/1	0.11	-	36,36,36,36	0
32	MG	A	3557	1/1	0.08	-	57,57,57,57	0
32	MG	A	3456	1/1	0.11	-	53,53,53,53	0
32	MG	A	3293	1/1	0.28	-	67,67,67,67	0
32	MG	R	202	1/1	0.29	-	34,34,34,34	0
32	MG	A	3471	1/1	0.08	-	30,30,30,30	0
32	MG	A	3443	1/1	0.25	-	42,42,42,42	0
32	MG	A	3542	1/1	0.14	-	82,82,82,82	0
32	MG	A	3130	1/1	0.37	-	47,47,47,47	0
32	MG	A	3050	1/1	1.01	-	56,56,56,56	0
32	MG	A	3105	1/1	0.29	-	53,53,53,53	0
32	MG	A	3263	1/1	0.18	-	54,54,54,54	0
32	MG	A	3220	1/1	0.23	-	32,32,32,32	0
32	MG	A	3270	1/1	0.53	-	50,50,50,50	0
32	MG	A	3572	1/1	0.05	-	35,35,35,35	0
32	MG	A	3248	1/1	0.54	-	59,59,59,59	0
32	MG	A	3277	1/1	0.52	-	58,58,58,58	0
32	MG	A	3517	1/1	0.14	-	56,56,56,56	0
32	MG	A	3449	1/1	0.15	-	90,90,90,90	0
33	ZN	Y	201	1/1	0.04	-	94,94,94,94	0
32	MG	A	3073	1/1	0.21	-	48,48,48,48	0
32	MG	A	3488	1/1	0.30	-	44,44,44,44	0
32	MG	A	3309	1/1	0.29	-	29,29,29,29	0
32	MG	A	3420	1/1	0.09	-	32,32,32,32	0
32	MG	A	3021	1/1	0.12	-	39,39,39,39	0
32	MG	A	3001	1/1	0.37	-	38,38,38,38	0
32	MG	A	3491	1/1	0.17	-	37,37,37,37	0
32	MG	A	3500	1/1	0.12	-	34,34,34,34	0
32	MG	A	3551	1/1	0.18	-	47,47,47,47	0
32	MG	8	102	1/1	0.51	-	45,45,45,45	0
32	MG	A	3160	1/1	0.55	-	56,56,56,56	0
32	MG	A	3422	1/1	0.15	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3584	1/1	0.30	-	95,95,95,95	0
32	MG	A	3219	1/1	0.22	-	54,54,54,54	0
32	MG	A	3058	1/1	0.43	-	60,60,60,60	0
32	MG	A	3095	1/1	0.71	-	38,38,38,38	0
32	MG	A	3078	1/1	0.21	-	37,37,37,37	0
32	MG	A	3110	1/1	0.45	-	59,59,59,59	0
32	MG	A	3044	1/1	0.59	-	49,49,49,49	0
32	MG	B	206	1/1	0.20	-	58,58,58,58	0
32	MG	A	3028	1/1	0.36	-	66,66,66,66	0
32	MG	A	3313	1/1	0.36	-	69,69,69,69	0
32	MG	A	3508	1/1	0.10	-	49,49,49,49	0
32	MG	A	3391	1/1	0.07	-	47,47,47,47	0
32	MG	A	3589	1/1	0.13	-	83,83,83,83	0
32	MG	A	3470	1/1	0.05	-	38,38,38,38	0
32	MG	A	3195	1/1	0.81	-	44,44,44,44	0
32	MG	A	3143	1/1	0.29	-	48,48,48,48	0
32	MG	A	3266	1/1	0.30	-	47,47,47,47	0
32	MG	A	3070	1/1	0.84	-	58,58,58,58	0
32	MG	A	3253	1/1	0.55	-	56,56,56,56	0
32	MG	E	302	1/1	0.21	-	21,21,21,21	0
32	MG	A	3131	1/1	0.29	-	62,62,62,62	0
32	MG	A	3128	1/1	0.59	-	36,36,36,36	0
32	MG	A	3579	1/1	0.49	-	63,63,63,63	0
32	MG	A	3250	1/1	0.25	-	64,64,64,64	0
32	MG	A	3380	1/1	0.24	-	54,54,54,54	0
