



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:06 AM GMT

PDB ID : 3PIP  
Title : Crystal structure of the synergistic antibiotic pair lankamycin and lankacidin in complex with the large ribosomal subunit  
Authors : Belousoff, M.J.; Shapira, T.; Bashan, A.; Zimmerman, E.; Kinashi, H.; Rozenberg, H.; Yonath, A.  
Deposited on : 2010-11-07  
Resolution : 3.45 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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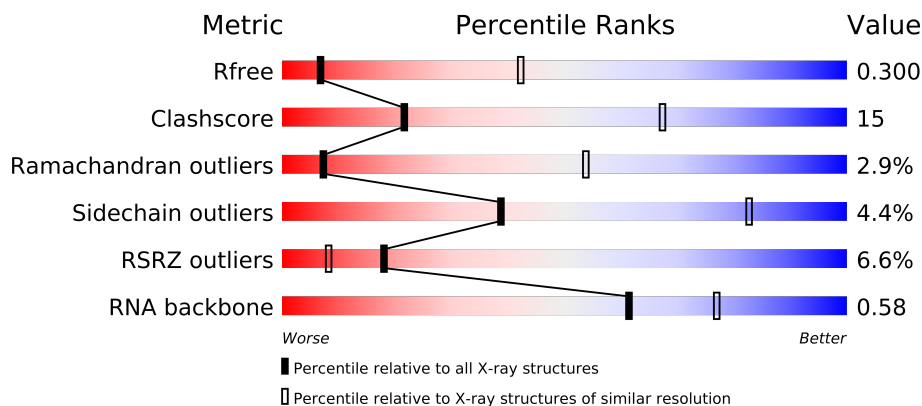
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
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 3.45 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))
$R_{free}$	66092	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)
RNA backbone	1838	1004 (4.10-2.76)

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	X	2880	
2	Y	123	
3	A	274	
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	

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Mol	Chain	Length	Quality of chain
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	
30	4	37	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
31	LC2	X	2881	-	X
32	LMA	X	2882	-	X
33	MG	X	2883	-	X
33	MG	X	2884	-	X
33	MG	X	2885	-	X
33	MG	X	2886	-	X
33	MG	X	2887	-	X
33	MG	X	2888	-	X
33	MG	X	2890	-	X
33	MG	X	2891	-	X
33	MG	X	2892	-	X
33	MG	X	2893	-	X
33	MG	X	2894	-	X
33	MG	X	2895	-	X
33	MG	X	2898	-	X
33	MG	X	2899	-	X
33	MG	X	2900	-	X
33	MG	X	2901	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	X	2903	-	X
33	MG	X	2904	-	X
33	MG	X	2905	-	X
33	MG	X	2906	-	X
33	MG	X	2907	-	X
33	MG	X	2908	-	X
33	MG	X	2910	-	X
33	MG	X	2911	-	X
33	MG	X	2913	-	X
33	MG	X	2914	-	X
33	MG	X	2915	-	X
33	MG	X	2917	-	X
33	MG	X	2918	-	X
33	MG	X	2919	-	X
33	MG	X	2920	-	X
33	MG	X	2922	-	X
33	MG	X	2925	-	X
33	MG	X	2926	-	X
33	MG	X	2927	-	X
33	MG	X	2929	-	X
33	MG	X	2931	-	X
33	MG	X	2932	-	X
33	MG	X	2933	-	X
33	MG	X	2934	-	X
33	MG	X	2935	-	X
33	MG	X	2937	-	X
33	MG	X	2938	-	X
33	MG	X	2939	-	X
33	MG	X	2942	-	X
33	MG	X	2948	-	X
33	MG	X	2949	-	X
33	MG	X	2950	-	X
33	MG	X	2951	-	X
33	MG	X	2952	-	X
33	MG	X	2953	-	X
34	K	X	2955	-	X
34	K	X	2956	-	X
34	K	X	2957	-	X
35	NA	X	2958	-	X
35	NA	X	2959	-	X
35	NA	X	2960	-	X
35	NA	X	2961	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	X	2962	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 83963 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 RIBOSOMAL 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2644	Total	C	N	O	P	0	0	0
			56750	25314	10473	18320	2643			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	253	Total	C	N	O	S	0	0	0
			1920	1196	382	340	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1394	889	244	254	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	63	Total	C	N	O	S	0	0	0
			451	280	82	86	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	134	Total	C	N	O	S	0	0	0
			1005	616	203	186				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	126	Total	C	N	O	S	0	0	0
			1004	633	197	172	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			714	452	130	130	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			537	334	110	93				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

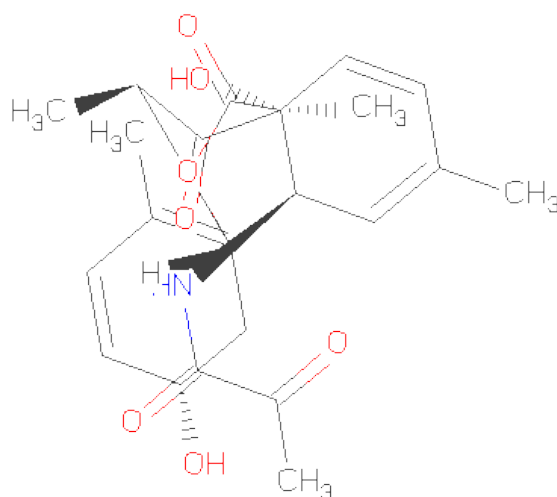
- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 30 is a protein called 50S ribosomal protein L36.

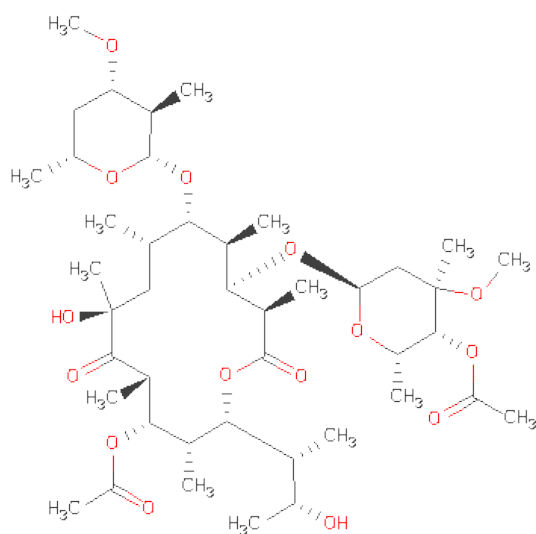
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	37	Total	C	N	O	S	0	0	0
			297	179	66	47	5			

- Molecule 31 is N-[(1S,2R,3E,5E,7S,9E,11E,13S,15R,19R)-7,13-DIHYDROXY-1,4,10,19-TE TRAMETHYL-17,18-DIOXO-16-OXABICYCLO[13.2.2]NONADECA-3,5,9,11-TETRAEN-2-YL]-2-OXOPROPANAMIDE (three-letter code: LC2) (formula: C<sub>25</sub>H<sub>33</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	X	1	Total	C	N	O	0	0
			33	25	1	7		

- Molecule 32 is LANKAMYCIN (three-letter code: LMA) (formula: C<sub>43</sub>H<sub>74</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			58	43	15		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	71	Total	Mg	0	0
			71	71		
33	I	1	Total	Mg	0	0
			1	1		
33	U	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	X	4	Total	K	0	0
			4	4		

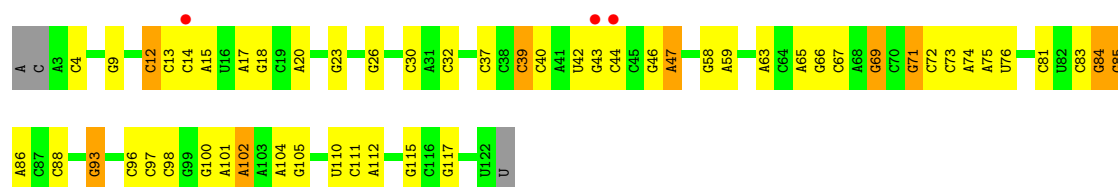
- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	X	5	Total	Na	0	0
			5	5		



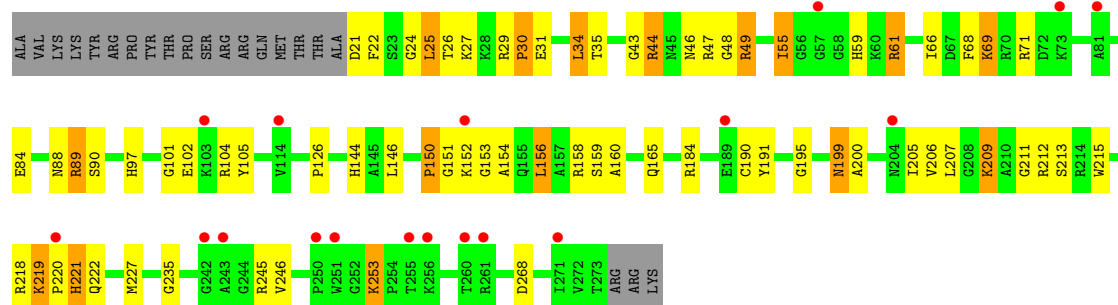
A1851	U1766	C1700	G1559	C1466	C1308	G1243	U1177	G1098	U1023	G953	A886	U810
G1852	G1767	C1701	G1562	U1467	G1309	G1246	C1178	A1099	G1028	U954	A886	G811
C1853	U1768	C1702	U1563	U1469	C1310	G1249	A1179	U1100	C1029	G955	G887	G812
A1867	U1769	C1703	U1564	U1470	C1311	G1250	A1180	U1101	U1030	A956	G888	
A1868	U1770	U1704	U1565	G1471	U1312	G1249	C1181	U1030	C1031	G957	C889	A816
	C1772	U1705	G1566	G1472	U1313	A1260	U1182	G1104	A1032	G958	U890	U816
G1874	G1773	U1706		U1473	A1314	G1251	C1183		A1033	C959	A	A817
	C1774	U1707	C1570	U1474	A1315	C1252	G	U1108	U1034	U960	G	G818
A1884	U1775	U1709	G1571	U1475	G1316	G1253	C		U1035	G961	G	C819
	A1776	U1710	C1572	G1476	G1317	A1254	G	A1114	G1036	C962	G	U820
G1888	U1777	C1711	U1573	U1477	A1318	G1255	A	C1115	U1037	G963	G	A821
G	U1778	G1713	A1574	U1478	G1324	U1256	A	U1119	U1038	A964	C	
G	C1779		C1575	G1479	U1325	G1258	C	G1120		A966	C	U824
C	A1780	A1714	G1576	U1480	U1326	A1259	A	G1123	G1041	U967	U	C825
C	A1781	U1715	G1577	U1481	C1327	U1260	G	U1044	U1044	C968	A	U826
U	A1782	G1716	U1578	U1482	C1328	G1261	U1194	G1128	G1045	C969	C	C828
U		U1717	U1579	U1483	U1329	U1262	U1195	A1129	U1046	C970	C	C829
A	U1789	U1718	A1582	G1488	G1330	G1263	U1196	U1130	G1047	A971	A	C830
A	C1790	G1719	A1583	U1489	G1331	C1264	U1197	U1131		C972	G	G831
C	C1791	G1720	U1584	U1490	G1332	G1265	C1198	C1135	U1051	U974	U	A832
U	C1792	G1721	G1584	G1494	G1333	G1266	U1199	G1136	G1052	U975	U	A833
A	A1793	G1722	A1585	G1495	A1334	U1267	G1200	A1137	G1053	U976	A	U834
U		G1723	A1586	G1496	G1335	U1268	G1201	U1138	C1054	C977	C	U835
A	C1801	U1724	U1592	C1497	G1336	G1269	U1202	A		G980	C	G836
A	A1802	C1725			G1337	C1270	U1203	U1141	U1058	C981	C	U837
C		C1726	U1601	C1506	G1338	C1271	A	U1142	A	C982		A911
C	G1806	G1730	G1602	C1514	G1341	G1272	G1204	G1143	G1058	G983		U838
G	A1807		U1605	U1521	U1342	U1273	G1205	A1144	A1059	C984		U839
C	G	U1733	A1606	C	C1343	U1276	G1209	G1145	G1060	U916	U	U840
U1909	U1810	G1735	C1607	U1521	C1344	G1277	C1210	G1146	A1061	U917	U	A942
A1910	A1811	C1736	A1608	C	G1345	U1278	G1211	G1147	G1062	A918		G843
A1911	U1812	U1737	G1609	A	C1346	G1279	U1212	G1148	C1063	G920		U844
G1912	A1813			U1526	U1347	U1280	U1213	G1149	C1064	A921		U845
		G1741	G1613	G1527	G1351	A1281	C1214	G1150		A922		G849
G1916	U1816		C1614	G1527	U1355	A1282	A1215	G1069	G1069	A923		U850
C1917	U1817	G1744	C1615	C1528	G1356	C1283	G1220	G1070	C924	C924		C851
G1918	U1818	C1745	C1616	C1529	U1357	G1284	C1221	C1152	U925	U925		G858
A1919	U1819	U1746	U1617	C1535	C1358	U1285	U1222	A1153	C997	C997		U859
A1920	U1820	G1747	G1536	C1536	C1359	U1286	G1223	G1154	A999	G927		U860
A1921	U1821	U1748	G1621	U1539	G1364	A1287	U1224	G1155	G1000	G928		G861
U1922	G1823	G1749	G1622	U1539	U1365	A1288	G1225	A1158	A1001			A862
U1923	C1824	A1751	A1624	C1540	U1366	A1289	U1226	U1159	U1005	G933		A863
C1924	C1825	U1752	U1625	U1543	A1366	U1291	A1227	C1160	C1006	G934		C864
		G1753	A1626	G1544	G1371	A1293	C1229	C1163	U1005			A865
U1927	C1828	U1754	C1627	G1545	U1378	U1294	U1232	A1166	C1006			A866
G1928	U1829	G1755	U1628	U1546	A1379	U1295	U1233	A1167	C1008			C867
U1929	C1830	G1756	C1629	C1549	U1380	G1296	U1234	G1086	G1009			U871
C1930	G1831	C1757	G1630	C1550	G1381	U1297	C1235	C1087	U1010			C872
G1931		U1758	C1631	U1551	U1382	U1298	C1236	C1088	A1011			U873
U1932		G1759	A1632	C1552	G1383	A1299	U1237	C1089	A1012			A874
G1933		U1760	C1633	C1553	U1384	A1300	G1238	C1090	C1016			G875
U1934	A1840	G1761	U1634	U1554	G1387	U1304	U1239	U1091	C1017			C878
A1935	U1841	C1762	G1635	U1555	U1388	C1305	A1239	U1092	C1018			U879
A1936	G1842	U1763	U1636	U1556	G1389	U1306	G1240	U1095	U1019			C880
U1937	U1843	G1764	U1637	A1556	C1388	U1307	U1241	A1096	A1020			G881
U1938	C1844		G1638					U1097	A1021			A883
U1939		C1765							A1022			C884





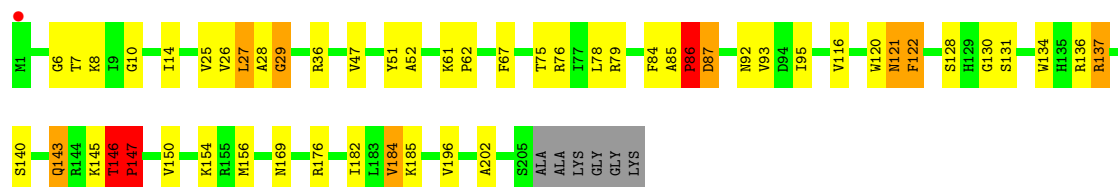
• Molecule 3: 50S ribosomal protein L2

Chain A:



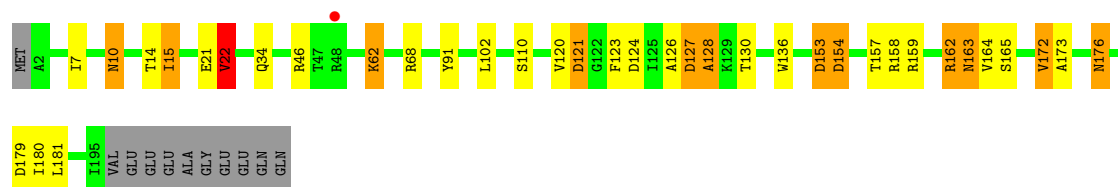
• Molecule 4: 50S ribosomal protein L3

Chain B:



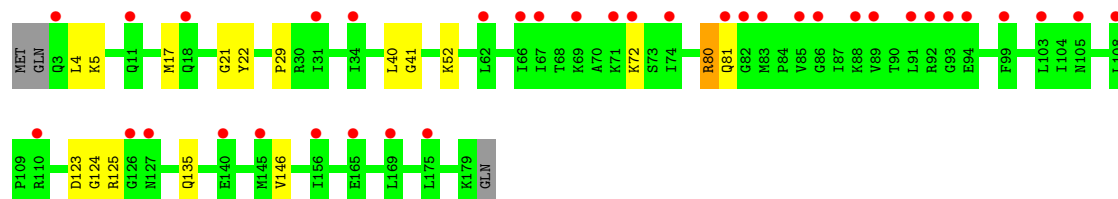
• Molecule 5: 50S ribosomal protein L4

Chain C:



• Molecule 6: 50S ribosomal protein L5

Chain D:



• Molecule 7: 50S ribosomal protein L6

Chain E:







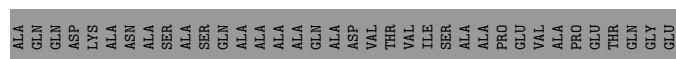
- Molecule 14: 50S ribosomal protein L18

Chain L:



- Molecule 15: 50S ribosomal protein L19

Chain M:



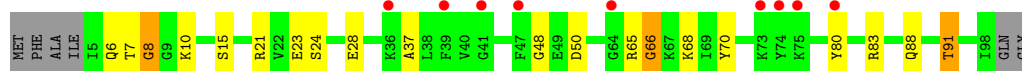
- Molecule 16: 50S ribosomal protein L20

Chain N:



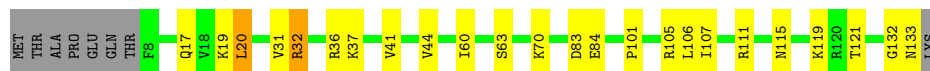
- Molecule 17: 50S ribosomal protein L21

Chain O:



- Molecule 18: 50S ribosomal protein L22

Chain P:



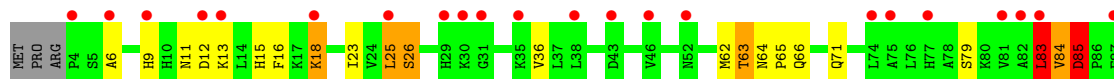
- Molecule 19: 50S ribosomal protein L23

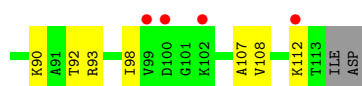
Chain Q:



- Molecule 20: 50S ribosomal protein L24

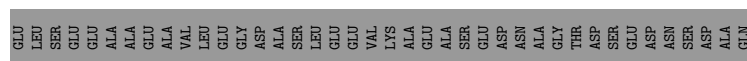
Chain R:





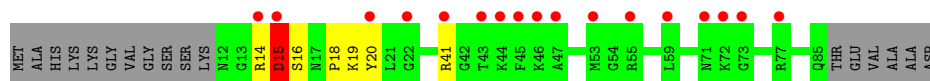
- Molecule 21: 50S ribosomal protein L25

Chain S:



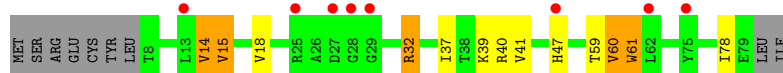
- Molecule 22: 50S ribosomal protein L27

Chain T:



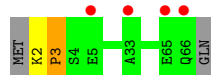
- Molecule 23: 50S ribosomal protein L28

Chain U:



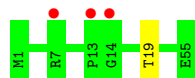
- Molecule 24: 50S ribosomal protein L29

Chain V:



- Molecule 25: 50S ribosomal protein L30

Chain W:



- Molecule 26: 50S ribosomal protein L32

Chain Z:



- Molecule 27: 50S ribosomal protein L33

Chain 1:



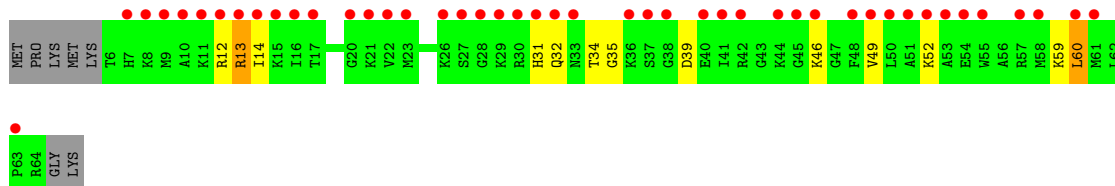
- Molecule 28: 50S ribosomal protein L34

Chain 2: 



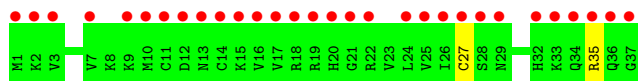
- Molecule 29: 50S ribosomal protein L35

Chain 3: 



- Molecule 30: 50S ribosomal protein L36

Chain 4: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.72Å 408.56Å 693.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.45 93.01 – 3.44	Depositor EDS
% Data completeness (in resolution range)	83.3 (20.00-3.45) 82.4 (93.01-3.44)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 3.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4.486)	Depositor
R, $R_{free}$	0.257 , 0.301 0.261 , 0.300	Depositor DCC
$R_{free}$ test set	2645 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 262327 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	83963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: NA, K, LC2, MG, LMA

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	X	1.17	260/63542 (0.4%)	1.58	1813/99100 (1.8%)
2	Y	0.80	1/2863 (0.0%)	1.13	21/4461 (0.5%)
3	A	0.65	0/1958	0.83	2/2638 (0.1%)
4	B	0.85	0/1567	0.93	2/2105 (0.1%)
5	C	0.84	0/1504	0.84	1/2036 (0.0%)
6	D	0.46	0/1413	0.56	0/1896
7	E	0.57	0/1308	0.60	0/1771
8	F	0.37	0/455	0.45	0/611
9	G	0.75	0/1138	0.82	0/1539
10	H	0.94	0/1007	0.99	0/1352
11	I	0.62	0/1016	0.71	0/1359
12	J	0.80	0/1113	0.80	0/1486
13	K	0.93	1/886 (0.1%)	1.01	0/1188
14	L	0.72	0/785	0.93	1/1048 (0.1%)
15	M	0.99	0/884	1.07	1/1186 (0.1%)
16	N	0.93	0/994	0.85	0/1323
17	O	0.77	0/750	0.81	0/1000
18	P	1.01	2/1017 (0.2%)	0.97	1/1362 (0.1%)
19	Q	0.66	0/725	0.69	0/974
20	R	0.66	0/835	0.72	1/1121 (0.1%)
21	S	0.51	0/1370	0.60	1/1862 (0.1%)
22	T	0.74	0/563	0.77	0/747
23	U	0.57	0/541	0.70	1/723 (0.1%)
24	V	0.67	0/529	0.63	0/704
25	W	0.60	0/426	0.71	0/568
26	Z	0.89	0/464	0.94	1/622 (0.2%)
27	1	0.32	0/438	0.60	0/583
28	2	0.57	0/387	0.54	0/509
29	3	0.22	0/468	0.38	0/614
30	4	0.69	1/298 (0.3%)	0.58	0/390
All	All	1.06	265/91244 (0.3%)	1.42	1846/136878 (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
7	E	0	4
8	F	0	3
9	G	0	8
10	H	0	2
11	I	0	1
12	J	0	1
All	All	0	19

All (265) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	616	U	C3'-C2'	-13.53	1.37	1.52
1	X	1775	A	O3'-P	-11.52	1.47	1.61
1	X	1299	A	N9-C4	-11.34	1.31	1.37
1	X	1260	A	N9-C4	-11.21	1.31	1.37
1	X	2669	C	N1-C6	-10.57	1.30	1.37
1	X	2524	G	N7-C5	-10.21	1.33	1.39
1	X	747	A	N9-C8	-9.54	1.30	1.37
1	X	1316	G	N3-C4	-9.29	1.28	1.35
1	X	581	A	N9-C4	-9.27	1.32	1.37
1	X	1635	G	N3-C4	-9.03	1.29	1.35
1	X	1290	A	N9-C8	-8.96	1.30	1.37
1	X	2486	C	C4-C5	-8.89	1.35	1.43
1	X	461	A	N7-C5	-8.61	1.34	1.39
1	X	2745	A	N9-C4	-8.54	1.32	1.37
1	X	542	A	N9-C4	-8.43	1.32	1.37
1	X	2799	C	N3-C4	-8.35	1.28	1.33
1	X	2381	A	C2'-C1'	-8.28	1.44	1.53
1	X	982	C	N1-C6	-8.23	1.32	1.37
1	X	2669	C	C2-O2	8.22	1.31	1.24
1	X	827	C	N1-C6	-7.90	1.32	1.37
1	X	583	C	C4-C5	-7.69	1.36	1.43
1	X	955	G	O3'-P	-7.68	1.51	1.61
1	X	691	C	N3-C4	-7.60	1.28	1.33
1	X	2826	C	N1-C6	-7.53	1.32	1.37
1	X	1284	G	N3-C4	-7.51	1.30	1.35
1	X	2540	A	N9-C4	-7.51	1.33	1.37
1	X	679	C	N1-C6	-7.50	1.32	1.37
1	X	1975	G	N3-C4	-7.41	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2314	A	N9-C8	-7.33	1.31	1.37
1	X	975	C	N1-C6	-7.25	1.32	1.37
1	X	1655	C	N1-C6	-7.24	1.32	1.37
1	X	754	G	C5-C4	-7.16	1.33	1.38
1	X	2531	U	N1-C6	-7.16	1.31	1.38
1	X	586	G	N7-C5	-7.09	1.34	1.39
1	X	2674	C	N1-C2	-7.07	1.33	1.40
1	X	2712	G	N3-C4	-7.06	1.30	1.35
1	X	1288	A	C5-C4	7.02	1.43	1.38
1	X	2790	C	N1-C6	-7.00	1.32	1.37
1	X	522	G	C5-C4	6.99	1.43	1.38
1	X	579	G	C5-C6	6.91	1.49	1.42
1	X	1333	G	N9-C4	-6.86	1.32	1.38
1	X	1333	G	N3-C4	-6.83	1.30	1.35
1	X	1621	C	C3'-C2'	-6.82	1.45	1.52
1	X	2696	A	C5-C4	-6.80	1.33	1.38
1	X	2312	A	N7-C5	-6.80	1.35	1.39
1	X	1246	G	C6-N1	-6.79	1.34	1.39
1	X	1770	U	N3-C4	-6.76	1.32	1.38
1	X	2382	C	O3'-P	6.76	1.69	1.61
1	X	1717	A	N3-C4	-6.71	1.30	1.34
1	X	1674	C	N1-C6	-6.70	1.33	1.37
1	X	1744	G	C6-N1	-6.69	1.34	1.39
1	X	2807	U	N1-C2	6.67	1.44	1.38
1	X	575	U	N1-C2	-6.65	1.32	1.38
1	X	2432	A	N7-C5	-6.65	1.35	1.39
1	X	836	G	N7-C5	-6.64	1.35	1.39
1	X	465	C	N1-C6	-6.61	1.33	1.37
1	X	1675	C	N1-C6	-6.58	1.33	1.37
1	X	1261	G	N7-C5	-6.58	1.35	1.39
1	X	569	C	C4-N4	-6.57	1.28	1.33
1	X	1672	A	N9-C4	-6.56	1.33	1.37
1	X	1986	G	O3'-P	-6.52	1.53	1.61
1	X	2226	A	N9-C4	-6.47	1.33	1.37
1	X	1292	A	N7-C5	6.46	1.43	1.39
1	X	2617	G	N9-C8	-6.44	1.33	1.37
1	X	740	A	N3-C4	-6.43	1.30	1.34
1	X	2486	C	N1-C6	-6.39	1.33	1.37
1	X	2807	U	C4-C5	6.38	1.49	1.43
1	X	1250	A	N9-C4	-6.34	1.34	1.37
1	X	2702	G	N9-C8	6.34	1.42	1.37
1	X	1265	G	N9-C8	-6.34	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	753	U	N1-C2	-6.33	1.32	1.38
1	X	2065	A	N7-C5	-6.30	1.35	1.39
1	X	1334	A	N7-C5	-6.29	1.35	1.39
2	Y	101	A	C6-N1	-6.29	1.31	1.35
1	X	2039	G	C2-N3	-6.27	1.27	1.32
1	X	2691	C	N3-C4	6.26	1.38	1.33
1	X	461	A	N9-C8	-6.25	1.32	1.37
1	X	1281	A	C6-N6	6.20	1.39	1.33
1	X	2694	G	N9-C4	6.19	1.43	1.38
1	X	2815	C	N1-C6	6.19	1.40	1.37
1	X	2352	A	N3-C4	-6.15	1.31	1.34
1	X	1332	G	N9-C8	-6.12	1.33	1.37
1	X	2054	A	C6-N1	-6.10	1.31	1.35
1	X	986	A	N9-C4	-6.09	1.34	1.37
1	X	499	G	N1-C2	-6.09	1.32	1.37
1	X	690	A	N3-C4	-6.09	1.31	1.34
1	X	2602	G	N9-C4	6.07	1.42	1.38
1	X	2515	G	N3-C4	-6.07	1.31	1.35
1	X	2398	U	C4-O4	6.07	1.28	1.23
1	X	571	U	N1-C2	-6.06	1.33	1.38
1	X	1629	G	N7-C5	-6.05	1.35	1.39
1	X	807	A	N9-C4	-6.05	1.34	1.37
1	X	2530	C	N1-C6	-6.04	1.33	1.37
1	X	1288	A	N9-C8	6.03	1.42	1.37
1	X	2759	U	N1-C6	-6.03	1.32	1.38
1	X	1166	A	N9-C4	6.02	1.41	1.37
1	X	157	G	P-O5'	-5.98	1.53	1.59
1	X	2218	G	C5-C6	-5.97	1.36	1.42
1	X	1653	C	N1-C6	-5.96	1.33	1.37
1	X	2555	G	N9-C4	-5.94	1.33	1.38
1	X	815	A	N9-C4	-5.94	1.34	1.37
1	X	1687	C	N1-C6	-5.90	1.33	1.37
1	X	1624	A	N3-C4	-5.90	1.31	1.34
1	X	1290	A	N9-C4	-5.89	1.34	1.37
1	X	2523	G	C6-N1	-5.86	1.35	1.39
1	X	1672	A	N3-C4	-5.84	1.31	1.34
1	X	1290	A	N3-C4	-5.84	1.31	1.34
1	X	841	G	N9-C4	-5.82	1.33	1.38
1	X	2495	G	N1-C2	-5.81	1.33	1.37
1	X	522	G	N1-C2	5.80	1.42	1.37
1	X	1699	A	C5-C6	-5.75	1.35	1.41
1	X	351	A	N3-C4	-5.74	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1671	A	N3-C4	5.73	1.38	1.34
1	X	1223	G	N3-C4	-5.73	1.31	1.35
1	X	1313	U	N3-C4	-5.72	1.33	1.38
1	X	2699	G	P-O5'	-5.72	1.54	1.59
1	X	2854	G	N9-C8	5.72	1.41	1.37
1	X	156	G	N9-C4	-5.71	1.33	1.38
1	X	2015	G	N9-C8	5.71	1.41	1.37
1	X	1700	C	N1-C6	-5.70	1.33	1.37
1	X	2574	G	C5-C4	-5.70	1.34	1.38
1	X	2258	G	N9-C8	-5.70	1.33	1.37
1	X	596	C	N1-C6	-5.70	1.33	1.37
1	X	2696	A	N7-C5	-5.69	1.35	1.39
1	X	174	A	C3'-O3'	-5.69	1.34	1.42
1	X	1268	U	O3'-P	-5.67	1.54	1.61
1	X	1761	G	C2-N2	-5.67	1.28	1.34
1	X	320	A	N9-C4	-5.66	1.34	1.37
1	X	1288	A	C6-N6	-5.66	1.29	1.33
1	X	2355	A	C5-C4	-5.65	1.34	1.38
1	X	2424	G	N9-C8	-5.65	1.33	1.37
1	X	1012	A	N9-C4	-5.63	1.34	1.37
1	X	950	G	N3-C4	-5.63	1.31	1.35
1	X	393	U	C4-O4	5.61	1.28	1.23
18	P	17	GLN	CD-OE1	5.61	1.36	1.24
1	X	1665	C	N1-C6	-5.60	1.33	1.37
1	X	322	A	N7-C5	5.60	1.42	1.39
1	X	2258	G	C6-N1	-5.59	1.35	1.39
1	X	1940	C	N1-C6	-5.59	1.33	1.37
1	X	1267	A	O3'-P	5.58	1.67	1.61
1	X	2688	G	N7-C5	5.58	1.42	1.39
1	X	1474	A	N9-C4	5.57	1.41	1.37
1	X	1334	A	N9-C4	-5.57	1.34	1.37
1	X	2492	G	P-O5'	-5.57	1.54	1.59
1	X	2014	A	N7-C5	-5.57	1.35	1.39
1	X	520	C	N1-C2	-5.56	1.34	1.40
1	X	1678	G	N7-C5	5.56	1.42	1.39
1	X	1985	G	O3'-P	-5.55	1.54	1.61
1	X	538	A	N9-C4	5.54	1.41	1.37
1	X	2527	G	C5-C4	-5.54	1.34	1.38
1	X	2007	G	C6-O6	5.53	1.29	1.24
1	X	513	A	C6-N1	-5.53	1.31	1.35
1	X	72	A	C6-N1	-5.53	1.31	1.35
1	X	1325	U	N1-C6	-5.52	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1282	A	C5-C6	-5.52	1.36	1.41
1	X	2039	G	N7-C5	-5.52	1.35	1.39
1	X	1287	A	C6-N1	-5.51	1.31	1.35
1	X	2498	U	P-O5'	-5.51	1.54	1.59
1	X	1673	C	N1-C6	-5.51	1.33	1.37
1	X	752	G	N3-C4	-5.48	1.31	1.35
1	X	1232	U	N1-C2	-5.48	1.33	1.38
1	X	1625	A	N9-C4	-5.48	1.34	1.37
1	X	718	A	N3-C4	-5.48	1.31	1.34
1	X	1278	A	C5-C6	-5.48	1.36	1.41
1	X	562	G	N9-C8	-5.46	1.34	1.37
1	X	2540	A	C5-C4	-5.46	1.34	1.38
1	X	2698	G	N7-C5	-5.45	1.35	1.39
1	X	1265	G	N7-C5	-5.45	1.35	1.39
1	X	2226	A	N3-C4	-5.45	1.31	1.34
1	X	991	A	C5-C6	-5.44	1.36	1.41
1	X	2680	U	C4-O4	5.44	1.27	1.23
1	X	542	A	N3-C4	-5.43	1.31	1.34
1	X	2802	C	N1-C2	-5.43	1.34	1.40
1	X	2815	C	C4-C5	5.43	1.47	1.43
1	X	1150	C	P-O5'	-5.43	1.54	1.59
1	X	970	A	N7-C5	-5.41	1.36	1.39
1	X	1968	G	N9-C8	-5.40	1.34	1.37
1	X	1172	U	N1-C2	-5.40	1.33	1.38
1	X	1678	G	C6-N1	-5.40	1.35	1.39
1	X	2825	A	C6-N1	-5.40	1.31	1.35
1	X	928	G	N7-C5	-5.40	1.36	1.39
1	X	168	A	N3-C4	-5.39	1.31	1.34
1	X	1778	U	N1-C2	-5.38	1.33	1.38
1	X	1298	G	N9-C8	-5.38	1.34	1.37
1	X	1260	A	N3-C4	-5.38	1.31	1.34
1	X	1670	G	C5-C4	-5.38	1.34	1.38
1	X	462	G	C6-O6	5.36	1.28	1.24
1	X	2042	A	N7-C5	-5.36	1.36	1.39
1	X	1449	C	N1-C6	5.36	1.40	1.37
1	X	1665	C	N3-C4	-5.36	1.30	1.33
1	X	2674	C	N3-C4	-5.34	1.30	1.33
1	X	1041	G	N9-C4	-5.34	1.33	1.38
1	X	2471	U	C4-O4	-5.32	1.19	1.23
1	X	947	C	N1-C6	-5.32	1.33	1.37
1	X	2596	C	C2-O2	5.30	1.29	1.24
1	X	2681	A	N9-C4	-5.30	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2634	G	N9-C8	-5.30	1.34	1.37
1	X	693	A	N9-C4	-5.29	1.34	1.37
1	X	1276	U	P-O5'	-5.29	1.54	1.59
1	X	572	G	N3-C4	-5.29	1.31	1.35
1	X	482	A	P-O5'	-5.27	1.54	1.59
1	X	1151	U	N1-C6	-5.27	1.33	1.38
1	X	2218	G	N7-C5	-5.26	1.36	1.39
1	X	991	A	N7-C5	-5.26	1.36	1.39
1	X	1333	G	N9-C8	5.25	1.41	1.37
1	X	2837	G	C5-C4	-5.25	1.34	1.38
1	X	536	A	N9-C4	5.24	1.41	1.37
1	X	1278	A	N3-C4	-5.24	1.31	1.34
1	X	841	G	N9-C8	5.24	1.41	1.37
1	X	1666	G	C8-N7	5.24	1.34	1.30
1	X	1942	G	N9-C4	-5.24	1.33	1.38
1	X	2520	A	P-O5'	-5.23	1.54	1.59
1	X	2229	G	C5-C6	5.23	1.47	1.42
1	X	1472	C	N3-C4	5.22	1.37	1.33
1	X	2540	A	C6-N6	-5.22	1.29	1.33
1	X	2508	G	C5-C6	-5.22	1.37	1.42
1	X	1282	A	N7-C5	-5.22	1.36	1.39
1	X	1287	A	N3-C4	-5.21	1.31	1.34
1	X	2303	C	N1-C6	-5.21	1.34	1.37
1	X	1938	U	C2'-C1'	-5.20	1.47	1.53
1	X	1270	C	N3-C4	-5.19	1.30	1.33
1	X	2372	A	N7-C5	-5.19	1.36	1.39
1	X	2823	G	N9-C8	-5.19	1.34	1.37
1	X	24	G	N7-C5	-5.18	1.36	1.39
1	X	2673	G	C5-C4	-5.18	1.34	1.38
1	X	2244	C	N1-C6	-5.18	1.34	1.37
1	X	538	A	C2'-C1'	5.18	1.59	1.53
1	X	2039	G	C5-C6	-5.16	1.37	1.42
1	X	2693	U	N3-C4	-5.16	1.33	1.38
1	X	1337	G	O3'-P	-5.16	1.54	1.61
1	X	461	A	C6-N1	5.16	1.39	1.35
1	X	691	C	N1-C6	-5.15	1.34	1.37
1	X	1761	G	C5-C4	-5.14	1.34	1.38
1	X	1952	A	N3-C4	-5.14	1.31	1.34
1	X	523	A	N9-C8	-5.13	1.33	1.37
1	X	920	G	C5-C4	-5.13	1.34	1.38
1	X	1265	G	C6-N1	5.13	1.43	1.39
13	K	88	ALA	CA-CB	-5.12	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	703	A	N3-C4	-5.11	1.31	1.34
1	X	745	C	N1-C6	-5.11	1.34	1.37
1	X	1778	U	C4-O4	-5.11	1.19	1.23
1	X	2348	A	N9-C4	-5.11	1.34	1.37
1	X	2745	A	C5-C6	-5.11	1.36	1.41
1	X	522	G	N9-C8	5.11	1.41	1.37
1	X	1813	A	N7-C5	-5.10	1.36	1.39
1	X	2812	A	N7-C5	-5.10	1.36	1.39
1	X	1054	C	N1-C6	-5.10	1.34	1.37
1	X	2015	G	C8-N7	5.09	1.34	1.30
1	X	584	A	N3-C4	-5.07	1.31	1.34
1	X	522	G	P-O5'	-5.07	1.54	1.59
1	X	718	A	N9-C4	-5.07	1.34	1.37
1	X	1278	A	N7-C5	-5.06	1.36	1.39
30	4	27	CYS	CB-SG	5.06	1.90	1.82
18	P	31	VAL	CB-CG1	-5.06	1.42	1.52
1	X	1650	A	P-O5'	-5.05	1.54	1.59
1	X	1240	G	N9-C8	-5.05	1.34	1.37
1	X	1778	U	C2-O2	-5.04	1.17	1.22
1	X	1246	G	C5-C4	-5.04	1.34	1.38
1	X	2856	U	N1-C2	-5.04	1.34	1.38
1	X	1763	G	N9-C8	-5.02	1.34	1.37
1	X	755	C	N1-C6	-5.02	1.34	1.37
1	X	1671	A	N9-C4	5.02	1.40	1.37
1	X	743	A	N3-C4	-5.02	1.31	1.34
1	X	762	A	C5-C6	-5.01	1.36	1.41
1	X	2331	A	N3-C4	-5.00	1.31	1.34

