



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 PM GMT

PDB ID : 4IOA  
Title : Crystal structure of compound 4e bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*  
Authors : Han, S.; Marr, E.S.  
Deposited on : 2013-01-07  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

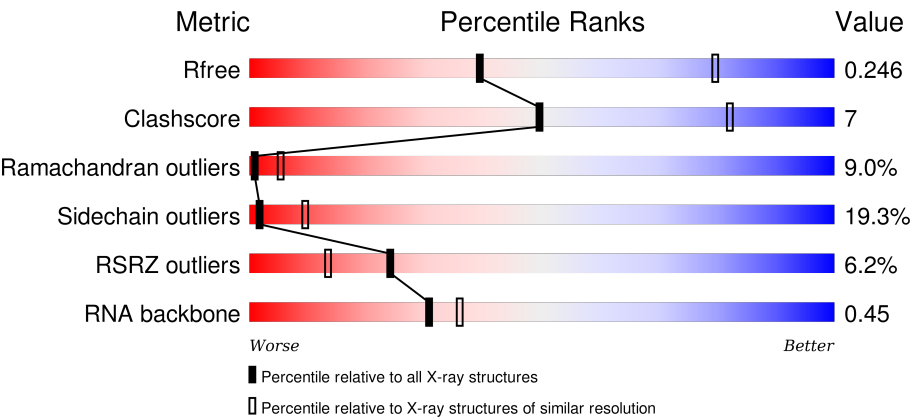
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2880	<div><div>3%</div><div><div></div><div>36%</div><div>34%</div><div>19%</div><div>•</div><div>7%</div></div></div>
2	Y	123	<div><div>2%</div><div><div></div><div>40%</div><div>42%</div><div>15%</div><div>••</div></div></div>
3	A	274	<div><div>2%</div><div><div></div><div>48%</div><div>30%</div><div>8%</div><div>•</div><div>12%</div></div></div>
4	B	211	<div><div>%</div><div><div></div><div>67%</div><div>21%</div><div>9%</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
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	

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Mol	Chain	Length	Quality of chain
30	4	37	<div> <div>97%</div> <div>73%</div> <div>24%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	2902	-	-	-	X
31	MG	X	2908	-	-	-	X
31	MG	X	2916	-	-	-	X
31	MG	X	2919	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2926	-	-	-	X
31	MG	X	2928	-	-	-	X
31	MG	Y	201	-	-	-	X

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	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	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	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
			1400	892	247	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	71	Total	C	N	O	S	0	0	0
			503	310	91	99	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	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- 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	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	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
			726	458	136	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	84	Total	C	N	O	S	0	0	0
			625	393	122	109	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
			552	341	116	95				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- 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	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

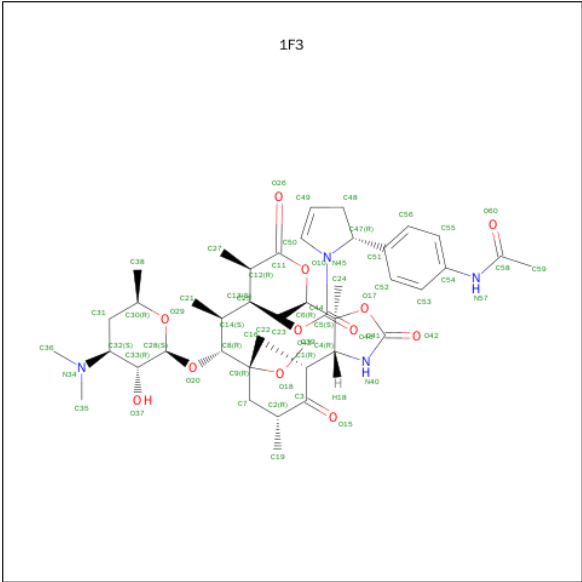
- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	30	Total Mg 30 30	0	0
31	Y	5	Total Mg 5 5	0	0

- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15R,15AR)-4-ETHYL-11-METHOXY-3-A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{{3,4,6-TRIDEOXY-3-(DIMETHYL AMINO)-BETA-D-XYLO-HEXOPYRANOSYL}OXY}TETRADECAHYDRO-2H-OXA CYCLOTETRADECINO[4,3-D][1,3]OXAZOL-8-YL (2R)-2-[4-(ACETYLAMINO)PHEN YL]-2,3-DIHYDRO-1H-PYRROLE-1-CARBOXYLATE (three-letter code: 1F3) (formula: C<sub>44</sub>H<sub>66</sub>N<sub>4</sub>O<sub>12</sub>).

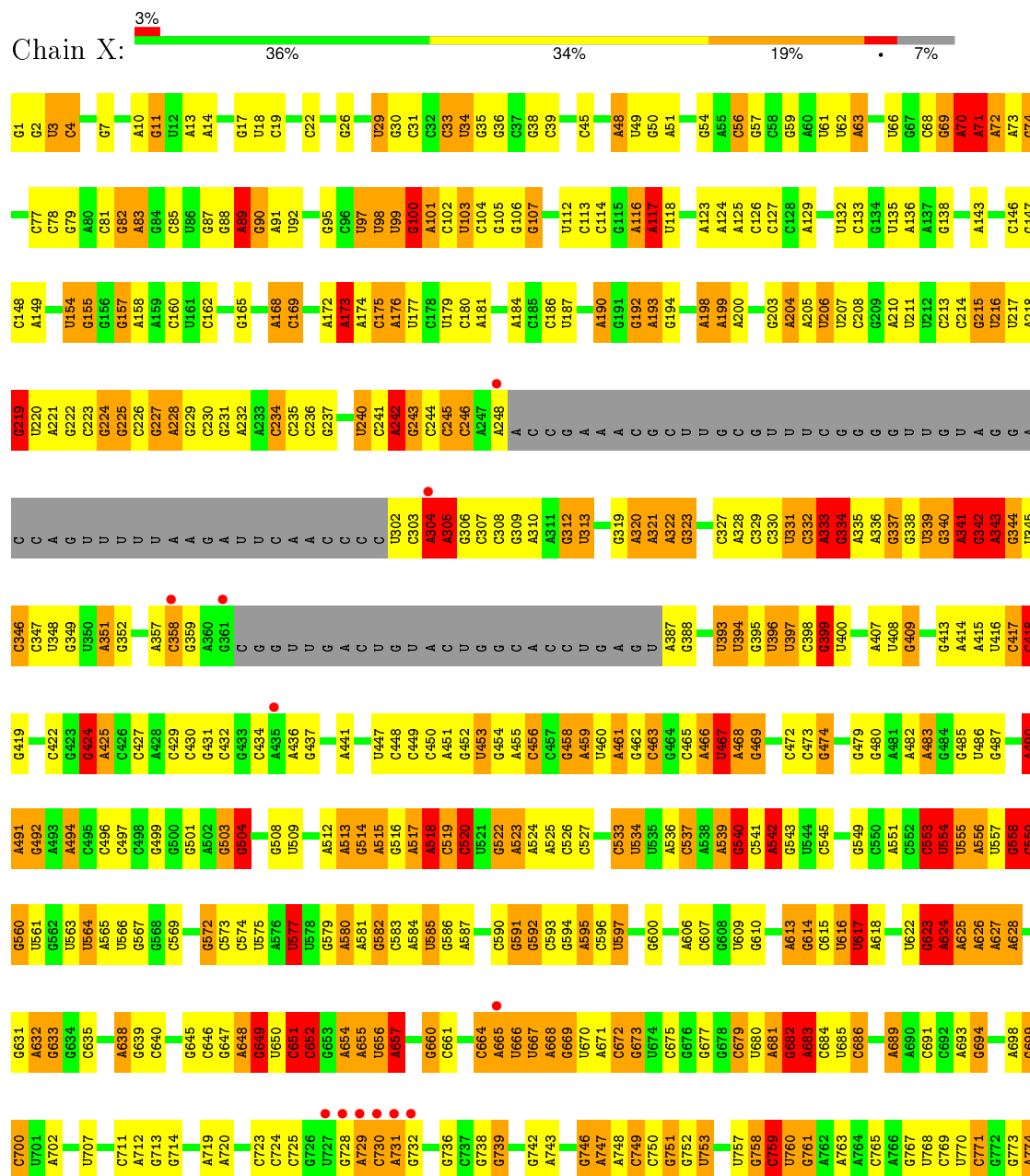


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			60	44	4	12		

### 3 Residue-property plots

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

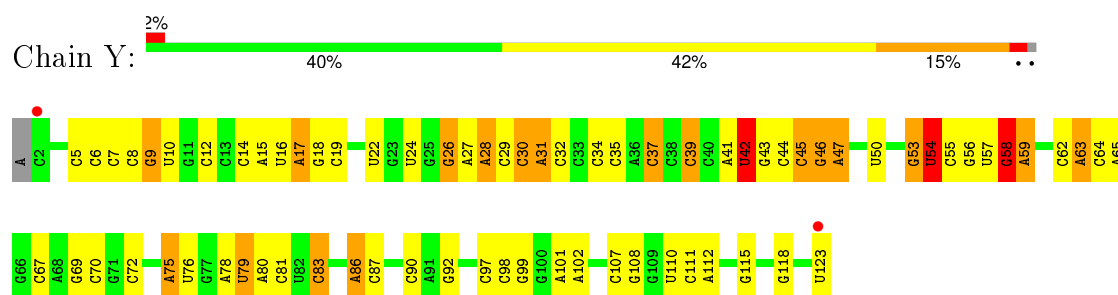
#### • Molecule 1: 23S ribosomal RNA



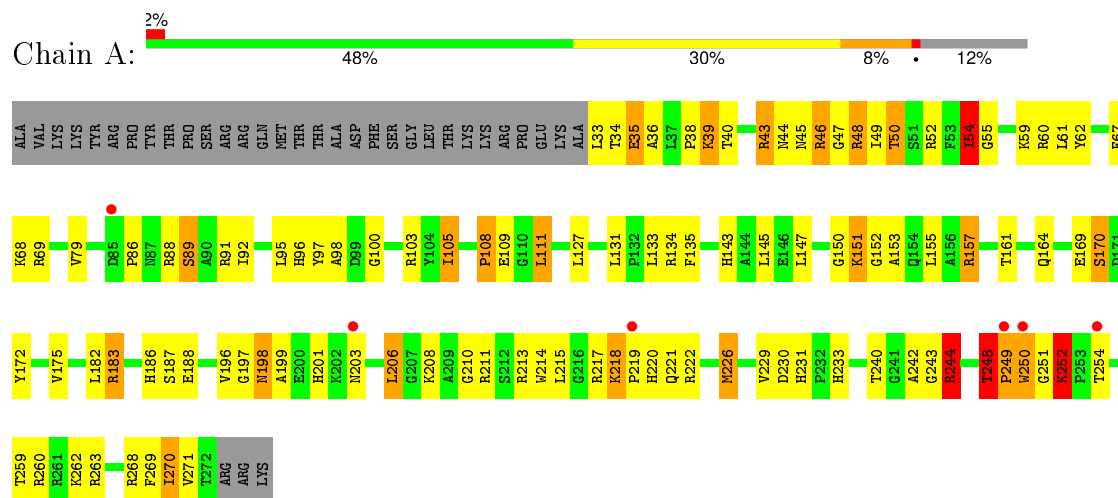
G1790	C1791	G1720	U1847	U1564	A1493	U1342	G1273	C1190	G1117	U1056	A984	U	A838	U776
C1792	G1793	G1721	C1648	A1567	G1494	C1343	G1274	G1191	G1118	A1057	G985	A	U839	G776
A1793	G1794	G1722	U1651	U1422	G1495	C1344	C1275	A1192	U1119	G1058	A986	C	U840	A777
C1794	G1795	U1723	G1652	C1422	G1496	G1345	U1276	U1194	G1121	A1059	U	C	G841	G778
A1796	G1724	G1725	U1571	U1426	C1497	C1346	G1277	U1195	G1122	C1060	A990	A911	G842	U779
			C1855	G1427	U1499	C1347	A1278	U1210	G1123	C1063	C993	U917	G844	G781
			U1656	G1572	U1500	G1350	G1279	U1199	U1124	C1064	A994	A922	U845	U784
			A1657	A1574	A1428	G1351	U1280	G1200	A1065	G1066	A995	A923	U846	U785
			C1575	U1430	U1505	G1352	A1281	G1201	C1127	G1067	A999	A924	C847	U786
			G1576	U1431	U1506	A1353	A1282	U1202	G1128	A1068	C998	C926	C851	A787
			G1579	U1432	A1507	A1354	G1283	U1130	U1129	G1069	A999	C927	U852	G788
			G1580	U1433	A1508	A1355	G1284	C1210	U1130	G1070	G1000	C928	U853	G789
			C1581	U1434	A1509	G1356	A1285		G1131	U1071	A1001	U931	U857	A790
			C1582	A1437	A1510	U1357	U1286	C1218	C1132	U1072	A1002	G931	U858	G792
			A1583	G1438	U1513	C1358	A1287	G1219	G1133	G1073	A1003	C937	U859	G793
			A1584	U1443	U1514	U1359	A1288	G1220	C1134	G1074	U1004	G938	U860	A794
			A1585	A1441	U1515	C1363	A1289	G1221	G1135	G1075	U1005	G939	U861	A795
			A1586	C1442	G1519	U1364	A1290	G1222	U1141	U1076	C1006	G940	U862	A796
			A1669	G1443	U1520	U1365	G1291	G1223	A1137	U1077	A1007	G941	U863	A797
			C1593	U1444	U1521	A1367	A1292	G1225	A1138	A1078	C942	U941	U864	A798
			U1594	A1445	U1522	G1368	U1297	A1297	U1139	G1079	U866	U942	U866	G798
			C1598	U1446	A1523	U1373	G1298	G1229	U1141	A1080	U1010	U943	U867	C799
			G1599	U1447	U1524	A1378	A1299	C1230	G1142	A1081	A1011	A944	U868	U800
			U1600	A1448	U1525	A1379	A1300	A1231	A1143	G1082	A1012	G945	U869	A801
			C1673	C1451	U1526	U1380	U1301	U1232	U1144	C1083	G1013	U946	U870	A802
			C1674	U1454	G1527	G1381	U1302	A1233	C1145	A1084	G1014	C947	U871	A803
			C1675	U1454	G1528	U1382	U1303	C1234	G1146	G1085	C948	U949	U872	C804
			G1678	U1454	G1529	U1383	U1304	C1235	G1149	G1086	C1016	G949	U873	C805
			U1679	A1458	U1530	U1384	U1305	G1236	C1150	A1087	C1017	G950	A874	A806
			U1680	U1459	U1531	C1385	U1306	G1237	C1151	A1088	C1018	G951	U875	C809
			G1683	G1460	A1532	U1385	U1307	A1238	U1151	C1089	U1019	A952	U876	U810
			G1684	C1461	U1533	U1386	U1308	A1239	C1152	C1090	A1022	G953	G877	G811
			A1685	C1461	G1534	U1387	U1310	G1240	A1153	C1091	U1023	U954	C878	G812
			C1686	U1465	U1535	U1388	C1311	G1241	A1154	U1092	G1024	G955	A879	A813
			U1687	C1466	C1536	G1390	G1312	A1242	G1155	U1093	U	G956	C880	G814
			U1688	U1467	U1539	A1391	U1313	C1243	U1161	C1094	G1028	G957	U881	G815
			U1689	A1468	C1540	U1392	U1314	U1244	U1162	A1095	C1029	G958	C882	A816
			G1692	U1470	G1541	C1396	U1315	G1245	C1164	A1096	U1030	C959	A883	U817
			C1693	G1471	U1542	U1397	C1319	U1247	U1167	A1098	C1031	A964	C884	C818
			A1694	C1472	G1543	U1398	G1324	G1248	C1168	U1099	A1032	U967	C889	C819
			U1695	U1473	G1544	C1399	U1325	A1249	C1169	G1100	G1033	G967	U890	U820
			C1696	A1474	U1545	U1403	U1326	A1250	U1170	U1101	U1034	C963	A891	G821
			U1699	U1475	G1546	C1404	C1327	C1251	G1171	G1102	G1035	C969	G	G822
			C1700	U1476	U1547	U1405	U1328	C1253	U1172	C1103	G1036	A970	G	U823
			G1703	G1477	C1549	A1406	U1329	G1254	G1173	G1104	U1037	A971	G	U824
			U1703	U1478	U1550	G1407	G1330	A1255	G1174	U1105	U1038	C972	G	C825
			C1703	U1482	U1551	A1408	U1333	C1256	C1181	A1106	A1043	U973	G	U826
			C1703	G1483	G1552	U1409	G1334	U1257	U1182	A1107	U1044	U974	C	C827
			U1710	U1483	G1553	U1410	A1334	U1257	U1182	U1108	C828	C975	C	C828
			C1711	C1487	G1554	C1411	A1335	G1263	C1183	A1109	U1044	C976	U	C829
			G1712	G1488	U1555	U1412	G1336	U1264	G1184	C1111	C1049	G977	A	C830
			G1713	C1489	G1556	U1413	G1337	G1265	G1185	C1112	U1051	U978	C	G831
			U1714	U1490	G1557	U1414	G1338	G1266	G1186	U1113	C1062	A979	C	A832
			C1715	C1491	G1558	U1415	U1339	G1267	G1187	C1114	G1063	G980	A	A833
			G1716	U1492	U1563	U1416	G1340	U1268	A1188	A1115	C1064	C981	G	G834
			U1717	A1492	U1563	C1417	G1341	G1269	G1189	U1116	A1055	C982	C	U835