32	MG	A	3350	1/1	0.63	-	61,61,61,61	0
32	MG	A	3365	1/1	0.11	-	52,52,52,52	0
32	MG	A	3440	1/1	0.19	-	75,75,75,75	0
32	MG	A	3326	1/1	0.32	-	41,41,41,41	0
32	MG	A	3025	1/1	0.31	-	55,55,55,55	0
32	MG	A	3286	1/1	0.49	-	54,54,54,54	0
32	MG	A	3138	1/1	0.30	-	60,60,60,60	0
32	MG	A	3547	1/1	0.14	-	58,58,58,58	0
32	MG	A	3417	1/1	0.13	-	37,37,37,37	0
32	MG	A	3023	1/1	0.36	-	67,67,67,67	0
32	MG	A	3531	1/1	0.13	-	28,28,28,28	0
32	MG	A	3243	1/1	0.34	-	67,67,67,67	0
32	MG	A	3196	1/1	0.31	-	34,34,34,34	0
32	MG	A	3179	1/1	0.25	-	26,26,26,26	0
32	MG	A	3278	1/1	0.22	-	42,42,42,42	0
32	MG	A	3479	1/1	0.26	-	56,56,56,56	0
32	MG	A	3294	1/1	0.69	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3289	1/1	0.37	-	33,33,33,33	0
32	MG	A	3381	1/1	0.14	-	45,45,45,45	0
32	MG	A	3370	1/1	0.14	-	32,32,32,32	0
32	MG	A	3178	1/1	0.34	-	46,46,46,46	0
32	MG	A	3339	1/1	0.25	-	38,38,38,38	0
32	MG	A	3553	1/1	0.15	-	56,56,56,56	0
32	MG	A	3323	1/1	0.24	-	46,46,46,46	0
32	MG	A	3182	1/1	0.22	-	54,54,54,54	0
32	MG	A	3406	1/1	0.08	-	73,73,73,73	0
32	MG	A	3109	1/1	0.41	-	30,30,30,30	0
32	MG	A	3153	1/1	0.30	-	44,44,44,44	0
32	MG	A	3433	1/1	0.59	-	81,81,81,81	0
32	MG	A	3245	1/1	0.46	-	49,49,49,49	0
32	MG	A	3351	1/1	0.10	-	49,49,49,49	0
32	MG	A	3342	1/1	0.33	-	54,54,54,54	0
32	MG	A	3529	1/1	0.52	-	116,116,116,116	0
32	MG	A	3172	1/1	0.21	-	70,70,70,70	0
32	MG	A	3198	1/1	0.25	-	66,66,66,66	0
32	MG	A	3390	1/1	0.24	-	41,41,41,41	0
32	MG	A	3268	1/1	0.55	-	57,57,57,57	0
33	ZN	5	101	1/1	0.05	-	69,69,69,69	0
32	MG	A	3586	1/1	0.21	-	75,75,75,75	0
32	MG	A	3254	1/1	0.40	-	52,52,52,52	0
32	MG	A	3378	1/1	0.14	-	42,42,42,42	0
32	MG	A	3304	1/1	0.25	-	35,35,35,35	0
32	MG	A	3181	1/1	0.56	-	57,57,57,57	0
32	MG	A	3386	1/1	0.08	-	51,51,51,51	0
32	MG	O	201	1/1	0.26	-	39,39,39,39	0
32	MG	A	3566	1/1	0.15	-	104,104,104,104	0
32	MG	A	3186	1/1	0.26	-	59,59,59,59	0
32	MG	A	3136	1/1	0.65	-	60,60,60,60	0
32	MG	A	3283	1/1	0.14	-	33,33,33,33	0
32	MG	A	3064	1/1	0.21	-	42,42,42,42	0
32	MG	A	3494	1/1	0.32	-	83,83,83,83	0
32	MG	A	3462	1/1	0.14	-	75,75,75,75	0
32	MG	A	3011	1/1	0.51	-	62,62,62,62	0
32	MG	A	3102	1/1	0.28	-	54,54,54,54	0
32	MG	A	3429	1/1	0.19	-	70,70,70,70	0