All (1846) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	29	ARG	C-N-CD	-19.10	78.58	120.60
1	X	1678	G	N1-C6-O6	-18.90	108.56	119.90
1	X	2486	C	C5-C6-N1	17.23	129.62	121.00
1	X	2815	C	C6-N1-C2	17.04	127.12	120.30
14	L	54	ALA	CB-CA-C	16.51	134.87	110.10
1	X	2486	C	O5'-P-OP1	-16.31	91.02	105.70
1	X	747	A	C8-N9-C4	15.93	112.17	105.80
1	X	2815	C	C5-C6-N1	-15.67	113.17	121.00
1	X	1282	A	N1-C6-N6	14.72	127.43	118.60
1	X	1674	C	C6-N1-C2	14.58	126.13	120.30
1	X	1290	A	N7-C8-N9	13.97	120.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2565	C	C6-N1-C2	-13.92	114.73	120.30
1	X	2550	C	C6-N1-C2	-13.26	115.00	120.30
1	X	491	A	C8-N9-C4	13.16	111.06	105.80
1	X	2034	A	C8-N9-C4	-13.14	100.54	105.80
1	X	545	C	C6-N1-C2	13.09	125.53	120.30
1	X	841	G	C5-N7-C8	-12.85	97.88	104.30
1	X	1292	A	C8-N9-C4	12.70	110.88	105.80
1	X	579	G	C4-C5-N7	-12.46	105.82	110.80
1	X	982	C	C5-C6-N1	12.42	127.21	121.00
1	X	1670	G	N7-C8-N9	-12.17	107.01	113.10
1	X	2008	C	N3-C4-C5	-12.14	117.04	121.90
1	X	527	C	C6-N1-C2	-12.10	115.46	120.30
1	X	1991	C	C5-C4-N4	11.94	128.56	120.20
1	X	1991	C	N3-C4-N4	-11.90	109.67	118.00
1	X	1305	C	C6-N1-C2	11.86	125.04	120.30
1	X	2802	C	N1-C2-O2	-11.85	111.79	118.90
1	X	174	A	P-O3'-C3'	-11.76	105.59	119.70
1	X	1333	G	N3-C4-C5	11.73	134.47	128.60
1	X	1770	U	C5-C6-N1	-11.71	116.84	122.70
1	X	2371	A	C8-N9-C4	-11.71	101.11	105.80
1	X	850	C	N3-C4-C5	-11.63	117.25	121.90
1	X	1678	G	C5-C6-O6	11.57	135.54	128.60
1	X	37	C	C6-N1-C2	-11.52	115.69	120.30
1	X	1676	U	P-O3'-C3'	-11.50	105.90	119.70
1	X	2524	G	C8-N9-C4	-11.47	101.81	106.40
1	X	805	G	N1-C6-O6	-11.37	113.08	119.90
1	X	2039	G	N1-C6-O6	11.35	126.71	119.90
1	X	1771	A	C8-N9-C4	-11.35	101.26	105.80
1	X	2486	C	C6-N1-C2	-11.32	115.77	120.30
1	X	2008	C	C6-N1-C2	-11.31	115.78	120.30
1	X	1993	G	N1-C6-O6	11.30	126.68	119.90
1	X	2034	A	N9-C4-C5	11.30	110.32	105.80
1	X	1235	C	C6-N1-C2	11.21	124.78	120.30
1	X	496	C	C6-N1-C2	11.15	124.76	120.30
1	X	2807	U	C5-C6-N1	-11.14	117.13	122.70
1	X	1290	A	C5-N7-C8	-11.10	98.35	103.90
1	X	57	G	C8-N9-C4	-11.04	101.98	106.40
1	X	1255	A	N1-C6-N6	-11.02	111.99	118.60
1	X	2347	C	C6-N1-C2	11.01	124.70	120.30
1	X	1667	A	N1-C6-N6	11.00	125.20	118.60
1	X	761	G	C8-N9-C4	10.99	110.79	106.40
1	X	1665	C	C5-C6-N1	-10.98	115.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2229	G	N1-C6-O6	-10.96	113.32	119.90
1	X	1995	G	N1-C2-N2	-10.92	106.37	116.20
1	X	830	C	C6-N1-C2	10.90	124.66	120.30
1	X	2855	C	N3-C2-O2	10.90	129.53	121.90
1	X	1708	C	C6-N1-C2	10.82	124.63	120.30
1	X	1288	A	C8-N9-C4	-10.79	101.48	105.80
1	X	2825	A	C8-N9-C4	-10.75	101.50	105.80
1	X	579	G	C5-C6-O6	10.74	135.05	128.60
1	X	2655	C	C6-N1-C2	10.70	124.58	120.30
1	X	1702	C	C6-N1-C2	10.62	124.55	120.30
1	X	1773	C	C6-N1-C2	10.60	124.54	120.30
1	X	1991	C	C5-C6-N1	-10.56	115.72	121.00
1	X	2303	C	C6-N1-C2	10.56	124.53	120.30
1	X	1937	G	C8-N9-C4	10.54	110.62	106.40
1	X	2035	G	N1-C6-O6	-10.49	113.60	119.90
1	X	1333	G	N3-C4-N9	-10.47	119.72	126.00
1	X	2672	U	N3-C2-O2	-10.46	114.88	122.20
1	X	1670	G	C8-N9-C4	10.44	110.58	106.40
1	X	504	G	N1-C6-O6	10.43	126.16	119.90
1	X	1993	G	C2-N3-C4	-10.38	106.71	111.90
1	X	2811	G	C8-N9-C4	10.38	110.55	106.40
1	X	841	G	C4-C5-N7	10.31	114.92	110.80
1	X	806	A	N1-C6-N6	-10.31	112.42	118.60
1	X	1670	G	C5-N7-C8	10.24	109.42	104.30
1	X	481	A	N1-C6-N6	10.24	124.74	118.60
1	X	1009	C	C6-N1-C2	10.19	124.38	120.30
1	X	2540	A	C8-N9-C4	10.19	109.88	105.80
1	X	2229	G	C5-C6-O6	10.17	134.70	128.60
1	X	985	G	C8-N9-C4	-10.15	102.34	106.40
1	X	1674	C	C5-C6-N1	-10.13	115.94	121.00
1	X	985	G	C5-N7-C8	-10.12	99.24	104.30
1	X	1298	G	C8-N9-C4	10.12	110.45	106.40
1	X	520	C	N1-C2-O2	-10.11	112.83	118.90
1	X	982	C	O4'-C1'-N1	10.11	116.29	108.20
1	X	2034	A	C2-N3-C4	10.06	115.63	110.60
1	X	2523	G	N1-C6-O6	-10.03	113.88	119.90
1	X	522	G	N1-C6-O6	10.02	125.91	119.90
1	X	1201	G	C8-N9-C4	-10.02	102.39	106.40
1	X	1663	C	N1-C2-O2	9.99	124.89	118.90
1	X	1288	A	N7-C8-N9	9.99	118.79	113.80
1	X	1699	A	N1-C6-N6	9.97	124.58	118.60
1	X	985	G	N7-C8-N9	9.96	118.08	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1680	U	C5-C6-N1	-9.91	117.75	122.70
1	X	1242	A	C8-N9-C4	9.90	109.76	105.80
1	X	2634	G	C8-N9-C4	9.87	110.35	106.40
1	X	2486	C	C5'-C4'-O4'	9.85	120.92	109.10
1	X	1333	G	C2-N3-C4	-9.84	106.98	111.90
1	X	2056	C	C6-N1-C2	9.83	124.23	120.30
1	X	1535	C	C6-N1-C2	9.81	124.22	120.30
1	X	2815	C	C2-N3-C4	-9.78	115.01	119.90
1	X	2035	G	C5-C6-O6	9.77	134.46	128.60
1	X	309	G	C4-C5-N7	9.75	114.70	110.80
1	X	537	C	C5-C4-N4	9.73	127.01	120.20
1	X	1411	C	C6-N1-C2	9.71	124.19	120.30
1	X	2039	G	C6-C5-N7	-9.68	124.59	130.40
1	X	2524	G	C5-C6-O6	-9.67	122.80	128.60
1	X	1770	U	N3-C4-O4	-9.62	112.67	119.40
1	X	358	C	C6-N1-C2	-9.61	116.45	120.30
1	X	1995	G	N3-C2-N2	9.61	126.63	119.90
1	X	1721	G	C8-N9-C4	9.60	110.24	106.40
1	X	2815	C	N3-C4-C5	9.59	125.74	121.90
1	X	1166	A	C8-N9-C4	-9.55	101.98	105.80
1	X	2039	G	C4-C5-N7	9.55	114.62	110.80
1	X	2553	G	C8-N9-C4	-9.54	102.58	106.40
1	X	2014	A	C8-N9-C4	-9.54	101.98	105.80
1	X	2015	G	C5-N7-C8	-9.51	99.54	104.30
1	X	1944	C	C6-N1-C2	9.50	124.10	120.30
2	Y	20	A	C8-N9-C4	9.48	109.59	105.80
1	X	752	G	N9-C4-C5	9.48	109.19	105.40
1	X	581	A	C8-N9-C4	9.47	109.59	105.80
1	X	752	G	C8-N9-C4	-9.47	102.61	106.40
1	X	2782	G	C8-N9-C4	9.44	110.18	106.40
1	X	1666	G	C8-N9-C4	9.44	110.17	106.40
1	X	1631	C	C6-N1-C2	9.43	124.07	120.30
1	X	985	G	C4-C5-N7	9.39	114.56	110.80
1	X	527	C	N3-C4-C5	-9.37	118.15	121.90
1	X	15	G	C4-C5-N7	-9.36	107.06	110.80
1	X	2486	C	C4-C5-C6	-9.33	112.74	117.40
1	X	50	G	C8-N9-C4	9.33	110.13	106.40
1	X	594	G	N1-C6-O6	-9.30	114.32	119.90
1	X	742	G	C8-N9-C4	-9.30	102.68	106.40
1	X	2725	C	C6-N1-C2	9.28	124.01	120.30
1	X	2745	A	C5-N7-C8	-9.27	99.27	103.90
1	X	2371	A	N9-C4-C5	9.23	109.49	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	747	A	N7-C8-N9	-9.23	109.18	113.80
1	X	1773	C	N1-C2-O2	9.23	124.44	118.90
1	X	717	G	C8-N9-C4	9.22	110.09	106.40
1	X	1717	A	N9-C4-C5	9.21	109.49	105.80
1	X	1744	G	N1-C6-O6	-9.21	114.37	119.90
1	X	821	A	C8-N9-C4	9.20	109.48	105.80
1	X	1289	A	C3'-C2'-C1'	9.19	108.85	101.50
1	X	1158	A	C8-N9-C4	9.14	109.46	105.80
1	X	2807	U	N3-C4-O4	-9.14	113.00	119.40
1	X	538	A	C2-N3-C4	9.12	115.16	110.60
1	X	537	C	N3-C4-N4	-9.11	111.62	118.00
1	X	1779	C	N1-C2-O2	-9.08	113.45	118.90
1	X	479	G	N1-C6-O6	9.08	125.35	119.90
1	X	2247	A	N1-C6-N6	9.07	124.05	118.60
1	X	1678	G	C6-N1-C2	-9.05	119.67	125.10
1	X	2440	C	C5-C6-N1	-9.05	116.47	121.00
1	X	833	A	N1-C6-N6	9.00	124.00	118.60
1	X	1469	U	O4'-C1'-N1	8.99	115.39	108.20
1	X	2825	A	N9-C4-C5	8.98	109.39	105.80
1	X	1931	G	N1-C6-O6	8.97	125.28	119.90
1	X	522	G	C2-N3-C4	-8.96	107.42	111.90
1	X	1664	G	N1-C6-O6	8.96	125.28	119.90
1	X	31	C	N1-C2-O2	-8.95	113.53	118.90
1	X	1792	C	C6-N1-C2	8.95	123.88	120.30
1	X	2688	G	C8-N9-C4	8.93	109.97	106.40
1	X	1201	G	N9-C4-C5	8.92	108.97	105.40
1	X	1992	G	N1-C6-O6	-8.91	114.55	119.90
1	X	533	C	C6-N1-C2	8.91	123.86	120.30
1	X	491	A	N7-C8-N9	-8.90	109.35	113.80
1	X	465	C	C6-N1-C2	8.88	123.85	120.30
1	X	1466	C	C3'-C2'-C1'	8.88	108.60	101.50
1	X	479	G	C5-C6-O6	-8.86	123.28	128.60
1	X	2508	G	C5-C6-O6	-8.85	123.29	128.60
2	Y	101	A	N1-C6-N6	-8.85	113.29	118.60
1	X	2024	U	C6-N1-C2	8.84	126.30	121.00
1	X	2540	A	N1-C2-N3	-8.84	124.88	129.30
1	X	236	C	C6-N1-C2	-8.84	116.77	120.30
1	X	841	G	N7-C8-N9	8.83	117.52	113.10
1	X	1282	A	C5-C6-N6	-8.82	116.64	123.70
1	X	492	G	C2-N3-C4	-8.81	107.49	111.90
1	X	806	A	C5-C6-N6	8.79	130.73	123.70
1	X	1678	G	C5-C6-N1	8.79	115.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2468	G	N7-C8-N9	-8.78	108.71	113.10
1	X	1471	G	C8-N9-C4	8.76	109.91	106.40
1	X	2459	C	N1-C2-O2	-8.75	113.65	118.90
1	X	1467	U	O4'-C1'-N1	-8.75	101.20	108.20
1	X	2697	G	N3-C2-N2	8.75	126.02	119.90
1	X	357	A	N1-C6-N6	8.73	123.84	118.60
1	X	1332	G	C8-N9-C4	8.72	109.89	106.40
1	X	1998	A	N1-C6-N6	-8.72	113.37	118.60
1	X	1242	A	C5-C6-N1	8.70	122.05	117.70
1	X	1771	A	N9-C4-C5	8.69	109.28	105.80
1	X	2003	A	C8-N9-C4	-8.69	102.32	105.80
1	X	2431	C	N3-C4-C5	8.66	125.37	121.90
1	X	1288	A	C5-N7-C8	-8.66	99.57	103.90
1	X	1135	C	N1-C2-O2	-8.65	113.71	118.90
1	X	2520	A	N1-C6-N6	-8.65	113.41	118.60
1	X	1016	C	C6-N1-C2	-8.64	116.84	120.30
1	X	1149	G	N1-C6-O6	-8.64	114.72	119.90
1	X	1278	A	C4-C5-C6	8.64	121.32	117.00
1	X	829	C	C2-N3-C4	-8.63	115.58	119.90
1	X	1699	A	C2-N3-C4	-8.63	106.28	110.60
1	X	1717	A	N1-C6-N6	-8.61	113.43	118.60
1	X	2042	A	N1-C6-N6	8.61	123.77	118.60
1	X	2488	G	C5-C6-N1	8.60	115.80	111.50
1	X	2674	C	N1-C2-O2	-8.59	113.75	118.90
1	X	2655	C	N3-C4-C5	8.58	125.33	121.90
1	X	1770	U	C6-N1-C2	8.58	126.15	121.00
1	X	1246	G	N1-C6-O6	-8.57	114.75	119.90
1	X	2555	G	C8-N9-C4	8.57	109.83	106.40
1	X	2856	U	N1-C2-N3	8.55	120.03	114.90
1	X	2627	G	N3-C2-N2	-8.55	113.92	119.90
1	X	2347	C	N1-C2-O2	-8.54	113.77	118.90
1	X	2508	G	C4-C5-N7	8.51	114.20	110.80
1	X	2576	G	N1-C6-O6	8.51	125.01	119.90
1	X	1251	G	C8-N9-C4	-8.50	103.00	106.40
1	X	2039	G	C2-N3-C4	-8.50	107.65	111.90
1	X	1467	U	C5'-C4'-O4'	-8.50	98.90	109.10
1	X	937	C	C6-N1-C2	8.47	123.69	120.30
1	X	1333	G	C5-N7-C8	-8.47	100.06	104.30
1	X	347	C	C6-N1-C2	8.46	123.69	120.30
1	X	596	C	C5-C6-N1	-8.46	116.77	121.00
1	X	1665	C	C6-N1-C2	8.45	123.68	120.30
1	X	1664	G	C5-C6-O6	-8.45	123.53	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1994	U	N3-C2-O2	8.45	128.11	122.20
1	X	1617	G	N1-C6-O6	8.44	124.97	119.90
1	X	2496	C	C6-N1-C2	8.43	123.67	120.30
1	X	2515	G	N1-C6-O6	-8.43	114.84	119.90
1	X	31	C	N3-C2-O2	8.42	127.80	121.90
1	X	2393	G	N1-C6-O6	8.41	124.95	119.90
1	X	2565	C	C5-C6-N1	8.40	125.20	121.00
1	X	2751	C	C6-N1-C2	8.39	123.66	120.30
1	X	409	G	C8-N9-C4	-8.36	103.05	106.40
1	X	2023	C	C6-N1-C2	8.36	123.64	120.30
1	X	1246	G	N9-C4-C5	8.35	108.74	105.40
1	X	508	G	N1-C6-O6	8.34	124.91	119.90
1	X	2519	C	C6-N1-C2	-8.34	116.96	120.30
1	X	2434	G	N1-C6-O6	-8.34	114.90	119.90
1	X	1678	G	N1-C2-N2	-8.33	108.70	116.20
1	X	1778	U	N3-C4-O4	-8.33	113.57	119.40
1	X	1721	G	N9-C4-C5	-8.32	102.07	105.40
1	X	597	U	C5-C6-N1	-8.32	118.54	122.70
1	X	1673	C	N3-C2-O2	8.32	127.72	121.90
1	X	870	C	N1-C2-O2	-8.31	113.91	118.90
1	X	2440	C	C6-N1-C2	8.31	123.62	120.30
1	X	761	G	N9-C4-C5	-8.30	102.08	105.40
1	X	2397	A	C8-N9-C4	8.30	109.12	105.80
1	X	1725	C	C6-N1-C2	-8.25	117.00	120.30
1	X	2035	G	C4-C5-N7	-8.25	107.50	110.80
1	X	2218	G	N1-C6-O6	8.24	124.85	119.90
1	X	2408	G	N9-C4-C5	8.24	108.70	105.40
1	X	1722	G	C8-N9-C4	8.23	109.69	106.40
1	X	1991	C	C4-C5-C6	8.23	121.52	117.40
1	X	864	C	C6-N1-C2	-8.22	117.01	120.30
1	X	2569	A	C8-N9-C4	8.20	109.08	105.80
1	X	2616	U	N3-C4-O4	8.20	125.14	119.40
1	X	2431	C	C6-N1-C2	8.20	123.58	120.30
1	X	2754	C	N3-C4-C5	-8.19	118.62	121.90
1	X	323	G	C8-N9-C4	-8.18	103.13	106.40
1	X	837	U	C5-C6-N1	-8.18	118.61	122.70
1	X	2856	U	N1-C2-O2	-8.18	117.07	122.80
1	X	1966	C	C6-N1-C2	8.18	123.57	120.30
2	Y	88	C	N1-C2-O2	-8.18	114.00	118.90
1	X	2799	C	N1-C2-O2	-8.17	114.00	118.90
1	X	2853	U	C6-N1-C2	8.16	125.90	121.00
1	X	545	C	C5-C6-N1	-8.15	116.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1669	A	O4'-C1'-N9	-8.13	101.69	108.20
1	X	2754	C	C6-N1-C2	-8.13	117.05	120.30
1	X	492	G	C8-N9-C4	8.11	109.64	106.40
1	X	2218	G	C6-C5-N7	-8.11	125.53	130.40
1	X	1225	G	C8-N9-C4	8.11	109.64	106.40
1	X	2669	C	N1-C2-O2	8.10	123.76	118.90
1	X	2408	G	C8-N9-C4	-8.10	103.16	106.40
1	X	1646	G	N1-C6-O6	8.09	124.75	119.90
1	X	479	G	N9-C4-C5	-8.08	102.17	105.40
1	X	2356	A	N1-C6-N6	8.08	123.45	118.60
1	X	2015	G	C4-C5-N7	8.08	114.03	110.80
1	X	1927	U	N3-C2-O2	-8.08	116.55	122.20
1	X	521	U	C6-N1-C2	8.06	125.84	121.00
1	X	2495	G	N3-C2-N2	8.05	125.54	119.90
1	X	2694	G	N3-C4-C5	-8.05	124.57	128.60
1	X	2827	G	N3-C2-N2	8.04	125.53	119.90
1	X	37	C	C5-C6-N1	8.04	125.02	121.00
1	X	456	C	C6-N1-C2	-8.04	117.08	120.30
1	X	2009	U	C5-C6-N1	8.03	126.71	122.70
1	X	2347	C	N3-C2-O2	8.02	127.51	121.90
1	X	2836	U	C5-C6-N1	8.02	126.71	122.70
1	X	1235	C	N3-C4-C5	8.01	125.11	121.90
1	X	2807	U	C6-N1-C2	8.01	125.81	121.00
1	X	569	C	N3-C4-C5	8.00	125.10	121.90
1	X	2745	A	C4-C5-N7	8.00	114.70	110.70
1	X	1942	G	C8-N9-C4	8.00	109.60	106.40
1	X	829	C	N3-C4-C5	8.00	125.10	121.90
1	X	1993	G	C5-C6-N1	-7.99	107.51	111.50
1	X	2802	C	N3-C2-O2	7.98	127.49	121.90
1	X	2435	C	C6-N1-C2	7.98	123.49	120.30
1	X	15	G	C5-C6-O6	7.97	133.38	128.60
1	X	1278	A	N1-C6-N6	7.97	123.38	118.60
1	X	2696	A	N7-C8-N9	-7.96	109.82	113.80
1	X	2468	G	C5-N7-C8	7.95	108.28	104.30
1	X	533	C	C5-C6-N1	-7.95	117.03	121.00
1	X	1678	G	N3-C4-C5	-7.94	124.63	128.60
1	X	29	U	C5-C4-O4	-7.94	121.14	125.90
1	X	850	C	C6-N1-C2	-7.94	117.13	120.30
1	X	1255	A	N9-C4-C5	7.93	108.97	105.80
1	X	863	C	C6-N1-C2	-7.92	117.13	120.30
1	X	555	U	C5-C6-N1	-7.92	118.74	122.70
1	X	2619	G	C5-N7-C8	-7.92	100.34	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1699	A	C5-C6-N1	-7.91	113.74	117.70
1	X	1965	U	N3-C2-O2	-7.90	116.67	122.20
1	X	1104	G	C8-N9-C4	-7.89	103.24	106.40
1	X	1656	U	C5-C6-N1	-7.88	118.76	122.70
1	X	1246	G	C4-C5-N7	-7.87	107.65	110.80
1	X	886	A	C8-N9-C4	-7.85	102.66	105.80
1	X	1242	A	C5-C6-N6	-7.83	117.44	123.70
1	X	594	G	N9-C4-C5	7.82	108.53	105.40
1	X	1242	A	N9-C4-C5	-7.82	102.67	105.80
1	X	34	U	C5-C6-N1	-7.81	118.79	122.70
1	X	1927	U	N1-C2-N3	7.81	119.58	114.90
1	X	1136	G	N1-C6-O6	-7.80	115.22	119.90
1	X	2495	G	N3-C4-C5	-7.80	124.70	128.60
1	X	816	U	C6-N1-C2	-7.80	116.32	121.00
1	X	1038	U	N3-C2-O2	-7.80	116.74	122.20
1	X	508	G	N3-C4-C5	7.79	132.50	128.60
1	X	1379	A	C8-N9-C4	7.78	108.91	105.80
1	X	2311	U	N3-C2-O2	-7.77	116.76	122.20
1	X	2827	G	N3-C4-N9	7.77	130.66	126.00
1	X	2687	G	C8-N9-C4	7.77	109.51	106.40
1	X	981	C	C4'-C3'-C2'	-7.76	94.83	102.60
1	X	1467	U	C5'-C4'-C3'	7.76	128.41	116.00
1	X	1665	C	C4-C5-C6	7.76	121.28	117.40
1	X	2002	A	C8-N9-C4	7.75	108.90	105.80
1	X	2797	G	N3-C4-C5	-7.75	124.73	128.60
1	X	1210	C	N1-C2-O2	-7.74	114.25	118.90
1	X	1041	G	N3-C4-N9	-7.73	121.36	126.00
1	X	1678	G	C4-C5-N7	-7.71	107.71	110.80
1	X	2393	G	C5-C6-O6	-7.71	123.97	128.60
1	X	1290	A	C8-N9-C4	-7.70	102.72	105.80
1	X	583	C	C5-C6-N1	7.70	124.85	121.00
1	X	2540	A	N7-C8-N9	-7.69	109.95	113.80
1	X	1292	A	N7-C8-N9	-7.68	109.96	113.80
1	X	555	U	C2-N3-C4	-7.67	122.40	127.00
1	X	1937	G	N7-C8-N9	-7.66	109.27	113.10
1	X	518	A	C8-N9-C4	-7.66	102.74	105.80
1	X	1278	A	C6-C5-N7	-7.66	126.94	132.30
1	X	1472	C	C6-N1-C2	7.65	123.36	120.30
1	X	1744	G	C5-C6-O6	7.65	133.19	128.60
1	X	2434	G	C8-N9-C4	-7.65	103.34	106.40
1	X	2243	C	N3-C4-C5	-7.64	118.85	121.90
1	X	2832	G	N1-C6-O6	7.64	124.48	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1813	A	C8-N9-C4	-7.63	102.75	105.80
1	X	2560	G	C8-N9-C4	-7.63	103.35	106.40
1	X	2466	G	C8-N9-C4	-7.63	103.35	106.40
1	X	2523	G	C5-C6-O6	7.63	133.18	128.60
1	X	746	G	C8-N9-C1'	-7.62	117.10	127.00
1	X	1617	G	C5-C6-O6	-7.62	124.03	128.60
1	X	2382	C	P-O3'-C3'	-7.61	110.57	119.70
1	X	570	G	C8-N9-C4	7.61	109.44	106.40
1	X	2007	G	C4-C5-N7	-7.61	107.76	110.80
1	X	1286	U	C6-N1-C2	-7.59	116.44	121.00
1	X	2431	C	N1-C2-O2	-7.58	114.35	118.90
1	X	2486	C	O4'-C1'-N1	7.57	114.26	108.20
1	X	2748	C	N1-C2-O2	-7.57	114.36	118.90
1	X	1647	U	N1-C2-N3	7.57	119.44	114.90
1	X	31	C	C6-N1-C2	7.54	123.32	120.30
1	X	50	G	N9-C4-C5	-7.54	102.39	105.40
1	X	572	G	C8-N9-C4	-7.54	103.39	106.40
1	X	583	C	N3-C4-N4	7.53	123.27	118.00
1	X	2753	C	C6-N1-C2	-7.53	117.29	120.30
1	X	1308	C	C6-N1-C2	-7.53	117.29	120.30
1	X	1481	U	N1-C2-O2	-7.52	117.53	122.80
1	X	829	C	C6-N1-C2	7.52	123.31	120.30
1	X	1305	C	C5-C6-N1	-7.51	117.24	121.00
1	X	1278	A	C8-N9-C4	-7.51	102.80	105.80
1	X	2446	C	C6-N1-C2	7.51	123.30	120.30
1	X	471	A	C8-N9-C4	7.50	108.80	105.80
1	X	591	G	C8-N9-C4	7.50	109.40	106.40
1	X	2524	G	C6-C5-N7	-7.50	125.90	130.40
1	X	982	C	C4-C5-C6	-7.50	113.65	117.40
1	X	2855	C	N1-C2-O2	-7.50	114.40	118.90
1	X	2848	A	C6-N1-C2	-7.49	114.11	118.60
1	X	2560	G	N7-C8-N9	7.48	116.84	113.10
1	X	156	G	C8-N9-C4	7.47	109.39	106.40
1	X	175	C	C6-N1-C2	7.47	123.29	120.30
1	X	1172	U	N1-C2-O2	-7.46	117.57	122.80
1	X	1779	C	N3-C2-O2	7.46	127.12	121.90
1	X	2619	G	C4-C5-N7	7.45	113.78	110.80
1	X	1404	C	C6-N1-C2	7.45	123.28	120.30
1	X	2007	G	C5-N7-C8	7.44	108.02	104.30
1	X	805	G	C5-C6-O6	7.43	133.06	128.60
1	X	1449	C	C6-N1-C2	-7.43	117.33	120.30
1	X	1154	A	C2-N3-C4	7.42	114.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2694	G	C8-N9-C4	-7.42	103.43	106.40
1	X	1631	C	C5-C6-N1	-7.41	117.29	121.00
1	X	597	U	N1-C2-O2	-7.41	117.61	122.80
1	X	715	U	N1-C2-N3	7.41	119.35	114.90
1	X	2708	U	P-O3'-C3'	-7.41	110.81	119.70
1	X	1928	G	N1-C6-O6	-7.41	115.46	119.90
1	X	508	G	C8-N9-C4	7.40	109.36	106.40
1	X	1994	U	N1-C2-O2	-7.40	117.62	122.80
1	X	1289	A	C4'-C3'-C2'	-7.40	95.20	102.60
1	X	481	A	C5-C6-N6	-7.39	117.78	123.70
1	X	2259	G	C2-N3-C4	-7.39	108.20	111.90
1	X	309	G	C5-C6-O6	-7.38	124.17	128.60
1	X	1735	G	C8-N9-C4	-7.38	103.45	106.40
1	X	2798	A	C2-N3-C4	-7.37	106.91	110.60
1	X	1941	C	C6-N1-C2	7.37	123.25	120.30
1	X	2559	U	C6-N1-C2	7.36	125.42	121.00
1	X	2698	G	N1-C6-O6	7.36	124.32	119.90
1	X	1933	G	C8-N9-C4	-7.36	103.46	106.40
1	X	2495	G	N1-C2-N2	-7.35	109.59	116.20
1	X	1470	G	OP1-P-OP2	-7.34	108.59	119.60
1	X	2627	G	C2-N3-C4	-7.34	108.23	111.90
1	X	1718	A	C8-N9-C4	-7.33	102.87	105.80
1	X	755	C	C4-C5-C6	7.33	121.07	117.40
1	X	2617	G	N3-C4-N9	7.33	130.40	126.00
1	X	2587	G	C8-N9-C4	-7.33	103.47	106.40
1	X	2547	C	C6-N1-C2	7.31	123.23	120.30
1	X	2495	G	N3-C4-N9	7.31	130.39	126.00
1	X	2617	G	C8-N9-C4	7.31	109.32	106.40
1	X	2652	G	C8-N9-C4	7.31	109.32	106.40
1	X	2034	A	N1-C6-N6	-7.31	114.22	118.60
1	X	2693	U	N1-C2-N3	7.29	119.28	114.90
1	X	661	C	C6-N1-C2	-7.29	117.38	120.30
1	X	1766	U	C5-C6-N1	-7.28	119.06	122.70
1	X	1778	U	C2-N3-C4	-7.28	122.63	127.00
1	X	1578	U	C6-N1-C2	7.28	125.37	121.00
1	X	2347	C	C2-N1-C1'	-7.28	110.79	118.80
1	X	2703	C	N3-C4-C5	-7.28	118.99	121.90
1	X	538	A	C5-C6-N1	7.28	121.34	117.70
1	X	2663	U	P-O3'-C3'	7.27	128.43	119.70
1	X	812	G	C8-N9-C4	-7.27	103.49	106.40
1	X	187	U	N1-C2-O2	-7.26	117.72	122.80
1	X	2827	G	N3-C4-C5	-7.26	124.97	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2617	G	C5-N7-C8	7.26	107.93	104.30
1	X	830	C	C5-C6-N1	-7.25	117.38	121.00
1	X	2468	G	N1-C6-O6	-7.25	115.55	119.90
1	X	1272	G	N1-C6-O6	-7.23	115.56	119.90
1	X	1773	C	C6-N1-C1'	-7.23	112.13	120.80
1	X	70	A	C8-N9-C4	-7.23	102.91	105.80
1	X	1009	C	C5-C6-N1	-7.22	117.39	121.00
1	X	1285	A	C2-N3-C4	-7.22	106.99	110.60
1	X	1644	G	C8-N9-C4	7.21	109.28	106.40
1	X	2355	A	C8-N9-C4	7.21	108.68	105.80
1	X	1053	G	P-O3'-C3'	7.21	128.35	119.70
1	X	2474	G	N1-C6-O6	-7.21	115.57	119.90
1	X	2488	G	C5-C6-O6	-7.21	124.28	128.60
1	X	2567	G	C8-N9-C4	-7.21	103.52	106.40
1	X	1758	C	C6-N1-C2	-7.20	117.42	120.30
1	X	2856	U	N3-C4-C5	-7.20	110.28	114.60
1	X	1240	G	C8-N9-C4	7.20	109.28	106.40
1	X	1675	C	N1-C2-O2	-7.20	114.58	118.90
1	X	2807	U	N1-C2-O2	7.19	127.83	122.80
1	X	1667	A	C5-C6-N6	-7.19	117.95	123.70
1	X	1773	C	N3-C4-C5	7.18	124.77	121.90
1	X	15	G	N9-C4-C5	7.18	108.27	105.40
1	X	2838	U	C5-C6-N1	-7.17	119.11	122.70
1	X	1778	U	N1-C2-O2	-7.17	117.78	122.80
1	X	2559	U	N3-C2-O2	7.17	127.22	122.20
1	X	955	G	OP2-P-O3'	7.16	120.96	105.20
1	X	2211	U	C6-N1-C2	7.16	125.30	121.00
1	X	2015	G	N7-C8-N9	7.16	116.68	113.10
1	X	508	G	C5-C6-O6	-7.15	124.31	128.60
1	X	2437	G	N9-C4-C5	-7.15	102.54	105.40
1	X	2019	C	N1-C2-O2	-7.15	114.61	118.90
1	X	2508	G	N1-C6-O6	7.15	124.19	119.90
1	X	1333	G	C4-C5-N7	7.15	113.66	110.80
1	X	1469	U	N1-C2-O2	7.14	127.80	122.80
1	X	1722	G	N9-C4-C5	-7.14	102.54	105.40
1	X	768	U	C5-C4-O4	-7.14	121.62	125.90
1	X	175	C	N3-C4-C5	7.14	124.75	121.90
1	X	562	G	C8-N9-C4	7.13	109.25	106.40
1	X	1645	U	N3-C2-O2	7.12	127.19	122.20
1	X	2566	A	N1-C2-N3	7.12	132.86	129.30
1	X	1472	C	C5-C4-N4	-7.12	115.21	120.20
1	X	1466	C	O4'-C1'-N1	7.12	113.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	547	U	N1-C2-O2	-7.12	117.82	122.80
1	X	2014	A	N9-C4-C5	7.12	108.65	105.80
1	X	1741	G	C8-N9-C4	7.11	109.25	106.40
1	X	2699	G	N1-C6-O6	7.11	124.17	119.90
1	X	393	U	N3-C4-O4	7.10	124.37	119.40
1	X	598	U	N1-C2-O2	-7.09	117.84	122.80
1	X	2437	G	C4-C5-N7	7.08	113.63	110.80
1	X	2000	U	N1-C2-O2	-7.08	117.84	122.80
1	X	2811	G	N9-C4-C5	-7.08	102.57	105.40
1	X	670	U	C6-N1-C2	-7.08	116.75	121.00
1	X	479	G	C8-N9-C4	7.08	109.23	106.40
1	X	743	A	C2-N3-C4	-7.07	107.06	110.60
1	X	530	G	C8-N9-C4	7.07	109.23	106.40
1	X	693	A	C2-N3-C4	-7.06	107.07	110.60
1	X	1209	G	N3-C2-N2	-7.06	114.96	119.90
1	X	2553	G	N9-C4-C5	7.06	108.22	105.40
1	X	1287	A	C6-N1-C2	-7.06	114.37	118.60
1	X	745	C	N3-C2-O2	-7.05	116.96	121.90
1	X	970	A	N1-C6-N6	7.05	122.83	118.60
1	X	1300	A	C8-N9-C4	7.05	108.62	105.80
1	X	2496	C	C5-C6-N1	-7.05	117.48	121.00
1	X	2559	U	N1-C2-N3	-7.05	110.67	114.90
1	X	755	C	N3-C4-C5	-7.04	119.08	121.90
1	X	309	G	C5-N7-C8	-7.04	100.78	104.30
1	X	2657	G	C8-N9-C4	-7.04	103.59	106.40
1	X	1698	C	N1-C2-O2	-7.03	114.68	118.90
1	X	2226	A	C2-N3-C4	-7.03	107.08	110.60
1	X	57	G	N7-C8-N9	7.03	116.61	113.10
1	X	1332	G	C5-C6-O6	-7.03	124.38	128.60
1	X	2547	C	N3-C4-C5	7.03	124.71	121.90
1	X	2677	U	N1-C2-O2	-7.02	117.89	122.80
1	X	2243	C	C6-N1-C2	-7.01	117.49	120.30
1	X	165	G	C8-N9-C4	7.01	109.20	106.40
1	X	1771	A	N1-C6-N6	-7.01	114.39	118.60
1	X	494	A	C8-N9-C4	7.01	108.60	105.80
1	X	761	G	N3-C4-N9	7.01	130.21	126.00
1	X	1287	A	N1-C6-N6	-7.01	114.39	118.60
1	X	1032	A	C8-N9-C4	-7.00	103.00	105.80
1	X	9	U	N3-C2-O2	-7.00	117.30	122.20
1	X	21	A	C2-N3-C4	-7.00	107.10	110.60
1	X	1316	G	N9-C4-C5	7.00	108.20	105.40
1	X	2431	C	N3-C2-O2	7.00	126.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2457	A	N1-C6-N6	-6.99	114.41	118.60
1	X	1270	C	N1-C2-O2	-6.99	114.71	118.90
1	X	1917	C	C6-N1-C2	-6.98	117.51	120.30
1	X	773	G	C5-C6-N1	-6.98	108.01	111.50
1	X	1160	C	C6-N1-C2	-6.98	117.51	120.30
1	X	2260	C	N1-C2-O2	-6.98	114.71	118.90
1	X	2697	G	C2-N3-C4	6.97	115.39	111.90
1	X	18	U	C6-N1-C2	-6.97	116.82	121.00
1	X	1404	C	C5-C6-N1	-6.97	117.52	121.00
1	X	1985	G	C3'-C2'-C1'	-6.96	95.93	101.50
1	X	661	C	N3-C2-O2	-6.96	117.03	121.90
1	X	1272	G	C5-C6-O6	6.96	132.77	128.60
1	X	1770	U	C2-N3-C4	-6.96	122.83	127.00
1	X	2274	C	C6-N1-C2	6.95	123.08	120.30
1	X	1298	G	N7-C8-N9	-6.95	109.62	113.10
1	X	2025	A	C5-C6-N6	-6.95	118.14	123.70
1	X	2247	A	C5-C6-N6	-6.95	118.14	123.70
1	X	850	C	C5-C4-N4	6.95	125.06	120.20
1	X	1698	C	C6-N1-C2	6.94	123.08	120.30
1	X	465	C	N1-C2-O2	6.94	123.06	118.90
1	X	972	C	C6-N1-C2	-6.94	117.52	120.30
1	X	2652	G	N3-C4-C5	6.94	132.07	128.60
1	X	1818	G	N9-C4-C5	-6.94	102.62	105.40
1	X	2409	A	P-O3'-C3'	6.94	128.03	119.70
1	X	1053	G	O4'-C1'-N9	6.94	113.75	108.20
1	X	2559	U	C5-C4-O4	-6.93	121.74	125.90
1	X	579	G	N1-C6-O6	-6.93	115.74	119.90
1	X	691	C	C5-C6-N1	-6.93	117.53	121.00
1	X	1028	G	C8-N9-C4	6.93	109.17	106.40
1	X	1149	G	C5-C6-O6	6.93	132.76	128.60
1	X	1235	C	C5-C6-N1	-6.93	117.54	121.00
1	X	2498	U	N1-C2-O2	-6.93	117.95	122.80
1	X	1678	G	N3-C2-N2	6.92	124.75	119.90
1	X	2640	G	C5-C6-O6	-6.92	124.44	128.60
1	X	443	A	C8-N9-C4	6.92	108.57	105.80
1	X	1419	G	C8-N9-C4	6.92	109.17	106.40
1	X	2000	U	N3-C2-O2	6.92	127.05	122.20
1	X	1708	C	N3-C4-C5	6.92	124.67	121.90
1	X	2375	G	C8-N9-C4	6.91	109.17	106.40
1	X	2515	G	N3-C4-C5	-6.91	125.14	128.60
1	X	753	U	N1-C2-O2	-6.91	117.96	122.80
1	X	2660	C	C6-N1-C2	6.91	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1240	G	N9-C4-C5	-6.91	102.64	105.40
1	X	504	G	C4-C5-N7	6.91	113.56	110.80
1	X	1292	A	N1-C6-N6	-6.91	114.46	118.60
1	X	850	C	N1-C2-O2	-6.90	114.76	118.90
1	X	1343	C	N3-C4-C5	6.90	124.66	121.90
1	X	2434	G	N9-C4-C5	6.90	108.16	105.40
1	X	2818	G	N1-C6-O6	6.90	124.04	119.90
1	X	579	G	C5-N7-C8	6.89	107.75	104.30
1	X	50	G	N3-C4-C5	6.88	132.04	128.60
1	X	2034	A	N3-C4-C5	-6.88	121.98	126.80
1	X	1708	C	C5-C6-N1	-6.88	117.56	121.00
1	X	2617	G	N7-C8-N9	-6.88	109.66	113.10
1	X	491	A	N9-C4-C5	-6.88	103.05	105.80
1	X	2222	U	C5-C6-N1	-6.88	119.26	122.70
1	X	520	C	C6-N1-C2	-6.87	117.55	120.30
1	X	736	G	C8-N9-C4	6.87	109.15	106.40
1	X	1778	U	N3-C4-C5	6.87	118.72	114.60
1	X	2230	G	C4-C5-N7	6.87	113.55	110.80
1	X	2024	U	C5-C6-N1	-6.87	119.27	122.70
1	X	2038	C	C6-N1-C2	6.87	123.05	120.30
1	X	2267	A	C2-N3-C4	6.87	114.03	110.60
1	X	2848	A	N1-C2-N3	6.86	132.73	129.30
1	X	2230	G	C5-C6-O6	-6.85	124.49	128.60
1	X	190	A	C8-N9-C4	6.85	108.54	105.80
1	X	752	G	C4-C5-N7	-6.85	108.06	110.80
1	X	2748	C	N3-C2-O2	6.84	126.69	121.90
1	X	11	G	N1-C6-O6	6.83	124.00	119.90
1	X	1228	G	N9-C4-C5	6.83	108.13	105.40
1	X	1540	C	C6-N1-C2	-6.83	117.57	120.30
1	X	2495	G	C5-C6-N1	6.83	114.91	111.50
1	X	2745	A	C5-C6-N6	-6.83	118.24	123.70
1	X	1481	U	N3-C2-O2	6.83	126.98	122.20
1	X	806	A	C4-C5-N7	-6.83	107.29	110.70
1	X	2633	A	C5-C6-N1	6.83	121.11	117.70
1	X	1636	G	C8-N9-C4	6.82	109.13	106.40
1	X	1408	A	C8-N9-C4	-6.82	103.07	105.80
1	X	2704	U	N3-C2-O2	-6.82	117.43	122.20
1	X	423	G	C8-N9-C4	6.82	109.13	106.40
1	X	2425	G	N3-C2-N2	-6.81	115.13	119.90
1	X	2399	C	C6-N1-C2	6.81	123.03	120.30
1	X	322	A	C8-N9-C4	6.81	108.52	105.80
1	X	2619	G	N7-C8-N9	6.81	116.50	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1951	G	C8-N9-C4	-6.80	103.68	106.40
1	X	1982	C	C2-N3-C4	-6.80	116.50	119.90
1	X	1006	C	N1-C2-O2	6.79	122.98	118.90
1	X	1242	A	C4-C5-C6	-6.79	113.60	117.00
1	X	697	G	N3-C2-N2	-6.79	115.15	119.90
1	X	2451	G	C5-C6-N1	6.79	114.89	111.50
1	X	742	G	N7-C8-N9	6.79	116.49	113.10
1	X	2007	G	C5-C6-O6	6.78	132.67	128.60
1	X	541	C	C4-C5-C6	6.78	120.79	117.40
1	X	2522	G	C8-N9-C4	-6.78	103.69	106.40
1	X	1821	A	N1-C6-N6	6.78	122.67	118.60
1	X	797	A	C8-N9-C4	6.76	108.51	105.80
1	X	2634	G	N9-C4-C5	-6.76	102.69	105.40
1	X	549	G	C4-C5-N7	-6.76	108.09	110.80
1	X	1236	G	C4-C5-N7	6.76	113.50	110.80
1	X	1985	G	P-O3'-C3'	6.76	127.81	119.70
1	X	2009	U	C6-N1-C2	-6.76	116.94	121.00
1	X	2515	G	C5-C6-O6	6.76	132.66	128.60
1	X	2565	C	N3-C4-C5	-6.76	119.19	121.90
1	X	2687	G	N7-C8-N9	-6.76	109.72	113.10
1	X	2547	C	C2-N3-C4	-6.76	116.52	119.90
1	X	1166	A	C2-N3-C4	6.76	113.98	110.60
1	X	1253	C	C6-N1-C2	-6.75	117.60	120.30
1	X	2751	C	N3-C4-C5	6.75	124.60	121.90
1	X	1718	A	N9-C4-C5	6.75	108.50	105.80
1	X	2818	G	C5-C6-O6	-6.75	124.55	128.60
1	X	522	G	N3-C4-C5	6.74	131.97	128.60
1	X	1965	U	N1-C2-N3	6.74	118.95	114.90
1	X	2063	A	C8-N9-C4	-6.74	103.10	105.80
2	Y	101	A	N9-C4-C5	6.74	108.50	105.80
1	X	492	G	N3-C4-C5	6.74	131.97	128.60
1	X	1748	U	C5-C4-O4	-6.74	121.86	125.90
1	X	834	A	C4'-C3'-C2'	-6.73	95.87	102.60
1	X	524	A	C6-N1-C2	-6.73	114.56	118.60
1	X	2398	U	N3-C4-C5	-6.73	110.56	114.60
1	X	2266	A	C8-N9-C4	6.72	108.49	105.80
1	X	1993	G	N3-C2-N2	-6.72	115.19	119.90
1	X	2522	G	N9-C4-C5	6.72	108.09	105.40
1	X	2540	A	C4-C5-C6	-6.72	113.64	117.00
1	X	1359	G	N1-C6-O6	-6.72	115.87	119.90
1	X	2764	U	N3-C4-O4	-6.72	114.70	119.40
1	X	2003	A	N7-C8-N9	6.72	117.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	236	C	N3-C2-O2	-6.71	117.20	121.90
1	X	1703	C	C6-N1-C2	6.71	122.98	120.30
1	X	1931	G	C5-C6-O6	-6.71	124.58	128.60
1	X	661	C	N1-C2-O2	6.71	122.92	118.90
1	X	816	U	N3-C2-O2	-6.71	117.50	122.20
1	X	319	G	N3-C4-C5	6.71	131.95	128.60
1	X	82	G	N1-C6-O6	-6.70	115.88	119.90
1	X	137	A	C8-N9-C4	-6.70	103.12	105.80
1	X	752	G	C5-C6-N1	-6.70	108.15	111.50
1	X	2691	C	N3-C2-O2	6.69	126.58	121.90
1	X	323	G	N3-C4-C5	-6.69	125.25	128.60
1	X	480	G	C8-N9-C4	-6.69	103.72	106.40
1	X	1818	G	C8-N9-C4	6.69	109.08	106.40
1	X	2205	C	C6-N1-C2	6.69	122.97	120.30
1	X	991	A	N1-C6-N6	6.68	122.61	118.60
1	X	2008	C	C5-C6-N1	6.68	124.34	121.00
1	X	2815	C	C2-N1-C1'	-6.68	111.45	118.80
1	X	67	G	C4-C5-N7	6.68	113.47	110.80
1	X	1221	C	C6-N1-C2	-6.68	117.63	120.30
1	X	2832	G	C4-C5-N7	6.68	113.47	110.80
1	X	2065	A	C8-N9-C4	-6.67	103.13	105.80
1	X	1635	G	N1-C6-O6	6.67	123.90	119.90
1	X	2548	G	C5-N7-C8	6.67	107.63	104.30
1	X	1912	G	C8-N9-C4	-6.66	103.73	106.40
1	X	2555	G	N3-C4-C5	6.66	131.93	128.60
1	X	474	G	C8-N9-C4	6.66	109.06	106.40
1	X	541	C	C5-C6-N1	-6.66	117.67	121.00
1	X	591	G	N7-C8-N9	-6.65	109.77	113.10
1	X	1328	C	C6-N1-C2	-6.65	117.64	120.30
1	X	2608	A	C8-N9-C4	-6.65	103.14	105.80
1	X	2855	C	C5-C4-N4	-6.65	115.55	120.20
1	X	2490	U	C5-C6-N1	-6.64	119.38	122.70
1	X	692	C	C2-N3-C4	-6.63	116.58	119.90
1	X	771	C	C6-N1-C2	-6.63	117.65	120.30
1	X	2515	G	N9-C4-C5	6.63	108.05	105.40
1	X	2848	A	N9-C4-C5	6.62	108.45	105.80
1	X	2011	U	C5-C6-N1	-6.62	119.39	122.70
1	X	1469	U	C4-C5-C6	-6.62	115.73	119.70
1	X	689	A	N1-C6-N6	6.62	122.57	118.60
1	X	1680	U	C2-N3-C4	-6.61	123.03	127.00
1	X	2696	A	C8-N9-C4	6.61	108.44	105.80
1	X	883	A	N1-C2-N3	-6.60	126.00	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2253	A	N9-C4-C5	-6.60	103.16	105.80
1	X	829	C	C5-C6-N1	-6.59	117.70	121.00
1	X	2655	C	C5-C6-N1	-6.59	117.70	121.00
1	X	25	U	N3-C4-O4	6.59	124.01	119.40
1	X	2790	C	C5-C6-N1	-6.59	117.71	121.00
1	X	2859	U	C4'-C3'-C2'	-6.59	96.01	102.60
2	Y	101	A	C5-C6-N6	6.59	128.97	123.70
1	X	1615	C	C6-N1-C2	6.58	122.93	120.30
1	X	2520	A	C2-N3-C4	6.58	113.89	110.60
1	X	2485	U	C3'-C2'-C1'	6.58	106.76	101.50
1	X	2586	G	N1-C6-O6	-6.58	115.95	119.90
1	X	1747	G	C8-N9-C4	6.57	109.03	106.40
1	X	2757	G	C2-N3-C4	-6.57	108.61	111.90
1	X	166	G	C8-N9-C4	6.57	109.03	106.40
1	X	465	C	C6-N1-C1'	-6.57	112.92	120.80
1	X	2451	G	N1-C6-O6	-6.57	115.96	119.90
1	X	1944	C	N3-C4-C5	6.57	124.53	121.90
1	X	885	A	C8-N9-C4	-6.57	103.17	105.80
1	X	720	A	C2-N3-C4	-6.57	107.32	110.60
1	X	1830	C	C6-N1-C2	6.56	122.93	120.30
1	X	1968	G	C8-N9-C4	6.56	109.03	106.40
1	X	841	G	C8-N9-C4	-6.56	103.78	106.40
1	X	2008	C	N3-C4-N4	6.56	122.59	118.00
1	X	2466	G	N7-C8-N9	6.56	116.38	113.10
1	X	2712	G	N1-C6-O6	-6.56	115.97	119.90
1	X	1009	C	C2-N3-C4	-6.55	116.62	119.90
1	X	596	C	C4-C5-C6	6.55	120.67	117.40
1	X	1656	U	C6-N1-C2	6.55	124.93	121.00
1	X	2853	U	C5-C6-N1	-6.55	119.42	122.70
1	X	1017	C	C6-N1-C2	-6.55	117.68	120.30
1	X	2711	G	N1-C6-O6	-6.54	115.97	119.90
1	X	2485	U	C4-C5-C6	-6.54	115.78	119.70
1	X	2049	C	C6-N1-C2	-6.54	117.69	120.30
1	X	1009	C	N3-C4-C5	6.53	124.51	121.90
1	X	25	U	C5-C4-O4	-6.53	121.98	125.90
1	X	1260	A	C2-N3-C4	-6.53	107.34	110.60
1	X	2704	U	N1-C2-N3	6.53	118.82	114.90
1	X	579	G	N9-C4-C5	6.52	108.01	105.40
1	X	479	G	C4-C5-N7	6.52	113.41	110.80
1	X	858	G	C8-N9-C4	6.52	109.01	106.40
1	X	2792	C	C6-N1-C2	6.52	122.91	120.30
1	X	2347	C	C5-C6-N1	-6.51	117.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2623	A	N7-C8-N9	-6.51	110.54	113.80
1	X	1986	G	P-O3'-C3'	-6.51	111.89	119.70
1	X	833	A	N1-C2-N3	-6.50	126.05	129.30
1	X	1270	C	C2-N1-C1'	-6.50	111.65	118.80
1	X	1959	U	N3-C2-O2	-6.50	117.65	122.20
1	X	1256	C	N3-C2-O2	-6.50	117.35	121.90
1	X	1332	G	N9-C4-C5	-6.49	102.80	105.40
1	X	1467	U	N1-C1'-C2'	6.49	122.44	114.00
1	X	2237	C	C6-N1-C2	6.49	122.90	120.30
1	X	918	A	C8-N9-C4	6.49	108.40	105.80
1	X	1762	C	C6-N1-C2	-6.49	117.70	120.30
1	X	401	G	N9-C4-C5	6.49	108.00	105.40
1	X	787	A	C8-N9-C4	6.49	108.39	105.80
1	X	1246	G	C5-C6-O6	6.49	132.49	128.60
1	X	1717	A	C5-C6-N6	6.48	128.88	123.70
1	X	1480	G	N1-C6-O6	6.48	123.79	119.90
1	X	752	G	C5-C6-O6	6.48	132.49	128.60
1	X	1828	C	N3-C4-C5	6.48	124.49	121.90
1	X	34	U	C6-N1-C2	6.48	124.89	121.00
1	X	1304	U	C2-N3-C4	-6.47	123.11	127.00
1	X	1135	C	N3-C2-O2	6.47	126.43	121.90
1	X	323	G	N9-C4-C5	6.47	107.99	105.40
1	X	1916	G	C8-N9-C4	-6.47	103.81	106.40
1	X	1771	A	N7-C8-N9	6.47	117.03	113.80
1	X	1449	C	C5-C6-N1	6.46	124.23	121.00
1	X	1991	C	C2-N1-C1'	-6.46	111.70	118.80
1	X	338	G	C8-N9-C4	-6.45	103.82	106.40
1	X	1770	U	N3-C4-C5	6.45	118.47	114.60
1	X	2847	G	C5-C6-O6	-6.45	124.73	128.60
1	X	1664	G	N3-C4-C5	6.44	131.82	128.60
1	X	32	C	C6-N1-C2	6.44	122.88	120.30
1	X	2822	U	N3-C2-O2	6.44	126.71	122.20
1	X	1673	C	N1-C2-O2	-6.43	115.04	118.90
1	X	2543	A	N9-C4-C5	6.43	108.37	105.80
1	X	2419	C	C5-C6-N1	-6.43	117.78	121.00
1	X	2258	G	N3-C4-N9	6.42	129.85	126.00
1	X	357	A	C2-N3-C4	-6.41	107.39	110.60
1	X	18	U	C5-C6-N1	6.41	125.90	122.70
1	X	751	G	N1-C6-O6	6.40	123.74	119.90
1	X	1240	G	N3-C4-N9	6.40	129.84	126.00
1	X	762	A	N1-C6-N6	6.40	122.44	118.60
1	X	2627	G	C5-C6-N1	-6.40	108.30	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1471	G	N7-C8-N9	-6.40	109.90	113.10
1	X	2540	A	N9-C4-C5	-6.40	103.24	105.80
1	X	528	G	N9-C4-C5	-6.39	102.84	105.40
1	X	2759	U	N3-C4-O4	6.39	123.88	119.40
1	X	693	A	C8-N9-C4	6.39	108.36	105.80
1	X	2588	U	C6-N1-C2	6.39	124.83	121.00
1	X	1673	C	C6-N1-C2	6.38	122.85	120.30
1	X	2195	C	C6-N1-C2	6.38	122.85	120.30
1	X	2468	G	C4-C5-N7	-6.38	108.25	110.80
1	X	340	G	C8-N9-C4	6.38	108.95	106.40
1	X	504	G	C6-C5-N7	-6.38	126.57	130.40
1	X	522	G	C5-C6-N1	-6.38	108.31	111.50
1	X	596	C	C6-N1-C2	6.38	122.85	120.30
1	X	773	G	C2-N3-C4	-6.38	108.71	111.90
1	X	1653	C	N1-C2-O2	-6.38	115.07	118.90
1	X	2835	A	C5-C6-N1	-6.38	114.51	117.70
1	X	1304	U	N3-C4-C5	6.37	118.42	114.60
1	X	1163	C	C6-N1-C2	-6.37	117.75	120.30
1	X	762	A	C4-C5-N7	6.36	113.88	110.70
1	X	1647	U	N3-C4-C5	-6.36	110.78	114.60
1	X	2468	G	C8-N9-C4	6.36	108.94	106.40
1	X	2651	U	N3-C2-O2	6.36	126.66	122.20
1	X	2672	U	N1-C2-O2	6.36	127.25	122.80
1	X	1309	G	N3-C2-N2	6.36	124.35	119.90
1	X	2035	G	N3-C4-C5	-6.36	125.42	128.60
1	X	2008	C	N1-C2-O2	-6.36	115.09	118.90
1	X	1715	A	C5-C6-N6	-6.35	118.62	123.70
1	X	1773	C	C5-C6-N1	-6.35	117.82	121.00
1	X	2524	G	N1-C6-O6	6.34	123.71	119.90
1	X	1470	G	O5'-P-OP2	6.34	118.31	110.70
1	X	1702	C	N3-C4-C5	6.34	124.44	121.90
1	X	2760	G	C8-N9-C4	6.34	108.94	106.40
1	X	1409	U	C6-N1-C2	6.34	124.80	121.00
1	X	1777	A	N7-C8-N9	6.34	116.97	113.80
1	X	950	G	N9-C4-C5	6.34	107.94	105.40
1	X	2655	C	C2-N3-C4	-6.34	116.73	119.90
1	X	2039	G	C5-C6-O6	-6.34	124.80	128.60
1	X	1806	G	C8-N9-C4	-6.33	103.87	106.40
1	X	2437	G	C5-C6-O6	-6.33	124.80	128.60
26	Z	4	HIS	C-N-CD	-6.33	106.67	120.60
1	X	1270	C	C6-N1-C1'	6.33	128.39	120.80
1	X	572	G	N9-C4-C5	6.32	107.93	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	575	U	N1-C2-O2	-6.32	118.37	122.80
1	X	434	C	C6-N1-C2	-6.32	117.77	120.30
1	X	2422	C	C6-N1-C2	-6.32	117.77	120.30
1	X	1766	U	C6-N1-C2	6.32	124.79	121.00
1	X	2422	C	N1-C2-O2	-6.32	115.11	118.90
1	X	2858	A	C4'-C3'-C2'	-6.32	96.28	102.60
1	X	2603	G	C8-N9-C4	-6.31	103.88	106.40
1	X	46	C	C6-N1-C2	-6.31	117.78	120.30
1	X	1679	U	C5-C6-N1	-6.31	119.55	122.70
1	X	1761	G	N1-C2-N3	6.31	127.68	123.90
1	X	1824	C	C6-N1-C2	6.30	122.82	120.30
1	X	2836	U	C6-N1-C2	-6.30	117.22	121.00
1	X	536	A	C2-N3-C4	6.30	113.75	110.60
1	X	827	C	N1-C2-O2	6.30	122.68	118.90
1	X	1018	C	C5-C6-N1	-6.30	117.85	121.00
1	X	985	G	C6-C5-N7	-6.30	126.62	130.40
1	X	2812	A	C2-N3-C4	-6.30	107.45	110.60
1	X	1992	G	C5-C6-O6	6.29	132.38	128.60
1	X	2350	G	N9-C4-C5	6.29	107.92	105.40
1	X	972	C	N3-C4-C5	-6.29	119.38	121.90
1	X	2654	A	C8-N9-C4	6.29	108.32	105.80
1	X	1255	A	C5-C6-N6	6.29	128.73	123.70
1	X	2638	G	C8-N9-C4	-6.29	103.89	106.40
1	X	1299	A	N3-C4-N9	-6.29	122.37	127.40
1	X	1963	G	N9-C4-C5	6.29	107.91	105.40
1	X	2374	C	C5-C4-N4	6.29	124.60	120.20
1	X	2033	C	N1-C2-O2	-6.28	115.13	118.90
1	X	2522	G	C5-C6-O6	6.28	132.37	128.60
1	X	570	G	N3-C2-N2	-6.28	115.51	119.90
1	X	1622	G	N1-C6-O6	-6.28	116.13	119.90
1	X	1054	C	C5-C6-N1	6.27	124.14	121.00
1	X	1236	G	N9-C4-C5	-6.27	102.89	105.40
1	X	1469	U	C5-C6-N1	6.27	125.84	122.70
1	X	527	C	N3-C4-N4	6.27	122.39	118.00
1	X	1675	C	N3-C4-C5	-6.27	119.39	121.90
1	X	804	C	C2-N3-C4	-6.26	116.77	119.90
1	X	1285	A	N1-C2-N3	6.26	132.43	129.30
1	X	1169	C	N1-C2-O2	6.26	122.65	118.90
1	X	2397	A	N9-C4-C5	-6.26	103.30	105.80
1	X	531	G	C8-N9-C4	6.25	108.90	106.40
1	X	536	A	C8-N9-C4	-6.25	103.30	105.80
1	X	2637	C	N3-C2-O2	6.25	126.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	549	G	N1-C6-O6	-6.25	116.15	119.90
1	X	393	U	N3-C4-C5	-6.25	110.85	114.60
1	X	594	G	C5-C6-O6	6.25	132.35	128.60
1	X	2698	G	C5-C6-O6	-6.24	124.86	128.60
1	X	1251	G	N7-C8-N9	6.24	116.22	113.10
1	X	2794	G	C5-C6-O6	-6.23	124.86	128.60
1	X	951	G	C8-N9-C4	6.23	108.89	106.40
1	X	2515	G	N1-C2-N2	-6.23	110.59	116.20
1	X	2566	A	C2-N3-C4	-6.22	107.49	110.60
1	X	1314	A	N1-C6-N6	-6.22	114.87	118.60
1	X	1229	C	C5-C4-N4	6.22	124.55	120.20
1	X	1451	C	C6-N1-C2	-6.22	117.81	120.30
1	X	166	G	N3-C4-C5	6.21	131.71	128.60
1	X	1628	C	N1-C2-O2	-6.21	115.17	118.90
1	X	489	A	N1-C6-N6	-6.21	114.88	118.60
1	X	1228	G	C5-C6-O6	6.21	132.32	128.60
1	X	2474	G	N3-C2-N2	6.21	124.25	119.90
1	X	1789	U	N3-C2-O2	-6.20	117.86	122.20
1	X	2693	U	C5-C4-O4	6.20	129.62	125.90
1	X	861	G	C8-N9-C4	-6.20	103.92	106.40
1	X	1256	C	C2-N3-C4	-6.20	116.80	119.90
1	X	686	C	N3-C4-C5	6.20	124.38	121.90
1	X	1333	G	N1-C6-O6	6.20	123.62	119.90
1	X	777	A	C1'-O4'-C4'	-6.19	104.94	109.90
1	X	761	G	N1-C2-N2	-6.19	110.63	116.20
1	X	1658	A	N1-C6-N6	6.19	122.31	118.60
1	X	1719	G	N1-C6-O6	-6.19	116.19	119.90
1	X	2862	G	C8-N9-C4	-6.19	103.92	106.40
1	X	1642	G	C2-N3-C4	-6.19	108.81	111.90
1	X	1721	G	N7-C8-N9	-6.19	110.00	113.10
1	X	2056	C	C5-C6-N1	-6.19	117.91	121.00
1	X	1998	A	C4-C5-N7	-6.19	107.61	110.70
1	X	2782	G	N9-C4-C5	-6.18	102.93	105.40
1	X	2712	G	C5-C6-O6	6.18	132.31	128.60
1	X	1982	C	N1-C2-N3	6.18	123.53	119.20
1	X	219	G	N3-C2-N2	6.17	124.22	119.90
1	X	743	A	N1-C2-N3	6.17	132.39	129.30
1	X	2690	A	N1-C6-N6	6.17	122.30	118.60
1	X	1442	C	N3-C4-C5	6.17	124.37	121.90
1	X	1297	A	C2-N3-C4	-6.16	107.52	110.60
1	X	2524	G	N3-C4-C5	-6.16	125.52	128.60
1	X	507	A	C8-N9-C4	6.16	108.26	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	U	40	ARG	N-CA-CB	6.16	121.68	110.60
1	X	1661	C	C6-N1-C2	6.15	122.76	120.30
1	X	2792	C	C2-N3-C4	-6.15	116.82	119.90
1	X	1282	A	N9-C4-C5	-6.15	103.34	105.80
1	X	2047	C	N1-C2-O2	-6.15	115.21	118.90
1	X	2674	C	N3-C2-O2	6.14	126.20	121.90
1	X	1019	U	C6-N1-C2	6.14	124.69	121.00
1	X	1835	C	N1-C2-O2	-6.14	115.22	118.90
1	X	1255	A	C8-N9-C4	-6.13	103.35	105.80
1	X	27	G	C2-N3-C4	6.13	114.97	111.90
1	X	394	U	C6-N1-C2	6.13	124.68	121.00
1	X	1304	U	N3-C4-O4	-6.13	115.11	119.40
1	X	480	G	N9-C4-C5	6.12	107.85	105.40
1	X	1317	G	C2-N3-C4	-6.12	108.84	111.90
1	X	1648	C	C6-N1-C2	6.12	122.75	120.30
1	X	2619	G	C8-N9-C4	-6.12	103.95	106.40
1	X	126	C	C6-N1-C2	6.12	122.75	120.30
1	X	2343	C	C6-N1-C2	6.12	122.75	120.30
1	X	889	C	N1-C2-O2	6.12	122.57	118.90
1	X	597	U	C2-N1-C1'	-6.11	110.36	117.70
1	X	1292	A	C5-C6-N1	6.11	120.75	117.70
1	X	2697	G	N1-C2-N3	-6.11	120.23	123.90
1	X	1357	U	N3-C2-O2	-6.11	117.92	122.20
1	X	747	A	N9-C4-C5	-6.11	103.36	105.80
1	X	1993	G	C6-C5-N7	-6.10	126.74	130.40
1	X	2068	C	C6-N1-C2	-6.10	117.86	120.30
1	X	1202	U	N1-C2-O2	-6.09	118.53	122.80
1	X	1398	G	C8-N9-C4	6.09	108.84	106.40