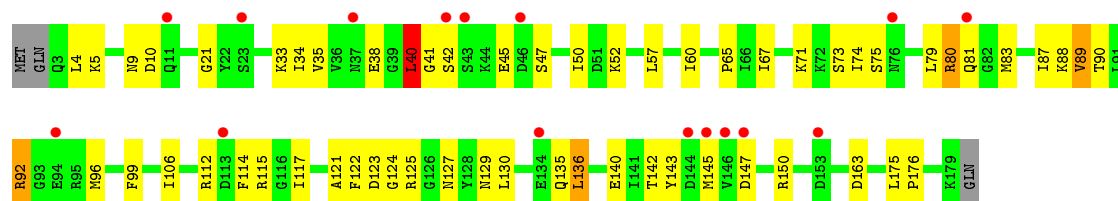
U2871	C2791	C2645	C2573	C2499	G2423	A2355	U2285	G2209	U2086	U1926	A1960
U2872	C2792	C2646	G2574	C2500	G2426	C2358	G2286	G2209	U2087	U1927	G1861
C2875	G2793	G2650	U2575	U2501	A2427	U2359	G2287	U2212	U2088	G1928	G1862
C2876	G2794	G2651	G2576	G2502	G2428	C2360	A2288	G2213	C2089	A1935	U1863
A2877	A2795	A2653	A2577	G2503	U2429	G2361	U2291	G2217	U2090	A1936	G1864
C	A2796	A2654	A2578	G2504	A2430	G2362	C2292	G2218	C	G1937	G1865
U	A2797	A2655	A2579	C2505	A2431	U2363	C2293	U2222	U	U1938	G1866
U	A2798	A2656	A2580	C2506	C2432	C2364	U2294	U2223	U	U1939	A1867
C2799	C2799	G2657	U2581	U2507	G2437	U2365	G2295	U2224	U	C1940	U1870
C2800	C2800	U2583	U2583	A2509	U2438	U2366	U2296	U2225	U	A2014	G1871
G2804	G2804	G2661	G2587	G2514	U2439	G2370	G2297	A2226	U	G2015	A1872
G2805	G2805	C2662	U2588	G2515	C2440	A2371	U2298	C2227	U	A2016	A1873
U2807	U2807	U2663	C2589	U2516	U2441	A2372	A2299	U2228	U	C1944	G1874
A2809	A2809	G2664	U2590	C2517	C2442	C2373	A2301	G2229	U	G1945	U1875
A2810	A2810	G2665	U2591	G2522	C2443	C2374	G2302	G2230	U	U1946	C1877
A2811	A2811	C2666	U2592	G2523	C2444	G2375	G2303	G2231	U	G1947	U1877
A2812	A2812	C2667	U2593	G2524	G2445	G2376	C2304	G2232	U	C1950	G1882
G2813	G2813	C2668	U2594	G2525	G2446	U2377	C2305	U2233	U	A2025	A1883
G2815	G2815	C2669	U2595	G2526	G2447	U2378	C2306	U2234	U	C2026	A1884
C2824	C2824	U2675	U2596	G2527	G2448	U2379	A2307	C2237	U	A1954	C1885
A2825	A2825	C2678	U2597	G2528	G2449	U2380	A2308	G2238	U	G1955	G1886
C2826	C2826	C2679	C2605	G2529	U2452	C2381	G2309	C2239	U	G1956	G1887
G2827	G2827	U2676	C2606	U2530	U2453	C2382	G2310	U2241	U	G1958	C1888
U2830	U2830	C2677	C2607	U2531	A2455	G2383	G2311	G2242	U	C1962	G
U2841	U2841	C2678	A2608	U2541	U2456	G2384	A2312	C2243	U	G1963	G
C2842	C2842	U2679	A2609	U2542	U2457	G2385	A2313	C2244	U	A1964	C
A2843	A2843	A2681	G2610	U2543	G2463	U2386	A2314	A2247	U	U1965	G
G2844	G2844	C2682	A2611	U2544	G2464	U2387	A2315	U2251	U	C1971	A
C2845	C2845	C2683	A2612	U2545	U2470	G2388	U2318	U2252	U	G1972	A
G2846	G2846	A2684	A2613	A2546	U2471	C2389	C2321	C2254	U	A1973	C
G2847	G2847	U2685	A2614	A2547	U2472	G2390	G2322	G2255	U	U1974	C
A2848	A2848	C2686	A2615	G2548	G2473	C2391	U2323	G2256	U	G1975	A
C2849	C2849	C2687	A2616	G2549	G2474	C2392	G2324	A2257	U	U1976	A
U2850	U2850	C2688	U2617	G2550	G2475	C2393	G2325	G2258	U	C1977	A
G2851	G2851	A2691	U2618	G2551	A2476	U2394	A2326	G2261	U	U1978	A
C2852	C2852	C2689	A2619	G2552	G2477	U2395	C2327	G2262	U	C1979	A
G2853	G2853	A2692	G2620	G2553	U2478	U2396	G2328	C2263	U	A1980	G
U2854	U2854	C2690	G2621	G2554	C2479	A2401	G2329	C2264	U	G1981	G
C2855	C2855	C2691	G2622	G2555	G2481	U2402	G2330	A2265	U	A1982	U
U2856	U2856	U2692	U2623	G2556	U2482	U2403	G2331	A2266	U	G1983	C
C2857	C2857	U2693	U2624	A2557	G2483	A2404	U2332	A2267	U	A1984	C
A2858	A2858	C2694	C2624	G2558	G2484	A2405	G2333	U2270	U	G1985	U1909
U2859	U2859	G2695	C2625	G2559	G2485	C2406	G2334	U2271	U	G1986	A1910
C2860	C2860	U2696	U2625	G2560	G2486	G2407	U2335	G2272	U	G1987	A1911
U2861	U2861	U2697	U2626	G2561	G2487	U2408	G2336	G2273	U	A1988	G1912
C2864	C2864	C2705	U2627	U2562	U2488	U2409	C2337	C2274	U	C1989	G1913
G2865	G2865	U2706	U2628	U2563	C2489	U2410	G2344	U2275	U	U1990	U1914
A2866	A2866	U2707	A2630	U2564	U2490	A2414	U2345	U2276	U	G1991	C
G2867	G2867	G2708	A2631	G2565	C2491	U2415	G2346	C2277	U	G1992	C1917
C2868	C2868	U2709	U2632	U2566	G2492	U2416	C2347	U2278	U	G1993	G1918
U2869	U2869	C2710	U2633	G2567	G2493	U2417	A2348	U2279	U	U1994	A1919
G2711	G2711	A2641	A2634	U2568	U2494	A2418	G2349	A2281	U	G1995	A1920
G2712	G2712	C2642	U2635	A2569	G2495	C2419	G2350	G2282	U	A1996	U1921
C2790	C2790	A2713	C2643	U2570	G2496	U2420	G2351	G2283	U	A1997	U1922
					U2498	C2421	G2352	G2284	U	A1998	U1923
						C2422	G2354	U2284	U	U1999	G1924
									U	U2000	C1925

- Molecule 2: 5S ribosomal RNA

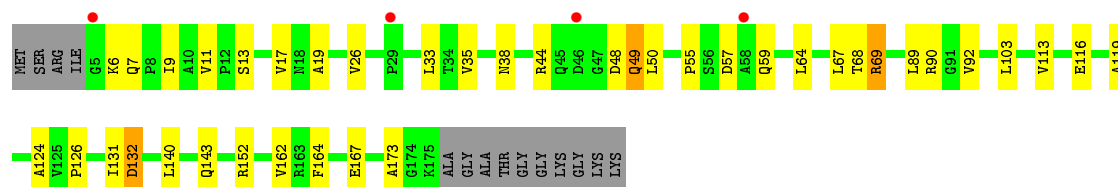


• Molecule 3: 50S ribosomal protein L2

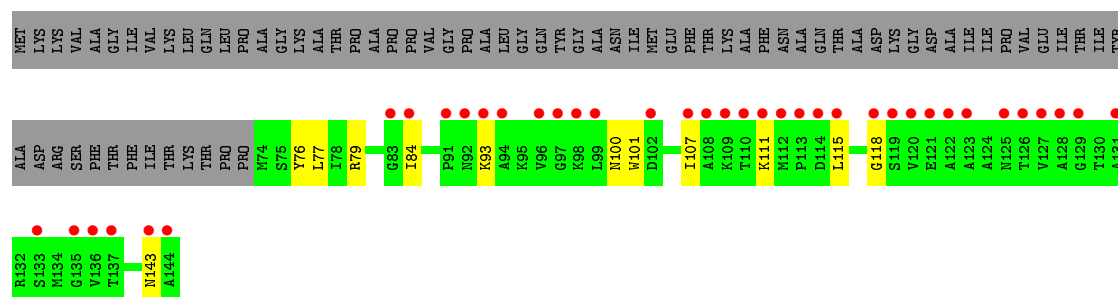
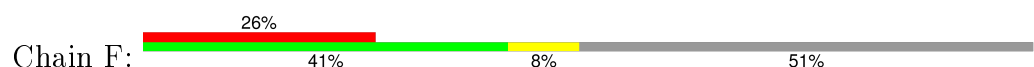




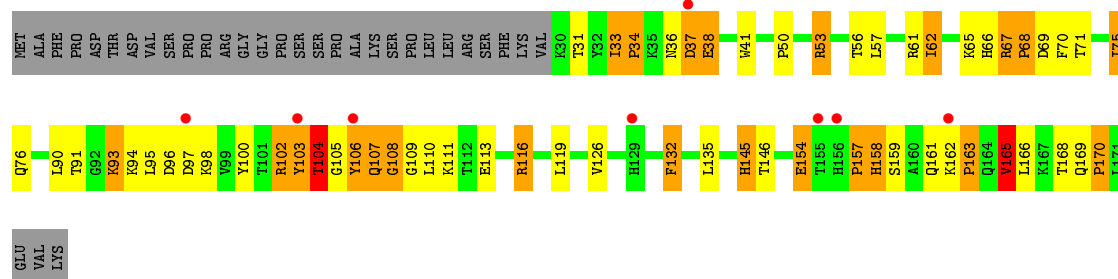
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L11

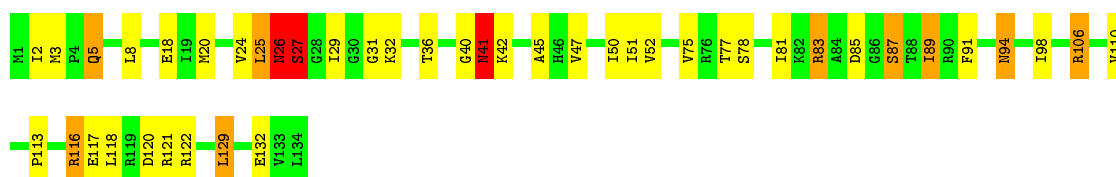


• Molecule 9: 50S ribosomal protein L13

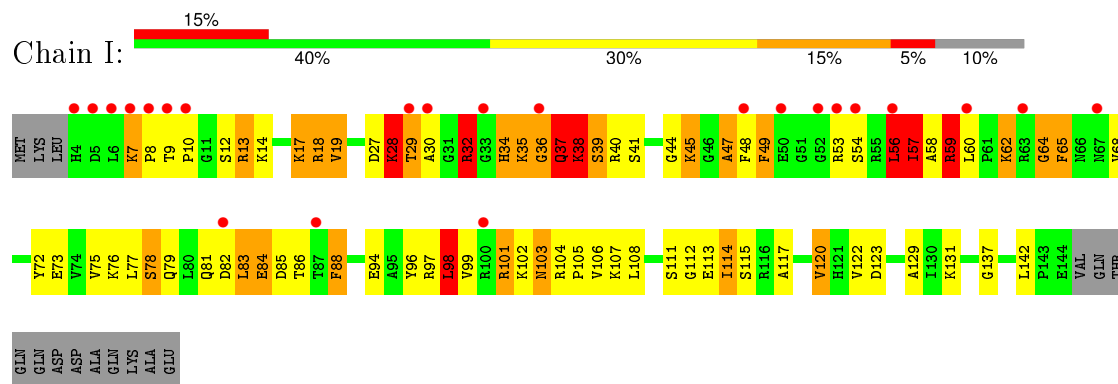


• Molecule 10: 50S ribosomal protein L14

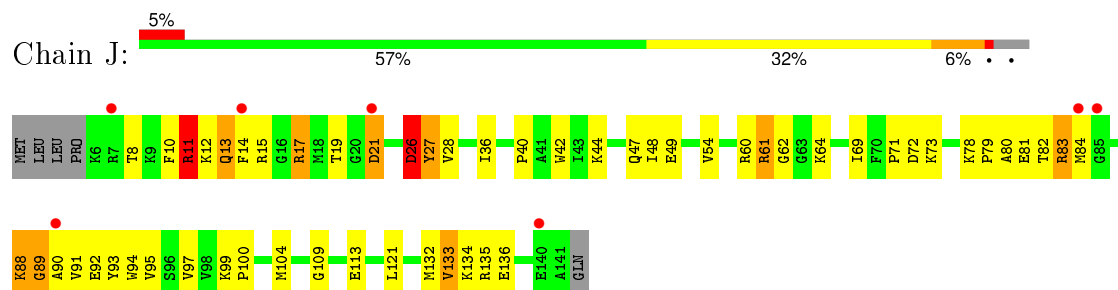




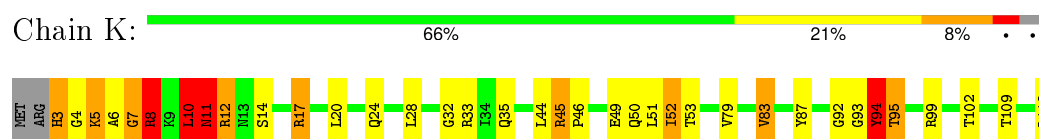
- Molecule 11: 50S ribosomal protein L15



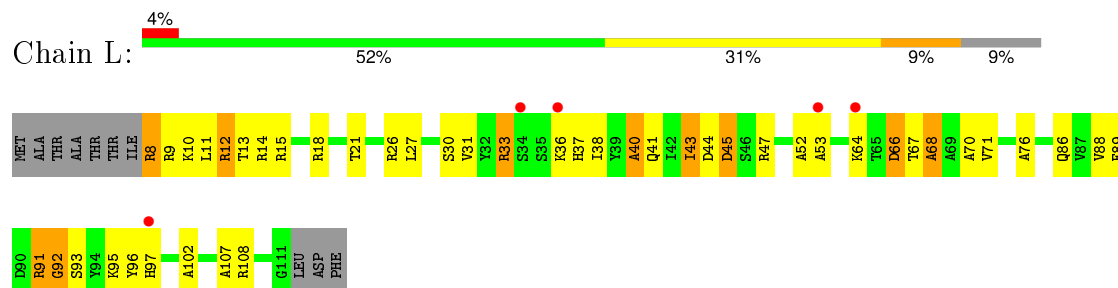
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