32	MG	A	3117	1/1	0.80	-	49,49,49,49	0
32	MG	A	3534	1/1	0.14	-	63,63,63,63	0
32	MG	A	3068	1/1	0.73	-	68,68,68,68	0
32	MG	A	3013	1/1	0.44	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3148	1/1	0.44	-	58,58,58,58	0
32	MG	A	3267	1/1	0.41	-	64,64,64,64	0
32	MG	A	3190	1/1	0.28	-	37,37,37,37	0
32	MG	A	3375	1/1	0.10	-	33,33,33,33	0
32	MG	A	3163	1/1	0.66	-	51,51,51,51	0
32	MG	A	3477	1/1	0.39	-	52,52,52,52	0
32	MG	A	3498	1/1	0.16	-	58,58,58,58	0
32	MG	A	3441	1/1	0.26	-	41,41,41,41	0
32	MG	A	3235	1/1	0.44	-	58,58,58,58	0
32	MG	A	3192	1/1	0.37	-	58,58,58,58	0
32	MG	A	3108	1/1	0.33	-	59,59,59,59	0
32	MG	Q	201	1/1	0.87	-	40,40,40,40	0
32	MG	A	3486	1/1	0.11	-	79,79,79,79	0
32	MG	A	3216	1/1	0.37	-	51,51,51,51	0
32	MG	A	3264	1/1	0.57	-	38,38,38,38	0
32	MG	A	3158	1/1	0.41	-	35,35,35,35	0
32	MG	A	3123	1/1	0.77	-	45,45,45,45	0
32	MG	A	3246	1/1	0.12	-	49,49,49,49	0
32	MG	A	3311	1/1	0.34	-	43,43,43,43	0
32	MG	A	3106	1/1	0.28	-	50,50,50,50	0
32	MG	A	3170	1/1	0.51	-	51,51,51,51	0
32	MG	A	3363	1/1	0.04	-	31,31,31,31	0
32	MG	A	3004	1/1	0.39	-	46,46,46,46	0
32	MG	A	3100	1/1	0.21	-	46,46,46,46	0
32	MG	A	3396	1/1	0.17	-	51,51,51,51	0
32	MG	A	3086	1/1	0.50	-	55,55,55,55	0
32	MG	A	3356	1/1	0.07	-	33,33,33,33	0
32	MG	A	3521	1/1	0.39	-	79,79,79,79	0
32	MG	A	3276	1/1	0.25	-	44,44,44,44	0
32	MG	B	201	1/1	0.18	-	43,43,43,43	0
32	MG	A	3515	1/1	0.28	-	69,69,69,69	0
32	MG	A	3535	1/1	0.37	-	87,87,87,87	0
32	MG	A	3472	1/1	0.20	-	30,30,30,30	0
32	MG	A	3048	1/1	0.56	-	40,40,40,40	0
32	MG	A	3101	1/1	0.23	-	37,37,37,37	0
32	MG	A	3187	1/1	0.40	-	51,51,51,51	0
32	MG	A	3475	1/1	0.12	-	87,87,87,87	0
32	MG	A	3010	1/1	0.22	-	38,38,38,38	0
32	MG	A	3033	1/1	0.24	-	37,37,37,37	0
32	MG	A	3548	1/1	0.20	-	62,62,62,62	0
32	MG	A	3504	1/1	0.07	-	80,80,80,80	0
32	MG	A	3213	1/1	0.34	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3285	1/1	0.21	-	39,39,39,39	0
32	MG	A	3389	1/1	0.08	-	35,35,35,35	0
32	MG	A	3006	1/1	0.52	-	42,42,42,42	0
32	MG	A	3077	1/1	0.26	-	36,36,36,36	0
32	MG	A	3024	1/1	0.47	-	40,40,40,40	0
32	MG	A	3157	1/1	0.46	-	39,39,39,39	0
32	MG	A	3384	1/1	0.10	-	60,60,60,60	0
32	MG	A	3575	1/1	0.16	-	29,29,29,29	0

## 6.5 Other polymers

There are no such residues in this entry.