1	X	1664	G	C4-C5-N7	6.09	113.24	110.80
1	X	878	C	N3-C4-C5	6.09	124.34	121.90
1	X	1699	A	C8-N9-C4	6.09	108.24	105.80
1	X	735	G	C8-N9-C4	6.09	108.83	106.40
1	X	2617	G	N1-C6-O6	-6.09	116.25	119.90
1	X	2651	U	C6-N1-C2	6.09	124.65	121.00
1	X	29	U	N3-C4-O4	6.08	123.66	119.40
1	X	2603	G	N7-C8-N9	6.08	116.14	113.10
1	X	2855	C	N3-C4-N4	6.08	122.26	118.00
1	X	1993	G	N3-C4-C5	6.08	131.64	128.60
1	X	2688	G	C2-N3-C4	-6.08	108.86	111.90
1	X	2496	C	C2-N3-C4	-6.08	116.86	119.90
1	X	1644	G	N7-C8-N9	-6.07	110.06	113.10
1	X	2711	G	C5-C6-N1	6.07	114.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1294	G	C8-N9-C4	-6.07	103.97	106.40
1	X	1711	C	N3-C4-C5	6.07	124.33	121.90
1	X	1710	U	C5-C4-O4	-6.06	122.26	125.90
1	X	2015	G	C8-N9-C4	-6.06	103.97	106.40
1	X	2035	G	C2-N3-C4	6.06	114.93	111.90
1	X	2764	U	C5-C6-N1	-6.06	119.67	122.70
1	X	70	A	N7-C8-N9	6.05	116.83	113.80
1	X	2490	U	N1-C2-N3	6.05	118.53	114.90
1	X	504	G	C2-N3-C4	-6.05	108.87	111.90
1	X	583	C	C6-N1-C2	-6.05	117.88	120.30
1	X	1285	A	C5-C6-N1	-6.05	114.67	117.70
1	X	2550	C	C5-C4-N4	6.05	124.43	120.20
1	X	1318	A	C8-N9-C4	6.04	108.22	105.80
1	X	1629	G	N3-C2-N2	6.04	124.13	119.90
1	X	2371	A	N7-C8-N9	6.04	116.82	113.80
1	X	231	G	C8-N9-C4	-6.04	103.98	106.40
1	X	579	G	C6-C5-N7	6.04	134.02	130.40
1	X	2751	C	C5-C6-N1	-6.04	117.98	121.00
1	X	1721	G	N3-C2-N2	6.03	124.12	119.90
1	X	1939	U	C5-C6-N1	6.03	125.72	122.70
1	X	2034	A	N7-C8-N9	6.03	116.81	113.80
1	X	2437	G	C8-N9-C4	6.03	108.81	106.40
1	X	2605	C	C5-C6-N1	-6.03	117.99	121.00
1	X	2026	C	N1-C2-O2	-6.02	115.29	118.90
1	X	1235	C	C2-N3-C4	-6.02	116.89	119.90
1	X	2039	G	C5-C6-N1	-6.02	108.49	111.50
1	X	2637	C	C6-N1-C2	6.02	122.71	120.30
1	X	581	A	N7-C8-N9	-6.02	110.79	113.80
1	X	761	G	N3-C2-N2	6.01	124.11	119.90
1	X	1963	G	C8-N9-C4	-6.00	104.00	106.40
1	X	1998	A	C6-N1-C2	-6.00	115.00	118.60
1	X	1035	G	N3-C4-C5	-6.00	125.60	128.60
1	X	769	C	C5-C4-N4	-6.00	116.00	120.20
1	X	1472	C	N3-C4-C5	6.00	124.30	121.90
1	X	1636	G	N9-C4-C5	-6.00	103.00	105.40
1	X	581	A	C2-N3-C4	-6.00	107.60	110.60
1	X	1357	U	C6-N1-C2	-6.00	117.40	121.00
1	X	1173	G	N1-C6-O6	-6.00	116.30	119.90
1	X	2230	G	N1-C6-O6	6.00	123.50	119.90
1	X	1255	A	C4-C5-N7	-5.99	107.70	110.70
1	X	1210	C	N3-C2-O2	5.99	126.09	121.90
1	X	527	C	C5-C6-N1	5.99	123.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	937	C	N3-C2-O2	5.99	126.09	121.90
1	X	2433	G	C8-N9-C4	5.99	108.80	106.40
1	X	2229	G	C4-C5-N7	-5.99	108.41	110.80
1	X	2682	C	C6-N1-C2	-5.98	117.91	120.30
1	X	841	G	N3-C4-C5	5.98	131.59	128.60
1	X	1699	A	C6-C5-N7	-5.98	128.11	132.30
1	X	15	G	N3-C2-N2	-5.98	115.72	119.90
1	X	2008	C	C2-N3-C4	5.98	122.89	119.90
1	X	1239	A	N9-C4-C5	-5.98	103.41	105.80
1	X	2039	G	C5-N7-C8	-5.98	101.31	104.30
1	X	808	C	C6-N1-C2	5.98	122.69	120.30
1	X	2701	A	N1-C2-N3	5.97	132.29	129.30
1	X	2745	A	C5-C6-N1	5.97	120.69	117.70
1	X	2049	C	N3-C2-O2	-5.97	117.72	121.90
1	X	2811	G	N7-C8-N9	-5.97	110.11	113.10
1	X	2828	C	C4-C5-C6	-5.97	114.42	117.40
1	X	2383	C	C6-N1-C2	-5.97	117.91	120.30
1	X	2331	A	N9-C4-C5	5.96	108.19	105.80
1	X	582	G	N1-C6-O6	5.96	123.48	119.90
1	X	771	C	N3-C2-O2	-5.96	117.73	121.90
1	X	1166	A	N3-C4-C5	-5.96	122.63	126.80
1	X	2862	G	N7-C8-N9	5.96	116.08	113.10
1	X	1477	C	C6-N1-C2	-5.95	117.92	120.30
1	X	1617	G	C8-N9-C4	5.95	108.78	106.40
1	X	571	U	N1-C2-O2	-5.95	118.64	122.80
1	X	753	U	N3-C4-C5	-5.95	111.03	114.60
1	X	1222	G	C8-N9-C4	5.95	108.78	106.40
1	X	2000	U	N3-C4-O4	5.95	123.56	119.40
1	X	1955	G	C8-N9-C4	5.95	108.78	106.40
1	X	2055	G	N3-C4-C5	-5.95	125.63	128.60
1	X	2258	G	C8-N9-C4	5.95	108.78	106.40
1	X	549	G	N9-C4-C5	5.94	107.78	105.40
1	X	2211	U	C5-C6-N1	-5.94	119.73	122.70
1	X	2335	U	N3-C2-O2	-5.94	118.04	122.20
1	X	963	G	C8-N9-C4	5.93	108.77	106.40
1	X	2037	A	N1-C6-N6	-5.93	115.04	118.60
1	X	717	G	N7-C8-N9	-5.93	110.13	113.10
1	X	1262	U	C5-C4-O4	-5.93	122.34	125.90
1	X	2024	U	C2-N3-C4	-5.93	123.44	127.00
1	X	1260	A	N3-C4-N9	-5.93	122.66	127.40
1	X	1404	C	C2-N3-C4	-5.93	116.94	119.90
1	X	1698	C	C5-C6-N1	-5.93	118.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1939	U	N1-C2-O2	-5.93	118.65	122.80
1	X	816	U	N1-C2-N3	5.92	118.45	114.90
1	X	67	G	N3-C2-N2	5.92	124.04	119.90
1	X	474	G	N7-C8-N9	-5.92	110.14	113.10
1	X	1570	C	C6-N1-C2	5.91	122.67	120.30
1	X	972	C	N3-C2-O2	-5.91	117.76	121.90
1	X	1678	G	C2-N3-C4	5.91	114.86	111.90
1	X	2035	G	C5-N7-C8	5.91	107.25	104.30
1	X	697	G	N3-C4-N9	-5.91	122.46	126.00
1	X	1763	G	C8-N9-C4	5.91	108.76	106.40
1	X	2824	C	C2-N3-C4	-5.91	116.95	119.90
1	X	2459	C	N3-C2-O2	5.91	126.03	121.90
1	X	1241	G	C8-N9-C4	5.90	108.76	106.40
1	X	387	A	N1-C6-N6	5.90	122.14	118.60
1	X	2703	C	C6-N1-C1'	5.90	127.88	120.80
1	X	327	C	C6-N1-C2	-5.90	117.94	120.30
1	X	1647	U	C4-C5-C6	5.90	123.24	119.70
1	X	521	U	C5-C6-N1	-5.89	119.75	122.70
1	X	985	G	C5-C6-O6	-5.89	125.06	128.60
1	X	1614	C	N1-C2-O2	-5.89	115.36	118.90
1	X	1635	G	N3-C4-N9	-5.89	122.46	126.00
1	X	2597	G	N3-C4-C5	-5.89	125.65	128.60
1	X	1983	G	N7-C8-N9	-5.89	110.16	113.10
1	X	2253	A	C8-N9-C4	5.89	108.16	105.80
1	X	1317	G	N3-C4-C5	5.88	131.54	128.60
1	X	2576	G	C5-C6-O6	-5.88	125.07	128.60
1	X	608	G	N1-C6-O6	-5.88	116.37	119.90
1	X	1041	G	C5-C6-O6	5.88	132.13	128.60
1	X	1717	A	C4-C5-N7	-5.88	107.76	110.70
1	X	2531	U	C2-N3-C4	-5.88	123.47	127.00
1	X	2054	A	N1-C6-N6	-5.88	115.07	118.60
1	X	859	U	N1-C2-O2	-5.88	118.69	122.80
1	X	2848	A	N1-C6-N6	-5.88	115.07	118.60
1	X	2751	C	N3-C4-N4	-5.88	113.89	118.00
1	X	10	A	C8-N9-C4	5.87	108.15	105.80
1	X	1260	A	N1-C6-N6	-5.87	115.08	118.60
1	X	1343	C	N1-C2-O2	-5.87	115.38	118.90
2	Y	42	U	C6-N1-C2	5.87	124.53	121.00
1	X	1939	U	N3-C4-O4	5.87	123.51	119.40
1	X	2524	G	N7-C8-N9	5.87	116.03	113.10
1	X	12	U	N3-C4-C5	-5.86	111.08	114.60
1	X	807	A	C8-N9-C4	5.86	108.14	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2825	A	N7-C8-N9	5.86	116.73	113.80
1	X	1229	C	N1-C2-N3	5.86	123.30	119.20
1	X	2022	C	N3-C4-C5	-5.86	119.56	121.90
1	X	14	A	C2-N3-C4	-5.86	107.67	110.60
1	X	1304	U	C5-C6-N1	-5.86	119.77	122.70
1	X	2753	C	C5-C6-N1	5.86	123.93	121.00
1	X	833	A	C5-C6-N6	-5.85	119.02	123.70
1	X	2218	G	C8-N9-C4	-5.85	104.06	106.40
1	X	2540	A	C5-C6-N1	5.85	120.63	117.70
1	X	806	A	C5-N7-C8	5.85	106.83	103.90
1	X	57	G	N9-C4-C5	5.85	107.74	105.40
1	X	1699	A	N9-C4-C5	-5.84	103.46	105.80
1	X	1616	C	C5-C6-N1	-5.84	118.08	121.00
1	X	2540	A	C2-N3-C4	5.84	113.52	110.60
1	X	2812	A	N1-C2-N3	5.84	132.22	129.30
1	X	2847	G	N1-C6-O6	5.84	123.41	119.90
1	X	1777	A	C5-N7-C8	-5.84	100.98	103.90
1	X	2268	G	C4-C5-N7	-5.84	108.46	110.80
1	X	2559	U	N3-C4-C5	5.84	118.10	114.60
1	X	1313	U	C5-C6-N1	-5.84	119.78	122.70
1	X	1398	G	N9-C4-C5	-5.83	103.07	105.40
1	X	1960	A	C8-N9-C4	5.83	108.13	105.80
1	X	2794	G	N1-C6-O6	5.83	123.40	119.90
1	X	746	G	C4-N9-C1'	5.83	134.09	126.50
1	X	1010	U	C5-C6-N1	-5.83	119.78	122.70
1	X	786	U	C5-C6-N1	-5.83	119.78	122.70
1	X	1006	C	N3-C2-O2	-5.83	117.82	121.90
1	X	2704	U	C5-C4-O4	5.83	129.40	125.90
1	X	157	G	N3-C4-N9	-5.83	122.50	126.00
1	X	2807	U	N3-C4-C5	5.83	118.10	114.60
1	X	2331	A	N1-C6-N6	-5.82	115.11	118.60
1	X	2440	C	C2-N1-C1'	-5.82	112.39	118.80
1	X	619	A	C8-N9-C4	-5.82	103.47	105.80
1	X	1781	C	N3-C4-C5	5.82	124.23	121.90
1	X	2453	C	C6-N1-C2	-5.82	117.97	120.30
2	Y	93	G	N1-C6-O6	5.82	123.39	119.90
1	X	2640	G	C4-C5-N7	5.82	113.13	110.80
1	X	496	C	C5-C6-N1	-5.82	118.09	121.00
1	X	1874	G	C8-N9-C4	-5.82	104.07	106.40
1	X	2745	A	C4-C5-C6	-5.82	114.09	117.00
1	X	1654	A	N1-C6-N6	-5.82	115.11	118.60
1	X	2800	C	N1-C2-O2	5.82	122.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	525	A	C2-N3-C4	5.81	113.51	110.60
1	X	1706	A	C6-N1-C2	5.81	122.09	118.60
1	X	2543	A	C8-N9-C4	-5.81	103.47	105.80
1	X	1777	A	C8-N9-C4	-5.81	103.48	105.80
1	X	2486	C	O4'-C1'-C2'	-5.81	99.99	105.80
1	X	981	C	N1-C1'-C2'	5.80	121.55	114.00
1	X	2524	G	C4-C5-N7	5.80	113.12	110.80
1	X	2627	G	N3-C4-N9	-5.80	122.52	126.00
1	X	2210	C	N1-C2-O2	-5.80	115.42	118.90
1	X	330	C	C6-N1-C2	-5.80	117.98	120.30
1	X	569	C	C6-N1-C2	5.80	122.62	120.30
1	X	2853	U	N3-C4-C5	5.80	118.08	114.60
1	X	1272	G	N7-C8-N9	-5.80	110.20	113.10
1	X	1290	A	C2-N3-C4	-5.79	107.70	110.60
1	X	2782	G	N7-C8-N9	-5.79	110.20	113.10
1	X	755	C	N1-C2-N3	5.79	123.25	119.20
1	X	1711	C	C6-N1-C2	5.79	122.62	120.30
1	X	2798	A	N1-C6-N6	5.79	122.07	118.60
1	X	837	U	C2-N3-C4	-5.79	123.53	127.00
1	X	841	G	N3-C4-N9	-5.79	122.53	126.00
1	X	1678	G	C6-C5-N7	5.79	133.87	130.40
1	X	219	G	C5-C6-N1	5.79	114.39	111.50
1	X	744	C	C4-C5-C6	5.78	120.29	117.40
1	X	2861	A	N1-C6-N6	5.78	122.07	118.60
1	X	30	G	C8-N9-C4	-5.78	104.09	106.40
1	X	461	A	N1-C6-N6	5.78	122.07	118.60
1	X	1647	U	C5-C4-O4	5.78	129.37	125.90
1	X	1636	G	C4-C5-N7	5.77	113.11	110.80
1	X	1670	G	C4-C5-N7	-5.77	108.49	110.80
1	X	2471	U	C5-C6-N1	-5.77	119.81	122.70
1	X	875	G	N1-C6-O6	5.77	123.36	119.90
1	X	744	C	N1-C2-N3	5.77	123.24	119.20
1	X	2007	G	N1-C6-O6	-5.77	116.44	119.90
1	X	1459	U	N1-C2-O2	-5.77	118.76	122.80
1	X	323	G	C4-C5-N7	-5.76	108.49	110.80
1	X	1262	U	N3-C4-O4	5.76	123.43	119.40
1	X	2555	G	N9-C4-C5	-5.76	103.10	105.40
1	X	2828	C	C5-C6-N1	5.76	123.88	121.00
1	X	2510	A	N1-C6-N6	5.76	122.06	118.60
1	X	2701	A	C2-N3-C4	-5.76	107.72	110.60
1	X	504	G	C5-C6-O6	-5.76	125.15	128.60
1	X	484	G	N1-C6-O6	5.75	123.35	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	12	U	N3-C4-O4	5.75	123.42	119.40
1	X	864	C	C5-C6-N1	5.75	123.88	121.00
1	X	2003	A	N1-C2-N3	5.75	132.18	129.30
1	X	777	A	O4'-C1'-N9	5.75	112.80	108.20
1	X	1283	C	C5-C6-N1	-5.75	118.13	121.00
1	X	2352	A	N1-C6-N6	-5.75	115.15	118.60
1	X	2687	G	C5-C6-O6	5.75	132.05	128.60
1	X	464	G	C5-C6-O6	5.75	132.05	128.60
1	X	761	G	N7-C8-N9	-5.74	110.23	113.10
1	X	2055	G	N1-C6-O6	-5.74	116.45	119.90
1	X	967	G	C2-N3-C4	5.74	114.77	111.90
1	X	35	G	C5-C6-O6	5.74	132.04	128.60
1	X	1747	G	N7-C8-N9	-5.74	110.23	113.10
1	X	109	A	C8-N9-C4	5.73	108.09	105.80
1	X	818	G	N1-C6-O6	5.73	123.34	119.90
1	X	886	A	N7-C8-N9	5.73	116.67	113.80
1	X	1985	G	C4'-C3'-C2'	-5.73	96.87	102.60
1	X	2228	U	N3-C4-O4	5.73	123.41	119.40
1	X	2267	A	C5-C6-N1	5.73	120.56	117.70
1	X	2701	A	C5-C6-N6	5.73	128.28	123.70
1	X	530	G	N3-C4-C5	5.73	131.46	128.60
1	X	1173	G	N9-C4-C5	5.73	107.69	105.40
1	X	1756	C	N1-C2-O2	-5.72	115.47	118.90
1	X	1479	G	N1-C6-O6	5.72	123.33	119.90
1	X	187	U	N3-C2-O2	5.72	126.20	122.20
1	X	1345	G	N1-C6-O6	-5.72	116.47	119.90
1	X	1751	A	N7-C8-N9	-5.72	110.94	113.80
1	X	2226	A	N1-C2-N3	5.71	132.16	129.30
1	X	2363	G	C5-C6-N1	-5.71	108.64	111.50
1	X	332	C	C6-N1-C2	5.71	122.58	120.30
1	X	2827	G	N1-C2-N2	-5.71	111.06	116.20
1	X	2363	G	N1-C6-O6	5.71	123.33	119.90
1	X	2495	G	C6-N1-C2	-5.71	121.67	125.10
1	X	2818	G	C6-C5-N7	-5.71	126.98	130.40
1	X	322	A	N7-C8-N9	-5.70	110.95	113.80
1	X	1294	G	N7-C8-N9	5.70	115.95	113.10
1	X	1616	C	C6-N1-C2	5.70	122.58	120.30
1	X	2484	G	C8-N9-C4	-5.70	104.12	106.40
1	X	58	C	N1-C2-O2	-5.70	115.48	118.90
1	X	1687	C	C2-N3-C4	-5.70	117.05	119.90
1	X	2515	G	C8-N9-C4	-5.70	104.12	106.40
1	X	2673	G	C4-C5-N7	5.70	113.08	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	507	A	N1-C6-N6	-5.70	115.18	118.60
1	X	545	C	N3-C4-C5	5.70	124.18	121.90
1	X	549	G	C5-C6-O6	5.70	132.02	128.60
1	X	570	G	N1-C2-N2	5.70	121.33	116.20
1	X	780	U	P-O3'-C3'	5.70	126.54	119.70
1	X	1256	C	C5-C6-N1	-5.70	118.15	121.00
1	X	1636	G	N3-C4-C5	5.70	131.45	128.60
1	X	2039	G	N1-C2-N3	5.69	127.32	123.90
1	X	537	C	N3-C2-O2	-5.69	117.92	121.90
1	X	179	U	C5-C6-N1	-5.69	119.86	122.70
1	X	1853	C	N1-C2-O2	-5.69	115.49	118.90
1	X	1675	C	N3-C2-O2	5.69	125.88	121.90
1	X	2055	G	C4-C5-N7	-5.69	108.53	110.80
1	X	2381	A	C3'-C2'-C1'	5.68	106.04	101.50
1	X	2448	A	C8-N9-C4	-5.68	103.53	105.80
1	X	27	G	N3-C2-N2	5.68	123.87	119.90
1	X	715	U	N1-C2-O2	-5.68	118.83	122.80
1	X	1666	G	N7-C8-N9	-5.67	110.26	113.10
1	X	2315	A	C8-N9-C4	5.67	108.07	105.80
1	X	1641	C	C6-N1-C2	5.67	122.57	120.30
1	X	1932	G	N1-C6-O6	-5.67	116.50	119.90
1	X	499	G	N3-C2-N2	5.67	123.87	119.90
1	X	686	C	C6-N1-C2	5.67	122.57	120.30
1	X	1968	G	N7-C8-N9	-5.67	110.27	113.10
1	X	1572	C	N3-C4-C5	-5.67	119.63	121.90
1	X	2753	C	N3-C4-N4	5.67	121.97	118.00
1	X	1316	G	N1-C2-N3	5.67	127.30	123.90
1	X	1773	C	N3-C2-O2	-5.66	117.94	121.90
1	X	1514	C	C6-N1-C2	-5.66	118.03	120.30
1	X	2856	U	C6-N1-C2	-5.66	117.60	121.00
1	X	1018	C	C2-N3-C4	-5.66	117.07	119.90
1	X	1678	G	C5-N7-C8	5.66	107.13	104.30
1	X	1707	A	C8-N9-C4	5.66	108.06	105.80
1	X	2072	C	N1-C2-O2	-5.66	115.50	118.90
1	X	536	A	N3-C4-C5	-5.65	122.84	126.80
1	X	2550	C	N3-C4-C5	-5.65	119.64	121.90
1	X	1166	A	N7-C8-N9	5.65	116.63	113.80
1	X	2440	C	N3-C4-N4	-5.65	114.04	118.00
1	X	566	U	N3-C4-O4	5.65	123.35	119.40
1	X	1616	C	C2-N3-C4	-5.65	117.08	119.90
1	X	211	U	N3-C2-O2	-5.65	118.25	122.20
1	X	634	G	N3-C2-N2	-5.65	115.95	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2515	G	N3-C2-N2	5.65	123.85	119.90
1	X	2656	G	C8-N9-C4	5.65	108.66	106.40
1	X	2729	A	N1-C6-N6	-5.65	115.21	118.60
1	X	1958	G	C8-N9-C4	5.64	108.66	106.40
1	X	1494	G	N3-C4-N9	-5.64	122.62	126.00
1	X	1943	A	C8-N9-C4	5.64	108.06	105.80
1	X	746	G	C4-C5-C6	5.64	122.18	118.80
1	X	2352	A	C6-N1-C2	-5.64	115.22	118.60
1	X	1927	U	C2-N3-C4	-5.63	123.62	127.00
1	X	1938	U	C6-N1-C2	5.63	124.38	121.00
1	X	2771	C	C6-N1-C2	-5.63	118.05	120.30
1	X	689	A	C5-C6-N6	-5.63	119.20	123.70
1	X	2328	G	C8-N9-C4	-5.63	104.15	106.40
1	X	1306	U	C2-N3-C4	-5.63	123.62	127.00
1	X	1330	G	C8-N9-C4	5.63	108.65	106.40
1	X	456	C	N3-C4-C5	-5.62	119.65	121.90
1	X	746	G	C5-C6-N1	-5.62	108.69	111.50
1	X	1966	C	N3-C2-O2	5.62	125.83	121.90
1	X	981	C	C6-N1-C2	-5.62	118.05	120.30
1	X	1287	A	N3-C4-C5	-5.62	122.87	126.80
1	X	496	C	N3-C4-C5	5.62	124.15	121.90
1	X	688	A	C5-C6-N6	-5.62	119.20	123.70
1	X	572	G	N7-C8-N9	5.62	115.91	113.10
1	X	1789	U	C6-N1-C2	-5.62	117.63	121.00
1	X	1411	C	C5-C6-N1	-5.62	118.19	121.00
1	X	1272	G	C4-C5-N7	-5.61	108.56	110.80
1	X	1406	A	N1-C6-N6	-5.61	115.23	118.60
1	X	2464	G	C5-C6-O6	-5.61	125.23	128.60
1	X	504	G	C5-C6-N1	-5.61	108.69	111.50
1	X	701	U	C5-C4-O4	5.61	129.27	125.90
1	X	12	U	N1-C2-O2	-5.61	118.87	122.80
1	X	2441	U	N3-C4-O4	-5.61	115.47	119.40
1	X	2764	U	C2-N3-C4	-5.61	123.63	127.00
1	X	1993	G	N1-C2-N3	5.61	127.26	123.90
1	X	1292	A	N9-C4-C5	-5.61	103.56	105.80
1	X	1300	A	C5-C6-N6	-5.61	119.22	123.70
1	X	2329	C	N3-C4-C5	5.61	124.14	121.90
1	X	2578	G	N1-C6-O6	5.61	123.26	119.90
1	X	1212	U	N1-C2-O2	-5.60	118.88	122.80
1	X	861	G	N9-C4-C5	5.60	107.64	105.40
1	X	21	A	N3-C4-C5	5.60	130.72	126.80
1	X	2845	C	C4'-C3'-C2'	-5.60	97.00	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2617	G	N3-C4-C5	-5.60	125.80	128.60
1	X	1653	C	N3-C4-N4	5.60	121.92	118.00
1	X	1715	A	N1-C6-N6	5.60	121.96	118.60
2	Y	102	A	N1-C6-N6	5.60	121.96	118.60
1	X	2350	G	C8-N9-C4	-5.59	104.17	106.40
1	X	1045	G	C8-N9-C4	5.59	108.64	106.40
1	X	638	A	C2-N3-C4	5.59	113.39	110.60
1	X	724	C	C6-N1-C2	-5.59	118.06	120.30
1	X	883	A	C8-N9-C4	5.58	108.03	105.80
1	X	2233	C	C5-C6-N1	-5.58	118.21	121.00
1	X	2763	U	C5-C4-O4	5.58	129.25	125.90
1	X	2792	C	C5-C6-N1	-5.58	118.21	121.00
1	X	22	C	C4-C5-C6	5.58	120.19	117.40
1	X	1228	G	C8-N9-C4	-5.58	104.17	106.40
1	X	1706	A	N1-C6-N6	5.57	121.94	118.60
1	X	220	U	C5-C4-O4	5.57	129.24	125.90
1	X	32	C	C5-C6-N1	-5.57	118.21	121.00
1	X	186	C	C6-N1-C2	5.57	122.53	120.30
1	X	1702	C	C5-C6-N1	-5.57	118.21	121.00
1	X	1572	C	C6-N1-C2	-5.57	118.07	120.30
1	X	1645	U	N1-C2-O2	-5.57	118.90	122.80
1	X	850	C	C4-C5-C6	5.56	120.18	117.40
1	X	953	G	C8-N9-C4	-5.56	104.17	106.40
1	X	346	C	C4-C5-C6	5.56	120.18	117.40
1	X	821	A	N1-C6-N6	5.56	121.94	118.60
1	X	1273	G	C8-N9-C4	5.56	108.62	106.40
1	X	762	A	C5-C6-N6	-5.56	119.25	123.70
1	X	821	A	N9-C4-C5	-5.56	103.58	105.80
1	X	1771	A	N3-C4-C5	-5.56	122.91	126.80
1	X	1173	G	C5-C6-O6	5.56	131.94	128.60
1	X	1172	U	C5-C4-O4	5.56	129.23	125.90
1	X	2553	G	C4-C5-N7	-5.55	108.58	110.80
1	X	2524	G	C6-N1-C2	-5.55	121.77	125.10
1	X	169	C	C5-C6-N1	-5.55	118.23	121.00
1	X	1577	G	N1-C6-O6	-5.55	116.57	119.90
1	X	1312	G	C5-N7-C8	-5.54	101.53	104.30
1	X	306	G	C8-N9-C4	-5.54	104.18	106.40
1	X	502	A	N1-C2-N3	5.54	132.07	129.30
1	X	1158	A	N9-C4-C5	-5.54	103.58	105.80
1	X	2605	C	C2-N3-C4	-5.54	117.13	119.90
1	X	2745	A	N3-C4-C5	5.54	130.68	126.80
1	X	1458	A	C8-N9-C4	5.54	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1286	U	N1-C2-N3	5.54	118.22	114.90
1	X	2431	C	C2-N3-C4	-5.54	117.13	119.90
1	X	2441	U	C5-C6-N1	-5.54	119.93	122.70
1	X	2616	U	N3-C4-C5	-5.54	111.28	114.60
1	X	479	G	C6-C5-N7	-5.53	127.08	130.40
1	X	697	G	C8-N9-C4	-5.53	104.19	106.40
1	X	2640	G	N1-C6-O6	5.53	123.22	119.90
1	X	2694	G	N3-C4-N9	5.53	129.32	126.00
2	Y	81	C	N3-C4-N4	5.53	121.87	118.00
1	X	613	A	C4-C5-C6	-5.53	114.23	117.00
1	X	697	G	N9-C4-C5	5.53	107.61	105.40
1	X	1718	A	N1-C2-N3	5.53	132.07	129.30
1	X	2326	C	C5-C6-N1	5.53	123.77	121.00
1	X	2810	A	C8-N9-C4	5.53	108.01	105.80
1	X	606	A	C5-C6-N1	-5.53	114.94	117.70
1	X	1759	A	N1-C6-N6	5.53	121.92	118.60
1	X	1138	A	C6-N1-C2	-5.53	115.28	118.60
1	X	58	C	C6-N1-C2	-5.53	118.09	120.30
1	X	1624	A	N9-C4-C5	5.53	108.01	105.80
1	X	1653	C	N3-C4-C5	-5.53	119.69	121.90
1	X	174	A	C4'-C3'-C2'	5.52	108.12	102.60
2	Y	81	C	C6-N1-C2	-5.52	118.09	120.30
1	X	1085	G	C8-N9-C4	-5.52	104.19	106.40
1	X	1267	A	N1-C6-N6	-5.52	115.29	118.60
1	X	1578	U	N1-C2-N3	-5.52	111.59	114.90
1	X	339	U	C6-N1-C2	-5.52	117.69	121.00
1	X	835	U	N1-C2-N3	5.52	118.21	114.90
1	X	1617	G	N9-C4-C5	-5.52	103.19	105.40
1	X	2468	G	C6-C5-N7	5.51	133.71	130.40
1	X	1346	C	C5-C4-N4	-5.51	116.34	120.20
1	X	2657	G	N3-C2-N2	-5.51	116.04	119.90
1	X	527	C	C2-N1-C1'	5.51	124.86	118.80
1	X	691	C	N3-C4-N4	-5.51	114.14	118.00
1	X	981	C	C3'-C2'-C1'	5.51	105.91	101.50
4	B	121	ASN	N-CA-C	-5.51	96.12	111.00
1	X	1172	U	C2-N1-C1'	-5.51	111.09	117.70
1	X	583	C	C5-C4-N4	-5.50	116.35	120.20
1	X	508	G	N9-C4-C5	-5.50	103.20	105.40
1	X	1944	C	C5-C6-N1	-5.50	118.25	121.00
1	X	2687	G	N1-C6-O6	-5.50	116.60	119.90
1	X	584	A	N9-C4-C5	5.50	108.00	105.80
1	X	1983	G	N1-C6-O6	-5.49	116.60	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	100	G	N1-C6-O6	5.49	123.19	119.90
1	X	2790	C	N3-C4-N4	-5.49	114.16	118.00
1	X	746	G	N1-C2-N3	5.49	127.19	123.90
1	X	883	A	C2-N3-C4	5.49	113.34	110.60
1	X	1383	C	C6-N1-C2	5.49	122.50	120.30
1	X	2631	C	C6-N1-C2	5.49	122.50	120.30
1	X	2693	U	N3-C4-O4	-5.49	115.56	119.40
1	X	1627	C	C6-N1-C2	-5.49	118.11	120.30
1	X	1666	G	N9-C4-C5	-5.49	103.21	105.40
1	X	755	C	C6-N1-C2	-5.48	118.11	120.30
1	X	2618	A	C8-N9-C4	-5.48	103.61	105.80
1	X	2060	A	C2-N3-C4	5.48	113.34	110.60
1	X	2679	G	N9-C4-C5	-5.48	103.21	105.40
1	X	1663	C	C5-C4-N4	-5.47	116.37	120.20
2	Y	42	U	N3-C2-O2	5.47	126.03	122.20
1	X	177	U	C6-N1-C2	-5.47	117.72	121.00
1	X	692	C	C5-C6-N1	-5.47	118.27	121.00
1	X	2617	G	C5-C6-N1	5.47	114.23	111.50
1	X	806	A	C6-C5-N7	5.46	136.13	132.30
1	X	2024	U	N3-C4-C5	5.46	117.88	114.60
1	X	991	A	C5-C6-N6	-5.46	119.33	123.70
1	X	1256	C	N1-C2-N3	5.46	123.02	119.20
1	X	1962	C	N1-C2-O2	-5.46	115.62	118.90
1	X	2020	G	N3-C2-N2	5.46	123.72	119.90
2	Y	93	G	C8-N9-C4	-5.46	104.22	106.40
1	X	1169	C	C6-N1-C2	5.46	122.48	120.30
1	X	1966	C	C2-N1-C1'	-5.45	112.80	118.80
1	X	2025	A	C4-C5-N7	5.45	113.43	110.70
1	X	2504	G	N1-C6-O6	-5.45	116.63	119.90
1	X	1635	G	C8-N9-C4	-5.45	104.22	106.40
1	X	659	G	C8-N9-C4	5.45	108.58	106.40
1	X	1768	U	N1-C2-N3	5.45	118.17	114.90
1	X	2362	G	N3-C4-C5	5.45	131.32	128.60
1	X	21	A	C4-C5-N7	5.45	113.42	110.70
1	X	1396	C	C2-N1-C1'	-5.45	112.81	118.80
1	X	2559	U	C4-C5-C6	-5.45	116.43	119.70
1	X	2807	U	N3-C2-O2	-5.45	118.39	122.20
1	X	1578	U	N3-C2-O2	5.45	126.01	122.20
1	X	2548	G	C4-C5-N7	-5.44	108.62	110.80
1	X	2751	C	C2-N1-C1'	-5.44	112.81	118.80
1	X	2824	C	N3-C4-N4	-5.44	114.19	118.00
2	Y	47	A	C8-N9-C4	-5.44	103.62	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1334	A	N1-C6-N6	5.44	121.86	118.60
1	X	1563	U	N3-C4-C5	5.44	117.86	114.60
1	X	2495	G	C5-C6-O6	-5.44	125.34	128.60
2	Y	32	C	C6-N1-C2	5.44	122.48	120.30
1	X	1033	G	N3-C4-C5	-5.44	125.88	128.60
1	X	1311	C	N3-C2-O2	-5.44	118.09	121.90
1	X	1940	C	C6-N1-C2	5.44	122.47	120.30
1	X	22	C	N1-C2-N3	5.43	123.00	119.20
1	X	502	A	N1-C6-N6	-5.43	115.34	118.60
1	X	1283	C	C2-N1-C1'	-5.43	112.82	118.80
1	X	1314	A	C8-N9-C4	-5.43	103.63	105.80
1	X	2848	A	C4-C5-C6	5.43	119.72	117.00
1	X	570	G	N3-C4-C5	5.43	131.31	128.60
1	X	2809	A	C5-C6-N1	5.43	120.41	117.70
1	X	999	A	N1-C6-N6	-5.43	115.34	118.60
1	X	2832	G	C5-C6-O6	-5.43	125.34	128.60
1	X	1613	G	C8-N9-C4	5.42	108.57	106.40
1	X	2805	G	C5-N7-C8	5.42	107.01	104.30
1	X	502	A	C4-C5-N7	-5.42	107.99	110.70
1	X	2054	A	N9-C4-C5	5.42	107.97	105.80
1	X	2550	C	N1-C2-N3	5.42	123.00	119.20
1	X	225	G	N3-C4-C5	5.42	131.31	128.60
1	X	2799	C	N1-C2-N3	5.42	122.99	119.20
1	X	342	G	N1-C6-O6	5.42	123.15	119.90
1	X	2498	U	N1-C2-N3	5.42	118.15	114.90
1	X	223	C	N1-C2-O2	-5.42	115.65	118.90
1	X	1242	A	N7-C8-N9	-5.42	111.09	113.80
1	X	1764	A	C4'-C3'-C2'	-5.42	97.19	102.60
1	X	357	A	C5-C6-N1	-5.41	114.99	117.70
1	X	2003	A	N9-C4-C5	5.41	107.97	105.80
1	X	2013	A	C8-N9-C4	5.41	107.97	105.80
1	X	2696	A	C5-N7-C8	5.41	106.61	103.90
1	X	1225	G	N9-C4-C5	-5.41	103.23	105.40
1	X	1299	A	N3-C4-C5	5.41	130.59	126.80
1	X	2363	G	C8-N9-C4	5.41	108.56	106.40
1	X	2651	U	N1-C2-O2	-5.41	119.01	122.80
1	X	2656	G	N7-C8-N9	-5.41	110.39	113.10
1	X	231	G	N9-C4-C5	5.41	107.56	105.40
1	X	1939	U	N3-C2-O2	5.41	125.98	122.20
1	X	1998	A	N9-C4-C5	5.41	107.96	105.80
1	X	528	G	C4-C5-N7	5.40	112.96	110.80
1	X	508	G	C4-C5-N7	5.40	112.96	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	923	A	C2-N3-C4	5.40	113.30	110.60
1	X	1467	U	C4'-C3'-C2'	-5.40	97.20	102.60
1	X	597	U	N3-C2-O2	5.40	125.98	122.20
1	X	872	G	N3-C4-N9	5.40	129.24	126.00
1	X	1656	U	C2-N3-C4	-5.40	123.76	127.00
1	X	2444	C	C6-N1-C2	-5.40	118.14	120.30
1	X	2876	C	C6-N1-C2	5.40	122.46	120.30
1	X	1260	A	C5-C6-N6	5.40	128.02	123.70
1	X	1007	A	N9-C4-C5	5.40	107.96	105.80
1	X	2755	A	C8-N9-C4	5.40	107.96	105.80
1	X	522	G	N3-C4-N9	-5.39	122.76	126.00
1	X	530	G	C5-C6-N1	-5.39	108.80	111.50
1	X	593	C	C6-N1-C2	-5.39	118.14	120.30
1	X	1203	A	C5-C6-N1	-5.39	115.00	117.70
1	X	973	U	N1-C2-N3	5.39	118.14	114.90
1	X	1621	C	C3'-C2'-O2'	-5.39	97.66	113.30
1	X	2230	G	C5-N7-C8	-5.39	101.60	104.30
1	X	2682	C	N3-C4-C5	-5.39	119.74	121.90
1	X	2253	A	C2-N3-C4	-5.39	107.91	110.60
1	X	2464	G	C4-C5-N7	5.39	112.96	110.80
1	X	797	A	N9-C4-C5	-5.38	103.65	105.80
1	X	1325	U	N3-C4-C5	-5.38	111.37	114.60
1	X	1705	U	N1-C2-O2	-5.38	119.03	122.80
1	X	2412	A	N1-C6-N6	-5.38	115.37	118.60
1	X	1992	G	N7-C8-N9	-5.38	110.41	113.10
1	X	592	G	N1-C6-O6	5.38	123.13	119.90
1	X	1966	C	C5-C6-N1	-5.38	118.31	121.00
1	X	2247	A	N9-C4-C5	-5.38	103.65	105.80
1	X	493	A	C8-N9-C4	5.37	107.95	105.80
1	X	1028	G	N9-C4-C5	-5.37	103.25	105.40
1	X	695	G	C8-N9-C4	5.37	108.55	106.40
1	X	1641	C	N3-C4-C5	5.37	124.05	121.90
1	X	2222	U	C2-N3-C4	-5.37	123.78	127.00
1	X	1778	U	C5-C6-N1	-5.36	120.02	122.70
1	X	2705	A	P-O3'-C3'	5.36	126.14	119.70
1	X	818	G	C5-C6-O6	-5.36	125.38	128.60
1	X	806	A	N7-C8-N9	-5.36	111.12	113.80
1	X	2527	G	N1-C6-O6	-5.36	116.69	119.90
1	X	2678	C	C4-C5-C6	5.36	120.08	117.40
1	X	1452	U	N3-C4-O4	5.36	123.15	119.40
1	X	1998	A	N7-C8-N9	-5.36	111.12	113.80
1	X	2038	C	C2-N1-C1'	-5.36	112.91	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1236	G	C8-N9-C4	5.35	108.54	106.40
1	X	580	A	N1-C2-N3	5.35	131.98	129.30
1	X	2042	A	C8-N9-C4	5.35	107.94	105.80
1	X	2425	G	N1-C2-N2	5.35	121.02	116.20
1	X	1664	G	N9-C4-C5	-5.35	103.26	105.40
1	X	1718	A	C2-N3-C4	-5.35	107.92	110.60
1	X	2611	A	C8-N9-C4	5.35	107.94	105.80
1	X	686	C	C4-C5-C6	-5.34	114.73	117.40
1	X	1236	G	C5-C6-N1	5.34	114.17	111.50
2	Y	63	A	N9-C4-C5	5.34	107.94	105.80
1	X	745	C	C4-C5-C6	5.34	120.07	117.40
1	X	850	C	C6-N1-C1'	5.34	127.21	120.80
1	X	1673	C	N3-C4-N4	5.34	121.74	118.00
1	X	2855	C	C6-N1-C2	5.34	122.44	120.30
1	X	401	G	N3-C4-N9	-5.34	122.80	126.00
1	X	2835	A	C2-N3-C4	-5.34	107.93	110.60
1	X	510	G	N1-C6-O6	-5.34	116.70	119.90
1	X	1366	A	C8-N9-C4	5.34	107.94	105.80
1	X	156	G	N3-C4-C5	5.33	131.27	128.60
1	X	1991	C	C2-N3-C4	-5.33	117.23	119.90
1	X	660	G	C8-N9-C4	-5.33	104.27	106.40
1	X	1181	C	C6-N1-C2	5.33	122.43	120.30
1	X	1332	G	N1-C6-O6	5.33	123.10	119.90
1	X	484	G	C8-N9-C4	-5.33	104.27	106.40
1	X	2486	C	P-O5'-C5'	5.33	129.43	120.90
1	X	121	G	C8-N9-C4	5.33	108.53	106.40
1	X	1937	G	N9-C4-C5	-5.33	103.27	105.40
1	X	1958	G	N9-C4-C5	-5.33	103.27	105.40
1	X	2019	C	N3-C2-O2	5.32	125.63	121.90
1	X	2623	A	C5-N7-C8	5.32	106.56	103.90
1	X	2864	C	C5-C6-N1	-5.32	118.34	121.00
1	X	12	U	N3-C2-O2	5.32	125.92	122.20
1	X	566	U	C5-C6-N1	5.32	125.36	122.70
1	X	583	C	N3-C2-O2	5.32	125.62	121.90
1	X	739	G	N3-C4-C5	-5.32	125.94	128.60
1	X	1459	U	N3-C2-O2	5.32	125.92	122.20
1	X	787	A	N9-C4-C5	-5.32	103.67	105.80
1	X	1752	U	N3-C2-O2	-5.32	118.48	122.20
1	X	1445	A	N9-C4-C5	-5.31	103.67	105.80
1	X	2362	G	C4-C5-N7	5.31	112.93	110.80
1	X	158	A	N1-C6-N6	-5.31	115.41	118.60
1	X	1768	U	C6-N1-C2	-5.31	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	805	G	C6-C5-N7	5.31	133.59	130.40
1	X	175	C	N3-C2-O2	5.31	125.62	121.90
1	X	2021	G	C5-C6-N1	-5.31	108.84	111.50
1	X	1158	A	N7-C8-N9	-5.31	111.15	113.80
1	X	2856	U	C4-C5-C6	5.31	122.88	119.70
1	X	329	C	C6-N1-C2	-5.30	118.18	120.30
1	X	2258	G	N1-C2-N2	-5.30	111.43	116.20
1	X	2823	G	N1-C2-N3	5.30	127.08	123.90
1	X	318	G	N7-C8-N9	-5.30	110.45	113.10
1	X	2678	C	C5-C6-N1	-5.30	118.35	121.00
1	X	2815	C	N3-C4-N4	-5.30	114.29	118.00
1	X	1041	G	N9-C4-C5	5.30	107.52	105.40
1	X	744	C	N1-C2-O2	-5.30	115.72	118.90
1	X	1543	G	C8-N9-C4	-5.30	104.28	106.40
1	X	549	G	N3-C4-C5	-5.29	125.95	128.60
1	X	1948	C	C6-N1-C2	5.29	122.42	120.30
1	X	2513	A	C2-N3-C4	-5.29	107.95	110.60
1	X	2621	G	N3-C2-N2	-5.29	116.20	119.90
1	X	1672	A	N1-C6-N6	5.29	121.77	118.60
1	X	1396	C	C6-N1-C2	5.29	122.42	120.30
1	X	2244	C	N3-C2-O2	-5.29	118.20	121.90
1	X	2303	C	C5-C6-N1	-5.28	118.36	121.00
1	X	2790	C	C2-N3-C4	-5.28	117.26	119.90
1	X	219	G	N3-C4-N9	5.28	129.17	126.00
1	X	739	G	C2-N3-C4	5.28	114.54	111.90
1	X	1667	A	C6-C5-N7	-5.28	128.60	132.30
1	X	2508	G	N9-C4-C5	-5.28	103.29	105.40
1	X	1038	U	N1-C2-N3	5.28	118.07	114.90
1	X	1752	U	N1-C2-N3	5.28	118.07	114.90
1	X	1766	U	N1-C2-O2	-5.28	119.11	122.80
1	X	2243	C	C4-C5-C6	5.28	120.04	117.40
1	X	1135	C	C2-N1-C1'	-5.27	113.00	118.80
1	X	872	G	N3-C4-C5	-5.27	125.96	128.60
1	X	923	A	N1-C2-N3	-5.27	126.66	129.30
1	X	937	C	N1-C2-O2	-5.27	115.74	118.90
1	X	1203	A	C6-N1-C2	5.27	121.76	118.60
1	X	2025	A	N1-C6-N6	5.27	121.76	118.60
1	X	2241	U	C5-C6-N1	-5.27	120.06	122.70
1	X	915	C	C6-N1-C2	5.27	122.41	120.30
1	X	1571	G	C8-N9-C4	-5.27	104.29	106.40
1	X	1983	G	C5-N7-C8	5.27	106.94	104.30
1	X	569	C	C5-C4-N4	-5.27	116.51	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1306	U	C5-C6-N1	-5.27	120.07	122.70
1	X	2849	C	N1-C2-O2	-5.27	115.74	118.90
1	X	971	A	N1-C6-N6	-5.27	115.44	118.60
1	X	2585	C	N1-C2-O2	-5.27	115.74	118.90
1	X	791	G	N1-C6-O6	-5.26	116.74	119.90
1	X	21	A	C5-N7-C8	-5.26	101.27	103.90
1	X	1256	C	C4-C5-C6	5.26	120.03	117.40
1	X	1749	G	C1'-O4'-C4'	-5.26	105.69	109.90
1	X	317	U	N1-C2-O2	-5.26	119.12	122.80
1	X	828	C	C6-N1-C2	5.26	122.40	120.30
1	X	850	C	N1-C2-N3	5.26	122.88	119.20
1	X	2209	G	N9-C4-C5	5.26	107.50	105.40
1	X	746	G	N1-C2-N2	-5.26	111.47	116.20
1	X	237	G	C8-N9-C4	-5.25	104.30	106.40
1	X	529	U	N1-C2-N3	5.25	118.05	114.90
1	X	1671	A	N9-C4-C5	-5.25	103.70	105.80
1	X	2833	C	N1-C2-O2	5.25	122.05	118.90
1	X	10	A	N9-C4-C5	-5.25	103.70	105.80
1	X	504	G	N3-C4-C5	5.25	131.23	128.60
1	X	691	C	N1-C2-O2	-5.25	115.75	118.90
1	X	1282	A	C8-N9-C4	5.25	107.90	105.80
1	X	787	A	N1-C6-N6	5.25	121.75	118.60
1	X	1678	G	N7-C8-N9	-5.25	110.48	113.10
1	X	2848	A	N3-C4-C5	-5.25	123.13	126.80
1	X	340	G	N3-C2-N2	5.24	123.57	119.90
1	X	458	G	N9-C4-C5	5.24	107.50	105.40
1	X	1282	A	C6-C5-N7	-5.24	128.63	132.30
1	X	2290	A	C8-N9-C4	5.24	107.90	105.80
1	X	818	G	N9-C4-C5	-5.24	103.30	105.40
1	X	2809	A	C6-N1-C2	-5.24	115.46	118.60
1	X	2757	G	N1-C2-N3	5.24	127.04	123.90
1	X	586	G	N1-C6-O6	5.24	123.04	119.90
1	X	1104	G	N3-C4-C5	-5.24	125.98	128.60
1	X	1998	A	C5-N7-C8	5.24	106.52	103.90
1	X	1953	A	C8-N9-C4	-5.23	103.71	105.80
1	X	2259	G	N1-C2-N3	5.23	127.04	123.90
1	X	1351	G	C8-N9-C4	5.23	108.49	106.40
1	X	1470	G	O4'-C1'-N9	5.23	112.38	108.20
1	X	2412	A	C5-C6-N1	5.23	120.31	117.70
1	X	2233	C	C6-N1-C2	5.23	122.39	120.30
1	X	2392	G	N3-C4-C5	5.23	131.22	128.60
1	X	457	C	C6-N1-C2	-5.23	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2634	G	N7-C8-N9	-5.23	110.49	113.10
1	X	1622	G	N1-C2-N2	-5.22	111.50	116.20
1	X	2700	U	C4'-C3'-C2'	-5.22	97.38	102.60
1	X	1033	G	C4-C5-N7	-5.22	108.71	110.80
1	X	1212	U	C5-C6-N1	-5.22	120.09	122.70
1	X	2466	G	N1-C6-O6	5.22	123.03	119.90
1	X	1395	A	C8-N9-C4	-5.22	103.71	105.80
1	X	2398	U	C4-C5-C6	5.22	122.83	119.70
1	X	1480	G	C5-C6-O6	-5.22	125.47	128.60
1	X	2051	U	C2-N3-C4	-5.22	123.87	127.00
1	X	2676	G	N3-C4-C5	-5.22	125.99	128.60
1	X	41	G	C8-N9-C4	5.22	108.49	106.40
1	X	2356	A	C5-C6-N6	-5.22	119.53	123.70
1	X	2247	A	N1-C2-N3	-5.22	126.69	129.30
1	X	2848	A	C4-C5-N7	-5.22	108.09	110.70
1	X	1009	C	C6-N1-C1'	-5.21	114.55	120.80
1	X	174	A	C3'-C2'-C1'	-5.21	97.33	101.50
1	X	917	U	C6-N1-C2	-5.21	117.87	121.00
1	X	2522	G	N1-C2-N3	5.21	127.03	123.90
1	X	471	A	C2-N3-C4	-5.21	108.00	110.60
1	X	1922	U	N3-C2-O2	-5.20	118.56	122.20
1	X	2566	A	C6-C5-N7	-5.20	128.66	132.30
1	X	2690	A	C2-N3-C4	-5.20	108.00	110.60
1	X	2031	A	N7-C8-N9	-5.20	111.20	113.80
1	X	2473	G	N1-C6-O6	-5.20	116.78	119.90
1	X	1129	A	C8-N9-C4	-5.20	103.72	105.80
1	X	2850	U	N1-C2-O2	-5.20	119.16	122.80
1	X	1060	C	C6-N1-C2	-5.19	118.22	120.30
1	X	1951	G	N3-C4-C5	-5.19	126.00	128.60
1	X	462	G	N1-C6-O6	5.19	123.02	119.90
1	X	1654	A	N1-C2-N3	5.19	131.90	129.30
1	X	2669	C	N3-C2-O2	-5.19	118.27	121.90
1	X	1780	A	C4-C5-C6	5.19	119.59	117.00
1	X	2832	G	C6-C5-N7	-5.19	127.29	130.40
1	X	440	U	C5-C4-O4	5.19	129.01	125.90
1	X	1325	U	N3-C4-O4	5.19	123.03	119.40
1	X	2348	A	C2-N3-C4	-5.19	108.01	110.60
1	X	1041	G	C2-N3-C4	-5.19	109.31	111.90
1	X	1284	G	C5-C6-O6	5.18	131.71	128.60
1	X	2039	G	N3-C2-N2	-5.18	116.27	119.90
1	X	2415	G	N3-C2-N2	-5.18	116.27	119.90
5	C	46	ARG	NE-CZ-NH1	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2698	G	N3-C2-N2	-5.18	116.27	119.90
3	A	253	LYS	C-N-CD	-5.18	109.20	120.60
1	X	2261	G	N1-C6-O6	-5.18	116.79	119.90
1	X	2441	U	C2-N3-C4	-5.18	123.89	127.00
2	Y	96	C	C6-N1-C2	-5.18	118.23	120.30
1	X	1771	A	C2-N3-C4	5.17	113.19	110.60
1	X	2613	A	C8-N9-C4	5.17	107.87	105.80
4	B	146	THR	C-N-CD	-5.17	109.22	120.60
1	X	2258	G	C5-C6-N1	5.17	114.09	111.50
15	M	42	GLY	N-CA-C	-5.17	100.17	113.10
1	X	1654	A	C5-C6-N6	5.17	127.84	123.70
1	X	2523	G	N9-C4-C5	5.17	107.47	105.40
1	X	1297	A	N1-C6-N6	5.17	121.70	118.60
1	X	1396	C	N3-C2-O2	5.17	125.52	121.90
2	Y	39	C	C6-N1-C2	5.17	122.37	120.30
1	X	470	U	N3-C4-O4	-5.17	115.78	119.40
1	X	597	U	C6-N1-C2	5.17	124.10	121.00
1	X	2329	C	C2-N3-C4	-5.17	117.32	119.90
1	X	15	G	N1-C6-O6	-5.16	116.80	119.90
1	X	1288	A	N1-C2-N3	5.16	131.88	129.30
1	X	1928	G	C5-C6-O6	5.16	131.70	128.60
1	X	1995	G	N1-C2-N3	5.16	127.00	123.90
1	X	2798	A	C4-C5-N7	5.16	113.28	110.70
1	X	528	G	N3-C4-N9	5.16	129.09	126.00
1	X	1334	A	C4-C5-C6	5.16	119.58	117.00
1	X	2812	A	C4-C5-C6	5.16	119.58	117.00
1	X	146	C	C6-N1-C2	5.16	122.36	120.30
1	X	767	G	N3-C2-N2	5.15	123.51	119.90
1	X	1964	A	C4'-C3'-C2'	-5.15	97.45	102.60
1	X	1716	G	C5-N7-C8	5.15	106.88	104.30
1	X	1306	U	N3-C4-O4	-5.15	115.80	119.40
1	X	90	G	N1-C6-O6	-5.15	116.81	119.90
1	X	1625	A	C5-N7-C8	-5.15	101.33	103.90
1	X	939	C	C6-N1-C2	5.14	122.36	120.30
1	X	1355	A	C2-N3-C4	-5.14	108.03	110.60
1	X	1466	C	C5'-C4'-O4'	-5.14	102.93	109.10
1	X	985	G	N1-C6-O6	5.14	122.98	119.90
1	X	2336	G	C5-C6-N1	-5.14	108.93	111.50
1	X	2725	C	C5-C6-N1	-5.14	118.43	121.00
1	X	720	A	C5-C6-N1	-5.14	115.13	117.70
1	X	1818	G	N3-C4-N9	5.14	129.08	126.00
1	X	704	G	C8-N9-C4	5.14	108.45	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	827	C	N3-C4-N4	-5.14	114.40	118.00
1	X	2207	G	C8-N9-C4	5.14	108.45	106.40
1	X	489	A	C5-C6-N6	5.14	127.81	123.70
1	X	536	A	N9-C4-C5	5.14	107.86	105.80
1	X	70	A	C5-N7-C8	-5.13	101.33	103.90
1	X	634	G	C4-C5-N7	-5.13	108.75	110.80
1	X	2640	G	C8-N9-C4	5.13	108.45	106.40
1	X	594	G	C8-N9-C4	-5.13	104.35	106.40
1	X	660	G	N3-C4-N9	-5.13	122.92	126.00
1	X	2827	G	C2-N3-C4	5.12	114.46	111.90
1	X	659	G	N7-C8-N9	-5.12	110.54	113.10
1	X	1726	C	N1-C2-O2	-5.12	115.83	118.90
1	X	1718	A	C4-C5-C6	5.12	119.56	117.00
1	X	2219	U	N3-C4-C5	-5.12	111.53	114.60
1	X	2790	C	C5-C4-N4	5.12	123.78	120.20
1	X	213	C	C6-N1-C2	5.12	122.35	120.30
1	X	2415	G	N1-C2-N2	5.12	120.81	116.20
1	X	995	A	C1'-O4'-C4'	-5.11	105.81	109.90
1	X	1316	G	N3-C4-N9	-5.11	122.93	126.00
1	X	1717	A	C8-N9-C4	-5.11	103.75	105.80
1	X	445	A	C8-N9-C4	-5.11	103.76	105.80
1	X	524	A	C5-C6-N1	5.11	120.25	117.70
1	X	1228	G	C4-C5-N7	-5.11	108.76	110.80
1	X	1579	G	N1-C6-O6	5.11	122.97	119.90
1	X	2209	G	C8-N9-C4	-5.11	104.36	106.40
20	R	85	ASP	C-N-CD	-5.11	109.36	120.60
21	S	90	GLU	C-N-CD	-5.11	109.36	120.60
1	X	1017	C	N1-C2-O2	-5.11	115.83	118.90
1	X	2548	G	N3-C4-C5	-5.11	126.05	128.60
1	X	2551	A	N1-C6-N6	-5.11	115.53	118.60
1	X	812	G	N9-C4-C5	5.11	107.44	105.40
1	X	1205	G	N1-C2-N3	5.11	126.96	123.90
1	X	2703	C	N1-C2-O2	-5.11	115.84	118.90
1	X	168	A	N1-C2-N3	5.10	131.85	129.30
1	X	955	G	O3'-P-O5'	-5.10	94.30	104.00
1	X	1766	U	N3-C2-O2	5.10	125.77	122.20
1	X	2669	C	N3-C4-C5	-5.10	119.86	121.90
1	X	787	A	C2-N3-C4	-5.10	108.05	110.60
1	X	1976	U	C4'-C3'-C2'	-5.10	97.50	102.60
1	X	2703	C	C2-N1-C1'	-5.10	113.19	118.80
1	X	736	G	N7-C8-N9	-5.10	110.55	113.10
1	X	339	U	C5-C4-O4	5.10	128.96	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1665	C	C6-N1-C1'	-5.10	114.68	120.80
1	X	462	G	C5-C6-N1	-5.10	108.95	111.50
1	X	2489	C	N1-C2-N3	5.09	122.77	119.20
1	X	102	C	C6-N1-C2	5.09	122.34	120.30
1	X	2035	G	N9-C4-C5	5.09	107.44	105.40
1	X	1311	C	N1-C2-O2	5.09	121.95	118.90
2	Y	12	C	C6-N1-C2	5.09	122.34	120.30
1	X	27	G	N3-C4-C5	-5.09	126.06	128.60
1	X	751	G	C5-C6-O6	-5.09	125.55	128.60
1	X	982	C	C2-N1-C1'	5.09	124.40	118.80
1	X	1479	G	C5-C6-O6	-5.09	125.55	128.60
1	X	1539	U	N3-C4-O4	5.09	122.96	119.40
1	X	2602	G	C2-N3-C4	5.09	114.44	111.90
1	X	613	A	N9-C4-C5	-5.09	103.77	105.80
1	X	953	G	N3-C4-C5	-5.09	126.06	128.60
1	X	2520	A	C4-C5-N7	-5.09	108.16	110.70
1	X	1241	G	N3-C4-N9	5.08	129.05	126.00
2	Y	101	A	C4-C5-N7	-5.08	108.16	110.70
1	X	948	C	C6-N1-C2	5.08	122.33	120.30
1	X	1232	U	N1-C2-O2	-5.08	119.24	122.80
1	X	2036	G	N1-C6-O6	5.08	122.95	119.90
1	X	973	U	N1-C2-O2	-5.08	119.24	122.80
1	X	94	C	C6-N1-C2	5.08	122.33	120.30
1	X	1563	U	C6-N1-C2	5.08	124.05	121.00
1	X	2055	G	C5-N7-C8	5.08	106.84	104.30
1	X	217	U	C6-N1-C2	5.08	124.05	121.00
1	X	530	G	C2-N3-C4	-5.08	109.36	111.90
1	X	833	A	C5-N7-C8	-5.08	101.36	103.90
1	X	115	G	N9-C4-C5	-5.07	103.37	105.40
1	X	670	U	N3-C2-O2	-5.07	118.65	122.20
1	X	2267	A	C8-N9-C4	-5.07	103.77	105.80
1	X	2757	G	C5-C6-N1	-5.07	108.96	111.50
1	X	581	A	N3-C4-C5	5.07	130.35	126.80
1	X	1965	U	C6-N1-C2	-5.07	117.96	121.00
1	X	2660	C	N3-C4-N4	-5.07	114.45	118.00
1	X	2443	C	N3-C4-C5	-5.07	119.87	121.90
1	X	2793	G	C8-N9-C4	5.07	108.43	106.40
1	X	1705	U	N3-C4-O4	-5.07	115.85	119.40
1	X	2243	C	N1-C2-N3	5.07	122.75	119.20
1	X	2688	G	N7-C8-N9	-5.07	110.57	113.10
1	X	1656	U	N3-C4-C5	5.06	117.64	114.60
2	Y	69	G	C4-C5-N7	-5.06	108.77	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1672	A	N3-C4-N9	-5.06	123.35	127.40
1	X	1911	A	C8-N9-C4	-5.06	103.78	105.80
1	X	2019	C	C6-N1-C2	-5.06	118.28	120.30
1	X	2647	G	C8-N9-C4	-5.06	104.38	106.40
1	X	2039	G	N9-C4-C5	-5.06	103.38	105.40
1	X	1238	A	N1-C6-N6	-5.06	115.56	118.60
1	X	2274	C	N3-C2-O2	5.06	125.44	121.90
1	X	2640	G	N3-C4-C5	5.06	131.13	128.60
1	X	529	U	C6-N1-C2	-5.06	117.97	121.00
1	X	1912	G	N7-C8-N9	5.06	115.63	113.10
1	X	1991	C	C6-N1-C1'	5.06	126.87	120.80
1	X	3	U	N3-C2-O2	5.05	125.74	122.20
1	X	236	C	N1-C2-O2	5.05	121.93	118.90
1	X	602	C	N3-C2-O2	5.05	125.44	121.90
18	P	36	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	X	744	C	N3-C4-C5	-5.05	119.88	121.90
1	X	30	G	N9-C4-C5	5.05	107.42	105.40
1	X	1033	G	C5-C6-O6	5.05	131.63	128.60
1	X	2234	G	C5-C6-N1	5.05	114.03	111.50
1	X	2766	U	N3-C4-C5	5.05	117.63	114.60
1	X	1759	A	C5-C6-N6	-5.05	119.66	123.70
1	X	2303	C	C6-N1-C1'	-5.05	114.75	120.80
1	X	165	G	N9-C4-C5	-5.04	103.38	105.40
1	X	1584	G	C4-C5-N7	5.04	112.82	110.80
1	X	1710	U	C6-N1-C2	5.04	124.03	121.00
1	X	2798	A	C5-C6-N1	-5.04	115.18	117.70
1	X	160	C	C6-N1-C2	-5.04	118.28	120.30
1	X	488	A	C5-C6-N1	-5.04	115.18	117.70
1	X	583	C	N1-C2-O2	-5.04	115.88	118.90
1	X	1296	G	C5-C6-O6	5.04	131.62	128.60
1	X	2553	G	C5-N7-C8	5.04	106.82	104.30
1	X	2508	G	C6-C5-N7	-5.04	127.38	130.40
1	X	1041	G	N3-C4-C5	5.04	131.12	128.60
1	X	1316	G	C5-C6-O6	5.04	131.62	128.60
1	X	1780	A	C8-N9-C4	-5.04	103.78	105.80
1	X	1828	C	N3-C4-N4	-5.04	114.47	118.00
1	X	1844	C	C6-N1-C2	-5.04	118.28	120.30
1	X	2412	A	C4-C5-C6	-5.04	114.48	117.00
1	X	531	G	N7-C8-N9	-5.04	110.58	113.10
1	X	2219	U	C6-N1-C2	-5.03	117.98	121.00
1	X	2244	C	N1-C2-O2	5.03	121.92	118.90
1	X	2434	G	C5-C6-O6	5.03	131.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	143	A	C8-N9-C4	5.03	107.81	105.80
1	X	2010	G	N3-C4-N9	5.03	129.02	126.00
1	X	2355	A	N7-C8-N9	-5.03	111.28	113.80
1	X	2679	G	C8-N9-C4	5.03	108.41	106.40
1	X	1242	A	C4-C5-N7	5.03	113.21	110.70
1	X	320	A	C8-N9-C4	5.03	107.81	105.80
1	X	1982	C	C4-C5-C6	5.03	119.91	117.40
1	X	1933	G	N9-C4-C5	5.02	107.41	105.40
1	X	1958	G	N1-C6-O6	5.02	122.91	119.90
1	X	2565	C	N3-C2-O2	-5.02	118.38	121.90
1	X	1584	G	N1-C6-O6	5.02	122.91	119.90
1	X	2587	G	N9-C4-C5	5.02	107.41	105.40
1	X	885	A	N9-C4-C5	5.02	107.81	105.80
1	X	1325	U	C6-N1-C2	-5.02	117.99	121.00
1	X	309	G	N9-C4-C5	-5.02	103.39	105.40
1	X	471	A	N9-C4-C5	-5.02	103.79	105.80
1	X	1240	G	N7-C8-N9	-5.02	110.59	113.10
1	X	1399	C	C6-N1-C2	5.02	122.31	120.30
1	X	1214	C	C6-N1-C2	-5.01	118.29	120.30
1	X	2550	C	C5-C6-N1	5.01	123.51	121.00
1	X	657	A	C8-N9-C4	-5.01	103.80	105.80
1	X	1635	G	C5-N7-C8	-5.01	101.79	104.30
1	X	2603	G	N3-C2-N2	-5.01	116.39	119.90
1	X	88	G	C4-C5-N7	5.01	112.80	110.80
1	X	1287	A	C2-N3-C4	5.01	113.10	110.60
1	X	2567	G	C4-C5-C6	5.00	121.80	118.80
1	X	547	U	N3-C2-O2	5.00	125.70	122.20
1	X	746	G	C2-N3-C4	-5.00	109.40	111.90
1	X	1698	C	N3-C2-O2	5.00	125.40	121.90