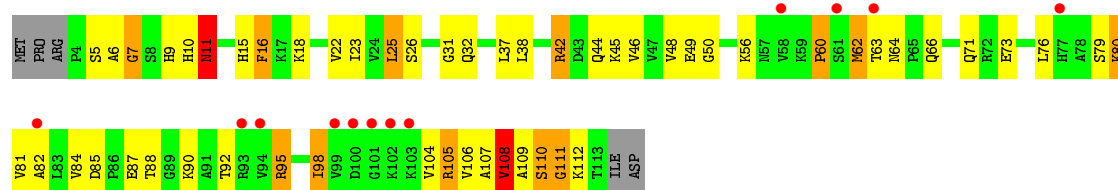


- Molecule 15: 50S ribosomal protein L19

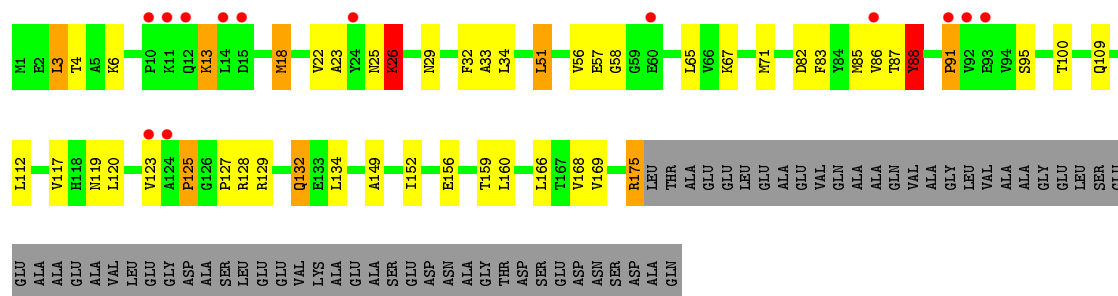








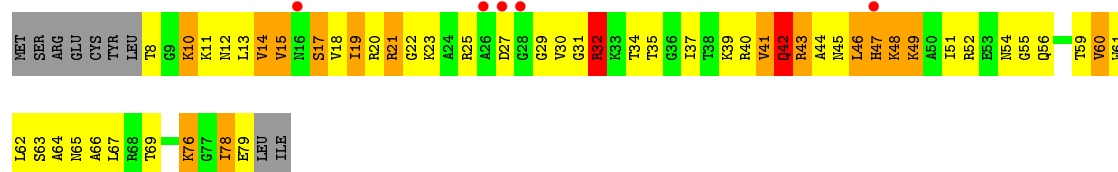
• Molecule 21: 50S ribosomal protein L25



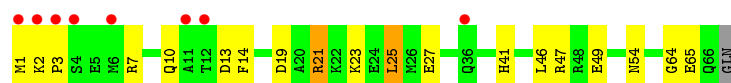
• Molecule 22: 50S ribosomal protein L27



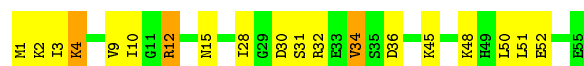
• Molecule 23: 50S ribosomal protein L28



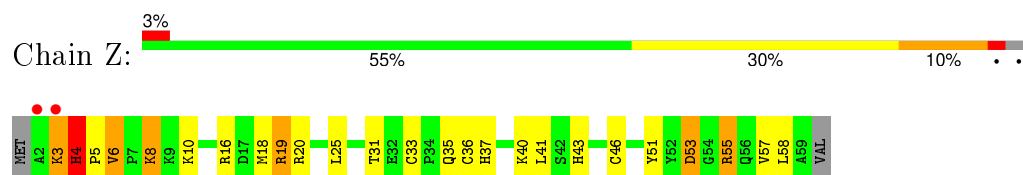
• Molecule 24: 50S ribosomal protein L29



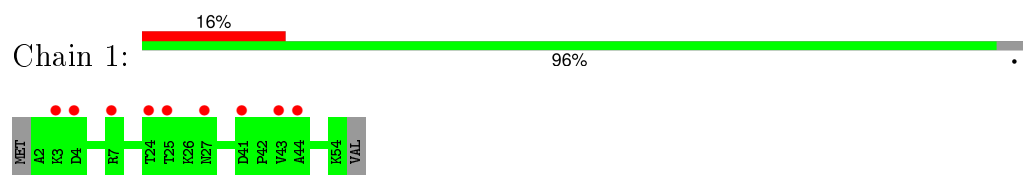
• Molecule 25: 50S ribosomal protein L30



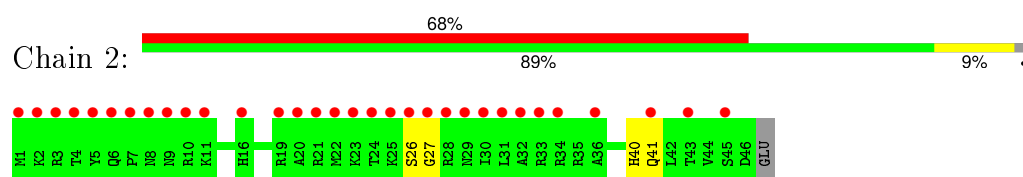
- Molecule 26: 50S ribosomal protein L32



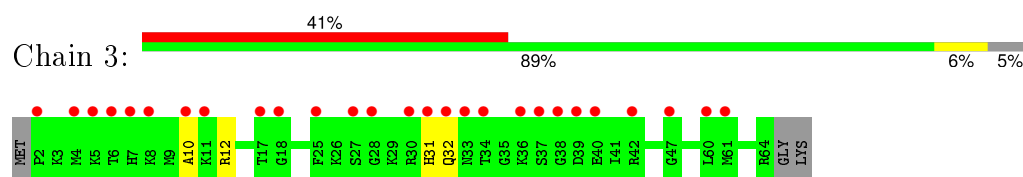
- Molecule 27: 50S ribosomal protein L33



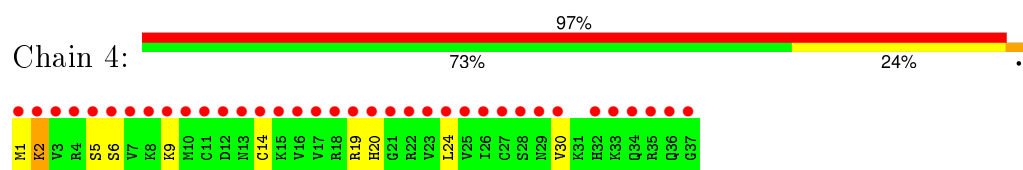
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.77Å 406.66Å 696.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.38 – 3.23	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 89.8 (30.38-3.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 3.24Å)	Xtriage
Refinement program	autobuster	Depositor
R, $R_{free}$	0.197 , 0.230 0.211 , 0.246	Depositor DCC
$R_{free}$ test set	17364 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.0	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 91.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 343784 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	83879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1F3

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	1.00	38/64561 (0.1%)	1.86	1965/100708 (2.0%)
2	Y	1.02	0/2904	1.68	66/4525 (1.5%)
3	A	0.62	0/1862	0.96	2/2510 (0.1%)
4	B	0.60	0/1567	0.96	2/2105 (0.1%)
5	C	0.63	0/1529	0.95	1/2070 (0.0%)
6	D	0.47	0/1419	0.67	0/1903
7	E	0.44	0/1308	0.68	0/1771
8	F	0.47	0/508	0.64	0/683
9	G	0.64	0/1138	1.01	4/1539 (0.3%)
10	H	0.55	0/1007	0.84	1/1352 (0.1%)
11	I	0.73	0/1081	1.11	8/1448 (0.6%)
12	J	0.65	0/1113	0.92	2/1486 (0.1%)
13	K	0.80	2/886 (0.2%)	0.99	3/1188 (0.3%)
14	L	0.57	0/785	0.95	1/1048 (0.1%)
15	M	0.65	1/884 (0.1%)	0.98	2/1186 (0.2%)
16	N	0.51	0/994	0.78	0/1323
17	O	0.56	0/750	0.96	1/1000 (0.1%)
18	P	0.56	0/1027	0.82	0/1373
19	Q	0.62	0/737	1.04	4/988 (0.4%)
20	R	0.64	0/835	0.99	0/1121
21	S	0.49	0/1370	0.73	0/1862
22	T	0.53	0/633	0.85	0/838
23	U	0.75	0/556	1.12	2/741 (0.3%)
24	V	0.47	0/537	0.69	0/714
25	W	0.46	0/426	0.79	0/568
26	Z	0.65	0/469	0.97	0/629
30	4	0.48	0/298	0.72	0/390
All	All	0.91	41/91184 (0.0%)	1.68	2064/137069 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	540	G	C2-N3	9.96	1.40	1.32
1	X	774	A	C5-C4	9.11	1.45	1.38
1	X	774	A	N7-C5	-7.92	1.34	1.39
1	X	2018	G	N9-C8	7.57	1.43	1.37
1	X	542	A	N7-C5	-7.47	1.34	1.39
1	X	1333	G	N9-C4	-6.86	1.32	1.38
1	X	537	C	N1-C2	6.71	1.46	1.40
1	X	774	A	N1-C2	6.70	1.40	1.34
1	X	540	G	N3-C4	6.67	1.40	1.35
1	X	1946	U	C1'-N1	6.67	1.58	1.48
1	X	774	A	N3-C4	6.56	1.38	1.34
13	K	3	HIS	CA-C	6.52	1.70	1.52
1	X	1980	A	N7-C5	-6.30	1.35	1.39
13	K	52	ILE	CG1-CD1	6.21	1.93	1.50
1	X	699	G	N9-C4	-6.18	1.33	1.38
15	M	29	PRO	CA-C	5.88	1.64	1.52
1	X	462	G	C6-O6	5.86	1.29	1.24
1	X	1468	A	N9-C4	5.79	1.41	1.37
1	X	343	A	N9-C4	5.76	1.41	1.37
1	X	796	A	N9-C4	-5.72	1.34	1.37
1	X	1467	U	C1'-N1	5.72	1.57	1.48
1	X	1288	A	C4'-C3'	-5.64	1.47	1.52
1	X	2485	U	N1-C2	5.64	1.43	1.38
1	X	434	C	C1'-N1	5.62	1.57	1.48
1	X	1688	U	C2-N3	5.54	1.41	1.37
1	X	2321	C	C1'-N1	5.41	1.56	1.48
1	X	540	G	C3'-O3'	5.38	1.49	1.42
1	X	537	C	C4-C5	5.34	1.47	1.43
1	X	868	U	C1'-N1	5.33	1.56	1.48
1	X	1223	G	C2-N3	5.30	1.36	1.32
1	X	2482	A	N3-C4	5.27	1.38	1.34
1	X	1688	U	N3-C4	5.25	1.43	1.38
1	X	327	C	C1'-N1	5.24	1.56	1.48
1	X	2485	U	C1'-N1	5.22	1.56	1.48
1	X	78	C	C1'-N1	5.21	1.56	1.48
1	X	358	C	C1'-N1	5.21	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2795	A	N3-C4	5.19	1.38	1.34
1	X	1522	C	C1'-N1	5.09	1.56	1.48
1	X	1688	U	C4-O4	5.05	1.27	1.23
1	X	559	C	C3'-O3'	5.03	1.49	1.42
1	X	2072	C	C1'-N1	5.03	1.56	1.48