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	E	125	VAL	Peptide
7	E	130	ARG	Sidechain
7	E	165	VAL	Peptide
7	E	174	GLY	Peptide
8	F	116	ASN	Peptide
8	F	117	ALA	Peptide
8	F	118	GLY	Peptide
9	G	110	LEU	Peptide

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Mol	Chain	Res	Type	Group
9	G	111	LYS	Peptide
9	G	170	PRO	Peptide
9	G	35	LYS	Peptide
9	G	36	ASN	Peptide
9	G	38	GLU	Peptide
9	G	85	ALA	Peptide
9	G	91	THR	Peptide
10	H	40	GLY	Peptide
10	H	41	ASN	Peptide
11	I	18	ARG	Peptide
12	J	83	ARG	Sidechain

## 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	X	56750	0	0	826	3
2	Y	2561	0	0	25	0
3	A	1920	0	0	70	0
4	B	1539	0	0	54	0
5	C	1481	0	0	34	0
6	D	1394	0	0	11	0
7	E	1286	0	0	5	0
8	F	451	0	0	6	0
9	G	1114	0	0	32	0
10	H	997	0	0	25	0
11	I	1005	0	0	23	0
12	J	1090	0	0	26	0
13	K	878	0	0	25	0
14	L	779	0	0	23	0
15	M	871	0	0	15	3
16	N	978	0	0	24	0
17	O	741	0	0	16	0
18	P	1004	0	0	17	0
19	Q	714	0	0	8	0
20	R	825	0	0	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	S	1345	0	0	8	0
22	T	556	0	0	10	0
23	U	537	0	0	7	0
24	V	525	0	0	2	0
25	W	424	0	0	1	0
26	Z	452	0	0	10	0
27	1	431	0	0	28	0
28	2	383	0	0	15	0
29	3	462	0	0	10	0
30	4	297	0	0	1	0
31	X	33	0	0	7	0
32	X	58	0	69	37	0
33	I	1	0	0	0	0
33	U	1	0	0	0	0
33	X	71	0	0	0	0
34	X	4	0	0	0	0
35	X	5	0	0	0	0
All	All	83963	0	69	1250	3

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 15.

All (1250) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:699:G:N2	28:2:5:TYR:CE1	1.89	1.39
3:A:66:ILE:CG2	3:A:68:PHE:CZ	2.19	1.24
1:X:2662:C:O2	10:H:82:LYS:NZ	1.71	1.22
1:X:2045:A:C6	32:X:2882:LMA:H27A	1.75	1.21
1:X:1391:A:N7	1:X:1393:G:C6	2.10	1.20
1:X:699:G:C8	28:2:11:LYS:CG	2.26	1.18
1:X:2427:A:N6	11:I:40:ARG:NH2	1.90	1.18
1:X:1692:C:O2	4:B:128:SER:O	1.62	1.17
32:X:2882:LMA:H34	32:X:2882:LMA:H56B	1.28	1.15
32:X:2882:LMA:C34	32:X:2882:LMA:H56B	1.75	1.15
1:X:1685:A:N6	1:X:1974:U:O2	1.82	1.12
9:G:35:LYS:CB	9:G:37:ASP:OD2	2.00	1.08
9:G:35:LYS:CG	9:G:37:ASP:OD2	2.03	1.06
1:X:1391:A:C5	1:X:1393:G:C5	2.43	1.06
17:O:21:ARG:NH2	17:O:88:GLN:OE1	1.86	1.05
1:X:1142:G:N2	9:G:101:THR:CG2	2.20	1.05
32:X:2882:LMA:H40	32:X:2882:LMA:H29B	1.37	1.03
21:S:129:ARG:NH2	21:S:156:GLU:OE1	1.93	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1391:A:C8	1:X:1393:G:O6	2.14	1.01
32:X:2882:LMA:H56A	32:X:2882:LMA:H12	1.42	0.99
1:X:2494:C:OP1	9:G:108:GLY:O	1.81	0.99
1:X:309:G:OP1	20:R:93:ARG:O	1.81	0.98
1:X:775:U:C5'	1:X:776:G:C2	2.45	0.98
1:X:348:U:OP2	20:R:93:ARG:NH2	1.98	0.97
1:X:699:G:N7	28:2:11:LYS:CG	2.28	0.96
1:X:2257:A:N6	22:T:15:ASP:OD1	1.99	0.95
1:X:775:U:C5'	1:X:776:G:N2	2.30	0.95
1:X:334:G:N2	5:C:162:ARG:NH2	2.15	0.94
32:X:2882:LMA:H12	32:X:2882:LMA:C56	1.99	0.93
1:X:123:A:O2'	28:2:13:ALA:O	1.89	0.91
1:X:1291:G:OP1	13:K:36:THR:OG1	1.89	0.90
27:1:28:ARG:CB	27:1:30:ASN:OD1	2.20	0.89
3:A:90:SER:O	3:A:199:ASN:ND2	2.05	0.89
32:X:2882:LMA:H56A	32:X:2882:LMA:H57	1.53	0.88
1:X:1391:A:C8	1:X:1393:G:C6	2.61	0.88
22:T:14:ARG:O	22:T:15:ASP:OD2	1.92	0.88
1:X:919:U:OP1	12:J:26:ASP:OD2	1.91	0.87
31:X:2881:LC2:C2	31:X:2881:LC2:C28	2.51	0.87
1:X:1391:A:C4	1:X:1393:G:N7	2.43	0.86
1:X:2664:G:OP1	10:H:90:ARG:NH1	2.08	0.86
1:X:1692:C:C2	4:B:128:SER:O	2.28	0.85
32:X:2882:LMA:H32	32:X:2882:LMA:O53	1.76	0.84
1:X:2350:G:O2'	27:1:46:LYS:CG	2.25	0.84
3:A:218:ARG:CG	3:A:219:LYS:N	2.39	0.84
14:L:39:TYR:O	14:L:54:ALA:O	1.96	0.84
1:X:2264:C:C5	27:1:28:ARG:NH1	2.46	0.83
32:X:2882:LMA:O9	32:X:2882:LMA:H32A	1.77	0.83
18:P:41:VAL:O	18:P:44:VAL:CG2	2.27	0.83
10:H:100:ASN:OD1	10:H:102:GLN:N	2.12	0.82
1:X:1685:A:N6	1:X:1974:U:C2	2.48	0.82
1:X:334:G:C2	5:C:162:ARG:NH2	2.48	0.82
1:X:2350:G:O2'	27:1:46:LYS:CB	2.28	0.81
3:A:26:THR:CG2	3:A:27:LYS:N	2.44	0.81
14:L:37:HIS:NE2	14:L:39:TYR:CZ	2.49	0.80
1:X:834:A:O2'	1:X:957:G:OP2	1.98	0.80
1:X:1685:A:O4'	1:X:1686:A:C2	2.35	0.80
14:L:21:THR:CG2	14:L:45:ASP:O	2.29	0.80
1:X:2045:A:C6	32:X:2882:LMA:C27	2.61	0.80
31:X:2881:LC2:C14	31:X:2881:LC2:O6	2.30	0.80
17:O:80:TYR:O	17:O:80:TYR:CG	2.34	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1391:A:C4'	1:X:1392:U:OP1	2.30	0.80
3:A:27:LYS:CE	3:A:205:ILE:CD1	2.59	0.80
3:A:84:GLU:OE2	3:A:105:TYR:CE2	2.34	0.80
1:X:845:U:OP1	11:I:38:LYS:NZ	2.14	0.79
32:X:2882:LMA:C34	32:X:2882:LMA:C56	2.60	0.79
1:X:1391:A:N7	1:X:1393:G:C5	2.47	0.79
1:X:2264:C:C5	27:1:28:ARG:CZ	2.66	0.79
1:X:1336:G:OP1	18:P:119:LYS:NZ	2.15	0.79
1:X:1691:G:N1	1:X:1972:G:O6	2.16	0.79
1:X:2045:A:N6	32:X:2882:LMA:H27A	1.97	0.78
1:X:309:G:OP1	20:R:93:ARG:CB	2.31	0.78
1:X:596:C:OP2	11:I:29:THR:CG2	2.31	0.78
3:A:66:ILE:CG2	3:A:68:PHE:CE2	2.66	0.78
16:N:25:TRP:CE3	16:N:26:GLY:N	2.52	0.78
1:X:587:A:OP1	1:X:1268:U:O2'	2.03	0.77
1:X:1142:G:C1'	9:G:103:TYR:CD2	2.67	0.77
1:X:1668:G:N2	1:X:1990:U:C2	2.53	0.77
1:X:1365:U:O2	1:X:1393:G:C2	2.38	0.77
1:X:2663:U:O4	1:X:2664:G:O6	2.02	0.77
3:A:102:GLU:OE2	3:A:104:ARG:NE	2.18	0.77
1:X:1365:U:O2	1:X:1393:G:N2	2.18	0.76
1:X:791:G:C2	1:X:800:U:O2	2.38	0.76
1:X:400:U:OP2	23:U:37:ILE:CD1	2.34	0.76
1:X:2426:G:C3'	1:X:2479:U:OP2	2.33	0.76
3:A:160:ALA:CB	3:A:199:ASN:CG	2.54	0.76
32:X:2882:LMA:C29	32:X:2882:LMA:H40	2.16	0.76
1:X:2855:C:O2'	13:K:90:ARG:NH1	2.19	0.75
1:X:1203:A:OP1	11:I:33:GLY:O	2.05	0.75
3:A:22:PHE:O	3:A:209:LYS:CG	2.35	0.75
1:X:1289:A:C2	1:X:1290:A:C5	2.74	0.75
32:X:2882:LMA:H34B	32:X:2882:LMA:H56B	1.66	0.75
3:A:30:PRO:C	3:A:31:GLU:OE1	2.26	0.74
4:B:78:LEU:O	4:B:79:ARG:CD	2.35	0.74
1:X:797:A:O2'	1:X:798:G:C8	2.40	0.74
1:X:2841:U:O2'	1:X:2842:C:P	2.46	0.74
1:X:309:G:OP1	20:R:93:ARG:C	2.26	0.74
3:A:160:ALA:CB	3:A:199:ASN:ND2	2.51	0.74
3:A:102:GLU:OE2	3:A:104:ARG:CZ	2.36	0.74
1:X:337:G:O2'	20:R:9:HIS:ND1	2.20	0.74
21:S:13:LYS:CE	21:S:33:ALA:CB	2.66	0.73
1:X:2015:G:C4'	1:X:2016:A:OP1	2.37	0.73
16:N:59:ARG:O	16:N:63:GLN:OE1	2.07	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1289:A:C2	1:X:1290:A:C4	2.77	0.72
1:X:2840:U:C4	1:X:2841:U:C5	2.77	0.72
17:O:21:ARG:O	17:O:91:THR:CG2	2.38	0.72
1:X:1684:G:O2'	1:X:1974:U:O4	2.08	0.71
6:D:123:ASP:OD1	6:D:125:ARG:N	2.23	0.71
12:J:27:TYR:O	12:J:28:VAL:CG2	2.39	0.71
1:X:1391:A:N7	1:X:1393:G:O6	2.17	0.71
1:X:958:G:O2'	1:X:995:A:N1	2.24	0.71
1:X:798:G:O2'	1:X:1770:U:C5'	2.39	0.71
4:B:84:PHE:CD2	4:B:84:PHE:O	2.44	0.71
1:X:2664:G:N2	1:X:2706:U:O2	2.24	0.71
1:X:703:A:O2'	1:X:793:G:OP1	2.09	0.71
1:X:699:G:O6	28:2:12:ARG:CA	2.39	0.70
3:A:55:ILE:CD1	3:A:55:ILE:N	2.54	0.70
4:B:121:ASN:O	4:B:122:PHE:CB	2.39	0.70
14:L:37:HIS:CD2	14:L:39:TYR:CE1	2.79	0.70
1:X:1290:A:OP1	13:K:40:LYS:NZ	2.24	0.70
1:X:2478:C:O5'	1:X:2478:C:C6	2.44	0.69
5:C:7:ILE:O	5:C:120:VAL:O	2.09	0.69
1:X:1391:A:C5	1:X:1393:G:N7	2.60	0.69
3:A:154:ALA:O	3:A:158:ARG:NH2	2.25	0.69
1:X:116:A:OP1	28:2:22:MET:SD	2.50	0.69
1:X:863:C:O2'	25:W:19:THR:OG1	2.09	0.69
32:X:2882:LMA:O9	32:X:2882:LMA:C32	2.41	0.69
1:X:1686:A:O2'	1:X:2528:G:OP1	2.11	0.69
1:X:919:U:OP1	12:J:26:ASP:CG	2.31	0.69
1:X:2012:A:C2	1:X:2016:A:C5	2.80	0.69
1:X:2045:A:N6	32:X:2882:LMA:H32B	2.08	0.68
11:I:83:LEU:O	11:I:84:GLU:CB	2.41	0.68
32:X:2882:LMA:C12	32:X:2882:LMA:C56	2.70	0.68
24:V:2:LYS:N	24:V:3:PRO:CD	2.56	0.68
17:O:21:ARG:NH2	17:O:88:GLN:CD	2.47	0.68
1:X:1750:A:O2'	1:X:2694:G:O2'	2.12	0.68
27:1:21:TYR:CD2	27:1:21:TYR:C	2.67	0.68
1:X:2272:A:OP2	14:L:18:ARG:NH1	2.26	0.68
1:X:2500:C:C6	1:X:2500:C:O5'	2.47	0.68
1:X:1817:U:C4'	3:A:253:LYS:CD	2.71	0.67
1:X:2571:G:C2	1:X:2582:G:C2	2.82	0.67
1:X:2692:A:C5'	1:X:2693:U:OP2	2.43	0.67
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.28	0.67
1:X:167:A:OP2	1:X:182:G:N2	2.27	0.67
32:X:2882:LMA:H56A	32:X:2882:LMA:C57	2.24	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:114:C:O2'	1:X:124:A:N3	2.27	0.67
14:L:37:HIS:CD2	14:L:39:TYR:CZ	2.82	0.67
1:X:2005:U:C6	1:X:2005:U:OP2	2.47	0.67
1:X:2238:G:C8	1:X:2406:C:N4	2.63	0.67
26:Z:4:HIS:CB	26:Z:5:PRO:CD	2.73	0.67
1:X:1686:A:C6	1:X:1977:C:O2	2.47	0.67
1:X:2663:U:O2'	10:H:88:THR:CG2	2.43	0.67
1:X:1404:C:C4	1:X:1406:A:C8	2.82	0.67
1:X:1773:C:N3	1:X:2565:C:N4	2.43	0.67
3:A:66:ILE:CG2	3:A:68:PHE:CE1	2.78	0.67
1:X:759:C:C2	32:X:2882:LMA:H37	2.29	0.66
3:A:30:PRO:O	3:A:31:GLU:OE1	2.13	0.66
1:X:824:U:C2'	11:I:30:ALA:CA	2.72	0.66
1:X:1265:G:O4'	16:N:33:ARG:CD	2.44	0.66
11:I:58:ALA:O	11:I:59:ARG:CB	2.43	0.66
1:X:2462:C:O2	12:J:125:LYS:NZ	2.28	0.66
1:X:851:C:O2	1:X:952:A:C2	2.48	0.66
1:X:1774:A:C2	1:X:2566:A:C5	2.84	0.66
12:J:105:PHE:C	12:J:106:GLU:OE2	2.33	0.66
2:Y:84:G:N1	2:Y:98:C:C2	2.64	0.66
11:I:18:ARG:CG	11:I:21:ARG:CB	2.74	0.66
3:A:159:SER:OG	3:A:160:ALA:N	2.28	0.65
1:X:1770:U:OP2	1:X:1775:A:N6	2.29	0.65
12:J:13:GLN:O	12:J:74:PRO:CG	2.44	0.65
1:X:1948:C:C5	1:X:1949:A:N7	2.65	0.65
11:I:55:ARG:O	11:I:57:ILE:N	2.29	0.65
1:X:2430:A:OP1	1:X:2476:A:N6	2.30	0.65
1:X:797:A:O2'	1:X:798:G:N7	2.29	0.65
1:X:834:A:C2'	1:X:957:G:OP2	2.45	0.65
1:X:2668:U:O2	1:X:2693:U:O5'	2.14	0.65
12:J:66:TYR:O	12:J:106:GLU:OE1	2.14	0.65
1:X:1445:A:C2	1:X:1579:G:C2	2.84	0.65
8:F:116:ASN:OD1	8:F:117:ALA:N	2.30	0.65
10:H:26:ASN:ND2	10:H:26:ASN:O	2.30	0.65
16:N:25:TRP:CE3	16:N:26:GLY:CA	2.80	0.65
1:X:1607:A:N3	1:X:1608:U:O4'	2.30	0.65
1:X:123:A:C5'	28:2:19:ARG:NH2	2.60	0.65
27:1:41:ASP:OD2	27:1:46:LYS:CD	2.44	0.65
1:X:748:A:N6	1:X:749:C:O2	2.30	0.65
1:X:626:A:O2'	5:C:176:ASN:OD1	2.15	0.65
1:X:2045:A:N6	32:X:2882:LMA:C32	2.60	0.64
4:B:47:VAL:CG2	4:B:84:PHE:O	2.45	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1704:G:N2	1:X:1719:G:C6	2.65	0.64
32:X:2882:LMA:H56A	32:X:2882:LMA:C12	2.22	0.64
1:X:818:G:N2	1:X:842:A:OP1	2.30	0.64
1:X:1939:U:O2	1:X:2531:U:OP1	2.15	0.64
1:X:992:A:C2	1:X:2011:U:O4'	2.51	0.64
1:X:2676:G:C2	1:X:2690:A:C2	2.86	0.64
4:B:87:ASP:OD2	4:B:87:ASP:N	2.30	0.64
1:X:1681:A:N6	1:X:1979:C:N4	2.46	0.64
21:S:155:PRO:CG	21:S:158:CYS:SG	2.86	0.64
18:P:32:ARG:CA	18:P:32:ARG:NE	2.61	0.64
1:X:2046:C:C5	1:X:2047:C:C4	2.85	0.64
1:X:1683:G:N2	1:X:1978:U:N3	2.45	0.64
5:C:162:ARG:CG	5:C:162:ARG:NH1	2.62	0.64
1:X:1265:G:O2'	1:X:1266:G:C8	2.51	0.64
1:X:2663:U:O4	1:X:2664:G:C6	2.51	0.63
1:X:1391:A:C6	1:X:1393:G:C4	2.86	0.63
1:X:540:G:C6	1:X:2005:U:O5'	2.51	0.63
1:X:998:C:N4	1:X:999:A:C6	2.66	0.63
1:X:2257:A:N6	22:T:15:ASP:CG	2.51	0.63
4:B:85:ALA:N	4:B:86:PRO:CD	2.60	0.63
1:X:2660:C:C2	1:X:2704:U:O4	2.52	0.63
1:X:1142:G:C1'	9:G:103:TYR:CE2	2.81	0.63
1:X:1008:G:C2	1:X:1170:U:O2	2.52	0.63
1:X:2007:G:N2	1:X:2023:C:C2	2.67	0.63
1:X:1816:G:O2'	3:A:253:LYS:CD	2.47	0.62
1:X:486:U:C2	1:X:492:G:N2	2.67	0.62
1:X:2720:A:N6	1:X:2721:A:C6	2.68	0.62
1:X:966:A:N6	1:X:967:G:C6	2.68	0.62
1:X:1142:G:N3	9:G:103:TYR:CD2	2.67	0.62
28:2:1:MET:O	28:2:2:LYS:C	2.36	0.62
1:X:717:G:N3	1:X:739:G:C2	2.67	0.62
32:X:2882:LMA:H34B	32:X:2882:LMA:C56	2.27	0.62
1:X:2264:C:OP2	27:1:28:ARG:NH1	2.33	0.62
9:G:162:LYS:N	9:G:163:PRO:CD	2.63	0.62
1:X:1673:C:C5'	4:B:136:ARG:CD	2.78	0.62
1:X:2060:A:O2'	1:X:2413:A:O2'	2.17	0.62
4:B:154:LYS:CE	4:B:156:MET:SD	2.88	0.62
1:X:67:G:N2	1:X:73:A:N3	2.48	0.62
1:X:2806:G:O2'	1:X:2859:U:OP1	2.18	0.62
1:X:1677:C:O2	1:X:1984:A:C2	2.52	0.61
1:X:679:C:C5'	11:I:49:PHE:CE1	2.82	0.61
4:B:136:ARG:CG	4:B:137:ARG:N	2.63	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:K:87:TYR:CE1	13:K:94:TYR:CD1	2.88	0.61
10:H:85:ASP:OD2	10:H:87:SER:N	2.33	0.61
19:Q:7:LEU:CD2	19:Q:7:LEU:C	2.69	0.61
1:X:1182:U:C4'	1:X:1183:C:OP1	2.47	0.61
1:X:2349:G:N2	27:1:46:LYS:NZ	2.48	0.61
1:X:1179:A:C2	1:X:1196:G:C2	2.88	0.61
1:X:2429:A:C6	1:X:2430:A:N6	2.69	0.61
12:J:81:GLU:O	12:J:82:THR:OG1	2.19	0.61
26:Z:52:TYR:O	26:Z:53:ASP:CB	2.48	0.61
1:X:1774:A:C2	1:X:2566:A:C4	2.89	0.61
2:Y:85:G:O6	2:Y:86:A:C6	2.53	0.61
1:X:2671:C:OP1	1:X:2846:G:C4'	2.49	0.61
9:G:132:PHE:CD2	9:G:145:HIS:CG	2.88	0.61
1:X:224:G:C2	1:X:229:G:C6	2.88	0.61
1:X:1277:G:O5'	1:X:1277:G:C8	2.54	0.61
1:X:1817:U:O4'	3:A:253:LYS:CD	2.49	0.61
1:X:2670:C:O2	1:X:2698:G:N2	2.34	0.61
1:X:1755:G:C6	1:X:1972:G:C2	2.89	0.60
1:X:2006:G:N2	1:X:2024:U:C2	2.69	0.60
1:X:459:A:N6	1:X:484:G:C4	2.69	0.60
1:X:746:G:N2	1:X:747:A:N6	2.49	0.60
1:X:2840:U:O4	1:X:2841:U:C4	2.54	0.60
1:X:1466:C:O2'	1:X:1467:U:O4'	2.19	0.60
1:X:494:A:C8	1:X:495:C:C5	2.88	0.60
1:X:2825:A:O4'	1:X:2843:A:C2	2.55	0.60
1:X:1701:C:C2	1:X:1722:G:N2	2.70	0.60
1:X:1223:G:C4'	1:X:1224:A:OP2	2.50	0.60
1:X:2805:G:O2'	1:X:2858:A:N1	2.33	0.60
1:X:1681:A:C2	1:X:2706:U:C1'	2.84	0.60
31:X:2881:LC2:C3	31:X:2881:LC2:C28	2.79	0.60
1:X:795:A:N1	3:A:227:MET:CE	2.64	0.60
1:X:2840:U:C4	1:X:2841:U:C4	2.89	0.60
1:X:1496:G:C4'	1:X:1497:C:OP1	2.50	0.60
1:X:219:G:N2	1:X:232:A:OP2	2.35	0.60
21:S:71:MET:N	21:S:71:MET:SD	2.74	0.60
1:X:1683:G:N2	1:X:1978:U:C4	2.70	0.60
1:X:1685:A:O4'	1:X:1686:A:N1	2.34	0.60
1:X:1998:A:C2	26:Z:5:PRO:O	2.53	0.60
1:X:749:C:C3'	1:X:749:C:C6	2.85	0.60
1:X:1674:C:OP1	4:B:136:ARG:O	2.20	0.60
2:Y:39:C:N3	14:L:97:HIS:NE2	2.50	0.60
10:H:19:ILE:CG1	10:H:19:ILE:O	2.49	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:788:G:O2'	1:X:789:G:OP2	2.20	0.60
1:X:2720:A:C6	1:X:2721:A:C6	2.89	0.60
1:X:1919:A:N7	1:X:1928:G:C6	2.70	0.60
27:1:12:MET:CG	27:1:27:ASN:OD1	2.50	0.60
1:X:2464:G:C4'	12:J:125:LYS:O	2.50	0.59
1:X:583:C:O2	4:B:145:LYS:NZ	2.35	0.59
1:X:1407:G:O6	1:X:1408:A:N6	2.34	0.59
1:X:793:G:C2	1:X:798:G:O6	2.55	0.59
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.35	0.59
1:X:693:A:C4	1:X:811:G:N2	2.70	0.59
1:X:2760:G:N1	9:G:128:GLU:OE2	2.35	0.59
1:X:2824:C:O4'	1:X:2843:A:C6	2.55	0.59
1:X:583:C:O2	4:B:145:LYS:CE	2.51	0.59
4:B:6:GLY:CA	4:B:27:LEU:O	2.50	0.59
1:X:611:C:O2'	1:X:615:C:OP1	2.21	0.59
11:I:57:ILE:O	29:3:12:ARG:CD	2.51	0.59
1:X:583:C:C2	4:B:145:LYS:NZ	2.71	0.59
1:X:709:A:C2	1:X:780:U:C2	2.90	0.59
17:O:21:ARG:NH2	17:O:88:GLN:NE2	2.51	0.59
1:X:1696:C:C6	1:X:1696:C:O5'	2.56	0.59
2:Y:84:G:C2	2:Y:98:C:O2	2.55	0.59
1:X:2500:C:N3	1:X:2501:U:C4	2.71	0.59
1:X:1194:U:O2'	1:X:1195:U:C6	2.55	0.59
32:X:2882:LMA:C54	32:X:2882:LMA:H34B	2.33	0.59
12:J:92:GLU:CG	12:J:93:TYR:CD2	2.86	0.59
1:X:2261:G:C4	1:X:2404:A:N6	2.71	0.58
1:X:2033:C:N4	1:X:2034:A:C6	2.71	0.58
3:A:59:HIS:O	3:A:61:ARG:N	2.36	0.58
10:H:23:ARG:CB	10:H:23:ARG:NH2	2.66	0.58
32:X:2882:LMA:H29B	32:X:2882:LMA:C40	2.14	0.58
1:X:1234:C:O2	1:X:1242:A:C2	2.56	0.58
20:R:84:VAL:CG2	20:R:84:VAL:O	2.51	0.58
1:X:2825:A:OP2	1:X:2843:A:N3	2.36	0.58
1:X:2841:U:C1'	1:X:2843:A:O4'	2.51	0.58
2:Y:84:G:O2'	2:Y:85:G:C5'	2.51	0.58
1:X:2034:A:C2	1:X:2593:A:C2	2.91	0.58
1:X:1724:C:C2	1:X:1747:G:N1	2.72	0.58
1:X:1724:C:C2	1:X:1747:G:C6	2.91	0.58
4:B:143:GLN:N	4:B:143:GLN:NE2	2.51	0.58
27:1:21:TYR:CD2	27:1:50:PHE:CZ	2.91	0.58
4:B:136:ARG:O	4:B:137:ARG:CB	2.51	0.58
1:X:76:C:C2	1:X:108:G:N2	2.72	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:796:A:C2	1:X:1769:U:O2'	2.57	0.58
1:X:775:U:C4'	1:X:776:G:C2	2.87	0.58
3:A:160:ALA:CA	3:A:199:ASN:CG	2.71	0.58
1:X:2793:G:N2	1:X:2804:G:C4	2.72	0.58
10:H:100:ASN:C	10:H:100:ASN:OD1	2.41	0.58
11:I:62:LYS:CD	29:3:12:ARG:C	2.72	0.58
1:X:67:G:N2	1:X:73:A:C4	2.72	0.58
23:U:32:ARG:NE	23:U:32:ARG:N	2.52	0.58
1:X:521:U:O4	1:X:522:G:N2	2.37	0.58
1:X:2533:U:C4	1:X:2534:U:O4	2.56	0.57
2:Y:85:G:C6	2:Y:86:A:C5	2.92	0.57
1:X:500:G:N7	18:P:70:LYS:NZ	2.51	0.57
11:I:49:PHE:CD1	11:I:50:GLU:N	2.72	0.57
1:X:860:U:C2'	1:X:860:U:O2	2.50	0.57
1:X:1681:A:C6	1:X:2706:U:C6	2.93	0.57
1:X:2754:C:N4	1:X:2755:A:N6	2.52	0.57
1:X:2040:A:N6	1:X:2041:A:N6	2.52	0.57
1:X:851:C:C2	1:X:952:A:N1	2.73	0.57
20:R:62:MET:O	20:R:63:THR:CB	2.53	0.57
1:X:1972:G:C5	1:X:1973:C:C4	2.91	0.57
1:X:615:C:O2'	1:X:670:U:O2'	2.23	0.57
1:X:2711:G:OP1	4:B:169:ASN:CG	2.43	0.57
3:A:150:PRO:CD	3:A:190:CYS:SG	2.92	0.57
20:R:18:LYS:O	20:R:36:VAL:O	2.21	0.57
15:M:103:LYS:O	15:M:104:LEU:CB	2.51	0.57
1:X:331:U:O2	5:C:162:ARG:NH2	2.38	0.57
1:X:1215:A:C2	1:X:1258:G:C2	2.93	0.57
1:X:1975:G:O2'	1:X:1980:A:N6	2.38	0.56
1:X:832:A:N3	1:X:1203:A:C2	2.73	0.56
5:C:126:ALA:O	5:C:127:ASP:CB	2.52	0.56
1:X:1823:G:C2	1:X:1958:G:C2	2.93	0.56
2:Y:66:G:C6	2:Y:67:C:N3	2.73	0.56
27:1:8:ILE:CG1	27:1:30:ASN:ND2	2.68	0.56
1:X:760:U:C4	1:X:2592:U:C5	2.92	0.56
1:X:1989:C:O2'	1:X:2798:A:O2'	2.22	0.56
1:X:1974:U:C3'	1:X:1974:U:C6	2.87	0.56
4:B:121:ASN:O	4:B:122:PHE:CD2	2.58	0.56
5:C:120:VAL:O	5:C:121:ASP:CB	2.52	0.56
6:D:22:TYR:OH	6:D:29:PRO:CD	2.52	0.56
1:X:1650:A:N6	1:X:1652:G:C2	2.73	0.56
1:X:1333:G:N2	1:X:1344:C:N4	2.52	0.56
2:Y:83:C:C2'	2:Y:84:G:C5'	2.83	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1332:G:C6	1:X:1333:G:C6	2.93	0.56
3:A:44:ARG:N	3:A:44:ARG:CD	2.67	0.56
1:X:1033:G:C6	1:X:1151:U:C5	2.94	0.56
4:B:116:VAL:O	4:B:121:ASN:O	2.23	0.56
16:N:32:TYR:O	16:N:33:ARG:C	2.43	0.56
1:X:1006:C:OP2	16:N:54:LYS:NZ	2.38	0.56
27:1:13:GLU:O	27:1:52:GLU:O	2.23	0.56
1:X:208:C:N4	1:X:209:G:N2	2.53	0.56
32:X:2882:LMA:C32	32:X:2882:LMA:O53	2.50	0.56
1:X:955:G:C5'	1:X:955:G:N3	2.69	0.56
1:X:1682:A:C8	1:X:1682:A:O5'	2.59	0.56
22:T:14:ARG:O	22:T:15:ASP:CB	2.54	0.56
29:3:12:ARG:O	29:3:14:ILE:N	2.38	0.56
1:X:1441:A:C4'	1:X:1442:C:O5'	2.53	0.56
1:X:1296:G:N2	1:X:1299:A:C8	2.73	0.56
16:N:32:TYR:O	16:N:34:ASN:N	2.39	0.56
3:A:211:GLY:C	3:A:213:SER:N	2.59	0.56
1:X:577:U:C5'	1:X:956:A:N6	2.69	0.56
9:G:104:THR:OG1	9:G:106:TYR:O	2.24	0.56
1:X:1142:G:C4	9:G:103:TYR:CD2	2.94	0.55
1:X:494:A:N7	1:X:495:C:C4	2.74	0.55
5:C:128:ALA:O	5:C:130:THR:N	2.39	0.55
20:R:25:LEU:O	20:R:26:SER:CB	2.53	0.55
1:X:396:U:C4	1:X:398:C:C5	2.94	0.55
1:X:2282:G:C2	1:X:2293:G:C2	2.94	0.55
1:X:599:A:C2	1:X:681:A:C2	2.93	0.55
1:X:1605:A:C6	1:X:1606:C:N4	2.73	0.55
1:X:879:A:N3	1:X:879:A:C2'	2.69	0.55
1:X:1681:A:N7	1:X:1682:A:C6	2.75	0.55
22:T:14:ARG:O	22:T:15:ASP:CG	2.45	0.55
3:A:59:HIS:C	3:A:61:ARG:N	2.59	0.55
1:X:2707:G:N7	1:X:2708:U:C4	2.75	0.55
10:H:76:ARG:O	10:H:95:ALA:N	2.38	0.55
1:X:760:U:C4	1:X:2592:U:C4	2.94	0.55
7:E:156:ALA:O	7:E:157:TYR:CG	2.59	0.55
12:J:12:LYS:O	12:J:13:GLN:CB	2.54	0.55
1:X:2707:G:C2'	1:X:2708:U:O5'	2.55	0.55
5:C:153:ASP:O	5:C:154:ASP:CB	2.55	0.55
1:X:1947:G:C6	1:X:1950:C:C4	2.94	0.55
8:F:121:GLU:O	8:F:125:ASN:N	2.40	0.55
7:E:172:LYS:O	7:E:173:ALA:CB	2.55	0.55
1:X:2045:A:C5	32:X:2882:LMA:C27	2.90	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2593:A:O2'	1:X:2594:U:OP2	2.25	0.55
3:A:71:ARG:NH1	3:A:150:PRO:CA	2.70	0.55
1:X:1989:C:O2'	1:X:2798:A:C2'	2.55	0.55
1:X:525:A:N7	1:X:526:C:C4	2.75	0.55
1:X:1280:U:C5	1:X:1995:G:N2	2.75	0.55
1:X:2757:G:OP2	1:X:2761:A:O2'	2.25	0.55
5:C:172:VAL:O	5:C:173:ALA:C	2.45	0.55
1:X:2612:G:C2	1:X:2766:U:O2	2.59	0.55
1:X:1145:C:C6	1:X:1147:G:OP2	2.59	0.55
3:A:24:GLY:O	3:A:25:LEU:CB	2.55	0.54
1:X:748:A:N7	1:X:749:C:N3	2.56	0.54
1:X:177:U:O4	1:X:225:G:C2	2.60	0.54
1:X:17:G:C2	1:X:534:U:O2	2.60	0.54
1:X:832:A:C4	1:X:1203:A:C2	2.95	0.54
1:X:2040:A:C8	1:X:2040:A:O5'	2.60	0.54
12:J:135:ARG:O	12:J:136:GLU:CB	2.54	0.54
1:X:1978:U:O2	10:H:44:TYR:OH	2.25	0.54
1:X:2664:G:N2	1:X:2705:A:N7	2.56	0.54
1:X:1607:A:O2'	1:X:1608:U:C6	2.60	0.54
1:X:1928:G:N2	1:X:1929:U:C2	2.75	0.54
1:X:593:C:N4	1:X:594:G:C6	2.75	0.54
1:X:1365:U:C2	1:X:1393:G:N2	2.75	0.54
11:I:18:ARG:CB	11:I:21:ARG:CB	2.85	0.54
4:B:184:VAL:CG1	4:B:185:LYS:N	2.70	0.54
1:X:2552:C:OP1	1:X:2553:G:OP1	2.24	0.54
1:X:2475:C:N4	1:X:2476:A:N6	2.56	0.54
1:X:971:A:N6	12:J:83:ARG:NH2	2.55	0.54
1:X:33:C:O2	1:X:466:A:C2	2.61	0.54
1:X:958:G:O2'	1:X:995:A:C2	2.61	0.54
1:X:1704:G:N2	1:X:1719:G:O6	2.41	0.54
1:X:2494:C:OP1	9:G:108:GLY:C	2.44	0.54
1:X:2394:G:C2	1:X:2395:C:C2	2.96	0.54
1:X:2032:G:N2	1:X:2599:U:N3	2.56	0.54
1:X:459:A:C2	1:X:466:A:C8	2.96	0.54
5:C:157:THR:CG2	5:C:158:ARG:N	2.70	0.54
11:I:115:SER:OG	11:I:136:ALA:CB	2.55	0.54
1:X:318:G:O2'	1:X:319:G:C8	2.61	0.54
21:S:155:PRO:O	21:S:156:GLU:CB	2.55	0.54
1:X:45:C:OP2	1:X:192:G:C2'	2.56	0.54
1:X:995:A:OP2	1:X:996:C:N4	2.40	0.53
1:X:1405:A:N6	1:X:1406:A:N6	2.56	0.53
3:A:43:GLY:N	3:A:44:ARG:NH1	2.56	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2381:A:O2'	1:X:2382:C:C6	2.61	0.53
5:C:22:VAL:CG1	5:C:110:SER:OG	2.56	0.53
1:X:626:A:O2'	5:C:176:ASN:CG	2.46	0.53
1:X:2814:G:C4'	13:K:49:GLU:OE2	2.55	0.53
29:3:59:LYS:O	29:3:60:LEU:CB	2.56	0.53
1:X:2557:G:N2	1:X:2558:C:C2	2.77	0.53
1:X:2045:A:C5	32:X:2882:LMA:H27A	2.40	0.53
12:J:106:GLU:CD	12:J:106:GLU:N	2.62	0.53
1:X:224:G:N2	1:X:229:G:C6	2.77	0.53
1:X:172:A:C8	1:X:174:A:OP1	2.61	0.53
18:P:101:PRO:O	18:P:121:THR:CG2	2.56	0.53
10:H:116:ARG:NH1	15:M:38:LYS:CE	2.71	0.53
3:A:207:LEU:CA	3:A:212:ARG:NH1	2.71	0.53
1:X:16:G:C2	1:X:535:U:O2	2.62	0.53
1:X:2429:A:N6	1:X:2430:A:N6	2.57	0.53
4:B:176:ARG:NH2	15:M:19:ASP:OD2	2.41	0.53
15:M:34:ARG:NH1	15:M:88:VAL:CG2	2.70	0.53
1:X:2238:G:N7	1:X:2406:C:N4	2.57	0.53
21:S:87:THR:O	21:S:88:TYR:CB	2.55	0.53
1:X:562:G:C6	1:X:563:U:N3	2.76	0.53
1:X:2496:C:C5	1:X:2521:A:C8	2.97	0.53
1:X:131:C:C2	1:X:141:G:N2	2.77	0.53
3:A:160:ALA:CB	3:A:199:ASN:CB	2.87	0.53
1:X:1928:G:C2	1:X:1929:U:C2	2.96	0.53
1:X:131:C:O2	1:X:141:G:N2	2.42	0.53
1:X:2045:A:N6	32:X:2882:LMA:C27	2.70	0.53
1:X:1391:A:C4	1:X:1393:G:C8	2.97	0.53
1:X:1391:A:C8	1:X:1393:G:C5	2.95	0.53
27:1:31:THR:O	27:1:32:GLN:C	2.47	0.53
27:1:42:PRO:O	27:1:43:VAL:C	2.46	0.53
1:X:693:A:C6	1:X:811:G:C2	2.97	0.53
1:X:695:G:N2	1:X:809:C:C2	2.77	0.53
15:M:39:VAL:CG1	15:M:45:THR:OG1	2.57	0.53
1:X:827:C:OP1	17:O:83:ARG:N	2.42	0.53
3:A:71:ARG:NH1	3:A:151:GLY:N	2.57	0.52
10:H:76:ARG:NH1	10:H:113:PRO:O	2.42	0.52
1:X:2634:G:O2'	1:X:2635:U:C5	2.62	0.52
1:X:2378:G:C1'	27:1:22:TYR:OH	2.56	0.52
3:A:219:LYS:CD	3:A:219:LYS:C	2.76	0.52
1:X:845:U:OP1	11:I:41:SER:OG	2.27	0.52
1:X:793:G:N3	1:X:798:G:C6	2.77	0.52
15:M:102:ALA:O	15:M:103:LYS:CD	2.56	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1441:A:C1'	1:X:1442:C:OP2	2.57	0.52
1:X:177:U:O2'	1:X:178:C:O4'	2.26	0.52
3:A:144:HIS:ND1	3:A:195:GLY:O	2.42	0.52
1:X:1069:G:N3	8:F:116:ASN:ND2	2.57	0.52
2:Y:84:G:C2'	2:Y:85:G:O5'	2.58	0.52
11:I:62:LYS:CD	29:3:13:ARG:N	2.73	0.52
32:X:2882:LMA:H37B	32:X:2882:LMA:H35	1.91	0.52
1:X:758:G:O2'	1:X:759:C:OP1	2.28	0.52
1:X:1680:U:O2'	1:X:1681:A:O5'	2.28	0.52
1:X:2429:A:N1	1:X:2430:A:C6	2.78	0.52
2:Y:40:C:O4'	14:L:97:HIS:CE1	2.62	0.52
1:X:1918:G:C4	1:X:1945:C:N4	2.78	0.52
6:D:123:ASP:OD1	6:D:123:ASP:C	2.47	0.52
11:I:18:ARG:CG	11:I:21:ARG:CG	2.87	0.52
1:X:537:C:O2	1:X:538:A:C2	2.63	0.52
12:J:135:ARG:NH2	21:S:118:HIS:CD2	2.78	0.52
1:X:2032:G:N2	1:X:2599:U:C2	2.78	0.52
1:X:817:A:OP1	11:I:45:LYS:CG	2.57	0.52
10:H:28:GLY:O	10:H:35:THR:N	2.42	0.52
15:M:27:PHE:CG	15:M:27:PHE:O	2.63	0.52
1:X:1972:G:C6	1:X:1973:C:N3	2.78	0.52
1:X:2505:G:N1	1:X:2517:C:O2	2.43	0.52
1:X:1391:A:C6	1:X:1393:G:C5	2.96	0.52
1:X:2824:C:O2	1:X:2843:A:C8	2.63	0.52
1:X:700:C:C5	1:X:701:U:C4	2.98	0.52
1:X:2825:A:OP2	1:X:2843:A:C4	2.63	0.52
1:X:2222:U:O2	1:X:2413:A:C2	2.63	0.52
1:X:1447:U:O2	1:X:1577:G:C2	2.63	0.52
22:T:18:PRO:O	22:T:19:LYS:CG	2.58	0.52
1:X:507:A:OP2	18:P:19:LYS:NZ	2.43	0.52
5:C:102:LEU:O	5:C:102:LEU:CD2	2.58	0.52
12:J:54:VAL:CG2	12:J:125:LYS:NZ	2.73	0.51
1:X:883:A:C2	1:X:920:G:C6	2.98	0.51
1:X:1457:A:C2	1:X:1565:G:C2	2.98	0.51
1:X:1982:C:O2	1:X:2666:U:O2'	2.27	0.51
1:X:2625:U:OP2	1:X:2712:G:O2'	2.28	0.51
1:X:1332:G:C6	1:X:1333:G:O6	2.63	0.51
15:M:27:PHE:CD1	15:M:27:PHE:O	2.63	0.51
1:X:1425:G:C2	1:X:1607:A:N6	2.78	0.51
1:X:2505:G:C2	1:X:2517:C:O2	2.63	0.51
1:X:2529:G:C2	1:X:2538:C:O2	2.64	0.51
1:X:1693:A:C6	1:X:1694:A:C6	2.97	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2238:G:C8	1:X:2406:C:C4	2.99	0.51
11:I:62:LYS:CD	29:3:12:ARG:CA	2.89	0.51
1:X:2791:C:C2	1:X:2806:G:N2	2.79	0.51
18:P:37:LYS:NZ	18:P:63:SER:OG	2.43	0.51
1:X:5:A:C2	1:X:2873:G:C2	2.98	0.51
1:X:1692:C:N3	4:B:128:SER:O	2.43	0.51
1:X:693:A:C2	1:X:811:G:C2	2.98	0.51
1:X:2606:G:N2	1:X:2757:G:C4	2.79	0.51
1:X:695:G:N2	1:X:809:C:O2	2.43	0.51
1:X:2265:A:N1	27:1:38:LYS:NZ	2.58	0.51
1:X:331:U:O2'	5:C:162:ARG:NH1	2.43	0.51
3:A:199:ASN:O	3:A:200:ALA:C	2.47	0.51
1:X:2824:C:C4'	1:X:2825:A:OP2	2.58	0.51
1:X:2848:A:C2	13:K:7:GLY:N	2.78	0.51
1:X:1344:C:N4	1:X:1346:C:O2	2.44	0.51
1:X:2819:G:C2	1:X:2820:C:C2	2.99	0.51
1:X:2335:U:O2	1:X:2341:G:C2	2.63	0.51
14:L:37:HIS:CG	14:L:37:HIS:O	2.64	0.51
4:B:84:PHE:CG	4:B:84:PHE:O	2.61	0.51
9:G:132:PHE:CD2	9:G:145:HIS:CD2	2.97	0.51
1:X:1277:G:N2	1:X:1997:A:C8	2.79	0.51
1:X:859:U:O2'	1:X:860:U:C2	2.64	0.51
5:C:124:ASP:CG	5:C:136:TRP:CD1	2.84	0.51
1:X:2571:G:C2	1:X:2582:G:N1	2.79	0.51
1:X:2204:A:C4'	1:X:2205:C:O5'	2.59	0.51
23:U:59:THR:O	23:U:60:VAL:CG2	2.58	0.51
14:L:51:LEU:CD1	14:L:51:LEU:N	2.74	0.51
1:X:1473:U:O2	1:X:1474:A:N6	2.44	0.51
1:X:1605:A:C5	1:X:1606:C:N4	2.78	0.51
27:1:14:SER:OG	27:1:23:THR:N	2.44	0.51
1:X:1701:C:N3	1:X:1722:G:C2	2.79	0.51
1:X:1777:A:N3	1:X:1921:A:C6	2.78	0.51
1:X:1311:C:C2	1:X:1660:G:N2	2.79	0.51
1:X:748:A:N7	1:X:749:C:C4	2.79	0.50
1:X:583:C:N3	4:B:145:LYS:NZ	2.59	0.50
4:B:61:LYS:N	4:B:62:PRO:CD	2.74	0.50
16:N:91:ASN:O	16:N:93:LYS:N	2.44	0.50
1:X:938:G:O2'	1:X:939:C:C5'	2.59	0.50
1:X:860:U:C3'	1:X:860:U:O2	2.59	0.50
8:F:120:VAL:CG1	8:F:121:GLU:N	2.73	0.50
1:X:2427:A:OP1	1:X:2477:C:OP2	2.29	0.50
2:Y:84:G:C2	2:Y:98:C:C2	2.99	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:693:A:N1	1:X:811:G:C2	2.80	0.50
1:X:2711:G:OP1	4:B:169:ASN:CB	2.60	0.50
1:X:1920:A:C5	1:X:1922:U:O2	2.64	0.50
1:X:671:A:C6	1:X:672:C:C4	2.99	0.50
1:X:791:G:C2	1:X:800:U:C2	2.99	0.50
2:Y:23:G:C2	2:Y:65:A:C2	3.00	0.50
10:H:11:ALA:N	10:H:96:ALA:O	2.44	0.50
1:X:2014:A:C6	1:X:2477:C:C1'	2.95	0.50
1:X:2016:A:O2'	1:X:2018:G:OP2	2.29	0.50
1:X:2261:G:C2	1:X:2404:A:C5	2.99	0.50
1:X:2819:G:C5	1:X:2820:C:C4	3.00	0.50
13:K:84:ALA:N	13:K:85:PRO:CD	2.75	0.50
1:X:2797:G:O2'	1:X:2799:C:OP2	2.30	0.50
1:X:331:U:C2'	5:C:162:ARG:NH1	2.75	0.50
1:X:2840:U:O2'	1:X:2841:U:OP1	2.30	0.50
1:X:2005:U:OP2	1:X:2005:U:O4'	2.30	0.50
1:X:1265:G:O2'	1:X:1266:G:N9	2.45	0.50
1:X:1279:G:O2'	1:X:1995:G:O6	2.29	0.50
1:X:1656:U:C2'	1:X:1657:A:C5'	2.90	0.50
1:X:3:U:O2'	1:X:4:C:O5'	2.30	0.50
1:X:2314:A:O2'	1:X:2315:A:C8	2.65	0.50
1:X:756:C:OP1	4:B:130:GLY:CA	2.60	0.50
1:X:1696:C:O2	1:X:1972:G:N2	2.45	0.50
1:X:789:G:N2	1:X:2220:A:OP1	2.45	0.50
1:X:789:G:O2'	1:X:790:A:OP2	2.30	0.50
1:X:1021:A:OP1	16:N:66:ASN:ND2	2.44	0.50
1:X:2671:C:N3	1:X:2698:G:N2	2.60	0.50
15:M:26:ASP:O	15:M:26:ASP:OD2	2.30	0.50
1:X:2430:A:N1	31:X:2881:LC2:C15	2.75	0.50
1:X:1289:A:N1	1:X:1290:A:C6	2.79	0.50
4:B:85:ALA:O	4:B:86:PRO:O	2.29	0.50
1:X:780:U:O2'	1:X:781:G:O5'	2.30	0.50
1:X:2378:G:C2	1:X:2397:A:C2	3.00	0.50
1:X:980:G:C6	1:X:981:C:N3	2.80	0.50
1:X:30:G:O6	1:X:520:C:N4	2.45	0.50
1:X:2571:G:C5	1:X:2572:U:C4	3.00	0.49
2:Y:83:C:C2'	2:Y:84:G:O5'	2.60	0.49
1:X:693:A:C5	1:X:811:G:N2	2.80	0.49
1:X:2793:G:C2	1:X:2804:G:C2	2.99	0.49
1:X:1623:C:C4'	1:X:1624:A:O5'	2.60	0.49
1:X:1096:A:O4'	1:X:1097:A:OP1	2.30	0.49
9:G:36:ASN:O	9:G:38:GLU:O	2.30	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:608:G:C2	1:X:609:U:C2	3.00	0.49
18:P:107:ILE:CG2	18:P:107:ILE:O	2.60	0.49
5:C:123:PHE:CD2	5:C:123:PHE:C	2.85	0.49
1:X:1979:C:O4'	1:X:1979:C:OP1	2.30	0.49
8:F:116:ASN:OD1	8:F:117:ALA:CA	2.60	0.49
1:X:998:C:N4	1:X:999:A:C5	2.81	0.49
13:K:94:TYR:CE1	13:K:115:LEU:O	2.65	0.49
2:Y:39:C:C2	14:L:97:HIS:NE2	2.79	0.49
1:X:1096:A:C4'	1:X:1097:A:OP1	2.60	0.49
1:X:2510:A:N6	1:X:2511:G:C6	2.80	0.49
1:X:1288:A:C8	13:K:16:ALA:CB	2.94	0.49
9:G:93:LYS:N	9:G:93:LYS:CD	2.74	0.49
3:A:220:PRO:O	3:A:221:HIS:O	2.29	0.49
1:X:1141:U:C4	4:B:147:PRO:CD	2.95	0.49
1:X:309:G:P	20:R:93:ARG:CB	3.00	0.49