All (2064) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-38.76	78.89	109.90
1	X	1288	A	C5'-C4'-O4'	20.93	134.22	109.10
1	X	1716	G	P-O3'-C3'	19.09	142.60	119.70
1	X	1288	A	C4'-C3'-C2'	-19.04	83.56	102.60
1	X	2808	U	O4'-C1'-N1	17.91	122.53	108.20
1	X	1775	A	P-O3'-C3'	17.83	141.10	119.70
1	X	1333	G	N3-C4-N9	-17.19	115.69	126.00
1	X	774	A	N7-C8-N9	16.88	122.24	113.80
1	X	540	G	P-O3'-C3'	16.87	139.94	119.70
1	X	1631	C	O4'-C1'-N1	16.27	121.21	108.20
1	X	537	C	O4'-C1'-N1	16.23	121.18	108.20
1	X	1333	G	O4'-C1'-N9	15.97	120.98	108.20
1	X	1288	A	O4'-C1'-N9	15.69	120.75	108.20
1	X	2497	A	P-O3'-C3'	15.66	138.49	119.70
1	X	1473	U	P-O3'-C3'	15.41	138.20	119.70
1	X	1631	C	P-O3'-C3'	15.28	138.03	119.70
1	X	2705	A	P-O3'-C3'	15.27	138.03	119.70
1	X	774	A	N1-C6-N6	15.10	127.66	118.60
1	X	1475	U	P-O3'-C3'	14.90	137.59	119.70
1	X	994	A	P-O3'-C3'	14.88	137.56	119.70
1	X	343	A	O4'-C1'-N9	14.77	120.02	108.20
1	X	1278	A	O4'-C1'-N9	14.74	120.00	108.20
1	X	777	A	P-O3'-C3'	14.73	137.37	119.70
1	X	2014	A	P-O3'-C3'	14.71	137.36	119.70
1	X	2706	U	P-O3'-C3'	14.71	137.35	119.70
1	X	399	G	P-O3'-C3'	14.67	137.30	119.70
1	X	774	A	C5-N7-C8	-14.57	96.61	103.90
1	X	1812	U	C1'-O4'-C4'	-14.53	98.27	109.90
1	X	540	G	N3-C4-N9	14.43	134.66	126.00
1	X	1249	G	P-O3'-C3'	14.41	136.99	119.70
1	X	1482	U	O4'-C1'-N1	14.39	119.71	108.20
1	X	802	A	P-O3'-C3'	14.30	136.86	119.70
1	X	100	G	P-O3'-C3'	13.66	136.10	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1409	U	P-O3'-C3'	13.51	135.91	119.70
1	X	176	A	P-O3'-C3'	13.47	135.86	119.70
1	X	2564	U	P-O3'-C3'	13.40	135.78	119.70
1	X	98	U	P-O3'-C3'	13.38	135.75	119.70
1	X	1570	C	O4'-C1'-N1	13.37	118.90	108.20
1	X	2736	U	P-O3'-C3'	13.23	135.58	119.70
1	X	774	A	C8-N9-C4	-13.23	100.51	105.80
1	X	774	A	C6-C5-N7	-13.06	123.16	132.30
1	X	1019	U	P-O3'-C3'	12.92	135.21	119.70
1	X	2404	A	P-O3'-C3'	12.91	135.20	119.70
1	X	1811	A	P-O3'-C3'	12.85	135.11	119.70
1	X	1820	G	P-O3'-C3'	12.84	135.11	119.70
1	X	1037	U	C1'-O4'-C4'	-12.83	99.63	109.90
1	X	1333	G	N3-C4-C5	12.79	135.00	128.60
1	X	540	G	N3-C2-N2	12.78	128.84	119.90
1	X	540	G	C4-C5-N7	12.77	115.91	110.80
1	X	1152	C	P-O3'-C3'	12.75	135.00	119.70
1	X	33	C	P-O3'-C3'	12.69	134.92	119.70
1	X	2018	G	P-O3'-C3'	12.67	134.91	119.70
1	X	1938	U	P-O3'-C3'	12.59	134.81	119.70
1	X	1561	A	P-O3'-C3'	12.59	134.80	119.70
1	X	1037	U	O4'-C1'-N1	12.53	118.22	108.20
1	X	2706	U	O4'-C1'-N1	12.51	118.21	108.20
1	X	1233	A	P-O3'-C3'	12.46	134.65	119.70
1	X	334	G	P-O3'-C3'	12.35	134.52	119.70
1	X	2371	A	O4'-C1'-N9	12.29	118.04	108.20
1	X	1467	U	P-O3'-C3'	-12.28	104.96	119.70
1	X	1963	G	P-O3'-C3'	12.27	134.42	119.70
1	X	469	G	O4'-C1'-N9	12.21	117.97	108.20
1	X	1055	A	P-O3'-C3'	12.18	134.31	119.70
1	X	467	U	C1'-O4'-C4'	-12.17	100.16	109.90
1	X	554	U	O4'-C1'-N1	12.06	117.84	108.20
1	X	1468	A	O4'-C1'-N9	12.06	117.84	108.20
1	X	1283	C	P-O3'-C3'	11.99	134.09	119.70
1	X	2770	A	P-O3'-C3'	11.98	134.07	119.70
1	X	683	A	P-O3'-C3'	11.94	134.03	119.70
1	X	1468	A	C8-N9-C4	-11.93	101.03	105.80
1	X	2608	A	P-O3'-C3'	11.85	133.92	119.70
1	X	2204	A	P-O3'-C3'	11.75	133.81	119.70
1	X	99	U	P-O3'-C3'	11.75	133.80	119.70
1	X	2312	A	P-O3'-C3'	11.72	133.77	119.70
1	X	1031	C	P-O3'-C3'	11.72	133.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1467	U	C5-C6-N1	11.71	128.56	122.70
1	X	774	A	C4-C5-N7	11.67	116.53	110.70
1	X	48	A	P-O3'-C3'	11.63	133.66	119.70
1	X	969	U	P-O3'-C3'	11.57	133.58	119.70
1	X	780	U	P-O3'-C3'	11.54	133.54	119.70
1	X	594	G	P-O3'-C3'	11.50	133.50	119.70
1	X	1790	G	P-O3'-C3'	11.48	133.48	119.70
2	Y	16	U	P-O3'-C3'	11.39	133.37	119.70
1	X	2589	C	P-O3'-C3'	11.37	133.34	119.70
1	X	1468	A	O4'-C1'-C2'	-11.17	94.63	105.80
1	X	2298	U	P-O3'-C3'	11.10	133.01	119.70
1	X	1975	G	P-O3'-C3'	11.09	133.01	119.70
1	X	2088	U	P-O3'-C3'	11.08	133.00	119.70
1	X	2498	U	P-O3'-C3'	11.08	132.99	119.70
1	X	1574	A	C4'-C3'-C2'	-11.06	91.54	102.60
1	X	514	G	P-O3'-C3'	11.05	132.96	119.70
1	X	537	C	N3-C2-O2	-11.05	114.17	121.90
1	X	2261	G	P-O3'-C3'	10.97	132.86	119.70
1	X	1333	G	C8-N9-C1'	10.96	141.25	127.00
1	X	1096	A	P-O3'-C3'	10.93	132.82	119.70
1	X	1574	A	O4'-C1'-N9	10.80	116.84	108.20
1	X	1669	A	O4'-C4'-C3'	-10.80	93.20	104.00
1	X	540	G	C6-C5-N7	-10.78	123.93	130.40
1	X	2596	C	O4'-C1'-N1	10.78	116.83	108.20
1	X	1186	G	P-O3'-C3'	10.71	132.55	119.70
1	X	656	U	O4'-C1'-N1	10.61	116.69	108.20
1	X	825	C	P-O3'-C3'	-10.58	107.01	119.70
1	X	1194	U	P-O3'-C3'	10.55	132.36	119.70
1	X	540	G	C5-C6-O6	-10.52	122.29	128.60
1	X	1688	U	N3-C4-O4	10.51	126.76	119.40
1	X	553	C	P-O3'-C3'	10.50	132.30	119.70
1	X	71	A	P-O3'-C3'	10.50	132.30	119.70
1	X	1850	G	P-O3'-C3'	10.48	132.28	119.70
1	X	664	C	P-O3'-C3'	10.47	132.27	119.70
1	X	1333	G	N3-C2-N2	-10.46	112.58	119.90
1	X	699	G	C5-N7-C8	-10.42	99.09	104.30
1	X	540	G	N3-C4-C5	-10.41	123.39	128.60
1	X	2551	A	P-O3'-C3'	10.37	132.15	119.70
1	X	342	G	P-O3'-C3'	10.37	132.14	119.70
1	X	537	C	C1'-O4'-C4'	-10.36	101.61	109.90
1	X	2769	C	C1'-O4'-C4'	-10.35	101.62	109.90
1	X	540	G	C5-C6-N1	10.34	116.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1496	G	P-O3'-C3'	10.31	132.07	119.70
1	X	458	G	P-O3'-C3'	10.29	132.05	119.70
1	X	939	C	C5'-C4'-O4'	10.29	121.45	109.10
1	X	518	A	P-O3'-C3'	10.27	132.02	119.70
1	X	814	G	O4'-C1'-N9	-10.25	100.00	108.20
1	X	1033	G	P-O3'-C3'	10.25	132.00	119.70
1	X	1053	G	P-O3'-C3'	10.19	131.93	119.70
1	X	542	A	C8-N9-C4	-10.17	101.73	105.80
1	X	540	G	C3'-C2'-C1'	10.15	109.62	101.50
1	X	1139	A	C1'-O4'-C4'	-10.13	101.80	109.90
1	X	803	C	P-O3'-C3'	10.09	131.81	119.70
1	X	83	A	P-O3'-C3'	10.08	131.79	119.70
1	X	2426	G	P-O3'-C3'	10.06	131.78	119.70
1	X	554	U	P-O3'-C3'	10.05	131.76	119.70
1	X	1632	A	P-O3'-C3'	10.01	131.71	119.70
1	X	2795	A	P-O3'-C3'	9.97	131.67	119.70
1	X	175	C	P-O3'-C3'	9.97	131.66	119.70
1	X	805	G	O4'-C1'-N9	-9.96	100.23	108.20
1	X	632	A	O4'-C1'-N9	9.93	116.14	108.20
1	X	2769	C	O4'-C1'-N1	9.90	116.12	108.20
1	X	1552	C	P-O3'-C3'	9.89	131.56	119.70
1	X	655	A	P-O3'-C3'	9.85	131.52	119.70
1	X	480	G	C5-C6-O6	-9.83	122.70	128.60
1	X	1812	U	O4'-C1'-N1	9.79	116.03	108.20
1	X	2418	A	P-O3'-C3'	9.78	131.43	119.70
1	X	1333	G	N9-C4-C5	9.76	109.31	105.40
1	X	1482	U	C1'-O4'-C4'	-9.76	102.09	109.90
1	X	814	G	P-O3'-C3'	9.75	131.40	119.70
1	X	2330	G	P-O3'-C3'	9.73	131.38	119.70
1	X	1442	C	P-O3'-C3'	9.72	131.36	119.70
1	X	2633	A	P-O3'-C3'	9.71	131.35	119.70
1	X	666	U	O4'-C1'-N1	9.67	115.94	108.20
1	X	558	G	P-O3'-C3'	9.66	131.30	119.70
1	X	73	A	P-O3'-C3'	9.66	131.29	119.70
1	X	2691	C	O4'-C1'-C2'	-9.66	96.14	105.80
1	X	1182	U	P-O3'-C3'	9.65	131.29	119.70
1	X	699	G	N3-C4-C5	9.63	133.42	128.60
1	X	759	C	C5-C6-N1	9.62	125.81	121.00
1	X	689	A	C5-N7-C8	-9.61	99.09	103.90
1	X	554	U	C1'-O4'-C4'	-9.61	102.22	109.90
1	X	1575	C	P-O3'-C3'	9.58	131.19	119.70
1	X	689	A	O4'-C1'-N9	9.56	115.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	3	U	P-O3'-C3'	9.55	131.16	119.70
1	X	542	A	C3'-C2'-C1'	9.55	109.14	101.50
1	X	1613	G	C1'-O4'-C4'	-9.54	102.27	109.90
1	X	691	C	O4'-C1'-N1	9.49	115.79	108.20
1	X	1333	G	C4-N9-C1'	-9.49	114.17	126.50
1	X	169	C	O4'-C1'-N1	9.48	115.79	108.20
1	X	542	A	N7-C8-N9	9.45	118.53	113.80
2	Y	26	G	P-O3'-C3'	9.43	131.02	119.70
1	X	1288	A	C3'-C2'-C1'	-9.40	93.98	101.50
1	X	841	G	O4'-C1'-N9	9.39	115.72	108.20
1	X	540	G	N7-C8-N9	9.39	117.79	113.10
1	X	2229	G	P-O3'-C3'	9.38	130.96	119.70
1	X	1288	A	O4'-C4'-C3'	-9.36	94.64	104.00
1	X	1664	G	O5'-P-OP2	9.35	121.92	110.70
1	X	1601	U	P-O3'-C3'	9.35	130.92	119.70
1	X	1975	G	C2'-C3'-O3'	9.35	130.07	109.50
1	X	1633	C	O4'-C1'-N1	9.28	115.63	108.20
1	X	1412	C	C3'-C2'-C1'	-9.28	94.08	101.50
1	X	2051	U	O4'-C1'-N1	9.23	115.58	108.20
1	X	1086	C	P-O3'-C3'	9.22	130.76	119.70
1	X	540	G	C5-N7-C8	-9.21	99.70	104.30
1	X	2669	C	N1-C2-O2	9.17	124.40	118.90
1	X	638	A	P-O3'-C3'	9.13	130.66	119.70
1	X	1689	U	O4'-C1'-N1	9.12	115.50	108.20
1	X	1345	G	P-O3'-C3'	9.12	130.64	119.70
1	X	2703	C	O4'-C1'-N1	9.10	115.48	108.20
1	X	699	G	N3-C4-N9	-9.09	120.55	126.00
1	X	1754	G	P-O3'-C3'	9.07	130.58	119.70
1	X	763	A	P-O3'-C3'	9.07	130.58	119.70
1	X	1459	U	P-O3'-C3'	9.06	130.58	119.70
1	X	467	U	O4'-C1'-N1	9.06	115.45	108.20
1	X	789	G	P-O3'-C3'	9.06	130.57	119.70
1	X	1574	A	C1'-O4'-C4'	-9.06	102.66	109.90
1	X	3	U	C3'-C2'-C1'	-9.03	94.27	101.50
1	X	2554	C	O4'-C1'-N1	9.01	115.41	108.20
1	X	666	U	C1'-O4'-C4'	-9.01	102.69	109.90
1	X	198	A	P-O3'-C3'	8.99	130.48	119.70
1	X	537	C	N1-C2-O2	8.99	124.29	118.90
1	X	1799	A	C1'-O4'-C4'	-8.97	102.72	109.90
1	X	1154	A	P-O3'-C3'	8.96	130.45	119.70
1	X	483	A	P-O3'-C3'	-8.95	108.96	119.70
1	X	2018	G	N3-C4-N9	-8.93	120.64	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2672	U	O4'-C1'-N1	8.93	115.34	108.20
1	X	796	A	C5-N7-C8	-8.92	99.44	103.90
1	X	1184	G	P-O3'-C3'	8.91	130.39	119.70
1	X	515	A	P-O3'-C3'	8.89	130.37	119.70
1	X	1137	A	P-O3'-C3'	8.89	130.37	119.70
1	X	2222	U	O4'-C1'-N1	8.89	115.31	108.20
1	X	2018	G	N9-C1'-C2'	8.86	125.52	114.00
1	X	341	A	P-O3'-C3'	8.84	130.31	119.70
1	X	2475	C	O4'-C1'-N1	8.82	115.26	108.20
1	X	574	C	O4'-C1'-N1	8.82	115.26	108.20
1	X	1830	C	P-O3'-C3'	8.82	130.28	119.70
1	X	2671	C	O4'-C1'-N1	8.82	115.25	108.20
1	X	689	A	N7-C8-N9	8.81	118.20	113.80
1	X	559	C	N1-C1'-C2'	8.80	125.44	114.00
1	X	2706	U	C4'-C3'-C2'	8.78	111.38	102.60
1	X	1746	A	O4'-C1'-N9	8.78	115.23	108.20
1	X	2689	C	P-O3'-C3'	8.78	130.24	119.70
1	X	418	C	C1'-O4'-C4'	-8.75	102.90	109.90
1	X	774	A	C5-C6-N1	-8.74	113.33	117.70
1	X	841	G	C8-N9-C4	-8.74	102.90	106.40
1	X	1812	U	N1-C1'-C2'	8.73	125.34	114.00
1	X	1509	A	O4'-C1'-N9	8.72	115.17	108.20
1	X	1265	G	O4'-C1'-N9	-8.70	101.24	108.20
1	X	2782	G	C5-C6-O6	-8.70	123.38	128.60
1	X	686	C	O4'-C1'-N1	8.70	115.16	108.20
1	X	483	A	O4'-C1'-N9	8.68	115.14	108.20
1	X	1278	A	C3'-C2'-C1'	-8.65	94.58	101.50
1	X	540	G	N9-C4-C5	-8.65	101.94	105.40
1	X	625	A	P-O3'-C3'	8.64	130.07	119.70
1	X	1656	U	O4'-C1'-N1	8.64	115.11	108.20
1	X	1468	A	P-O3'-C3'	8.62	130.04	119.70
1	X	566	U	O4'-C1'-N1	8.61	115.08	108.20
1	X	758	G	C2'-C3'-O3'	8.60	128.43	109.50
1	X	540	G	N1-C2-N2	-8.59	108.47	116.20
1	X	953	G	O4'-C1'-N9	8.59	115.07	108.20