3:A:35:THR:O	3:A:105:TYR:OH	2.30	0.49
1:X:1747:G:O4'	1:X:1747:G:OP2	2.29	0.49
12:J:136:GLU:O	12:J:136:GLU:CG	2.58	0.49
1:X:2451:G:C5	1:X:2454:C:N4	2.81	0.49
3:A:25:LEU:O	3:A:26:THR:OG1	2.30	0.49
1:X:1607:A:O2'	1:X:1608:U:O5'	2.30	0.49
1:X:1466:C:C2'	1:X:1467:U:O4'	2.60	0.49
20:R:25:LEU:O	20:R:26:SER:OG	2.30	0.49
1:X:762:A:C2	1:X:766:A:O2'	2.65	0.49
1:X:1141:U:O2'	1:X:1142:G:O5'	2.30	0.49
1:X:123:A:O4'	1:X:123:A:OP1	2.30	0.49
1:X:221:A:C2	1:X:232:A:C4	3.01	0.49
13:K:33:ARG:C	13:K:34:ILE:CG2	2.81	0.49
1:X:1282:A:C2	1:X:1338:G:N2	2.81	0.49
15:M:33:VAL:CG2	15:M:51:GLU:CB	2.91	0.49
1:X:1238:A:OP1	17:O:68:LYS:NZ	2.46	0.49
1:X:2429:A:C6	1:X:2430:A:C6	3.01	0.49
1:X:1704:G:C2	1:X:1719:G:C6	3.01	0.49
1:X:1676:U:C2'	1:X:1677:C:O5'	2.58	0.49
1:X:1623:C:N4	1:X:1638:G:OP2	2.45	0.49
1:X:1545:G:C6	1:X:1559:G:N2	2.80	0.49
1:X:1823:G:C4	1:X:1958:G:N2	2.81	0.49
5:C:154:ASP:O	5:C:157:THR:CG2	2.61	0.49
1:X:2496:C:C5	1:X:2521:A:N7	2.81	0.49
18:P:19:LYS:O	18:P:20:LEU:CB	2.60	0.49
1:X:463:C:C2	1:X:465:C:C5	3.00	0.49
1:X:833:A:N3	1:X:954:U:O2'	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:R:85:ASP:O	20:R:85:ASP:OD1	2.30	0.49
1:X:2426:G:O2'	1:X:2427:A:OP2	2.30	0.49
1:X:789:G:C2	1:X:2220:A:OP1	2.65	0.49
1:X:2016:A:OP2	1:X:2016:A:O4'	2.30	0.49
12:J:137:VAL:C	12:J:138:TYR:CD2	2.86	0.49
1:X:1704:G:C2	1:X:1719:G:O6	2.66	0.49
1:X:76:C:C2	1:X:108:G:C2	3.00	0.49
1:X:888:G:N2	1:X:915:C:C2	2.80	0.49
1:X:2044:G:OP1	5:C:62:LYS:CG	2.60	0.49
3:A:25:LEU:CB	3:A:206:VAL:CG2	2.90	0.49
24:V:2:LYS:O	24:V:3:PRO:O	2.30	0.49
20:R:62:MET:O	20:R:63:THR:OG1	2.30	0.49
3:A:71:ARG:CG	3:A:191:TYR:CE1	2.96	0.49
3:A:97:HIS:CE1	3:A:101:GLY:CA	2.96	0.49
1:X:1391:A:O4'	1:X:1392:U:OP1	2.30	0.49
1:X:959:C:OP1	1:X:973:U:OP1	2.30	0.49
2:Y:84:G:O2'	2:Y:85:G:O5'	2.30	0.49
10:H:26:ASN:O	10:H:26:ASN:CG	2.47	0.49
1:X:708:G:C2	1:X:781:G:C2	3.01	0.49
1:X:681:A:C5	1:X:683:A:N7	2.80	0.49
17:O:23:GLU:O	17:O:24:SER:CB	2.60	0.49
9:G:70:PHE:CG	16:N:64:ARG:CG	2.96	0.49
13:K:80:MET:CA	13:K:80:MET:CE	2.89	0.49
32:X:2882:LMA:C34	32:X:2882:LMA:C54	2.91	0.48
1:X:2825:A:C2	13:K:61:HIS:CD2	3.01	0.48
1:X:2827:G:N2	1:X:2840:U:O2	2.45	0.48
1:X:780:U:O2'	1:X:781:G:O4'	2.30	0.48
19:Q:60:GLY:O	19:Q:61:LYS:O	2.30	0.48
5:C:163:ASN:O	5:C:163:ASN:ND2	2.45	0.48
3:A:55:ILE:O	3:A:55:ILE:CG2	2.60	0.48
2:Y:85:G:C6	2:Y:86:A:C6	3.01	0.48
1:X:1981:A:C4'	1:X:2704:U:O2'	2.61	0.48
1:X:2720:A:N6	1:X:2721:A:N1	2.60	0.48
1:X:594:G:N2	1:X:1269:G:C6	2.80	0.48
6:D:40:LEU:CD2	6:D:41:GLY:N	2.76	0.48
1:X:395:G:C2	1:X:406:G:C2	3.01	0.48
17:O:6:GLN:O	17:O:7:THR:OG1	2.30	0.48
3:A:49:ARG:NH1	3:A:49:ARG:N	2.61	0.48
1:X:2811:G:O2'	1:X:2812:A:O4'	2.31	0.48
19:Q:58:VAL:O	19:Q:75:ARG:N	2.46	0.48
1:X:1324:G:C4'	1:X:1325:U:OP1	2.60	0.48
3:A:90:SER:O	3:A:199:ASN:CG	2.50	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2840:U:O4	1:X:2841:U:O4	2.30	0.48
1:X:2581:A:OP2	1:X:2582:G:OP2	2.32	0.48
3:A:49:ARG:NH1	3:A:49:ARG:CB	2.76	0.48
9:G:141:GLY:O	9:G:144:MET:N	2.46	0.48
1:X:2762:G:C2	1:X:2763:U:C2	3.02	0.48
3:A:219:LYS:O	3:A:219:LYS:CD	2.61	0.48
4:B:120:TRP:CB	4:B:122:PHE:CE2	2.97	0.48
1:X:542:A:N6	1:X:2003:A:N3	2.61	0.48
1:X:1948:C:C6	1:X:1949:A:N7	2.81	0.48
1:X:681:A:C3'	1:X:681:A:C8	2.97	0.48
20:R:11:ASN:O	20:R:12:ASP:CB	2.60	0.48
18:P:60:ILE:O	18:P:60:ILE:CG2	2.58	0.48
3:A:66:ILE:CD1	3:A:89:ARG:CZ	2.92	0.48
1:X:1975:G:C1'	1:X:1976:U:OP2	2.62	0.48
1:X:2841:U:O2'	1:X:2842:C:OP2	2.30	0.48
1:X:958:G:N2	1:X:982:C:C2	2.81	0.48
1:X:2272:A:C5'	14:L:15:ARG:NH2	2.77	0.48
1:X:594:G:C2	1:X:1269:G:C6	3.02	0.48
1:X:585:U:O2'	1:X:2481:G:C6	2.66	0.48
1:X:1608:U:C5	1:X:1609:G:N7	2.81	0.48
1:X:2665:G:N2	1:X:2704:U:O2	2.46	0.48
1:X:2180:U:C5	1:X:2203:G:C6	3.01	0.48
10:H:3:MET:O	10:H:6:SER:CB	2.62	0.48
1:X:118:U:C2	1:X:143:A:C6	3.02	0.48
1:X:801:A:OP1	1:X:804:C:N4	2.47	0.48
1:X:2754:C:N4	1:X:2755:A:C6	2.82	0.48
1:X:2814:G:O4'	13:K:49:GLU:OE2	2.31	0.48
1:X:1693:A:N6	1:X:1694:A:C6	2.82	0.48
1:X:1545:G:N1	1:X:1559:G:C2	2.82	0.48
1:X:171:G:C2	1:X:179:U:O2	2.67	0.48
1:X:1910:A:C6	1:X:1911:A:N1	2.82	0.48
7:E:174:GLY:C	7:E:175:LYS:CG	2.81	0.48
12:J:137:VAL:O	12:J:138:TYR:CG	2.67	0.48
1:X:2707:G:O2'	1:X:2708:U:O5'	2.31	0.48
5:C:163:ASN:C	5:C:163:ASN:ND2	2.67	0.48
1:X:1387:G:C5	1:X:1388:C:C4	3.02	0.48
1:X:861:G:C6	1:X:943:U:O2	2.67	0.48
1:X:1141:U:O4	4:B:147:PRO:CD	2.62	0.47
27:1:8:ILE:C	27:1:9:ILE:CG2	2.81	0.47
27:1:8:ILE:O	27:1:9:ILE:CG2	2.61	0.47
1:X:959:C:C1'	1:X:995:A:C2	2.96	0.47
1:X:824:U:N3	1:X:1263:G:OP1	2.46	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:61:ARG:CD	3:A:88:ASN:OD1	2.62	0.47
1:X:1947:G:O2'	1:X:1950:C:OP1	2.32	0.47
1:X:525:A:C8	1:X:526:C:C5	3.02	0.47
3:A:220:PRO:O	3:A:221:HIS:C	2.53	0.47
1:X:2440:C:C5	1:X:2441:U:C5	3.02	0.47
1:X:2042:A:N1	32:X:2882:LMA:H29A	2.29	0.47
1:X:1441:A:C8	1:X:1442:C:C5	3.02	0.47
1:X:2658:A:C2	1:X:2709:C:N3	2.82	0.47
1:X:532:A:C6	1:X:533:C:N3	2.82	0.47
1:X:2728:A:C2	1:X:2737:A:C6	3.03	0.47
1:X:2485:U:OP2	1:X:2555:G:N1	2.47	0.47
1:X:1407:G:C6	1:X:1408:A:N6	2.82	0.47
1:X:2376:G:C2	1:X:2399:C:O2	2.68	0.47
1:X:921:A:N6	1:X:924:C:O2	2.47	0.47
2:Y:71:G:C6	2:Y:72:C:C2	3.03	0.47
31:X:2881:LC2:C16	31:X:2881:LC2:C14	2.93	0.47
1:X:611:C:N4	1:X:669:G:C6	2.82	0.47
13:K:54:THR:CG2	13:K:66:VAL:CG2	2.93	0.47
1:X:173:A:O2'	1:X:2051:U:C5	2.67	0.47
2:Y:9:G:C2	2:Y:117:G:C2	3.02	0.47
1:X:2539:C:N4	1:X:2540:A:N6	2.63	0.47
1:X:2046:C:C5	1:X:2047:C:N4	2.82	0.47
1:X:793:G:C2	1:X:798:G:C6	3.03	0.47
12:J:27:TYR:C	12:J:28:VAL:CG2	2.82	0.47
1:X:993:C:C5'	1:X:994:A:OP2	2.62	0.47
16:N:93:LYS:NZ	17:O:10:LYS:CE	2.78	0.47
1:X:2832:G:N2	1:X:2835:A:OP2	2.47	0.47
1:X:1092:U:C4'	8:F:122:ALA:CB	2.92	0.47
1:X:2274:C:OP2	14:L:11:LEU:CD2	2.63	0.47
1:X:410:A:OP1	23:U:47:HIS:CE1	2.68	0.47
1:X:668:A:O2'	1:X:669:G:O4'	2.31	0.47
13:K:87:TYR:CE1	13:K:94:TYR:CB	2.98	0.47
1:X:1392:U:C6	1:X:1392:U:O5'	2.67	0.47
1:X:1681:A:OP1	1:X:1682:A:OP2	2.33	0.47
1:X:1685:A:C4'	1:X:1686:A:C2	2.97	0.47
1:X:2258:G:O6	22:T:15:ASP:CG	2.53	0.47
1:X:331:U:C1'	5:C:162:ARG:NH1	2.78	0.47
1:X:2825:A:C6	1:X:2826:C:N3	2.83	0.47
4:B:120:TRP:O	4:B:122:PHE:CD2	2.68	0.47
1:X:2571:G:C6	1:X:2572:U:N3	2.83	0.47
1:X:2571:G:N1	1:X:2582:G:C6	2.83	0.47
1:X:182:G:C2'	1:X:183:U:OP2	2.61	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2594:U:C2'	1:X:2594:U:O2	2.61	0.47
2:Y:104:A:N6	2:Y:105:G:C6	2.83	0.47
1:X:1780:A:OP1	3:A:222:GLN:OE1	2.32	0.47
1:X:2400:G:O6	29:3:32:GLN:CG	2.63	0.47
26:Z:33:CYS:CB	26:Z:38:GLY:O	2.63	0.47
14:L:89:PHE:CZ	14:L:103:LEU:CD2	2.98	0.47
1:X:2447:G:O2'	1:X:2448:A:C8	2.67	0.47
1:X:2046:C:O2	1:X:2430:A:N1	2.48	0.47
14:L:39:TYR:O	14:L:54:ALA:C	2.54	0.47
1:X:2006:G:N2	1:X:2024:U:O2	2.48	0.47
1:X:709:A:C2	1:X:780:U:O2	2.68	0.47
1:X:2394:G:C6	1:X:2395:C:C4	3.03	0.47
20:R:85:ASP:OD1	20:R:85:ASP:C	2.52	0.47
1:X:510:G:N2	1:X:513:A:C8	2.83	0.47
1:X:2277:A:N6	1:X:2278:A:C2	2.83	0.47
28:2:15:THR:O	28:2:16:HIS:CB	2.62	0.47
1:X:1391:A:C1'	1:X:1392:U:O5'	2.63	0.47
1:X:2044:G:N2	31:X:2881:LC2:O2	2.48	0.47
1:X:751:G:O2'	1:X:752:G:O5'	2.32	0.47
1:X:579:G:C4'	1:X:994:A:C2	2.98	0.47
15:M:34:ARG:CD	15:M:88:VAL:CG2	2.93	0.47
32:X:2882:LMA:O57	18:P:111:ARG:NH2	2.48	0.47
6:D:4:LEU:CG	6:D:5:LYS:N	2.78	0.47
1:X:1730:G:C2	1:X:1737:G:C2	3.02	0.47
1:X:2430:A:C6	31:X:2881:LC2:C15	2.98	0.46
1:X:2676:G:N1	1:X:2690:A:C2	2.83	0.46
3:A:69:LYS:CD	3:A:69:LYS:N	2.78	0.46
9:G:103:TYR:N	9:G:103:TYR:CD1	2.82	0.46
1:X:123:A:C5'	28:2:19:ARG:NE	2.79	0.46
1:X:793:G:N1	1:X:795:A:C2	2.83	0.46
1:X:2580:C:O2'	1:X:2581:A:OP2	2.32	0.46
1:X:608:G:C6	1:X:609:U:C4	3.03	0.46
1:X:2502:G:C8	1:X:2502:G:O5'	2.68	0.46
1:X:584:A:OP2	1:X:2038:C:C5	2.68	0.46
1:X:1480:G:C2	1:X:1481:U:O2	2.68	0.46
1:X:314:G:C2	1:X:326:A:C2	3.03	0.46
1:X:791:G:N2	1:X:800:U:O2	2.48	0.46
1:X:540:G:C6	1:X:2005:U:C5'	2.98	0.46
10:H:116:ARG:C	10:H:118:LEU:N	2.67	0.46
1:X:26:G:C6	1:X:27:G:N1	2.84	0.46
1:X:2350:G:C6	1:X:2351:G:C5	3.03	0.46
1:X:1336:G:O6	1:X:1337:G:C6	2.68	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1674:C:OP1	4:B:134:TRP:O	2.33	0.46
1:X:2053:G:N2	1:X:2054:A:N3	2.63	0.46
1:X:748:A:C5	1:X:749:C:C2	3.04	0.46
1:X:2606:G:N2	1:X:2757:G:N3	2.64	0.46
1:X:2502:G:C2	1:X:2745:A:N6	2.83	0.46
23:U:14:VAL:O	23:U:15:VAL:CG2	2.63	0.46
1:X:115:G:C6	1:X:117:A:N6	2.84	0.46
2:Y:75:A:C6	2:Y:76:U:C2	3.03	0.46
4:B:92:ASN:OD1	4:B:92:ASN:N	2.46	0.46
1:X:1686:A:N6	1:X:1977:C:O2	2.48	0.46
1:X:2350:G:C6	1:X:2351:G:N7	2.84	0.46
1:X:1810:U:C5	3:A:158:ARG:CD	2.98	0.46
1:X:2033:C:N4	1:X:2034:A:N1	2.63	0.46
27:1:43:VAL:O	27:1:44:ALA:CB	2.62	0.46
1:X:986:A:C2	1:X:1001:A:C8	3.03	0.46
2:Y:30:C:N3	2:Y:58:G:N2	2.64	0.46
1:X:1202:U:O2	1:X:1202:U:C2'	2.62	0.46
1:X:746:G:N7	1:X:774:A:C6	2.84	0.46
20:R:18:LYS:N	20:R:18:LYS:CD	2.79	0.46
1:X:1371:G:C8	1:X:1384:G:O6	2.69	0.46
20:R:83:LEU:O	20:R:90:LYS:CE	2.64	0.46
1:X:1790:G:C4'	1:X:1791:C:O5'	2.64	0.46
1:X:919:U:OP1	12:J:26:ASP:OD1	2.34	0.46
1:X:2824:C:O4'	1:X:2843:A:C5	2.68	0.46
1:X:1677:C:C2	1:X:1984:A:C2	3.03	0.46
1:X:539:A:C6	1:X:2006:G:C4	3.04	0.46
1:X:478:G:C4	1:X:479:G:C8	3.04	0.46
1:X:2625:U:O4	1:X:2654:A:C2	2.68	0.46
1:X:26:G:C5	1:X:27:G:C6	3.04	0.46
17:O:48:GLY:O	17:O:50:ASP:N	2.49	0.46
1:X:24:G:C2	1:X:25:U:C2	3.04	0.46
1:X:2445:C:N4	1:X:2446:C:N4	2.64	0.46
1:X:1978:U:C2	1:X:1979:C:C5	3.03	0.46
1:X:708:G:N3	1:X:781:G:C2	2.84	0.46
19:Q:57:ASN:OD1	19:Q:57:ASN:N	2.49	0.46
1:X:2350:G:N1	1:X:2351:G:C5	2.84	0.45
1:X:2671:C:C5'	1:X:2845:C:O2	2.64	0.45
1:X:551:A:C2	1:X:562:G:C2	3.05	0.45
13:K:52:ILE:CG1	13:K:53:THR:N	2.79	0.45
18:P:83:ASP:O	18:P:84:GLU:C	2.54	0.45
4:B:182:ILE:CG2	4:B:182:ILE:O	2.64	0.45
1:X:802:A:C2	28:2:3:ARG:NH1	2.85	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2590:U:C1'	32:X:2882:LMA:H37B	2.46	0.45
1:X:1975:G:N2	1:X:1979:C:O2'	2.49	0.45
1:X:2840:U:N3	1:X:2841:U:C5	2.84	0.45
5:C:7:ILE:C	5:C:120:VAL:O	2.54	0.45
2:Y:85:G:N2	2:Y:97:C:C2	2.84	0.45
1:X:537:C:C5	1:X:2759:U:C2'	2.99	0.45
1:X:831:G:N2	1:X:1204:G:C6	2.84	0.45
4:B:26:VAL:CG1	4:B:196:VAL:CG2	2.95	0.45
1:X:759:C:N3	32:X:2882:LMA:H37	2.31	0.45
1:X:1467:U:C4	1:X:1473:U:N3	2.85	0.45
1:X:693:A:C2	1:X:811:G:N3	2.84	0.45
17:O:70:TYR:CD2	17:O:83:ARG:NH1	2.84	0.45
1:X:1745:C:N3	1:X:2696:A:O2'	2.48	0.45
1:X:1047:G:N3	1:X:1131:G:C2	2.85	0.45
1:X:2198:U:C4	1:X:2199:C:C2	3.04	0.45
1:X:1683:G:O5'	1:X:1683:G:C8	2.69	0.45
1:X:775:U:C4'	1:X:776:G:N3	2.79	0.45
1:X:845:U:C5	1:X:955:G:C6	3.05	0.45
1:X:2827:G:C6	1:X:2828:C:N3	2.85	0.45
1:X:2614:A:N1	1:X:2615:U:O2	2.50	0.45
1:X:2847:G:C2	1:X:2848:A:N6	2.84	0.45
16:N:86:ALA:C	16:N:88:ILE:N	2.70	0.45
1:X:610:G:N2	1:X:616:U:OP1	2.49	0.45
1:X:521:U:O4	1:X:522:G:C2	2.70	0.45
10:H:76:ARG:O	10:H:94:ASN:CA	2.65	0.45
13:K:33:ARG:O	13:K:34:ILE:CG2	2.65	0.45
1:X:2490:U:C4	1:X:2491:C:C4	3.04	0.45
1:X:2074:U:C4	1:X:2075:U:C4	3.04	0.45
1:X:697:G:C2	1:X:787:A:C2	3.05	0.45
1:X:758:G:C2'	1:X:759:C:OP1	2.65	0.45
4:B:131:SER:O	4:B:134:TRP:CD1	2.69	0.45
1:X:2754:C:C4	1:X:2755:A:C5	3.05	0.45
1:X:1715:A:C8	1:X:1717:A:O4'	2.69	0.45
1:X:1996:A:O2'	18:P:115:ASN:ND2	2.50	0.45
1:X:2063:A:O3'	23:U:39:LYS:CG	2.64	0.45
21:S:72:ASP:O	21:S:75:LYS:O	2.34	0.45
27:1:9:ILE:O	27:1:10:VAL:CG2	2.65	0.45
14:L:37:HIS:NE2	14:L:39:TYR:OH	2.49	0.45
5:C:158:ARG:O	5:C:159:ARG:C	2.55	0.45
1:X:1780:A:C5'	3:A:222:GLN:OE1	2.65	0.45
1:X:2053:G:C2	1:X:2054:A:C4	3.05	0.45
1:X:1456:C:C2	1:X:1566:G:N2	2.85	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1005:U:OP1	16:N:53:LYS:NZ	2.50	0.45
2:Y:73:C:N4	2:Y:74:A:C6	2.85	0.45
10:H:133:VAL:O	10:H:133:VAL:CG1	2.64	0.45
1:X:832:A:C2	1:X:1203:A:C2	3.05	0.44
22:T:18:PRO:C	22:T:19:LYS:CG	2.86	0.44
1:X:2550:C:O3'	4:B:146:THR:OG1	2.35	0.44
5:C:162:ARG:CB	5:C:162:ARG:NH1	2.80	0.44
26:Z:3:LYS:O	26:Z:4:HIS:C	2.55	0.44
1:X:67:G:N2	1:X:73:A:C2	2.86	0.44
1:X:1327:C:N4	1:X:1351:G:N1	2.65	0.44
1:X:555:U:C4	1:X:1243:G:N2	2.86	0.44
1:X:771:C:O2'	1:X:1964:A:N3	2.50	0.44
1:X:2727:G:C2	1:X:2736:U:C5	3.04	0.44
1:X:617:U:C5	1:X:631:G:C8	3.05	0.44
1:X:13:A:N3	1:X:15:G:C6	2.85	0.44
1:X:1677:C:C6	1:X:1677:C:C3'	3.01	0.44
1:X:760:U:C5	1:X:2592:U:C5	3.05	0.44
20:R:11:ASN:ND2	20:R:13:LYS:NZ	2.66	0.44
1:X:838:A:C2	1:X:839:U:C2	3.05	0.44
1:X:849:G:C5	1:X:850:C:C4	3.05	0.44
16:N:39:LEU:O	16:N:43:ALA:N	2.50	0.44
1:X:306:G:C6	1:X:355:G:C2	3.06	0.44
4:B:52:ALA:O	4:B:76:ARG:N	2.51	0.44
2:Y:66:G:C5	2:Y:67:C:C4	3.06	0.44
1:X:827:C:OP2	11:I:32:ARG:CZ	2.66	0.44
1:X:1851:A:C2	1:X:1867:A:C4	3.05	0.44
1:X:2426:G:O2'	1:X:2427:A:P	2.76	0.44
1:X:775:U:N3	1:X:1445:A:OP1	2.50	0.44
1:X:2046:C:C4	1:X:2047:C:C4	3.04	0.44
1:X:224:G:C2	1:X:229:G:N1	2.86	0.44
14:L:60:LYS:NZ	14:L:64:LYS:CE	2.81	0.44
1:X:1235:C:C2	1:X:1241:G:N2	2.86	0.44
1:X:777:A:OP2	3:A:215:TRP:CH2	2.70	0.44
1:X:81:C:C4	1:X:82:G:C6	3.06	0.44
5:C:180:ILE:CG2	5:C:181:LEU:N	2.80	0.44
1:X:2554:C:O2'	4:B:140:SER:CB	2.66	0.44
1:X:614:G:C5	1:X:615:C:C5	3.05	0.44
1:X:2272:A:P	14:L:18:ARG:NH1	2.90	0.44
1:X:540:G:C5	1:X:2005:U:C5'	3.00	0.44
16:N:14:HIS:CD2	16:N:32:TYR:CZ	3.06	0.44
1:X:2451:G:C4	1:X:2454:C:N4	2.86	0.44
2:Y:12:C:C5	2:Y:13:C:C4	3.06	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:93:VAL:C	4:B:95:ILE:N	2.71	0.44
3:A:66:ILE:CG2	3:A:89:ARG:NH2	2.81	0.44
3:A:21:ASP:C	3:A:22:PHE:CD2	2.90	0.44
23:U:60:VAL:CG2	23:U:61:TRP:N	2.80	0.44
1:X:2595:C:C6	1:X:2595:C:C3'	3.01	0.44
1:X:764:A:O5'	1:X:764:A:C8	2.70	0.44
14:L:45:ASP:OD2	14:L:46:SER:N	2.51	0.44
1:X:225:G:N7	1:X:227:G:N3	2.65	0.44
1:X:2496:C:C4	1:X:2521:A:C5	3.05	0.44
1:X:26:G:C6	1:X:27:G:C6	3.05	0.44
29:3:34:THR:OG1	29:3:35:GLY:N	2.51	0.44
1:X:2569:A:C2	1:X:2584:U:O2	2.70	0.44
1:X:649:G:N1	1:X:660:G:N1	2.65	0.44
1:X:1022:A:OP1	16:N:77:SER:N	2.50	0.44
1:X:2547:C:C6	1:X:2547:C:C3'	3.01	0.44
9:G:96:ASP:O	9:G:98:LYS:N	2.51	0.44
1:X:2754:C:C4	1:X:2755:A:N7	2.86	0.44
16:N:7:GLY:O	16:N:9:VAL:CG2	2.66	0.44
1:X:958:G:C2	1:X:982:C:N3	2.86	0.43
4:B:84:PHE:CE1	4:B:86:PRO:CB	3.00	0.43
1:X:2671:C:N3	1:X:2698:G:C2	2.86	0.43
1:X:494:A:C8	1:X:495:C:C6	3.06	0.43
1:X:1332:G:C5	1:X:1333:G:C6	3.06	0.43
1:X:2745:A:N3	1:X:2745:A:C3'	2.81	0.43
17:O:65:ARG:O	17:O:66:GLY:O	2.35	0.43
1:X:1726:C:C2	1:X:1741:G:N2	2.86	0.43
1:X:2637:C:N4	1:X:2638:G:C6	2.86	0.43
19:Q:12:ILE:O	19:Q:13:SER:CB	2.64	0.43
14:L:52:ALA:O	14:L:53:ALA:O	2.35	0.43
1:X:1030:U:O2	1:X:1155:G:N2	2.51	0.43
1:X:1222:G:N1	1:X:1251:G:C6	2.86	0.43
4:B:67:PHE:CZ	4:B:75:THR:CG2	3.01	0.43
1:X:1265:G:O2'	1:X:1266:G:C4	2.71	0.43
1:X:923:A:C5	12:J:12:LYS:CE	3.01	0.43
1:X:219:G:C2'	1:X:220:U:OP2	2.66	0.43
1:X:2394:G:C6	1:X:2395:C:N3	2.87	0.43
10:H:75:VAL:CG1	10:H:118:LEU:CD2	2.96	0.43
1:X:807:A:C2	1:X:808:C:C2	3.06	0.43
4:B:28:ALA:O	4:B:29:GLY:O	2.36	0.43
26:Z:42:SER:O	26:Z:44:HIS:CD2	2.72	0.43
1:X:775:U:C5'	1:X:776:G:N3	2.80	0.43
1:X:1473:U:O2	1:X:1474:A:C6	2.72	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2722:C:P	30:4:35:ARG:NH1	2.91	0.43
1:X:1571:G:C2	1:X:1572:C:C2	3.06	0.43
4:B:10:GLY:O	4:B:25:VAL:N	2.51	0.43
1:X:2345:A:N6	1:X:2346:G:C2	2.87	0.43
1:X:2621:G:OP1	9:G:110:LEU:CD1	2.66	0.43
9:G:84:ASN:N	9:G:153:GLY:O	2.52	0.43
27:1:11:LYS:N	27:1:11:LYS:CD	2.81	0.43
1:X:123:A:C2'	1:X:124:A:OP1	2.66	0.43
1:X:2653:A:N6	1:X:2654:A:C6	2.87	0.43
1:X:2400:G:OP1	27:1:4:ASP:CG	2.57	0.43
1:X:2659:C:O3'	4:B:8:LYS:NZ	2.51	0.43
1:X:2434:G:C6	1:X:2435:C:N4	2.87	0.43
6:D:17:MET:N	6:D:17:MET:SD	2.92	0.43
1:X:1298:G:C6	1:X:1342:U:C5	3.07	0.43
1:X:1437:A:C2	1:X:1592:U:O2	2.71	0.43
4:B:36:ARG:NH1	4:B:86:PRO:O	2.52	0.43
1:X:2043:A:O4'	1:X:2481:G:O4'	2.35	0.43
3:A:34:LEU:CG	3:A:34:LEU:O	2.66	0.43
19:Q:88:ILE:O	19:Q:88:ILE:CD1	2.66	0.43
1:X:1445:A:C2	1:X:1579:G:N3	2.87	0.43
9:G:70:PHE:CB	16:N:64:ARG:CG	2.96	0.43
1:X:29:U:C4'	16:N:11:ARG:NH1	2.81	0.43
14:L:37:HIS:CD2	14:L:39:TYR:OH	2.71	0.43
17:O:80:TYR:O	17:O:80:TYR:CD1	2.70	0.43
4:B:120:TRP:O	4:B:121:ASN:C	2.56	0.43
1:X:1008:G:C2	1:X:1170:U:C2	3.07	0.43
1:X:583:C:N4	1:X:2017:U:OP1	2.51	0.43
1:X:939:C:OP2	1:X:940:G:C8	2.72	0.43
1:X:1923:U:O2'	1:X:1924:C:OP2	2.36	0.43
1:X:870:C:O2	1:X:933:G:N2	2.52	0.43
7:E:171:LEU:N	7:E:171:LEU:CD1	2.81	0.43
1:X:1790:G:C6	1:X:1811:A:C5	3.07	0.43
1:X:1585:A:N1	1:X:1586:A:C2	2.87	0.43
1:X:2366:U:C1'	22:T:41:ARG:NH1	2.82	0.43
1:X:2013:A:C5'	1:X:2014:A:OP1	2.66	0.43
1:X:2475:C:N4	1:X:2476:A:C6	2.87	0.43
1:X:742:G:O6	1:X:1765:C:N3	2.52	0.43
1:X:2756:A:C4'	1:X:2757:G:O5'	2.67	0.43
1:X:2381:A:O2'	1:X:2382:C:C5	2.71	0.43
15:M:26:ASP:O	15:M:26:ASP:CG	2.57	0.43
1:X:463:C:O2	1:X:465:C:N4	2.51	0.43
1:X:2475:C:OP1	12:J:83:ARG:CB	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:851:C:C2	1:X:952:A:C2	3.06	0.43
1:X:1939:U:C5	1:X:1940:C:C4	3.06	0.43
1:X:2822:U:OP1	15:M:103:LYS:NZ	2.51	0.43
1:X:870:C:C2	1:X:933:G:N2	2.87	0.43
1:X:1935:A:C6	1:X:1936:A:N1	2.87	0.43
1:X:982:C:O2'	1:X:994:A:N3	2.52	0.42
1:X:538:A:O2'	1:X:539:A:C5'	2.67	0.42
9:G:169:GLN:NE2	9:G:171:LEU:C	2.73	0.42
16:N:45:TYR:O	16:N:49:ASP:OD1	2.37	0.42
1:X:2071:G:C2	1:X:2072:C:C2	3.07	0.42
1:X:961:G:C5	1:X:962:C:C4	3.07	0.42
3:A:268:ASP:C	3:A:268:ASP:OD1	2.57	0.42
1:X:995:A:P	1:X:996:C:C5	3.13	0.42
3:A:151:GLY:C	3:A:153:GLY:N	2.71	0.42
3:A:151:GLY:O	3:A:153:GLY:N	2.52	0.42
3:A:71:ARG:NH1	3:A:150:PRO:CB	2.82	0.42
1:X:2012:A:C2	1:X:2016:A:C6	3.06	0.42
1:X:1404:C:N4	1:X:1406:A:C8	2.87	0.42
1:X:1179:A:C2	1:X:1196:G:N2	2.87	0.42
1:X:221:A:C2	1:X:232:A:C5	3.07	0.42
1:X:45:C:C2	1:X:157:G:N2	2.87	0.42
17:O:7:THR:O	17:O:8:GLY:O	2.37	0.42
1:X:2657:G:N2	1:X:2710:C:O2	2.53	0.42
13:K:73:LYS:O	13:K:76:VAL:CG1	2.68	0.42
1:X:759:C:C4'	1:X:759:C:OP1	2.67	0.42
1:X:1683:G:C2'	1:X:1684:G:C5'	2.98	0.42
1:X:2825:A:OP2	1:X:2843:A:C2	2.71	0.42
1:X:2690:A:N6	1:X:2694:G:C4	2.88	0.42
1:X:1987:G:C6	1:X:1988:A:C5	3.07	0.42
9:G:104:THR:O	9:G:107:GLN:NE2	2.52	0.42
10:H:9:ASP:O	10:H:96:ALA:N	2.53	0.42
1:X:764:A:C3'	1:X:764:A:C8	3.02	0.42
1:X:1625:A:O2'	1:X:1632:A:O4'	2.37	0.42
1:X:188:G:C6	1:X:189:A:C6	3.06	0.42
16:N:28:ARG:O	16:N:35:ALA:CB	2.67	0.42
1:X:1937:G:N3	1:X:2530:C:C5'	2.82	0.42
3:A:184:ARG:NH1	3:A:184:ARG:CB	2.83	0.42
1:X:2636:A:C2	1:X:2644:A:C4	3.07	0.42
27:1:45:LYS:O	27:1:46:LYS:CB	2.67	0.42
1:X:171:G:C2	1:X:179:U:C2	3.06	0.42
1:X:1910:A:N6	1:X:1911:A:N1	2.68	0.42
1:X:1336:G:C6	1:X:1337:G:C5	3.08	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:3:13:ARG:CG	29:3:13:ARG:O	2.67	0.42
1:X:459:A:N7	1:X:484:G:C5	2.88	0.42
1:X:1344:C:C4	1:X:1346:C:C2	3.08	0.42
1:X:526:C:O2'	1:X:527:C:C5'	2.67	0.42
9:G:141:GLY:O	9:G:142:ARG:C	2.55	0.42
1:X:2445:C:C4	1:X:2446:C:N4	2.87	0.42
9:G:84:ASN:O	9:G:85:ALA:CB	2.67	0.42
1:X:2000:U:C4'	26:Z:8:LYS:O	2.68	0.42
6:D:52:LYS:NZ	6:D:135:GLN:OE1	2.53	0.42
18:P:133:ASN:N	18:P:133:ASN:OD1	2.52	0.42
28:2:12:ARG:O	28:2:15:THR:O	2.37	0.42
26:Z:3:LYS:N	26:Z:3:LYS:CD	2.82	0.42
1:X:1948:C:N4	1:X:1949:A:N6	2.68	0.42
5:C:176:ASN:CB	5:C:179:ASP:OD2	2.68	0.42
5:C:21:GLU:C	5:C:22:VAL:CG2	2.87	0.42
1:X:1177:U:C2	1:X:1198:C:O2	2.73	0.42
9:G:156:HIS:N	9:G:157:PRO:CD	2.82	0.42
1:X:1391:A:C1'	1:X:1392:U:P	3.08	0.42
4:B:121:ASN:O	4:B:122:PHE:CG	2.72	0.42
1:X:748:A:C5'	1:X:748:A:C8	3.02	0.42
13:K:94:TYR:CZ	13:K:115:LEU:O	2.72	0.42
1:X:681:A:C5	1:X:683:A:C8	3.08	0.42
1:X:13:A:C2	1:X:15:G:N1	2.88	0.42
1:X:649:G:N2	1:X:660:G:C2	2.88	0.42
9:G:84:ASN:O	9:G:151:TYR:O	2.38	0.42
1:X:180:C:C4	1:X:181:A:C5	3.08	0.42
1:X:2438:A:N6	1:X:2473:G:C2	2.88	0.42
1:X:1691:G:C6	1:X:1972:G:O6	2.73	0.42
1:X:1344:C:C4	1:X:1346:C:N3	2.88	0.42
4:B:93:VAL:O	4:B:95:ILE:N	2.53	0.42
1:X:2245:A:C2	1:X:2251:U:C5	3.08	0.42
1:X:2256:G:O3'	12:J:14:PHE:CD2	2.73	0.42
32:X:2882:LMA:HO57	18:P:111:ARG:NH2	2.17	0.42
1:X:1365:U:C2	1:X:1393:G:C2	3.07	0.42
1:X:611:C:O2	1:X:615:C:C5'	2.68	0.42
12:J:27:TYR:CB	12:J:137:VAL:CG2	2.98	0.42
1:X:2404:A:C4'	1:X:2405:A:OP2	2.68	0.42
1:X:593:C:OP2	16:N:10:ARG:NH1	2.52	0.42
1:X:671:A:C5	1:X:672:C:C4	3.08	0.42
13:K:79:VAL:O	13:K:84:ALA:CB	2.68	0.42
1:X:943:U:O2'	1:X:944:A:O4'	2.37	0.42
1:X:2244:C:C4	1:X:2245:A:C5	3.08	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:146:LEU:O	3:A:156:LEU:CB	2.68	0.42
14:L:33:ARG:NH1	14:L:99:ARG:O	2.53	0.42
1:X:750:C:C4'	1:X:779:U:O2'	2.68	0.42
1:X:768:U:C4	1:X:769:C:C4	3.08	0.42
27:1:9:ILE:C	27:1:10:VAL:CG2	2.88	0.41
3:A:90:SER:O	3:A:199:ASN:OD1	2.37	0.41
5:C:34:GLN:OE1	5:C:176:ASN:ND2	2.52	0.41
1:X:1473:U:O2'	1:X:1474:A:P	2.77	0.41
1:X:1299:A:C4'	1:X:1300:A:OP1	2.68	0.41
1:X:1790:G:C6	1:X:1811:A:N7	2.88	0.41
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.52	0.41
1:X:2727:G:N2	1:X:2736:U:C5	2.88	0.41
1:X:1200:G:C6	1:X:1201:G:C4	3.08	0.41
1:X:1225:G:C2'	1:X:1249:G:N2	2.83	0.41
14:L:93:SER:C	14:L:94:TYR:CD2	2.92	0.41
1:X:800:U:C5	1:X:804:C:N3	2.88	0.41
1:X:752:G:OP1	1:X:1775:A:N1	2.53	0.41
1:X:749:C:O5'	1:X:749:C:C6	2.73	0.41
1:X:2793:G:N3	1:X:2804:G:C2	2.88	0.41
1:X:983:G:O2'	1:X:984:A:OP1	2.38	0.41
1:X:461:A:N7	1:X:462:G:N7	2.68	0.41
1:X:572:G:C2	1:X:573:C:C2	3.08	0.41
1:X:590:C:OP1	16:N:31:GLN:CB	2.68	0.41
13:K:13:ASN:OD1	13:K:16:ALA:CB	2.69	0.41
12:J:64:LYS:CD	12:J:108:ALA:O	2.69	0.41
1:X:761:G:OP1	1:X:2591:C:N4	2.53	0.41
4:B:7:THR:OG1	4:B:51:TYR:OH	2.38	0.41
16:N:63:GLN:O	16:N:66:ASN:OD1	2.39	0.41
1:X:2003:A:C6	1:X:2005:U:C2	3.08	0.41
1:X:494:A:N7	1:X:495:C:C5	2.88	0.41
1:X:2766:U:O2'	4:B:62:PRO:O	2.39	0.41
28:2:39:ARG:O	28:2:40:HIS:CG	2.73	0.41
13:K:59:ASP:O	13:K:60:LEU:C	2.56	0.41
13:K:17:ARG:CG	13:K:18:VAL:N	2.83	0.41
1:X:654:A:C3'	1:X:654:A:N3	2.83	0.41
1:X:2671:C:O2	1:X:2822:U:O2'	2.38	0.41
1:X:594:G:N7	1:X:1264:C:N4	2.69	0.41
1:X:2450:A:N6	1:X:2451:G:C2	2.89	0.41
1:X:2728:A:C2	1:X:2737:A:C5	3.08	0.41
1:X:13:A:C2	1:X:15:G:C6	3.08	0.41
1:X:1488:G:C2	1:X:1536:G:C2	3.08	0.41
1:X:1129:A:C6	1:X:1130:U:N3	2.88	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:869:C:O2	1:X:934:G:C2	2.73	0.41
1:X:320:A:N3	1:X:340:G:O2'	2.53	0.41
1:X:788:G:O2'	1:X:789:G:P	2.79	0.41
1:X:2827:G:N1	1:X:2840:U:N3	2.69	0.41
1:X:2404:A:C8	1:X:2406:C:O2	2.74	0.41
1:X:2665:G:O5'	1:X:2665:G:C8	2.74	0.41
1:X:6:A:C1'	9:G:162:LYS:CG	2.99	0.41
20:R:63:THR:O	20:R:64:ASN:C	2.58	0.41
10:H:116:ARG:O	10:H:117:GLU:C	2.58	0.41
3:A:212:ARG:CG	3:A:212:ARG:O	2.68	0.41
27:1:43:VAL:CG2	27:1:43:VAL:O	2.69	0.41
1:X:984:A:C8	1:X:1202:U:C2	3.08	0.41
1:X:591:G:C6	1:X:592:G:C6	3.08	0.41
1:X:1175:A:C2	1:X:1176:U:C2	3.09	0.41
1:X:2560:G:C6	1:X:2589:C:C2	3.09	0.41
3:A:46:ASN:ND2	3:A:47:ARG:N	2.68	0.41
1:X:1142:G:N2	1:X:1143:A:N3	2.69	0.41
1:X:2571:G:N1	1:X:2582:G:N1	2.69	0.41
1:X:1987:G:C5	1:X:1988:A:C8	3.08	0.41
28:2:1:MET:CE	28:2:3:ARG:CZ	2.98	0.41
1:X:985:G:C8	1:X:1200:G:N2	2.89	0.41
20:R:15:HIS:ND1	20:R:16:PHE:CD2	2.88	0.41
19:Q:69:ILE:CD1	19:Q:70:GLY:N	2.83	0.41
1:X:872:G:O2'	1:X:873:U:OP2	2.39	0.41
1:X:2535:C:C5	1:X:2536:G:C5	3.09	0.41
11:I:73:GLU:OE1	11:I:73:GLU:N	2.53	0.41
1:X:1226:A:C4	1:X:1250:A:N3	2.88	0.41
20:R:92:THR:CB	20:R:107:ALA:O	2.69	0.41
1:X:2184:C:C4	1:X:2185:U:C4	3.08	0.41
1:X:1391:A:C2	1:X:1393:G:C8	3.09	0.41
1:X:2258:G:O6	22:T:15:ASP:CB	2.69	0.41
1:X:1774:A:OP1	1:X:1775:A:OP2	2.39	0.41
1:X:752:G:OP1	1:X:1775:A:C2	2.74	0.41
1:X:538:A:C4'	1:X:539:A:OP1	2.69	0.41
7:E:156:ALA:O	7:E:157:TYR:CD1	2.73	0.41
27:1:31:THR:O	27:1:33:ALA:N	2.54	0.41
1:X:980:G:C2	1:X:981:C:C2	3.09	0.41
1:X:573:C:C5	1:X:574:C:C5	3.09	0.41
1:X:469:G:C2'	28:2:39:ARG:O	2.69	0.41
1:X:1341:G:N2	1:X:1664:G:N1	2.69	0.41
1:X:1818:G:C6	1:X:1819:U:N3	2.89	0.41
5:C:14:THR:O	5:C:15:ILE:CB	2.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2857:C:OP1	13:K:96:ARG:NH2	2.54	0.41
1:X:997:C:C3'	1:X:997:C:C6	3.04	0.41
6:D:80:ARG:NE	6:D:80:ARG:N	2.69	0.41
32:X:2882:LMA:C51	32:X:2882:LMA:H21A	2.51	0.41
1:X:1289:A:C2	1:X:1290:A:C6	3.09	0.41
1:X:182:G:O2'	1:X:183:U:C5	2.74	0.41
1:X:851:C:C2	1:X:952:A:C6	3.09	0.41
11:I:57:ILE:O	29:3:12:ARG:NE	2.54	0.41
1:X:748:A:N7	1:X:749:C:C2	2.88	0.41
17:O:10:LYS:NZ	17:O:37:ALA:CB	2.84	0.41
1:X:196:A:N6	1:X:197:G:C6	2.89	0.41
1:X:2064:U:C5	1:X:2216:G:C2	3.09	0.41
1:X:841:G:C2'	1:X:841:G:N3	2.83	0.41
1:X:333:A:C5'	5:C:162:ARG:CG	2.99	0.40
1:X:2581:A:C2'	1:X:2582:G:O5'	2.69	0.40
1:X:1948:C:C4	1:X:1949:A:N7	2.89	0.40
1:X:2004:U:P	26:Z:12:SER:OG	2.79	0.40
1:X:916:U:C4	1:X:917:U:C4	3.09	0.40
32:X:2882:LMA:H4	32:X:2882:LMA:H7	1.88	0.40
1:X:2670:C:O4'	1:X:2847:G:C6	2.75	0.40
1:X:1335:A:N1	1:X:1346:C:O2'	2.54	0.40
1:X:2814:G:C1'	13:K:49:GLU:OE2	2.70	0.40
6:D:72:LYS:CA	6:D:81:GLN:O	2.70	0.40
1:X:754:G:C6	1:X:755:C:N4	2.90	0.40
3:A:66:ILE:CD1	3:A:89:ARG:NH2	2.83	0.40
1:X:1142:G:N3	9:G:103:TYR:CE2	2.89	0.40
10:H:28:GLY:O	10:H:35:THR:OG1	2.39	0.40
1:X:1920:A:C5	1:X:1922:U:C2	3.09	0.40
1:X:1096:A:C1'	1:X:1097:A:OP1	2.69	0.40
1:X:2555:G:N3	1:X:2555:G:C3'	2.84	0.40
19:Q:68:PHE:O	19:Q:69:ILE:CD1	2.70	0.40
15:M:24:LEU:CB	15:M:25:PRO:CD	2.99	0.40
20:R:65:PRO:O	20:R:66:GLN:C	2.57	0.40
1:X:2719:U:C5	1:X:2743:G:C6	3.09	0.40
10:H:1:MET:N	10:H:79:HIS:CB	2.84	0.40
9:G:90:LEU:CD1	9:G:90:LEU:N	2.85	0.40
6:D:123:ASP:OD1	6:D:124:GLY:N	2.54	0.40
1:X:486:U:O2	1:X:492:G:N2	2.54	0.40
1:X:965:G:O6	1:X:966:A:C6	2.74	0.40
1:X:1928:G:N1	1:X:1929:U:N3	2.70	0.40
1:X:1811:A:C4'	1:X:1812:U:O5'	2.70	0.40
1:X:1439:G:O2'	1:X:1440:G:O5'	2.39	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:R:23:ILE:CD1	20:R:23:ILE:C	2.90	0.40
1:X:309:G:OP1	20:R:93:ARG:CA	2.69	0.40
3:A:160:ALA:CA	3:A:199:ASN:CB	3.00	0.40
1:X:2571:G:N2	1:X:2582:G:C4	2.90	0.40
1:X:1724:C:C4	1:X:1747:G:O6	2.75	0.40
6:D:22:TYR:CZ	6:D:29:PRO:CD	3.05	0.40
1:X:1947:G:O6	1:X:1950:C:N4	2.54	0.40
1:X:513:A:OP1	1:X:514:G:N2	2.55	0.40
1:X:1621:C:O4'	1:X:1626:A:C6	2.75	0.40
1:X:1364:C:O2	1:X:1394:G:C2	2.75	0.40
1:X:1098:G:O6	1:X:1100:G:C2	2.74	0.40
5:C:164:VAL:CG2	5:C:165:SER:N	2.85	0.40
1:X:1688:U:C2	1:X:1690:U:OP2	2.74	0.40
18:P:106:LEU:CD2	18:P:106:LEU:C	2.89	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1552:C:O2	15:M:43:ASN:ND2[8_455]	0.99	1.21
1:X:1552:C:O2	15:M:43:ASN:CG[8_455]	1.93	0.27
1:X:1552:C:C2	15:M:43:ASN:ND2[8_455]	2.03	0.17