1	X	804	C	O4'-C1'-N1	8.58	115.07	108.20
1	X	2691	C	P-O3'-C3'	8.58	130.00	119.70
1	X	656	U	P-O3'-C3'	8.58	130.00	119.70
1	X	1938	U	C4'-C3'-C2'	8.58	111.18	102.60
1	X	216	U	O4'-C1'-N1	8.58	115.06	108.20
1	X	467	U	P-O3'-C3'	8.57	129.98	119.70
1	X	490	A	O4'-C1'-N9	8.56	115.05	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	54	U	O4'-C1'-N1	8.56	115.05	108.20
1	X	204	A	P-O3'-C3'	8.55	129.96	119.70
1	X	242	A	C4'-C3'-C2'	-8.55	94.05	102.60
1	X	788	G	P-O3'-C3'	8.53	129.93	119.70
1	X	1223	G	C3'-C2'-C1'	8.52	108.31	101.50
1	X	1399	C	O4'-C1'-N1	8.51	115.01	108.20
1	X	181	A	P-O3'-C3'	8.50	129.90	119.70
1	X	1974	U	O4'-C1'-N1	8.49	115.00	108.20
1	X	2594	U	C5-C6-N1	8.45	126.93	122.70
1	X	1602	G	P-O3'-C3'	8.45	129.84	119.70
1	X	1467	U	C4-C5-C6	-8.44	114.64	119.70
1	X	1278	A	C1'-O4'-C4'	-8.43	103.16	109.90
1	X	939	C	C1'-O4'-C4'	-8.42	103.16	109.90
1	X	1581	C	P-O3'-C3'	8.42	129.80	119.70
1	X	343	A	C8-N9-C4	-8.41	102.44	105.80
1	X	31	C	O4'-C1'-N1	8.40	114.92	108.20
1	X	2426	G	O4'-C1'-N9	8.40	114.92	108.20
1	X	537	C	N3-C4-N4	-8.38	112.13	118.00
1	X	1716	G	C4'-C3'-C2'	8.38	110.98	102.60
1	X	1441	A	P-O3'-C3'	8.37	129.75	119.70
1	X	2778	U	P-O3'-C3'	8.37	129.74	119.70
1	X	1469	U	N1-C1'-C2'	8.34	124.85	114.00
1	X	1574	A	C5'-C4'-O4'	8.34	119.11	109.10
1	X	2189	A	P-O3'-C3'	8.33	129.69	119.70
1	X	1953	A	P-O5'-C5'	-8.32	107.58	120.90
1	X	2018	G	C5'-C4'-C3'	-8.32	102.69	116.00
1	X	2685	A	N1-C6-N6	-8.32	113.61	118.60
1	X	1539	U	O4'-C1'-N1	8.31	114.85	108.20
1	X	1753	A	O4'-C1'-N9	8.30	114.84	108.20
1	X	2408	G	P-O5'-C5'	-8.30	107.62	120.90
1	X	2018	G	N3-C4-C5	8.30	132.75	128.60
1	X	2745	A	P-O3'-C3'	8.29	129.65	119.70
1	X	346	C	C6-N1-C2	-8.29	116.98	120.30
1	X	2191	A	O4'-C1'-N9	8.28	114.83	108.20
1	X	2867	G	N7-C8-N9	8.28	117.24	113.10
1	X	809	C	O4'-C1'-N1	8.27	114.82	108.20
1	X	2867	G	C5-N7-C8	-8.27	100.17	104.30
1	X	841	G	N7-C8-N9	8.26	117.23	113.10
1	X	358	C	O4'-C1'-N1	8.26	114.81	108.20
1	X	631	G	P-O5'-C5'	-8.25	107.70	120.90
1	X	346	C	O4'-C1'-N1	8.24	114.79	108.20
1	X	467	U	C2-N1-C1'	8.21	127.56	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	490	A	P-O3'-C3'	8.21	129.55	119.70
1	X	731	A	P-O3'-C3'	8.20	129.54	119.70
1	X	2710	C	P-O3'-C3'	-8.20	109.86	119.70
1	X	1523	A	P-O3'-C3'	8.20	129.53	119.70
1	X	1765	C	N1-C2-O2	8.19	123.81	118.90
1	X	1251	G	O4'-C1'-N9	8.18	114.75	108.20
1	X	2824	C	P-O3'-C3'	8.18	129.51	119.70
1	X	2491	C	O5'-P-OP2	-8.18	98.34	105.70
1	X	847	C	O4'-C1'-N1	8.17	114.74	108.20
1	X	593	C	O4'-C1'-N1	8.15	114.72	108.20
1	X	661	C	N1-C2-O2	8.15	123.79	118.90
1	X	2857	C	O4'-C1'-N1	8.12	114.69	108.20
1	X	469	G	P-O3'-C3'	8.12	129.44	119.70
1	X	2034	A	P-O3'-C3'	8.11	129.44	119.70
1	X	2867	G	C4-C5-N7	8.11	114.04	110.80
1	X	2487	G	O4'-C1'-N9	8.10	114.68	108.20
1	X	2730	A	P-O3'-C3'	8.10	129.42	119.70
1	X	1188	A	P-O3'-C3'	8.09	129.41	119.70
1	X	2298	U	O4'-C1'-N1	8.09	114.67	108.20
1	X	751	G	O4'-C4'-C3'	-8.08	95.92	104.00
1	X	597	U	O4'-C4'-C3'	-8.07	95.93	104.00
1	X	1232	U	O4'-C1'-N1	8.07	114.66	108.20
1	X	1712	G	N3-C2-N2	8.06	125.54	119.90
1	X	758	G	C3'-C2'-C1'	-8.06	95.05	101.50
1	X	1310	C	O4'-C1'-N1	8.05	114.64	108.20
1	X	1962	C	C3'-C2'-C1'	-8.05	95.06	101.50
1	X	99	U	O4'-C1'-N1	8.05	114.64	108.20
1	X	813	A	P-O3'-C3'	8.05	129.36	119.70
1	X	859	U	O4'-C1'-N1	8.05	114.64	108.20
1	X	526	C	O4'-C1'-N1	8.04	114.64	108.20
1	X	580	A	P-O3'-C3'	8.04	129.35	119.70
1	X	39	C	O4'-C1'-N1	8.03	114.62	108.20
1	X	1524	C	P-O3'-C3'	8.02	129.32	119.70
1	X	2667	C	P-O3'-C3'	8.02	129.32	119.70
1	X	739	G	O4'-C1'-N9	8.01	114.61	108.20
1	X	74	G	O4'-C4'-C3'	-8.00	96.00	104.00
1	X	542	A	N1-C2-N3	8.00	133.30	129.30
1	X	1468	A	C5-C6-N1	7.99	121.70	117.70
1	X	1710	U	P-O3'-C3'	7.99	129.29	119.70
1	X	117	A	P-O3'-C3'	7.99	129.28	119.70
1	X	313	U	O4'-C1'-N1	7.96	114.57	108.20
1	X	2854	G	C1'-O4'-C4'	-7.96	103.53	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2854	G	P-O3'-C3'	7.96	129.25	119.70
1	X	2859	U	O4'-C1'-N1	7.95	114.56	108.20
1	X	579	G	C4-C5-N7	-7.94	107.62	110.80
1	X	1314	A	P-O3'-C3'	7.94	129.22	119.70
1	X	542	A	C6-N1-C2	-7.93	113.84	118.60
1	X	1673	C	O4'-C1'-N1	7.93	114.54	108.20
1	X	2492	G	O4'-C1'-N9	7.93	114.54	108.20
1	X	1469	U	P-O3'-C3'	7.91	129.19	119.70
1	X	796	A	N1-C6-N6	7.91	123.35	118.60
1	X	841	G	N9-C1'-C2'	7.91	124.28	114.00
1	X	685	U	O4'-C1'-N1	7.90	114.52	108.20
1	X	165	G	O4'-C1'-N9	7.90	114.52	108.20
1	X	1139	A	O4'-C1'-N9	7.89	114.52	108.20
1	X	631	G	P-O3'-C3'	7.89	129.17	119.70
1	X	467	U	C4'-C3'-C2'	-7.89	94.71	102.60
1	X	699	G	N7-C8-N9	7.88	117.04	113.10
1	X	236	C	O4'-C1'-N1	7.88	114.50	108.20
1	X	2018	G	O4'-C1'-N9	7.87	114.50	108.20
1	X	100	G	O4'-C1'-N9	7.87	114.49	108.20
1	X	2258	G	C1'-O4'-C4'	-7.86	103.61	109.90
1	X	1679	U	N3-C2-O2	-7.85	116.70	122.20
1	X	307	C	O4'-C1'-N1	7.85	114.48	108.20
1	X	2009	U	O4'-C1'-N1	7.84	114.48	108.20
1	X	2810	A	P-O3'-C3'	7.84	129.11	119.70
1	X	554	U	N1-C1'-C2'	7.84	124.19	114.00
2	Y	42	U	O4'-C1'-N1	7.84	114.47	108.20
1	X	774	A	C5-C6-N6	-7.83	117.43	123.70
1	X	1775	A	C2'-C3'-O3'	7.83	126.73	109.50
1	X	1770	U	O4'-C4'-C3'	-7.83	96.17	104.00
1	X	1526	U	O4'-C1'-N1	7.82	114.46	108.20
1	X	2854	G	N9-C1'-C2'	7.82	124.16	114.00
1	X	868	U	O4'-C1'-N1	7.81	114.45	108.20
1	X	308	C	O4'-C1'-N1	7.81	114.45	108.20
1	X	864	C	O4'-C1'-N1	7.81	114.45	108.20
1	X	1161	U	O4'-C1'-N1	7.80	114.44	108.20
1	X	672	C	O4'-C4'-C3'	-7.80	96.20	104.00
1	X	1688	U	N3-C4-C5	-7.80	109.92	114.60
13	K	94	TYR	C-N-CA	7.79	141.19	121.70
1	X	2597	G	O4'-C1'-N9	7.78	114.42	108.20
1	X	2489	C	O4'-C1'-N1	7.78	114.42	108.20
1	X	2275	U	P-O3'-C3'	7.77	129.02	119.70
1	X	577	U	N3-C4-C5	-7.77	109.94	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1496	G	C3'-C2'-C1'	-7.76	95.29	101.50
1	X	2299	A	P-O3'-C3'	7.76	129.02	119.70
1	X	956	A	N1-C6-N6	7.75	123.25	118.60
1	X	1467	U	N1-C2-N3	-7.74	110.26	114.90
1	X	2043	A	O4'-C1'-N9	7.73	114.39	108.20
1	X	242	A	C1'-O4'-C4'	-7.73	103.72	109.90
1	X	312	G	P-O3'-C3'	7.72	128.97	119.70
1	X	526	C	C3'-C2'-C1'	-7.72	95.32	101.50
1	X	1829	C	O4'-C1'-N1	7.71	114.37	108.20
1	X	927	C	O4'-C1'-N1	7.70	114.36	108.20
1	X	1844	C	O4'-C1'-N1	7.68	114.35	108.20
1	X	1947	G	P-O3'-C3'	7.67	128.91	119.70
1	X	2813	G	O4'-C1'-N9	7.67	114.34	108.20
1	X	2062	U	O4'-C1'-N1	7.67	114.33	108.20
1	X	1561	A	C3'-C2'-C1'	-7.66	95.37	101.50
1	X	841	G	O4'-C4'-C3'	-7.66	96.34	104.00
1	X	462	G	C5-C6-N1	-7.66	107.67	111.50
1	X	1663	C	N1-C2-O2	7.64	123.49	118.90
1	X	1141	U	C2'-C3'-O3'	7.64	126.31	109.50
1	X	1674	C	O4'-C1'-N1	7.64	114.31	108.20
1	X	2501	U	C5'-C4'-C3'	-7.63	103.80	116.00
1	X	2018	G	C5-N7-C8	-7.62	100.49	104.30
1	X	2756	A	P-O3'-C3'	7.62	128.85	119.70
1	X	537	C	P-O3'-C3'	7.61	128.83	119.70
1	X	1976	U	P-O5'-C5'	-7.60	108.73	120.90
19	Q	60	GLY	C-N-CA	7.60	140.70	121.70
1	X	480	G	C4-C5-N7	7.59	113.84	110.80
1	X	1392	U	P-O3'-C3'	7.59	128.81	119.70
1	X	1468	A	C3'-C2'-C1'	-7.59	95.43	101.50
1	X	2000	U	O5'-P-OP2	-7.59	98.87	105.70
1	X	1279	G	C5-C6-O6	-7.58	124.05	128.60
1	X	2808	U	C1'-O4'-C4'	-7.57	103.84	109.90
1	X	2016	A	P-O3'-C3'	7.57	128.78	119.70
1	X	768	U	O4'-C1'-N1	7.57	114.25	108.20
1	X	1333	G	C8-N9-C4	-7.56	103.38	106.40
1	X	1607	A	P-O3'-C3'	7.56	128.77	119.70
1	X	1364	C	O4'-C1'-N1	7.55	114.24	108.20
1	X	699	G	C4-C5-N7	7.55	113.82	110.80
1	X	796	A	N7-C8-N9	7.55	117.58	113.80
1	X	2005	U	O4'-C1'-N1	7.54	114.24	108.20
1	X	1072	U	P-O3'-C3'	7.54	128.75	119.70
1	X	312	G	C1'-O4'-C4'	-7.54	103.87	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	246	C	O4'-C1'-N1	7.54	114.23	108.20
2	Y	30	C	O4'-C1'-N1	7.54	114.23	108.20
1	X	1963	G	C2'-C3'-O3'	7.53	126.08	109.50
1	X	2550	C	O4'-C1'-N1	7.53	114.22	108.20
1	X	1562	G	O4'-C1'-N9	7.51	114.21	108.20
1	X	520	C	P-O3'-C3'	7.51	128.71	119.70
1	X	2477	C	C5'-C4'-O4'	-7.50	100.10	109.10
1	X	759	C	C6-N1-C2	-7.49	117.31	120.30
1	X	2824	C	C2'-C3'-O3'	7.49	125.97	109.50
1	X	1466	C	C4'-C3'-C2'	-7.48	95.12	102.60
1	X	2370	G	C1'-O4'-C4'	-7.48	103.92	109.90
1	X	3	U	C2'-C3'-O3'	7.48	125.95	109.50
1	X	456	C	O4'-C1'-N1	7.48	114.18	108.20
1	X	774	A	C2-N3-C4	-7.48	106.86	110.60
1	X	1306	U	O4'-C1'-N1	7.48	114.18	108.20
1	X	418	C	C5'-C4'-O4'	7.46	118.05	109.10
1	X	1128	G	P-O3'-C3'	7.45	128.64	119.70
1	X	2031	A	O4'-C1'-N9	7.44	114.16	108.20
1	X	661	C	C4'-C3'-C2'	-7.44	95.16	102.60
1	X	1467	U	N1-C2-O2	7.44	128.01	122.80
1	X	408	U	P-O3'-C3'	7.43	128.62	119.70
1	X	394	U	O4'-C1'-N1	7.42	114.14	108.20
1	X	218	A	P-O3'-C3'	7.42	128.61	119.70
1	X	939	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	2206	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	346	C	N1-C1'-C2'	7.41	123.63	114.00
1	X	1917	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	1770	U	N3-C2-O2	-7.41	117.02	122.20
1	X	1429	A	C1'-O4'-C4'	-7.39	103.98	109.90
1	X	1988	A	P-O3'-C3'	7.39	128.57	119.70
1	X	503	G	O4'-C4'-C3'	-7.39	96.61	104.00
1	X	509	U	O4'-C1'-N1	7.38	114.11	108.20
1	X	796	A	C2-N3-C4	-7.38	106.91	110.60
1	X	537	C	C5-C6-N1	-7.38	117.31	121.00
1	X	429	C	O4'-C1'-N1	7.37	114.09	108.20
1	X	2193	C	O4'-C1'-N1	7.36	114.09	108.20
1	X	357	A	P-O3'-C3'	7.36	128.53	119.70
1	X	2392	G	O4'-C1'-N9	7.36	114.08	108.20
1	X	938	G	O4'-C1'-N9	7.35	114.08	108.20
1	X	1034	U	O4'-C1'-N1	7.35	114.08	108.20
1	X	826	U	O4'-C1'-N1	7.34	114.07	108.20
1	X	1265	G	P-O5'-C5'	7.34	132.64	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1656	U	P-O3'-C3'	7.34	128.50	119.70
1	X	68	C	O4'-C1'-N1	7.33	114.07	108.20
1	X	1336	G	C5-C6-O6	-7.33	124.20	128.60
1	X	192	G	P-O3'-C3'	7.33	128.50	119.70
1	X	838	A	OP1-P-O3'	7.33	121.31	105.20
1	X	89	A	P-O3'-C3'	7.32	128.49	119.70
1	X	765	C	P-O3'-C3'	7.32	128.48	119.70
1	X	2270	U	O4'-C1'-N1	7.32	114.06	108.20
2	Y	81	C	O4'-C1'-N1	7.32	114.05	108.20
1	X	174	A	P-O3'-C3'	7.31	128.48	119.70
1	X	2395	C	O4'-C1'-N1	7.30	114.04	108.20
1	X	777	A	C2'-C3'-O3'	7.29	125.53	109.50
1	X	1593	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	2752	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	1068	A	P-O3'-C3'	7.28	128.44	119.70
1	X	1470	G	P-O3'-C3'	-7.28	110.97	119.70
1	X	1044	U	P-O3'-C3'	7.27	128.43	119.70
1	X	661	C	O4'-C1'-N1	7.26	114.01	108.20