## 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	A	251/274 (92%)	207 (82%)	36 (14%)	8 (3%)	6	51
4	B	203/211 (96%)	174 (86%)	22 (11%)	7 (3%)	6	49
5	C	192/205 (94%)	153 (80%)	30 (16%)	9 (5%)	4	37
6	D	175/180 (97%)	146 (83%)	27 (15%)	2 (1%)	21	76
7	E	169/185 (91%)	147 (87%)	18 (11%)	4 (2%)	9	58
8	F	61/144 (42%)	51 (84%)	9 (15%)	1 (2%)	14	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	G	140/174 (80%)	118 (84%)	18 (13%)	4 (3%)	7	54
10	H	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
11	I	132/156 (85%)	96 (73%)	29 (22%)	7 (5%)	3	33
12	J	134/141 (95%)	107 (80%)	25 (19%)	2 (2%)	15	68
13	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	25	79
14	L	102/114 (90%)	81 (79%)	20 (20%)	1 (1%)	22	78
15	M	106/166 (64%)	94 (89%)	9 (8%)	3 (3%)	8	54
16	N	115/118 (98%)	106 (92%)	7 (6%)	2 (2%)	14	66
17	O	92/100 (92%)	77 (84%)	12 (13%)	3 (3%)	6	50
18	P	124/134 (92%)	109 (88%)	13 (10%)	2 (2%)	14	67
19	Q	91/95 (96%)	66 (72%)	20 (22%)	5 (6%)	3	32
20	R	108/115 (94%)	82 (76%)	20 (18%)	6 (6%)	3	31
21	S	173/237 (73%)	140 (81%)	28 (16%)	5 (3%)	7	54
22	T	72/91 (79%)	57 (79%)	12 (17%)	3 (4%)	4	41
23	U	70/81 (86%)	44 (63%)	21 (30%)	5 (7%)	2	24
24	V	63/67 (94%)	58 (92%)	4 (6%)	1 (2%)	14	67
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	55/60 (92%)	42 (76%)	12 (22%)	1 (2%)	13	65
27	1	51/55 (93%)	31 (61%)	15 (29%)	5 (10%)	1	14
28	2	44/47 (94%)	37 (84%)	7 (16%)	0	100	100
29	3	57/66 (86%)	37 (65%)	18 (32%)	2 (4%)	6	49
30	4	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3111/3558 (87%)	2556 (82%)	466 (15%)	89 (3%)	7	54

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	221	HIS
4	B	86	PRO
4	B	122	PHE
4	B	137	ARG
4	B	147	PRO
5	C	154	ASP
7	E	12	PRO

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Mol	Chain	Res	Type
12	J	13	GLN
12	J	136	GLU
15	M	29	PRO
16	N	94	VAL
20	R	83	LEU
21	S	91	PRO
21	S	156	GLU
23	U	15	VAL
23	U	60	VAL
24	V	3	PRO
27	1	9	ILE
27	1	44	ALA
29	3	60	LEU
3	A	30	PRO
3	A	89	ARG
5	C	15	ILE
5	C	121	ASP
6	D	21	GLY
14	L	53	ALA
15	M	17	GLU
17	O	8	GLY
18	P	132	GLY
19	Q	13	SER
19	Q	59	PRO
19	Q	61	LYS
19	Q	69	ILE
20	R	63	THR
21	S	26	LYS
21	S	88	TYR
22	T	16	SER
3	A	25	LEU
3	A	235	GLY
5	C	10	ASN
5	C	127	ASP
11	I	56	LEU
11	I	84	GLU
13	K	100	VAL
18	P	20	LEU
22	T	15	ASP
22	T	20	TYR
27	1	24	THR
27	1	34	LYS

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Mol	Chain	Res	Type
27	1	46	LYS
3	A	152	LYS
4	B	29	GLY
4	B	202	ALA
5	C	22	VAL
5	C	128	ALA
7	E	165	VAL
7	E	173	ALA
8	F	120	VAL
9	G	67	ARG
11	I	86	THR
11	I	88	PHE
15	M	28	ARG
16	N	8	ILE
17	O	66	GLY
19	Q	65	VAL
20	R	6	ALA
3	A	61	ARG
5	C	68	ARG
17	O	15	SER
20	R	26	SER
9	G	97	ASP
21	S	33	ALA
26	Z	7	PRO
29	3	13	ARG
6	D	146	VAL
9	G	163	PRO
20	R	98	ILE
3	A	48	GLY
7	E	7	GLN
9	G	52	GLY
11	I	19	VAL
11	I	68	VAL
20	R	108	VAL
23	U	14	VAL
23	U	18	VAL
5	C	172	VAL
11	I	114	ILE
23	U	41	VAL
4	B	14	ILE

### 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	A	194/215 (90%)	180 (93%)	14 (7%)	21	66
4	B	155/157 (99%)	147 (95%)	8 (5%)	32	78
5	C	154/163 (94%)	146 (95%)	8 (5%)	32	78
6	D	152/156 (97%)	151 (99%)	1 (1%)	91	97
7	E	136/144 (94%)	135 (99%)	1 (1%)	91	97
8	F	46/107 (43%)	46 (100%)	0	100	100
9	G	118/146 (81%)	111 (94%)	7 (6%)	28	74
10	H	103/103 (100%)	100 (97%)	3 (3%)	55	90
11	I	100/121 (83%)	93 (93%)	7 (7%)	21	67
12	J	110/115 (96%)	106 (96%)	4 (4%)	47	86
13	K	90/93 (97%)	85 (94%)	5 (6%)	30	76
14	L	74/82 (90%)	70 (95%)	4 (5%)	31	77
15	M	94/134 (70%)	90 (96%)	4 (4%)	40	83
16	N	96/97 (99%)	94 (98%)	2 (2%)	66	93
17	O	75/79 (95%)	73 (97%)	2 (3%)	57	90
18	P	108/115 (94%)	107 (99%)	1 (1%)	87	97
19	Q	73/76 (96%)	69 (94%)	4 (6%)	30	76
20	R	91/96 (95%)	83 (91%)	8 (9%)	14	55
21	S	149/192 (78%)	146 (98%)	3 (2%)	68	93
22	T	55/67 (82%)	54 (98%)	1 (2%)	71	93
23	U	54/66 (82%)	51 (94%)	3 (6%)	30	76
24	V	53/55 (96%)	53 (100%)	0	100	100
25	W	48/48 (100%)	48 (100%)	0	100	100
26	Z	51/53 (96%)	50 (98%)	1 (2%)	68	93
27	1	46/48 (96%)	36 (78%)	10 (22%)	1	8
28	2	39/40 (98%)	34 (87%)	5 (13%)	6	32
29	3	46/52 (88%)	41 (89%)	5 (11%)	9	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2545/2855 (89%)	2434 (96%)	111 (4%)	39	83

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

Mol	Chain	Res	Type
3	A	34	LEU
3	A	44	ARG
3	A	49	ARG
3	A	55	ILE
3	A	69	LYS
3	A	126	PRO
3	A	150	PRO
3	A	156	LEU
3	A	165	GLN
3	A	199	ASN
3	A	209	LYS
3	A	219	LYS
3	A	245	ARG
3	A	246	VAL
4	B	27	LEU
4	B	86	PRO
4	B	87	ASP
4	B	143	GLN
4	B	146	THR
4	B	147	PRO
4	B	150	VAL
4	B	184	VAL
5	C	10	ASN
5	C	22	VAL
5	C	62	LYS
5	C	91	TYR
5	C	153	ASP
5	C	162	ARG
5	C	163	ASN
5	C	176	ASN
6	D	80	ARG
7	E	84	THR
9	G	32	TYR
9	G	37	ASP
9	G	38	GLU
9	G	111	LYS

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Mol	Chain	Res	Type
9	G	112	THR
9	G	113	GLU
9	G	154	GLU
10	H	1	MET
10	H	21	CYS
10	H	23	ARG
11	I	17	LYS
11	I	32	ARG
11	I	45	LYS
11	I	48	PHE
11	I	49	PHE
11	I	59	ARG
11	I	88	PHE
12	J	64	LYS
12	J	103	VAL
12	J	135	ARG
12	J	139	ASP
13	K	3	HIS
13	K	5	LYS
13	K	36	THR
13	K	54	THR
13	K	94	TYR
14	L	42	ILE
14	L	60	LYS
14	L	89	PHE
14	L	91	ARG
15	M	5	ILE
15	M	28	ARG
15	M	31	ASP
15	M	103	LYS
16	N	22	LYS
16	N	63	GLN
17	O	28	GLU
17	O	91	THR
18	P	32	ARG
19	Q	7	LEU
19	Q	12	ILE
19	Q	57	ASN
19	Q	88	ILE
20	R	18	LYS
20	R	25	LEU
20	R	71	GLN

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Mol	Chain	Res	Type
20	R	79	SER
20	R	83	LEU
20	R	84	VAL
20	R	85	ASP
20	R	112	LYS
21	S	13	LYS
21	S	34	LEU
21	S	71	MET
22	T	15	ASP
23	U	32	ARG
23	U	61	TRP
23	U	78	ILE
26	Z	9	LYS
27	1	8	ILE
27	1	9	ILE
27	1	20	PHE
27	1	21	TYR
27	1	28	ARG
27	1	30	ASN
27	1	37	LEU
27	1	47	HIS
27	1	51	ARG
27	1	54	LYS
28	2	5	TYR
28	2	9	ASN
28	2	10	ARG
28	2	12	ARG
28	2	15	THR
29	3	31	HIS
29	3	39	ASP
29	3	46	LYS
29	3	49	VAL
29	3	52	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2630/2880 (91%)	470 (17%)	73 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Y	119/123 (96%)	22 (18%)	0
All	All	2749/3003 (91%)	492 (17%)	73 (2%)

All (492) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	14	A
1	X	34	U
1	X	35	G
1	X	39	C
1	X	45	C
1	X	49	U
1	X	59	G
1	X	63	A
1	X	68	C
1	X	70	A
1	X	74	G
1	X	76	C
1	X	83	A
1	X	87	G
1	X	88	G
1	X	89	A
1	X	90	G
1	X	98	U
1	X	100	G
1	X	101	A
1	X	118	U
1	X	123	A
1	X	124	A
1	X	129	A
1	X	136	A
1	X	155	G
1	X	158	A
1	X	173	A
1	X	174	A
1	X	177	U
1	X	178	C
1	X	182	G
1	X	183	U
1	X	193	A
1	X	199	A

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Mol	Chain	Res	Type
1	X	205	A
1	X	206	U
1	X	210	A
1	X	219	G
1	X	225	G
1	X	226	C
1	X	242	A
1	X	245	C
1	X	304	A
1	X	305	A
1	X	312	G
1	X	318	G
1	X	323	G
1	X	333	A
1	X	334	G
1	X	335	A
1	X	340	G
1	X	342	G
1	X	343	A
1	X	358	C
1	X	399	G
1	X	400	U
1	X	411	C
1	X	414	A
1	X	418	C
1	X	424	G
1	X	425	A
1	X	441	A
1	X	456	C
1	X	463	C
1	X	467	U
1	X	469	G
1	X	491	A
1	X	492	G
1	X	497	C
1	X	515	A
1	X	518	A
1	X	519	C
1	X	526	C
1	X	537	C
1	X	538	A
1	X	539	A

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Mol	Chain	Res	Type
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	556	A
1	X	557	U
1	X	558	G
1	X	559	C
1	X	572	G
1	X	581	A
1	X	583	C
1	X	584	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	636	G
1	X	648	A
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A
1	X	657	A
1	X	665	A
1	X	666	U
1	X	668	A
1	X	682	G
1	X	683	A
1	X	684	C
1	X	699	G
1	X	743	A
1	X	749	C
1	X	752	G
1	X	759	C
1	X	766	A
1	X	774	A

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Mol	Chain	Res	Type
1	X	777	A
1	X	778	G
1	X	781	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	796	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	816	U
1	X	818	G
1	X	819	C
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	844	G
1	X	859	U
1	X	860	U
1	X	862	A
1	X	879	A
1	X	919	U
1	X	921	A
1	X	922	A
1	X	926	C
1	X	939	C
1	X	940	G
1	X	944	A
1	X	952	A
1	X	955	G
1	X	956	A
1	X	957	G
1	X	969	U
1	X	970	A
1	X	972	C
1	X	984	A

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Mol	Chain	Res	Type
1	X	985	G
1	X	994	A
1	X	995	A
1	X	996	C
1	X	1006	C
1	X	1007	A
1	X	1016	C
1	X	1019	U
1	X	1023	U
1	X	1032	A
1	X	1033	G
1	X	1037	U
1	X	1044	U
1	X	1051	U
1	X	1054	C
1	X	1060	C
1	X	1070	G
1	X	1078	A
1	X	1079	G
1	X	1082	G
1	X	1087	C
1	X	1090	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1108	U
1	X	1115	C
1	X	1119	U
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1141	U
1	X	1142	G
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1167	A
1	X	1168	G
1	X	1183	C
1	X	1195	U

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Mol	Chain	Res	Type
1	X	1220	G
1	X	1223	G
1	X	1224	A
1	X	1250	A
1	X	1262	U
1	X	1265	G
1	X	1266	G
1	X	1268	U
1	X	1269	G
1	X	1279	G
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1299	A
1	X	1300	A
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1326	U
1	X	1331	G
1	X	1333	G
1	X	1334	A
1	X	1342	U
1	X	1359	G
1	X	1378	A
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1393	G
1	X	1398	G
1	X	1413	U
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1440	G
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U

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Mol	Chain	Res	Type
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1473	U
1	X	1475	U
1	X	1476	G
1	X	1482	U
1	X	1490	U
1	X	1497	C
1	X	1506	C
1	X	1528	C
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1570	C
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1582	A
1	X	1585	A
1	X	1601	U
1	X	1602	G
1	X	1608	U
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1632	A
1	X	1635	G
1	X	1648	C
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1669	A
1	X	1681	A
1	X	1685	A
1	X	1689	U
1	X	1691	G
1	X	1692	C
1	X	1710	U

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Mol	Chain	Res	Type
1	X	1712	G
1	X	1714	A
1	X	1716	G
1	X	1717	A
1	X	1735	G
1	X	1746	A
1	X	1747	G
1	X	1749	G
1	X	1750	A
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1765	C
1	X	1772	C
1	X	1775	A
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1793	A
1	X	1801	C
1	X	1802	A
1	X	1808	C
1	X	1812	U
1	X	1825	C
1	X	1831	G
1	X	1842	G
1	X	1868	A
1	X	1884	A
1	X	1910	A
1	X	1920	A
1	X	1922	U
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1928	G
1	X	1939	U
1	X	1946	U
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G

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Mol	Chain	Res	Type
1	X	1964	A
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1979	C
1	X	1980	A
1	X	2005	U
1	X	2006	G
1	X	2014	A
1	X	2015	G
1	X	2016	A
1	X	2017	U
1	X	2019	C
1	X	2026	C
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2047	C
1	X	2052	G
1	X	2057	U
1	X	2075	U
1	X	2083	G
1	X	2171	U
1	X	2181	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
1	X	2195	C
1	X	2196	U
1	X	2199	C
1	X	2200	G
1	X	2205	C
1	X	2218	G
1	X	2230	G
1	X	2238	G
1	X	2242	C
1	X	2246	A
1	X	2247	A
1	X	2262	C
1	X	2265	A

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Mol	Chain	Res	Type
1	X	2266	A
1	X	2272	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2298	U
1	X	2300	G
1	X	2301	A
1	X	2313	G
1	X	2316	G
1	X	2324	G
1	X	2326	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2386	G
1	X	2396	C
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2407	G
1	X	2408	G
1	X	2410	U
1	X	2420	C
1	X	2427	A
1	X	2428	U
1	X	2452	U
1	X	2455	A
1	X	2458	U
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2486	C
1	X	2497	A
1	X	2498	U
1	X	2499	C
1	X	2545	A
1	X	2546	G

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Mol	Chain	Res	Type
1	X	2552	C
1	X	2564	U
1	X	2565	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2591	C
1	X	2592	U
1	X	2602	G
1	X	2608	A
1	X	2609	G
1	X	2625	U
1	X	2634	G
1	X	2661	G
1	X	2668	U
1	X	2691	C
1	X	2692	A
1	X	2693	U
1	X	2700	U
1	X	2706	U
1	X	2707	G
1	X	2708	U
1	X	2709	C
1	X	2712	G
1	X	2713	A
1	X	2728	A
1	X	2730	A
1	X	2731	G
1	X	2732	C
1	X	2737	A
1	X	2744	A
1	X	2745	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2760	G
1	X	2761	A
1	X	2770	A
1	X	2771	C
1	X	2782	G
1	X	2795	A
1	X	2796	A

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Mol	Chain	Res	Type
1	X	2807	U
1	X	2808	U
1	X	2809	A
1	X	2825	A
1	X	2840	U
1	X	2841	U
1	X	2842	C
1	X	2843	A
1	X	2847	G
1	X	2850	U
1	X	2855	C
1	X	2858	A
1	X	2859	U
1	X	2868	G
2	Y	4	C
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	37	C
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	59	A
2	Y	69	G
2	Y	71	G
2	Y	84	G
2	Y	85	G
2	Y	93	G
2	Y	102	A
2	Y	110	U
2	Y	111	C
2	Y	112	A
2	Y	115	G

All (73) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	33	C
1	X	38	G

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Mol	Chain	Res	Type
1	X	48	A
1	X	173	A
1	X	182	G
1	X	192	G
1	X	334	G
1	X	342	G
1	X	466	A
1	X	538	A
1	X	583	C
1	X	631	G
1	X	682	G
1	X	777	A
1	X	780	U
1	X	788	G
1	X	789	G
1	X	795	A
1	X	802	A
1	X	803	C
1	X	843	G
1	X	969	U
1	X	995	A
1	X	1006	C
1	X	1031	C
1	X	1053	G
1	X	1096	A
1	X	1141	U
1	X	1182	U
1	X	1223	G
1	X	1261	G
1	X	1299	A
1	X	1313	U
1	X	1324	G
1	X	1337	G
1	X	1338	G
1	X	1391	A
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1496	G
1	X	1601	U
1	X	1607	A
1	X	1623	C

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Mol	Chain	Res	Type
1	X	1634	A
1	X	1691	G
1	X	1749	G
1	X	1750	A
1	X	1790	G
1	X	1811	A
1	X	1923	U
1	X	1938	U
1	X	1975	G
1	X	2005	U
1	X	2015	G
1	X	2044	G
1	X	2204	A
1	X	2245	A
1	X	2312	A
1	X	2404	A
1	X	2409	A
1	X	2426	G
1	X	2427	A
1	X	2485	U
1	X	2581	A
1	X	2705	A
1	X	2708	U
1	X	2736	U
1	X	2756	A
1	X	2824	C
1	X	2841	U
1	X	2842	C
1	X	2867	G

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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	X	2644/2880 (91%)	-0.05	74 (2%) 50 22	44, 115, 240, 575	0
2	Y	120/123 (97%)	-0.28	3 (2%) 54 24	108, 183, 252, 342	0
3	A	253/274 (92%)	0.53	18 (7%) 16 7	66, 158, 225, 423	0
4	B	205/211 (97%)	0.08	1 (0%) 88 63	35, 85, 159, 249	0
5	C	194/205 (94%)	-0.16	1 (0%) 88 63	61, 142, 250, 381	0
6	D	177/180 (98%)	1.17	36 (20%) 1 2	174, 255, 358, 427	0
7	E	171/185 (92%)	0.07	4 (2%) 57 26	87, 183, 269, 354	0
8	F	63/144 (43%)	3.20	46 (73%) 0 0	208, 334, 476, 516	0
9	G	142/174 (81%)	0.38	8 (5%) 24 10	73, 126, 257, 421	0
10	H	134/134 (100%)	-0.21	0 100 100	39, 71, 135, 248	0
11	I	134/156 (85%)	0.39	5 (3%) 39 16	75, 168, 261, 375	0
12	J	136/141 (96%)	0.50	8 (5%) 22 9	76, 135, 223, 388	0
13	K	113/116 (97%)	-0.03	0 100 100	32, 61, 101, 128	0
14	L	104/114 (91%)	0.01	4 (3%) 38 16	134, 193, 300, 325	0
15	M	108/166 (65%)	-0.15	0 100 100	32, 73, 138, 298	0
16	N	117/118 (99%)	0.21	1 (0%) 81 49	57, 116, 177, 328	0
17	O	94/100 (94%)	0.53	9 (9%) 8 5	82, 145, 271, 322	0
18	P	126/134 (94%)	-0.13	0 100 100	33, 84, 149, 226	0
19	Q	93/95 (97%)	0.81	13 (13%) 3 3	86, 134, 245, 329	0
20	R	110/115 (95%)	1.20	26 (23%) 1 2	93, 166, 332, 423	0
21	S	175/237 (73%)	0.19	9 (5%) 27 11	130, 202, 285, 326	0
22	T	74/91 (81%)	1.19	17 (22%) 1 2	112, 141, 201, 284	0
23	U	72/81 (88%)	0.81	8 (11%) 6 4	119, 188, 304, 349	0
24	V	65/67 (97%)	0.21	4 (6%) 20 9	116, 175, 235, 292	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	0.54	3 (5%) 24 10	97, 126, 181, 194	0
26	Z	57/60 (95%)	-0.23	0 100 100	44, 79, 182, 234	0
27	1	53/55 (96%)	1.79	21 (39%) 1 1	126, 192, 295, 403	0
28	2	46/47 (97%)	0.35	2 (4%) 34 14	72, 123, 258, 308	0
29	3	59/66 (89%)	2.93	45 (76%) 0 0	139, 213, 356, 435	0
30	4	37/37 (100%)	3.71	30 (81%) 0 0	152, 219, 307, 382	0
All	All	5931/6561 (90%)	0.23	396 (6%) 18 8	32, 131, 276, 575	0

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	12.7
8	F	94	ALA	8.5
30	4	24	LEU	8.4
30	4	15	LYS	8.3
8	F	99	LEU	8.1
8	F	113	PRO	7.1
8	F	95	LYS	6.9
1	X	2190	A	6.9
1	X	1089	C	6.7
8	F	111	LYS	6.6
8	F	110	THR	6.3
30	4	1	MET	6.3
2	Y	43	G	6.2
6	D	82	GLY	6.0
29	3	9	MET	5.9
27	1	6	PRO	5.9
29	3	7	HIS	5.7
29	3	10	ALA	5.6
8	F	98	LYS	5.6
24	V	66	GLN	5.6
30	4	34	GLN	5.6
1	X	665	A	5.5
30	4	28	SER	5.5
1	X	871	U	5.3
30	4	17	VAL	5.2
8	F	136	VAL	5.2
8	F	93	LYS	5.1
29	3	38	GLY	5.1
30	4	25	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
29	3	60	LEU	5.1
1	X	1086	C	5.0
20	R	102	LYS	5.0
1	X	1734	C	4.9
8	F	125	ASN	4.8
1	X	1063	C	4.8
1	X	1552	C	4.7
8	F	127	VAL	4.7
6	D	11	GLN	4.6
6	D	67	ILE	4.6
29	3	63	PRO	4.6
8	F	92	ASN	4.6
29	3	33	ASN	4.6
30	4	7	VAL	4.6
8	F	109	LYS	4.6
8	F	105	LEU	4.5
29	3	16	ILE	4.5
29	3	40	GLU	4.5
30	4	16	VAL	4.5
12	J	141	ALA	4.5
29	3	29	LYS	4.4
22	T	73	GLY	4.2
30	4	26	ILE	4.2
30	4	29	ASN	4.2
27	1	47	HIS	4.2
20	R	83	LEU	4.2
1	X	1114	A	4.2
6	D	83	MET	4.2
30	4	12	ASP	4.1
1	X	248	A	4.1
30	4	11	CYS	4.1
8	F	77	LEU	4.1
30	4	20	HIS	4.1
3	A	255	THR	4.1
20	R	100	ASP	4.1
30	4	35	ARG	4.1
8	F	90	THR	4.1
22	T	72	LYS	4.1
8	F	106	GLU	4.1
8	F	112	MET	4.1
29	3	20	GLY	4.1
30	4	21	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
27	1	13	GLU	4.0
30	4	2	LYS	4.0
2	Y	14	C	4.0
30	4	22	ARG	4.0
29	3	8	LYS	4.0
1	X	1095	A	4.0
8	F	78	ILE	4.0
3	A	251	TRP	3.9
20	R	112	LYS	3.9
6	D	34	ILE	3.9
29	3	61	MET	3.9
30	4	18	ARG	3.9
29	3	28	GLY	3.9
30	4	10	MET	3.8
8	F	114	ASP	3.8
29	3	12	ARG	3.8
29	3	46	LYS	3.8
27	1	23	THR	3.8
30	4	9	LYS	3.8
21	S	74	ARG	3.8
27	1	35	LEU	3.8
7	E	46	ASP	3.7
30	4	14	CYS	3.7
1	X	1090	C	3.7
1	X	1088	A	3.7
1	X	1115	C	3.7
11	I	61	PRO	3.7
3	A	250	PRO	3.7
1	X	1551	U	3.7
29	3	54	GLU	3.7
29	3	37	SER	3.7
1	X	558	G	3.6
12	J	133	VAL	3.6
30	4	13	ASN	3.6
19	Q	64	ARG	3.6
6	D	93	GLY	3.6
1	X	424	G	3.6
3	A	220	PRO	3.6
8	F	128	ALA	3.6
6	D	81	GLN	3.6
3	A	152	LYS	3.6
27	1	27	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
8	F	102	ASP	3.5
27	1	32	GLN	3.5
17	O	64	GLY	3.5
30	4	27	CYS	3.5
1	X	1733	U	3.5
17	O	74	TYR	3.5
6	D	69	LYS	3.5
29	3	14	ILE	3.5
6	D	3	GLN	3.5
29	3	13	ARG	3.5
8	F	107	ILE	3.4
19	Q	62	ARG	3.4
3	A	256	LYS	3.4
8	F	84	ILE	3.4
30	4	36	GLN	3.4
14	L	14	ARG	3.4
19	Q	49	ARG	3.4
1	X	1087	C	3.4
29	3	21	LYS	3.4
8	F	104	VAL	3.4
30	4	37	GLY	3.3
1	X	1091	C	3.3
11	I	60	LEU	3.3
6	D	74	ILE	3.3
6	D	94	GLU	3.3
7	E	37	TYR	3.3
27	1	40	TYR	3.3
1	X	1085	G	3.3
8	F	101	TRP	3.3
14	L	12	ARG	3.3
29	3	23	MET	3.3
6	D	140	GLU	3.2
27	1	31	THR	3.2
30	4	33	LYS	3.2
22	T	47	ALA	3.2
29	3	30	ARG	3.2
1	X	1397	A	3.2
6	D	103	LEU	3.2
1	X	1101	U	3.2
17	O	41	GLY	3.2
12	J	21	ASP	3.2
23	U	27	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
27	1	2	ALA	3.2
29	3	45	GLY	3.2
6	D	91	LEU	3.2
1	X	90	G	3.1
6	D	88	LYS	3.1
30	4	3	VAL	3.1
25	W	14	GLY	3.1
8	F	121	GLU	3.1
29	3	11	LYS	3.1
12	J	60	ARG	3.1
3	A	73	LYS	3.1
20	R	4	PRO	3.1
8	F	80	LYS	3.1
6	D	169	LEU	3.1
28	2	40	HIS	3.0
24	V	65	GLU	3.0
29	3	31	HIS	3.0
22	T	55	ARG	3.0
20	R	35	LYS	3.0
1	X	2275	U	3.0
8	F	76	TYR	3.0
29	3	44	LYS	3.0
20	R	82	ALA	2.9
8	F	132	ARG	2.9
29	3	41	ILE	2.9
22	T	71	ASN	2.9
8	F	123	ALA	2.9
11	I	62	LYS	2.9
21	S	92	VAL	2.9
27	1	45	LYS	2.9
30	4	19	ARG	2.9
1	X	514	G	2.9
27	1	26	LYS	2.9
27	1	11	LYS	2.9
20	R	74	LEU	2.9
1	X	2313	G	2.9
1	X	518	A	2.9
24	V	5	GLU	2.9
29	3	36	LYS	2.9
20	R	31	GLY	2.8
22	T	46	LYS	2.8
27	1	12	MET	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
23	U	75	TYR	2.8
29	3	26	LYS	2.8
1	X	2298	U	2.8
27	1	7	ARG	2.8
27	1	5	GLY	2.8
29	3	55	TRP	2.8
23	U	47	HIS	2.8
8	F	86	LYS	2.7
24	V	33	ALA	2.7
9	G	156	HIS	2.7
20	R	77	HIS	2.7
29	3	53	ALA	2.7
21	S	71	MET	2.7
19	Q	48	VAL	2.7
27	1	24	THR	2.7
29	3	42	ARG	2.7
8	F	103	GLN	2.7
1	X	2312	A	2.7
22	T	59	LEU	2.7
9	G	68	PRO	2.7
11	I	63	ARG	2.7
8	F	97	GLY	2.7
1	X	2276	C	2.6
22	T	43	THR	2.6
16	N	105	ALA	2.6
1	X	1098	G	2.6
9	G	97	ASP	2.6
6	D	156	ILE	2.6
29	3	27	SER	2.6
20	R	6	ALA	2.6
1	X	1224	A	2.6
3	A	57	GLY	2.6
19	Q	66	GLY	2.6
1	X	2274	C	2.6
20	R	46	VAL	2.6
22	T	41	ARG	2.6
6	D	86	GLY	2.6
1	X	1409	U	2.6
4	B	1	MET	2.6
6	D	105	ASN	2.6
6	D	85	VAL	2.6
1	X	2263	C	2.6

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Mol	Chain	Res	Type	RSRZ
29	3	48	PHE	2.6
22	T	20	TYR	2.6
1	X	1548	U	2.6
27	1	51	ARG	2.6
6	D	145	MET	2.6
3	A	243	ALA	2.5
6	D	126	GLY	2.5
6	D	110	ARG	2.5
8	F	120	VAL	2.5
23	U	25	ARG	2.5
1	X	1064	C	2.5
22	T	77	ARG	2.5
20	R	9	HIS	2.5
22	T	53	MET	2.5
1	X	1092	U	2.5
1	X	2295	C	2.5
1	X	209	G	2.5
23	U	29	GLY	2.5
8	F	131	ALA	2.5
1	X	1099	A	2.5
1	X	1062	G	2.5
1	X	1069	G	2.5
6	D	71	LYS	2.5
22	T	45	PHE	2.5
1	X	2299	A	2.4
1	X	559	C	2.4
12	J	114	GLN	2.4
8	F	91	PRO	2.4
1	X	200	A	2.4
1	X	1434	U	2.4
19	Q	94	GLN	2.4
14	L	11	LEU	2.4
8	F	89	SER	2.4
1	X	519	C	2.4
1	X	2326	C	2.4
25	W	13	PRO	2.4
20	R	75	ALA	2.4
6	D	127	ASN	2.4
20	R	29	HIS	2.4
8	F	129	GLY	2.4
29	3	32	GLN	2.4
1	X	1120	C	2.3

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Mol	Chain	Res	Type	RSRZ
7	E	47	GLY	2.3
8	F	81	ALA	2.3
1	X	2311	U	2.3
6	D	72	LYS	2.3
29	3	17	THR	2.3
17	O	80	TYR	2.3
1	X	2664	G	2.3
6	D	31	ILE	2.3
21	S	76	ARG	2.3
1	X	247	A	2.3
19	Q	65	VAL	2.3
20	R	38	LEU	2.3
21	S	68	ALA	2.3
6	D	66	ILE	2.3
9	G	53	ARG	2.3
3	A	114	VAL	2.3
12	J	68	ARG	2.3
8	F	87	GLY	2.3
20	R	52	ASN	2.3
1	X	2381	A	2.3
19	Q	27	PHE	2.3
8	F	130	THR	2.3
1	X	1553	G	2.3
20	R	81	VAL	2.3
3	A	261	ARG	2.3
8	F	79	ARG	2.3
17	O	73	LYS	2.3
27	1	38	LYS	2.2
3	A	260	THR	2.2
1	X	2325	A	2.2
23	U	13	LEU	2.2
20	R	30	LYS	2.2
29	3	22	VAL	2.2
3	A	189	GLU	2.2
1	X	1549	C	2.2
9	G	107	GLN	2.2
8	F	96	VAL	2.2
14	L	10	LYS	2.2
7	E	168	GLN	2.2
20	R	43	ASP	2.2
17	O	36	LYS	2.2
23	U	62	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	1074	G	2.2
1	X	99	U	2.2
1	X	1421	U	2.2
21	S	69	VAL	2.2
1	X	2732	C	2.2
6	D	92	ARG	2.2
19	Q	39	LYS	2.2
29	3	50	LEU	2.2
20	R	87	GLU	2.2
1	X	1077	U	2.2
8	F	108	ALA	2.2
1	X	1840	A	2.2
12	J	37	ALA	2.2
29	3	15	LYS	2.2
9	G	34	PRO	2.2
20	R	99	VAL	2.2
3	A	271	ILE	2.2
19	Q	3	HIS	2.2
21	S	15	ASP	2.2
21	S	14	LEU	2.1
30	4	32	HIS	2.1
1	X	1070	G	2.1
17	O	39	PHE	2.1
27	1	22	TYR	2.1
20	R	13	LYS	2.1
28	2	41	GLN	2.1
2	Y	44	C	2.1
6	D	165	GLU	2.1
29	3	52	LYS	2.1
1	X	341	A	2.1
19	Q	63	LYS	2.1
1	X	100	G	2.1
20	R	25	LEU	2.1
6	D	89	VAL	2.1
21	S	70	GLN	2.1
1	X	436	A	2.1
3	A	204	ASN	2.1
5	C	48	ARG	2.1
6	D	108	LEU	2.1
9	G	98	LYS	2.1
22	T	14	ARG	2.1
1	X	2265	A	2.1

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Mol	Chain	Res	Type	RSRZ
25	W	7	ARG	2.1
1	X	2294	U	2.1
3	A	81	ALA	2.1
22	T	15	ASP	2.1
29	3	49	VAL	2.1
8	F	100	ASN	2.1
3	A	242	GLY	2.1
29	3	58	MET	2.1
6	D	99	PHE	2.1
11	I	100	ARG	2.1
29	3	51	ALA	2.0
22	T	22	GLY	2.0
6	D	62	LEU	2.0
1	X	1556	A	2.0
6	D	18	GLN	2.0
6	D	175	LEU	2.0
17	O	47	PHE	2.0
3	A	103	LYS	2.0
27	1	8	ILE	2.0
20	R	12	ASP	2.0
29	3	57	ARG	2.0
1	X	1753	A	2.0
20	R	18	LYS	2.0
1	X	2336	G	2.0
17	O	75	LYS	2.0
22	T	44	LYS	2.0
19	Q	86	GLN	2.0
19	Q	47	GLY	2.0
9	G	100	TYR	2.0
12	J	20	GLY	2.0
1	X	2188	A	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
33	MG	X	2942	1/1	0.62	178.20	77,77,77,77	0
35	NA	X	2962	1/1	1.08	88.65	98,98,98,98	0
33	MG	X	2886	1/1	1.10	88.06	54,54,54,54	0
33	MG	X	2927	1/1	0.70	35.50	65,65,65,65	0
33	MG	X	2914	1/1	0.46	34.82	74,74,74,74	0
33	MG	X	2905	1/1	0.67	34.00	50,50,50,50	0
33	MG	X	2949	1/1	0.48	32.29	83,83,83,83	0
33	MG	X	2948	1/1	0.75	29.49	110,110,110,110	0
33	MG	X	2884	1/1	0.97	28.38	72,72,72,72	0
33	MG	X	2903	1/1	0.54	22.45	65,65,65,65	0
33	MG	X	2899	1/1	0.53	21.55	41,41,41,41	0
33	MG	X	2893	1/1	0.42	19.64	66,66,66,66	0
33	MG	X	2951	1/1	0.47	17.88	142,142,142,142	0
33	MG	X	2938	1/1	0.58	17.35	62,62,62,62	0
34	K	X	2957	1/1	0.56	16.64	82,82,82,82	0
33	MG	X	2925	1/1	0.58	16.19	80,80,80,80	0
33	MG	X	2898	1/1	0.37	15.98	19,19,19,19	0
33	MG	X	2931	1/1	0.66	15.22	72,72,72,72	0
33	MG	X	2883	1/1	0.53	15.16	23,23,23,23	0
33	MG	X	2937	1/1	0.45	13.91	109,109,109,109	0
33	MG	X	2913	1/1	0.39	13.89	63,63,63,63	0
33	MG	X	2933	1/1	0.34	13.58	83,83,83,83	0
33	MG	X	2908	1/1	0.65	13.54	80,80,80,80	0
33	MG	X	2885	1/1	0.49	12.47	68,68,68,68	0
33	MG	X	2934	1/1	0.38	12.15	56,56,56,56	0
35	NA	X	2958	1/1	0.53	11.95	48,48,48,48	0
33	MG	X	2888	1/1	0.53	11.24	51,51,51,51	0
34	K	X	2956	1/1	0.38	9.73	146,146,146,146	0
33	MG	X	2929	1/1	0.69	9.35	61,61,61,61	0
33	MG	X	2904	1/1	0.43	8.48	64,64,64,64	0
35	NA	X	2961	1/1	0.39	8.36	75,75,75,75	0
33	MG	X	2918	1/1	0.49	8.23	84,84,84,84	0
33	MG	X	2906	1/1	0.37	7.65	52,52,52,52	0
34	K	X	2955	1/1	0.19	7.56	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
33	MG	X	2939	1/1	0.52	7.22	54,54,54,54	0
33	MG	X	2920	1/1	0.37	7.07	100,100,100,100	0
33	MG	X	2917	1/1	0.26	6.74	104,104,104,104	0
33	MG	X	2895	1/1	0.28	6.58	26,26,26,26	0
32	LMA	X	2882	58/58	0.39	6.10	120,120,120,120	0
33	MG	X	2910	1/1	0.30	5.89	44,44,44,44	0
33	MG	X	2894	1/1	0.45	5.85	65,65,65,65	0
35	NA	X	2960	1/1	0.44	5.73	86,86,86,86	0
33	MG	X	2950	1/1	0.31	5.55	36,36,36,36	0
35	NA	X	2959	1/1	0.35	5.42	60,60,60,60	0
33	MG	X	2891	1/1	0.31	5.25	50,50,50,50	0
33	MG	X	2911	1/1	0.63	5.02	124,124,124,124	0
33	MG	X	2919	1/1	0.37	4.80	65,65,65,65	0
33	MG	X	2922	1/1	0.33	4.69	53,53,53,53	0
33	MG	X	2887	1/1	0.39	4.58	35,35,35,35	0
33	MG	X	2932	1/1	0.35	4.51	62,62,62,62	0
33	MG	X	2900	1/1	0.61	4.35	42,42,42,42	0
33	MG	X	2953	1/1	0.41	4.04	53,53,53,53	0
33	MG	X	2907	1/1	0.26	3.92	46,46,46,46	0
33	MG	X	2901	1/1	0.34	3.22	19,19,19,19	0
33	MG	X	2915	1/1	0.46	3.08	67,67,67,67	0
31	LC2	X	2881	33/33	0.32	3.05	49,106,118,122	0
33	MG	X	2935	1/1	0.24	2.73	36,36,36,36	0
33	MG	X	2926	1/1	0.41	2.57	67,67,67,67	0
33	MG	X	2892	1/1	0.28	2.54	71,71,71,71	0
33	MG	X	2890	1/1	0.36	2.17	59,59,59,59	0
33	MG	X	2952	1/1	0.30	2.02	59,59,59,59	0
33	MG	X	2940	1/1	0.30	1.90	71,71,71,71	0
33	MG	U	82	1/1	0.38	1.49	72,72,72,72	0
33	MG	X	2928	1/1	0.31	1.30	29,29,29,29	0
33	MG	X	2941	1/1	0.20	0.92	71,71,71,71	0
33	MG	X	2902	1/1	0.17	0.75	89,89,89,89	0
33	MG	X	2944	1/1	0.24	0.68	77,77,77,77	0
33	MG	X	2896	1/1	0.26	0.49	24,24,24,24	0
33	MG	X	2889	1/1	0.25	0.47	61,61,61,61	0
33	MG	X	2924	1/1	0.14	0.34	51,51,51,51	0
33	MG	X	2936	1/1	0.23	0.27	55,55,55,55	0
34	K	X	2954	1/1	0.23	0.27	70,70,70,70	0
33	MG	I	157	1/1	0.46	0.19	67,67,67,67	0
33	MG	X	2921	1/1	0.18	-0.01	61,61,61,61	0
33	MG	X	2916	1/1	0.19	-0.28	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	X	2923	1/1	0.17	-0.48	97,97,97,97	0
33	MG	X	2912	1/1	0.18	-0.49	62,62,62,62	0
33	MG	X	2930	1/1	0.20	-0.59	77,77,77,77	0
33	MG	X	2943	1/1	0.19	-0.83	43,43,43,43	0
33	MG	X	2897	1/1	0.16	-0.93	79,79,79,79	0
33	MG	X	2945	1/1	0.12	-1.35	67,67,67,67	0
33	MG	X	2946	1/1	0.15	-1.45	123,123,123,123	0
33	MG	X	2947	1/1	0.11	-2.26	56,56,56,56	0
33	MG	X	2909	1/1	0.15	-2.74	58,58,58,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.