1	X	1339	U	O4'-C1'-N1	7.26	114.01	108.20
1	X	661	C	N3-C2-O2	-7.26	116.82	121.90
1	X	926	C	O4'-C1'-N1	7.25	114.00	108.20
1	X	1334	A	O4'-C4'-C3'	-7.25	96.75	104.00
1	X	343	A	N7-C8-N9	7.24	117.42	113.80
1	X	2589	C	O4'-C1'-N1	-7.24	102.41	108.20
1	X	1770	U	C5-C6-N1	-7.24	119.08	122.70
1	X	59	G	P-O3'-C3'	7.23	128.37	119.70
1	X	742	G	P-O3'-C3'	7.22	128.37	119.70
1	X	1670	G	P-O3'-C3'	7.22	128.37	119.70
1	X	418	C	O4'-C1'-N1	7.22	113.98	108.20
1	X	2185	U	O4'-C1'-N1	7.22	113.97	108.20
1	X	2853	U	O4'-C1'-N1	7.21	113.97	108.20
1	X	1680	U	O4'-C4'-C3'	-7.21	96.79	104.00
1	X	882	C	O4'-C1'-N1	7.21	113.97	108.20
1	X	947	C	O4'-C1'-N1	7.21	113.96	108.20
1	X	1447	U	O4'-C1'-N1	7.20	113.96	108.20
1	X	2408	G	C5'-C4'-C3'	-7.20	104.47	116.00
1	X	843	G	P-O3'-C3'	7.20	128.34	119.70
1	X	518	A	N9-C1'-C2'	7.19	123.35	114.00
1	X	1333	G	C2-N3-C4	-7.19	108.31	111.90
1	X	1474	A	P-O3'-C3'	7.17	128.31	119.70
1	X	525	A	O4'-C1'-N9	7.17	113.94	108.20
1	X	1812	U	P-O3'-C3'	7.17	128.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	387	A	P-O3'-C3'	7.17	128.31	119.70
1	X	824	U	N1-C1'-C2'	7.16	123.31	114.00
1	X	2782	G	N1-C6-O6	7.16	124.19	119.90
1	X	1277	G	O4'-C1'-N9	7.15	113.92	108.20
1	X	514	G	O4'-C1'-N9	-7.14	102.48	108.20
1	X	2731	G	P-O3'-C3'	7.14	128.27	119.70
1	X	2668	U	C5-C4-O4	7.14	130.18	125.90
1	X	242	A	O4'-C4'-C3'	-7.14	96.86	104.00
1	X	517	A	P-O3'-C3'	7.14	128.26	119.70
1	X	1664	G	O5'-P-OP1	-7.14	99.28	105.70
1	X	2708	U	O4'-C1'-N1	7.14	113.91	108.20
1	X	1570	C	C1'-O4'-C4'	-7.13	104.19	109.90
1	X	714	G	O4'-C4'-C3'	-7.13	96.87	104.00
1	X	801	A	P-O3'-C3'	7.13	128.25	119.70
1	X	2217	G	P-O3'-C3'	7.13	128.25	119.70
1	X	2615	U	O4'-C1'-N1	7.13	113.90	108.20
1	X	1266	G	P-O3'-C3'	7.12	128.25	119.70
1	X	2744	A	O4'-C1'-N9	7.12	113.90	108.20
1	X	1467	U	C4'-C3'-O3'	7.12	127.24	113.00
1	X	540	G	C4-N9-C1'	7.12	135.75	126.50
1	X	542	A	C6-C5-N7	-7.12	127.32	132.30
1	X	1679	U	O4'-C4'-C3'	-7.12	96.88	104.00
1	X	1355	A	P-O3'-C3'	7.12	128.24	119.70
1	X	2408	G	C4'-C3'-C2'	7.12	109.72	102.60
1	X	617	U	N3-C2-O2	-7.10	117.23	122.20
1	X	2553	G	C5-C6-O6	-7.10	124.34	128.60
1	X	2808	U	C3'-C2'-C1'	-7.09	95.83	101.50
1	X	780	U	O4'-C1'-N1	7.09	113.87	108.20
1	X	1442	C	N1-C2-O2	7.09	123.15	118.90
1	X	494	A	N9-C1'-C2'	-7.08	104.21	112.00
1	X	1594	U	O4'-C1'-N1	7.07	113.86	108.20
1	X	1652	G	O4'-C1'-N9	-7.07	102.54	108.20
1	X	2485	U	O4'-C1'-N1	7.07	113.86	108.20
2	Y	17	A	O4'-C1'-N9	7.07	113.86	108.20
1	X	491	A	O4'-C1'-N9	-7.07	102.55	108.20
1	X	2872	U	O4'-C1'-N1	7.06	113.85	108.20
1	X	2808	U	C5'-C4'-O4'	7.06	117.57	109.10
1	X	1333	G	N1-C2-N2	7.06	122.55	116.20
1	X	537	C	C5'-C4'-O4'	7.06	117.57	109.10
1	X	2722	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	1221	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	666	U	P-O3'-C3'	7.05	128.16	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	711	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	1742	G	P-O3'-C3'	-7.05	111.24	119.70
1	X	1986	G	P-O3'-C3'	-7.04	111.25	119.70
1	X	2626	U	O4'-C1'-N1	7.04	113.84	108.20
1	X	2830	U	O4'-C1'-N1	7.04	113.83	108.20
1	X	1200	G	O4'-C1'-N9	7.04	113.83	108.20
1	X	1634	A	P-O3'-C3'	7.04	128.15	119.70
1	X	1651	U	O4'-C1'-N1	7.04	113.83	108.20
1	X	1935	A	P-O3'-C3'	7.04	128.15	119.70
1	X	845	U	O4'-C1'-N1	7.03	113.82	108.20
1	X	1302	C	O4'-C1'-N1	7.03	113.82	108.20
1	X	453	U	O4'-C1'-N1	7.02	113.82	108.20
1	X	761	G	C1'-O4'-C4'	-7.02	104.28	109.90
1	X	937	C	O4'-C1'-N1	7.02	113.82	108.20
1	X	227	G	O4'-C1'-N9	7.02	113.81	108.20
1	X	469	G	N3-C4-C5	-7.02	125.09	128.60
1	X	1071	U	P-O3'-C3'	7.01	128.11	119.70
1	X	2864	C	O4'-C1'-N1	7.01	113.81	108.20
1	X	1776	A	P-O3'-C3'	7.00	128.10	119.70
1	X	2669	C	O4'-C1'-C2'	-7.00	98.81	105.80
1	X	1946	U	N3-C2-O2	-6.99	117.31	122.20
1	X	1434	U	P-O3'-C3'	6.99	128.09	119.70
1	X	2039	G	C8-N9-C4	-6.97	103.61	106.40
1	X	592	G	O4'-C1'-N9	6.97	113.78	108.20
1	X	117	A	C1'-O4'-C4'	-6.97	104.33	109.90
1	X	474	G	O4'-C1'-N9	6.96	113.77	108.20
1	X	485	G	P-O3'-C3'	6.96	128.06	119.70
1	X	2698	G	C4'-C3'-C2'	-6.96	95.64	102.60
1	X	459	A	P-O3'-C3'	6.95	128.04	119.70
1	X	1434	U	C1'-O4'-C4'	-6.95	104.34	109.90
1	X	304	A	P-O5'-C5'	6.94	132.01	120.90
1	X	1550	C	O4'-C1'-N1	6.94	113.75	108.20
1	X	1997	A	N1-C6-N6	6.93	122.76	118.60
1	X	1434	U	O4'-C1'-N1	6.93	113.75	108.20
1	X	1663	C	OP1-P-O3'	6.93	120.45	105.20
1	X	835	U	N3-C2-O2	-6.93	117.35	122.20
1	X	2347	C	O4'-C1'-N1	6.93	113.74	108.20
1	X	2788	C	O4'-C1'-N1	6.92	113.74	108.20
1	X	751	G	C2'-C3'-O3'	6.92	124.78	113.70
1	X	1412	C	P-O3'-C3'	6.92	128.00	119.70
1	X	594	G	O4'-C1'-N9	6.92	113.73	108.20
1	X	1094	C	O4'-C1'-N1	6.91	113.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2581	A	P-O3'-C3'	6.91	127.99	119.70
1	X	467	U	C6-N1-C1'	-6.91	111.53	121.20
2	Y	37	C	O4'-C1'-N1	6.91	113.72	108.20
1	X	526	C	O5'-P-OP2	-6.90	99.49	105.70
1	X	1712	G	N3-C4-N9	6.90	130.14	126.00
1	X	308	C	P-O5'-C5'	6.90	131.94	120.90
1	X	2660	C	O4'-C1'-N1	6.90	113.72	108.20
1	X	2088	U	O4'-C1'-N1	6.90	113.72	108.20
1	X	1984	A	P-O5'-C5'	-6.89	109.87	120.90
1	X	2018	G	P-O5'-C5'	-6.89	109.87	120.90
1	X	585	U	O4'-C1'-N1	6.89	113.71	108.20
1	X	190	A	O4'-C1'-N9	6.89	113.71	108.20
1	X	305	A	O4'-C1'-N9	6.89	113.71	108.20
1	X	206	U	O4'-C1'-N1	6.88	113.71	108.20
13	K	7	GLY	C-N-CA	6.88	138.91	121.70
1	X	1865	C	O4'-C1'-N1	6.88	113.70	108.20
1	X	2043	A	P-O3'-C3'	6.88	127.95	119.70
1	X	2067	U	O4'-C1'-N1	6.87	113.70	108.20
1	X	413	G	C8-N9-C4	-6.86	103.66	106.40
1	X	650	U	O4'-C1'-N1	6.86	113.69	108.20
9	G	106	TYR	N-CA-CB	6.85	122.94	110.60
1	X	2075	U	P-O3'-C3'	6.85	127.92	119.70
1	X	469	G	C1'-O4'-C4'	-6.85	104.42	109.90
1	X	2523	G	O4'-C1'-N9	6.84	113.67	108.20
1	X	1432	G	O4'-C1'-N9	6.84	113.67	108.20
1	X	1249	G	C4'-C3'-C2'	6.84	109.44	102.60
1	X	334	G	C1'-O4'-C4'	-6.84	104.43	109.90
1	X	430	C	O4'-C1'-N1	6.84	113.67	108.20
1	X	2407	G	P-O3'-C3'	6.83	127.90	119.70
1	X	2423	G	O5'-P-OP2	-6.83	99.55	105.70
1	X	1680	U	O5'-P-OP2	-6.81	99.57	105.70
1	X	840	U	O4'-C1'-N1	6.81	113.65	108.20
1	X	796	A	C4-C5-N7	6.81	114.10	110.70
1	X	2208	U	O4'-C1'-N1	6.80	113.64	108.20
1	X	2799	C	O4'-C1'-N1	6.80	113.64	108.20
1	X	2082	C	O4'-C1'-N1	6.80	113.64	108.20
1	X	92	U	O4'-C1'-N1	6.79	113.63	108.20
1	X	2774	U	O4'-C1'-N1	6.79	113.63	108.20
1	X	539	A	C1'-O4'-C4'	-6.79	104.47	109.90
1	X	556	A	P-O3'-C3'	6.79	127.84	119.70
1	X	1787	U	O4'-C1'-N1	6.78	113.63	108.20
1	X	689	A	C2-N3-C4	-6.78	107.21	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	689	A	C4-C5-N7	6.78	114.09	110.70
2	Y	57	U	O4'-C1'-N1	6.78	113.62	108.20
1	X	1223	G	C6-C5-N7	-6.78	126.33	130.40
1	X	1771	A	P-O3'-C3'	6.77	127.83	119.70
1	X	2236	U	O4'-C1'-N1	6.77	113.62	108.20
1	X	1093	U	O4'-C1'-N1	6.77	113.61	108.20
1	X	1010	U	P-O5'-C5'	6.76	131.72	120.90
1	X	2671	C	O5'-P-OP2	-6.75	99.62	105.70
1	X	333	A	P-O3'-C3'	6.75	127.80	119.70
1	X	1279	G	C4-C5-N7	6.75	113.50	110.80
1	X	2038	C	OP2-P-O3'	6.75	120.05	105.20
1	X	2456	U	O4'-C1'-N1	6.75	113.60	108.20
1	X	759	C	C4'-C3'-C2'	6.75	109.34	102.60
1	X	730	C	P-O3'-C3'	6.74	127.79	119.70
1	X	1344	C	N1-C2-O2	6.74	122.94	118.90
1	X	943	U	O4'-C1'-N1	6.74	113.59	108.20
2	Y	55	C	O4'-C1'-N1	6.74	113.59	108.20
1	X	2408	G	C8-N9-C4	-6.74	103.70	106.40
1	X	1946	U	N1-C2-O2	6.73	127.51	122.80
1	X	981	C	O4'-C1'-N1	6.73	113.58	108.20
1	X	995	A	O4'-C1'-N9	6.73	113.58	108.20
1	X	1922	U	P-O3'-C3'	6.73	127.77	119.70
1	X	1664	G	P-O5'-C5'	6.73	131.66	120.90
1	X	1862	C	O4'-C1'-N1	6.73	113.58	108.20
1	X	1958	G	O4'-C4'-C3'	-6.71	97.29	104.00
1	X	1947	G	O4'-C1'-N9	-6.71	102.83	108.20
2	Y	16	U	N1-C1'-C2'	6.71	122.72	114.00
1	X	1522	C	C3'-C2'-C1'	-6.71	96.14	101.50
1	X	866	U	O4'-C1'-N1	6.70	113.56	108.20
1	X	1314	A	C4'-C3'-O3'	-6.70	95.33	109.40
1	X	1731	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	2373	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	418	C	C4'-C3'-C2'	-6.70	95.90	102.60
1	X	519	C	C6-N1-C2	-6.70	117.62	120.30
1	X	774	A	C6-N1-C2	6.70	122.62	118.60
1	X	1712	G	O4'-C1'-N9	6.69	113.55	108.20
1	X	632	A	P-O3'-C3'	6.69	127.73	119.70
1	X	1319	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1662	G	P-O3'-C3'	6.69	127.72	119.70
1	X	2478	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	948	C	P-O3'-C3'	-6.68	111.68	119.70
1	X	951	G	C3'-C2'-C1'	-6.68	96.15	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1804	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	564	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	1183	C	O4'-C1'-N1	6.67	113.53	108.20
1	X	2480	C	O4'-C1'-N1	6.67	113.53	108.20
1	X	533	C	O4'-C1'-N1	6.65	113.52	108.20
1	X	343	A	N9-C1'-C2'	6.65	122.65	114.00
1	X	1468	A	N7-C8-N9	6.65	117.13	113.80
1	X	2189	A	C8-N9-C4	-6.64	103.14	105.80
1	X	928	G	C5-C6-O6	-6.64	124.61	128.60
1	X	494	A	C3'-C2'-C1'	6.64	106.81	101.50
1	X	2501	U	O4'-C1'-N1	6.64	113.51	108.20
1	X	646	C	O4'-C1'-N1	6.64	113.51	108.20
1	X	1980	A	C5'-C4'-O4'	6.63	117.06	109.10
1	X	1712	G	N1-C2-N2	-6.63	110.24	116.20
1	X	1725	C	O4'-C1'-N1	6.62	113.50	108.20
1	X	35	G	O4'-C1'-N9	6.62	113.50	108.20
1	X	689	A	C1'-O4'-C4'	-6.62	104.60	109.90
1	X	1938	U	N1-C1'-C2'	6.62	122.60	114.00
1	X	2697	G	C2-N3-C4	6.62	115.21	111.90
1	X	989	G	O4'-C1'-N9	6.61	113.49	108.20
1	X	2735	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	613	A	P-O3'-C3'	6.61	127.63	119.70
1	X	677	G	C4'-C3'-C2'	-6.61	95.99	102.60
1	X	725	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	1288	A	C8-N9-C1'	-6.60	115.82	127.70
1	X	1469	U	N3-C2-O2	-6.60	117.58	122.20
1	X	1467	U	C4'-C3'-C2'	6.59	109.19	102.60
1	X	2181	A	C1'-O4'-C4'	-6.59	104.62	109.90
1	X	1120	C	P-O3'-C3'	6.59	127.61	119.70
1	X	2841	U	O4'-C1'-N1	6.59	113.47	108.20
1	X	2274	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	2734	U	O4'-C1'-N1	6.59	113.47	108.20
1	X	1325	U	P-O3'-C3'	6.58	127.60	119.70
1	X	1292	A	O4'-C1'-N9	6.58	113.46	108.20
1	X	2383	C	O4'-C1'-N1	6.58	113.46	108.20
1	X	467	U	O4'-C4'-C3'	-6.57	97.43	104.00
1	X	651	C	O4'-C1'-N1	6.57	113.46	108.20
1	X	97	U	O4'-C1'-N1	6.57	113.45	108.20
1	X	1683	G	O4'-C1'-N9	6.57	113.45	108.20
1	X	2431	C	O4'-C1'-N1	6.56	113.45	108.20
1	X	617	U	O4'-C1'-N1	6.56	113.45	108.20
1	X	1696	C	O4'-C1'-N1	6.56	113.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	788	G	C2'-C3'-O3'	6.56	124.19	113.70
1	X	1549	C	O4'-C1'-N1	6.55	113.44	108.20
1	X	1882	G	C3'-C2'-C1'	6.55	106.74	101.50
1	X	1412	C	C2'-C3'-O3'	6.54	124.17	113.70
1	X	575	U	O4'-C1'-N1	6.54	113.43	108.20
1	X	2239	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2708	U	P-O3'-C3'	-6.54	111.86	119.70
1	X	2860	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	1411	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	819	C	O5'-P-OP2	-6.53	99.82	105.70
1	X	1909	U	C2-N1-C1'	6.53	125.53	117.70
1	X	1403	U	P-O3'-C3'	6.53	127.53	119.70
1	X	1989	C	C1'-O4'-C4'	6.53	115.12	109.90
1	X	2804	G	C5-C6-N1	6.52	114.76	111.50
1	X	738	G	N7-C8-N9	6.52	116.36	113.10
1	X	2628	C	C3'-C2'-C1'	-6.52	96.29	101.50
1	X	527	C	N1-C2-O2	6.51	122.81	118.90
1	X	955	G	N9-C1'-C2'	6.51	122.47	114.00
1	X	2553	G	C5-N7-C8	-6.51	101.05	104.30
1	X	2482	A	C5'-C4'-O4'	6.50	116.90	109.10
1	X	746	G	N3-C4-C5	-6.50	125.35	128.60
1	X	1032	A	C5-N7-C8	-6.50	100.65	103.90
1	X	1992	G	OP1-P-OP2	-6.50	109.86	119.60
1	X	2797	G	N3-C4-N9	6.50	129.90	126.00
2	Y	54	U	P-O5'-C5'	6.49	131.29	120.90
1	X	2691	C	O4'-C1'-N1	6.49	113.39	108.20
1	X	2553	G	C4-C5-N7	6.48	113.39	110.80
1	X	2656	G	O4'-C1'-N9	6.48	113.38	108.20
1	X	114	C	O4'-C1'-N1	6.48	113.38	108.20
1	X	243	G	P-O5'-C5'	6.47	131.25	120.90
1	X	540	G	C4'-C3'-C2'	-6.47	96.13	102.60
1	X	234	C	O4'-C1'-N1	6.47	113.38	108.20
1	X	467	U	C3'-C2'-C1'	-6.47	96.33	101.50
1	X	591	G	O4'-C1'-N9	6.47	113.38	108.20
1	X	1752	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	2591	C	O4'-C1'-N1	6.47	113.38	108.20
1	X	549	G	O4'-C1'-N9	6.47	113.37	108.20
1	X	2437	G	O4'-C1'-N9	6.47	113.37	108.20
1	X	19	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	569	C	P-O3'-C3'	-6.46	111.94	119.70
1	X	796	A	C6-C5-N7	-6.46	127.78	132.30
1	X	1663	C	P-O3'-C3'	6.46	127.45	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1223	G	C4-C5-N7	6.46	113.38	110.80
1	X	160	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	648	A	P-O3'-C3'	6.46	127.45	119.70
1	X	483	A	C3'-C2'-C1'	-6.46	96.33	101.50
1	X	879	A	O4'-C1'-N9	-6.46	103.03	108.20
2	Y	70	C	O4'-C1'-N1	6.46	113.36	108.20
1	X	759	C	C5'-C4'-C3'	-6.45	105.68	116.00
1	X	1825	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	649	G	O4'-C1'-N9	6.45	113.36	108.20
1	X	689	A	C8-N9-C4	-6.45	103.22	105.80
1	X	2815	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	22	C	P-O3'-C3'	6.45	127.44	119.70
1	X	1811	A	C2'-C3'-O3'	6.45	124.01	113.70
1	X	1313	U	C1'-O4'-C4'	-6.44	104.75	109.90
1	X	1749	G	P-O3'-C3'	6.44	127.43	119.70
1	X	606	A	O4'-C4'-C3'	-6.43	97.57	104.00
1	X	1044	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	2726	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	1388	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	1413	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	2262	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	2591	C	C5-C6-N1	6.43	124.21	121.00
1	X	496	C	P-O3'-C3'	-6.42	111.99	119.70
1	X	2019	C	O4'-C1'-N1	6.42	113.34	108.20
1	X	774	A	C4-C5-C6	6.42	120.21	117.00
1	X	2530	C	O5'-P-OP2	-6.42	99.92	105.70
1	X	2426	G	C5'-C4'-C3'	-6.42	105.74	116.00
1	X	784	U	O4'-C1'-N1	6.41	113.33	108.20
1	X	665	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1570	C	N1-C2-O2	6.41	122.74	118.90
1	X	2782	G	C6-C5-N7	-6.41	126.56	130.40
1	X	1249	G	C2'-C3'-O3'	6.41	123.95	113.70
1	X	1561	A	C4'-C3'-O3'	6.41	125.81	113.00
1	X	1943	A	C4'-C3'-C2'	6.40	109.00	102.60
1	X	1768	U	N1-C2-O2	6.40	127.28	122.80
1	X	2675	U	O4'-C1'-N1	6.40	113.32	108.20
1	X	71	A	C4'-C3'-C2'	6.40	109.00	102.60
1	X	758	G	P-O3'-C3'	6.39	127.37	119.70
1	X	2452	U	O4'-C1'-N1	6.39	113.32	108.20
1	X	774	A	C5'-C4'-O4'	6.39	116.77	109.10
1	X	890	U	O4'-C1'-N1	6.39	113.31	108.20
1	X	2256	G	C8-N9-C4	-6.38	103.85	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	173	A	O4'-C1'-N9	6.37	113.30	108.20
1	X	1489	C	O4'-C1'-N1	6.37	113.30	108.20
1	X	1770	U	C1'-O4'-C4'	-6.37	104.80	109.90
1	X	2782	G	C4-C5-N7	6.37	113.35	110.80
1	X	2439	U	O4'-C1'-N1	6.37	113.29	108.20
1	X	841	G	C1'-O4'-C4'	-6.37	104.81	109.90
1	X	738	G	C8-N9-C4	-6.36	103.86	106.40
1	X	220	U	O4'-C1'-N1	6.36	113.29	108.20
1	X	483	A	C4'-C3'-C2'	6.36	108.96	102.60
1	X	504	G	O4'-C4'-C3'	-6.36	97.64	104.00
1	X	542	A	C5-N7-C8	-6.36	100.72	103.90
1	X	1468	A	N3-C4-C5	-6.36	122.35	126.80
1	X	2291	U	O4'-C1'-N1	6.35	113.28	108.20
1	X	869	C	O4'-C1'-N1	6.34	113.27	108.20
1	X	1764	A	N1-C6-N6	6.34	122.40	118.60
1	X	522	G	O4'-C1'-N9	6.33	113.27	108.20
1	X	1122	A	O4'-C1'-N9	6.33	113.26	108.20
1	X	1334	A	C3'-C2'-C1'	-6.33	96.44	101.50
1	X	2678	C	O4'-C1'-N1	6.32	113.26	108.20
1	X	66	U	O4'-C1'-N1	6.32	113.26	108.20
1	X	539	A	O4'-C1'-N9	6.32	113.26	108.20
1	X	858	G	O4'-C1'-N9	6.32	113.26	108.20
1	X	501	G	O4'-C1'-N9	6.32	113.25	108.20
1	X	540	G	C2-N3-C4	6.32	115.06	111.90
1	X	1831	G	C8-N9-C4	-6.31	103.87	106.40
1	X	1144	U	O4'-C1'-N1	6.31	113.25	108.20
11	I	28	LYS	C-N-CA	6.31	137.47	121.70
1	X	2500	C	O4'-C1'-N1	6.31	113.25	108.20
1	X	2795	A	O4'-C1'-N9	-6.30	103.16	108.20
1	X	537	C	C2-N3-C4	-6.30	116.75	119.90
1	X	656	U	P-O5'-C5'	6.30	130.98	120.90
1	X	2189	A	N7-C8-N9	6.30	116.95	113.80
1	X	1407	G	N9-C1'-C2'	6.29	122.18	114.00
1	X	399	G	C2'-C3'-O3'	6.29	123.76	113.70
1	X	579	G	O4'-C1'-N9	6.29	113.23	108.20
1	X	1278	A	N9-C1'-C2'	6.29	122.17	114.00
1	X	432	C	O4'-C1'-N1	6.28	113.23	108.20
1	X	1997	A	P-O3'-C3'	6.28	127.24	119.70
1	X	1247	U	O4'-C1'-N1	6.28	113.22	108.20
1	X	2482	A	N1-C2-N3	-6.28	126.16	129.30
1	X	2540	A	O4'-C1'-N9	6.28	113.22	108.20
1	X	878	C	N1-C2-O2	6.28	122.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	467	U	N1-C1'-C2'	6.28	122.16	114.00
1	X	2318	U	O4'-C1'-N1	6.28	113.22	108.20
1	X	2074	U	O4'-C1'-N1	6.27	113.22	108.20
1	X	1314	A	N9-C1'-C2'	6.26	122.14	114.00
1	X	1963	G	N3-C4-C5	-6.26	125.47	128.60
1	X	657	A	C3'-C2'-C1'	-6.26	96.49	101.50
1	X	434	C	P-O3'-C3'	6.26	127.21	119.70
1	X	729	A	P-O3'-C3'	6.25	127.21	119.70
1	X	2639	A	P-O3'-C3'	-6.25	112.19	119.70
1	X	237	G	O4'-C1'-N9	6.25	113.20	108.20
1	X	413	G	N7-C8-N9	6.25	116.23	113.10
1	X	559	C	C2'-C3'-O3'	6.25	123.69	113.70
1	X	2393	G	O4'-C1'-N9	6.25	113.20	108.20
1	X	2705	A	C4'-C3'-C2'	6.25	108.85	102.60
1	X	332	C	O4'-C1'-N1	6.25	113.20	108.20
1	X	1990	U	N3-C2-O2	-6.25	117.83	122.20
1	X	1001	A	O4'-C1'-N9	6.24	113.19	108.20
1	X	1111	C	O4'-C1'-N1	6.24	113.19	108.20
1	X	879	A	C4'-C3'-C2'	6.24	108.84	102.60
1	X	1051	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	187	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	1598	C	O4'-C1'-N1	6.24	113.19	108.20
1	X	2081	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	2594	U	C4-C5-C6	-6.24	115.96	119.70
1	X	2359	U	O4'-C1'-N1	6.23	113.19	108.20
1	X	780	U	C3'-C2'-C1'	-6.23	96.52	101.50
1	X	675	C	O4'-C1'-N1	6.22	113.18	108.20
1	X	2800	C	O4'-C1'-N1	6.22	113.18	108.20
1	X	1909	U	N1-C1'-C2'	6.22	122.08	114.00
1	X	1341	G	P-O3'-C3'	-6.21	112.25	119.70
1	X	2692	A	O5'-P-OP1	6.21	118.16	110.70
2	Y	83	C	N1-C2-O2	6.21	122.63	118.90
1	X	683	A	N9-C1'-C2'	6.21	122.07	114.00
1	X	1669	A	P-O5'-C5'	6.21	130.83	120.90
1	X	148	C	O4'-C1'-N1	6.21	113.17	108.20
1	X	1353	A	P-O3'-C3'	6.20	127.14	119.70
1	X	1373	G	O4'-C1'-N9	6.20	113.16	108.20
1	X	2181	A	O4'-C1'-N9	6.20	113.16	108.20
1	X	1991	C	P-O3'-C3'	-6.20	112.26	119.70
1	X	1624	A	C1'-O4'-C4'	-6.20	104.94	109.90
2	Y	45	C	N1-C2-O2	6.20	122.62	118.90
1	X	236	C	N1-C2-O2	6.19	122.62	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1621	C	O4'-C1'-N1	6.19	113.16	108.20
1	X	1288	A	N9-C1'-C2'	6.19	122.05	114.00
1	X	1819	U	O4'-C1'-N1	6.19	113.15	108.20
1	X	1882	G	P-O3'-C3'	6.19	127.13	119.70
1	X	2627	G	N1-C6-O6	6.19	123.61	119.90
1	X	595	A	O4'-C1'-N9	6.18	113.15	108.20
1	X	1953	A	C5'-C4'-O4'	6.18	116.52	109.10
1	X	956	A	C5-C6-N6	-6.18	118.75	123.70
1	X	346	C	C5-C6-N1	6.18	124.09	121.00
1	X	1075	C	O4'-C1'-N1	6.18	113.14	108.20
1	X	1288	A	C5'-C4'-C3'	6.18	125.89	116.00
1	X	857	U	O4'-C1'-N1	6.18	113.14	108.20
1	X	995	A	C3'-C2'-C1'	-6.18	96.56	101.50
1	X	1059	A	P-O3'-C3'	6.17	127.11	119.70
1	X	1467	U	N1-C1'-C2'	6.17	122.03	114.00
1	X	1983	G	P-O3'-C3'	6.17	127.11	119.70
1	X	2408	G	P-O3'-C3'	-6.17	112.30	119.70
1	X	2867	G	C6-C5-N7	-6.17	126.70	130.40
1	X	780	U	C2'-C3'-O3'	6.17	123.57	113.70
2	Y	87	C	O4'-C1'-N1	6.17	113.14	108.20
1	X	323	G	P-O5'-C5'	-6.17	111.03	120.90
1	X	2627	G	C5-C6-O6	-6.17	124.90	128.60
1	X	1505	U	O4'-C1'-N1	6.16	113.13	108.20
1	X	1579	G	O4'-C1'-N9	6.16	113.13	108.20
1	X	1006	C	P-O3'-C3'	6.16	127.09	119.70
1	X	169	C	N1-C2-O2	6.16	122.60	118.90
1	X	322	A	P-O3'-C3'	6.16	127.09	119.70
1	X	1338	G	C5-C6-O6	-6.16	124.90	128.60
1	X	1417	C	O4'-C1'-N1	6.16	113.13	108.20
1	X	1850	G	O4'-C1'-N9	6.16	113.13	108.20
1	X	1647	U	O4'-C1'-N1	6.16	113.12	108.20
1	X	393	U	O4'-C1'-N1	6.15	113.12	108.20
1	X	682	G	P-O3'-C3'	6.15	127.08	119.70
1	X	1398	G	O4'-C1'-N9	6.15	113.12	108.20
1	X	358	C	C6-N1-C2	-6.15	117.84	120.30
1	X	859	U	C5'-C4'-O4'	6.15	116.48	109.10
1	X	917	U	O4'-C1'-N1	6.15	113.12	108.20
1	X	1142	G	C1'-O4'-C4'	-6.14	104.98	109.90
1	X	796	A	C5-C6-N1	-6.14	114.63	117.70
1	X	1234	C	N1-C2-O2	6.14	122.58	118.90
1	X	542	A	C4-C5-C6	6.14	120.07	117.00
1	X	516	G	O4'-C1'-N9	6.14	113.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1981	A	O5'-P-OP2	-6.14	100.17	105.70
1	X	466	A	P-O3'-C3'	6.14	127.06	119.70
1	X	1032	A	N7-C8-N9	6.14	116.87	113.80
2	Y	32	C	C6-N1-C2	-6.14	117.84	120.30
1	X	193	A	O4'-C1'-N9	6.13	113.11	108.20
1	X	1467	U	C5-C4-O4	-6.13	122.22	125.90
2	Y	110	U	O4'-C1'-N1	6.13	113.11	108.20
1	X	2238	G	O4'-C1'-N9	6.13	113.11	108.20
1	X	2492	G	C8-N9-C4	-6.13	103.95	106.40
23	U	18	VAL	C-N-CA	6.13	137.03	121.70
1	X	387	A	C5'-C4'-O4'	6.13	116.45	109.10
1	X	982	C	O4'-C1'-N1	6.13	113.10	108.20
1	X	1496	G	C2'-C3'-O3'	6.13	123.50	113.70
1	X	2636	A	O4'-C1'-N9	6.13	113.10	108.20
1	X	321	A	P-O3'-C3'	6.12	127.05	119.70
1	X	1788	C	O4'-C1'-N1	6.12	113.10	108.20
1	X	1336	G	C5-C6-N1	6.12	114.56	111.50
1	X	244	C	O4'-C1'-N1	6.12	113.09	108.20
1	X	1468	A	N9-C1'-C2'	6.12	121.95	114.00
1	X	1792	C	P-O3'-C3'	6.12	127.04	119.70
1	X	2229	G	C8-N9-C4	-6.12	103.95	106.40
1	X	2809	A	P-O3'-C3'	6.12	127.04	119.70
1	X	2711	G	C5-C6-O6	-6.11	124.93	128.60
1	X	30	G	C8-N9-C4	-6.11	103.95	106.40
1	X	1017	C	O4'-C1'-N1	6.11	113.09	108.20
1	X	2312	A	O4'-C1'-N9	6.11	113.09	108.20
1	X	422	C	O4'-C1'-N1	6.11	113.08	108.20
1	X	29	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1380	C	O4'-C1'-N1	6.10	113.08	108.20
1	X	2844	G	O4'-C1'-N9	6.10	113.08	108.20
1	X	668	A	P-O3'-C3'	6.09	127.01	119.70
1	X	162	C	O4'-C1'-N1	6.09	113.07	108.20
19	Q	61	LYS	N-CA-C	6.09	127.45	111.00
1	X	707	U	O4'-C1'-N1	6.09	113.07	108.20
1	X	1181	C	O4'-C1'-N1	6.09	113.07	108.20
1	X	700	C	O4'-C1'-N1	6.09	113.07	108.20
1	X	1515	U	O4'-C1'-N1	6.09	113.07	108.20
9	G	103	TYR	C-N-CA	6.09	136.92	121.70
1	X	358	C	P-O5'-C5'	6.08	130.64	120.90
1	X	596	C	P-O5'-C5'	-6.08	111.17	120.90
1	X	2018	G	C1'-O4'-C4'	-6.08	105.03	109.90
1	X	396	U	C1'-O4'-C4'	-6.08	105.03	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	399	G	C4'-C3'-C2'	6.08	108.68	102.60
1	X	1540	C	O4'-C1'-N1	6.08	113.06	108.20
1	X	1142	G	O4'-C1'-C2'	-6.08	99.72	105.80
1	X	776	G	N9-C1'-C2'	6.08	121.90	114.00
1	X	1149	G	P-O3'-C3'	6.08	127.00	119.70
1	X	1233	A	C2'-C3'-O3'	6.08	123.43	113.70
1	X	1522	C	N1-C2-O2	6.08	122.55	118.90
1	X	135	U	O4'-C1'-N1	6.08	113.06	108.20
1	X	2554	C	N1-C2-O2	6.07	122.54	118.90
1	X	1466	C	O4'-C1'-N1	6.07	113.06	108.20
1	X	2414	A	P-O5'-C5'	6.07	130.61	120.90
1	X	618	A	O4'-C1'-N9	6.07	113.05	108.20
1	X	331	U	O4'-C1'-N1	6.06	113.05	108.20
1	X	113	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	1060	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	1758	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2039	G	C5-C6-O6	-6.06	124.97	128.60
1	X	2184	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	346	C	N3-C4-C5	-6.06	119.48	121.90
1	X	1006	C	N1-C1'-C2'	6.05	121.87	114.00
1	X	2336	G	O5'-P-OP2	-6.05	100.25	105.70
11	I	36	GLY	C-N-CA	6.05	136.83	121.70
1	X	1149	G	O4'-C1'-N9	6.05	113.04	108.20
1	X	1843	U	O4'-C1'-N1	6.05	113.04	108.20
1	X	1287	A	N1-C6-N6	-6.05	114.97	118.60
1	X	1353	A	O4'-C1'-N9	6.05	113.04	108.20
1	X	2661	G	O4'-C1'-N9	6.05	113.04	108.20
1	X	2685	A	C5-C6-N1	6.05	120.72	117.70
1	X	2281	C	O4'-C1'-N1	6.04	113.04	108.20
1	X	219	G	N9-C1'-C2'	6.04	121.85	114.00
1	X	90	G	N3-C4-C5	-6.04	125.58	128.60
1	X	473	C	OP2-P-O3'	6.04	118.48	105.20
1	X	1732	U	P-O3'-C3'	6.04	126.95	119.70
1	X	2295	C	O4'-C1'-N1	6.03	113.03	108.20
1	X	2799	C	C5-C4-N4	-6.03	115.98	120.20
1	X	1182	U	C2'-C3'-O3'	6.03	123.35	113.70
1	X	2264	C	O4'-C1'-N1	6.03	113.02	108.20
1	X	393	U	N3-C4-O4	6.03	123.62	119.40
1	X	833	A	N1-C6-N6	6.03	122.22	118.60
1	X	1333	G	C6-C5-N7	6.03	134.02	130.40
2	Y	54	U	C4'-C3'-C2'	-6.02	96.58	102.60
1	X	957	G	P-O3'-C3'	6.02	126.93	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2548	G	O4'-C4'-C3'	-6.02	97.98	104.00
1	X	1976	U	O4'-C1'-N1	6.02	113.01	108.20
1	X	2443	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	2325	A	P-O3'-C3'	6.01	126.91	119.70
1	X	2558	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	1655	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	1913	G	P-O3'-C3'	6.01	126.91	119.70
1	X	2363	G	O4'-C1'-N9	6.01	113.01	108.20
1	X	724	C	O4'-C1'-N1	6.00	113.00	108.20
1	X	1324	G	O4'-C1'-N9	6.00	113.00	108.20
1	X	577	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	2608	A	C1'-O4'-C4'	-6.00	105.10	109.90
2	Y	50	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	1548	U	O4'-C1'-N1	5.99	112.99	108.20
2	Y	7	C	O4'-C1'-N1	5.99	112.99	108.20
1	X	413	G	N3-C4-C5	-5.99	125.61	128.60
1	X	1946	U	C2-N1-C1'	5.99	124.89	117.70
1	X	1099	A	P-O3'-C3'	5.99	126.88	119.70
1	X	338	G	C8-N9-C4	-5.99	104.01	106.40
1	X	1541	G	C4'-C3'-C2'	-5.99	96.61	102.60
1	X	2408	G	OP1-P-OP2	-5.99	110.62	119.60
1	X	2645	C	N1-C2-O2	5.99	122.49	118.90
11	I	41	SER	N-CA-C	5.99	127.16	111.00
1	X	221	A	O4'-C1'-N9	5.98	112.99	108.20
1	X	1573	G	P-O3'-C3'	5.98	126.88	119.70
1	X	302	U	O4'-C1'-N1	5.98	112.98	108.20
1	X	1461	C	O4'-C1'-N1	5.98	112.98	108.20
1	X	2371	A	C8-N9-C4	-5.98	103.41	105.80
1	X	779	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	2193	C	O4'-C4'-C3'	-5.97	98.03	104.00
11	I	38	LYS	C-N-CA	5.97	136.63	121.70
1	X	223	C	O4'-C1'-N1	5.97	112.98	108.20
1	X	714	G	C3'-C2'-C1'	-5.97	96.72	101.50
1	X	2194	A	P-O3'-C3'	5.97	126.86	119.70
1	X	2775	U	O4'-C1'-N1	5.97	112.97	108.20
1	X	946	U	O4'-C1'-N1	5.97	112.97	108.20
1	X	1345	G	O5'-P-OP2	-5.97	100.33	105.70
1	X	2482	A	C2-N3-C4	5.97	113.58	110.60
1	X	2561	G	C4-C5-N7	5.96	113.19	110.80
1	X	1002	C	C6-N1-C2	-5.96	117.92	120.30
1	X	822	G	C4'-C3'-C2'	-5.96	96.64	102.60
1	X	1142	G	C3'-C2'-C1'	-5.96	96.73	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1030	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	2719	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	559	C	P-O3'-C3'	5.96	126.85	119.70
1	X	1950	C	O4'-C1'-N1	5.96	112.97	108.20
1	X	2683	C	O4'-C1'-N1	5.96	112.96	108.20
1	X	2408	G	N3-C4-C5	-5.95	125.62	128.60
1	X	2324	G	P-O3'-C3'	5.94	126.83	119.70
1	X	224	G	C5'-C4'-O4'	5.94	116.23	109.10
1	X	2258	G	C4'-C3'-C2'	-5.94	96.66	102.60
1	X	2858	A	O4'-C1'-N9	5.94	112.95	108.20
1	X	1336	G	C4-C5-N7	5.94	113.17	110.80
1	X	1530	U	O4'-C1'-N1	5.94	112.95	108.20
1	X	656	U	C1'-O4'-C4'	-5.94	105.15	109.90
1	X	2681	A	C5-C6-N1	5.94	120.67	117.70
15	M	28	ARG	N-CA-C	-5.93	94.98	111.00
1	X	1338	G	N3-C4-C5	-5.93	125.64	128.60
1	X	1350	G	C5-C6-O6	-5.93	125.04	128.60
2	Y	58	G	C3'-C2'-C1'	5.93	106.24	101.50
1	X	979	A	O4'-C1'-N9	5.93	112.94	108.20
1	X	2478	C	C6-N1-C2	-5.93	117.93	120.30
1	X	2552	C	C4'-C3'-C2'	-5.93	96.67	102.60
1	X	2576	G	O4'-C1'-N9	-5.93	103.46	108.20
1	X	1311	C	O4'-C1'-N1	5.92	112.94	108.20
2	Y	24	U	O4'-C1'-N1	5.92	112.94	108.20
1	X	2699	G	P-O3'-C3'	5.92	126.81	119.70
1	X	520	C	C4'-C3'-C2'	-5.92	96.68	102.60
1	X	2257	A	P-O5'-C5'	5.92	130.37	120.90
1	X	68	C	N1-C2-O2	5.92	122.45	118.90
1	X	2354	G	O4'-C4'-C3'	-5.92	98.08	104.00
1	X	242	A	P-O5'-C5'	5.92	130.36	120.90
1	X	567	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	1468	A	C6-N1-C2	-5.91	115.05	118.60
1	X	1805	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	841	G	C5-N7-C8	-5.91	101.35	104.30
1	X	1754	G	P-O5'-C5'	5.91	130.35	120.90
1	X	2406	C	P-O5'-C5'	5.91	130.35	120.90
1	X	2690	A	O4'-C1'-N9	5.91	112.93	108.20
1	X	865	A	O4'-C1'-N9	5.91	112.93	108.20
1	X	2382	C	C6-N1-C2	-5.91	117.94	120.30
1	X	825	C	P-O5'-C5'	5.91	130.35	120.90
1	X	1304	U	O4'-C1'-N1	5.91	112.92	108.20
1	X	1412	C	O4'-C4'-C3'	-5.91	98.09	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1667	A	O4'-C1'-N9	5.90	112.92	108.20
1	X	2578	G	P-O5'-C5'	5.90	130.35	120.90
1	X	2267	A	P-O3'-C3'	5.90	126.78	119.70
1	X	2854	G	O4'-C1'-C2'	-5.90	99.90	105.80
1	X	2045	A	C3'-C2'-C1'	5.90	106.22	101.50
1	X	2560	G	N3-C4-C5	-5.90	125.65	128.60
1	X	2593	A	P-O3'-C3'	5.90	126.78	119.70
1	X	1064	C	O4'-C1'-N1	5.90	112.92	108.20
1	X	154	U	O4'-C1'-N1	5.90	112.92	108.20
1	X	811	G	N1-C6-O6	-5.90	116.36	119.90
1	X	1454	U	N3-C4-O4	5.90	123.53	119.40
1	X	622	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2847	G	C8-N9-C4	-5.89	104.04	106.40
1	X	338	G	O4'-C1'-N9	5.89	112.91	108.20
1	X	1313	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2560	G	C5-C6-O6	-5.89	125.07	128.60
2	Y	22	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2692	A	P-O3'-C3'	5.88	126.76	119.70
1	X	466	A	P-O5'-C5'	5.88	130.31	120.90
1	X	681	A	C8-N9-C4	-5.88	103.45	105.80
1	X	2366	U	O4'-C1'-N1	5.88	112.91	108.20
1	X	2484	G	C8-N9-C4	-5.88	104.05	106.40
1	X	983	G	P-O3'-C3'	5.88	126.75	119.70
1	X	430	C	C5-C6-N1	5.88	123.94	121.00
1	X	1265	G	O5'-P-OP2	-5.87	100.42	105.70
1	X	955	G	N3-C4-C5	-5.87	125.67	128.60
1	X	1090	C	O4'-C1'-N1	5.87	112.89	108.20
1	X	2229	G	C5'-C4'-O4'	5.87	116.14	109.10
1	X	320	A	C2-N3-C4	5.87	113.53	110.60
1	X	431	G	O4'-C1'-N9	5.87	112.89	108.20
1	X	1338	G	N3-C4-N9	5.87	129.52	126.00
1	X	1468	A	C2-N3-C4	5.86	113.53	110.60
1	X	2018	G	N7-C8-N9	5.86	116.03	113.10
1	X	791	G	P-O3'-C3'	5.86	126.73	119.70
1	X	1922	U	N3-C2-O2	-5.86	118.10	122.20
1	X	2826	C	C4'-C3'-C2'	-5.86	96.75	102.60
1	X	2587	G	O4'-C1'-N9	5.85	112.88	108.20
1	X	1775	A	C4'-C3'-O3'	-5.85	97.11	109.40
1	X	2875	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	679	C	O4'-C1'-N1	5.84	112.87	108.20
1	X	2478	C	P-O3'-C3'	-5.84	112.69	119.70
2	Y	81	C	C5-C6-N1	5.84	123.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2258	G	O4'-C1'-N9	5.84	112.87	108.20
1	X	309	G	N7-C8-N9	5.84	116.02	113.10
1	X	515	A	O4'-C1'-N9	5.84	112.87	108.20
1	X	651	C	P-O3'-C3'	5.83	126.70	119.70
1	X	731	A	O4'-C1'-N9	5.83	112.87	108.20
1	X	1087	C	P-O5'-C5'	5.83	130.23	120.90
1	X	2025	A	O4'-C1'-N9	5.83	112.86	108.20
1	X	1472	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	1514	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	1243	G	O4'-C1'-N9	5.82	112.86	108.20
1	X	2422	C	O4'-C1'-N1	5.82	112.86	108.20
1	X	1288	A	N9-C4-C5	-5.82	103.47	105.80
1	X	1695	U	C5'-C4'-O4'	5.82	116.08	109.10
1	X	1703	C	C3'-C2'-C1'	-5.82	96.85	101.50
1	X	1115	C	O4'-C1'-N1	5.81	112.85	108.20
1	X	757	U	OP2-P-O3'	5.81	117.98	105.20
2	Y	67	C	P-O3'-C3'	5.81	126.67	119.70
1	X	424	G	P-O3'-C3'	5.81	126.67	119.70
1	X	2806	G	O4'-C1'-N9	5.81	112.85	108.20
1	X	1367	A	O4'-C1'-N9	5.81	112.84	108.20
1	X	1328	C	O4'-C1'-N1	5.80	112.84	108.20
1	X	1407	G	P-O3'-C3'	5.80	126.67	119.70
1	X	1344	C	N3-C4-C5	5.80	124.22	121.90
1	X	1244	U	O4'-C1'-N1	5.80	112.84	108.20
1	X	2303	C	N1-C2-O2	5.80	122.38	118.90
1	X	747	A	P-O3'-C3'	-5.80	112.74	119.70
1	X	2321	C	C6-N1-C2	-5.80	117.98	120.30
1	X	1781	C	C5'-C4'-O4'	5.79	116.06	109.10
1	X	1288	A	N1-C6-N6	5.79	122.07	118.60
1	X	1506	C	O4'-C1'-N1	5.79	112.83	108.20
1	X	1831	G	N7-C8-N9	5.79	116.00	113.10
1	X	2075	U	C1'-O4'-C4'	-5.79	105.27	109.90
1	X	2485	U	C2-N1-C1'	5.79	124.65	117.70
1	X	1286	U	P-O5'-C5'	5.78	130.15	120.90
1	X	1680	U	C2'-C3'-O3'	5.78	122.95	113.70
1	X	2315	A	P-O5'-C5'	5.78	130.15	120.90
1	X	437	G	O4'-C1'-N9	5.78	112.82	108.20
1	X	1469	U	C5'-C4'-O4'	5.78	116.04	109.10
1	X	2006	G	O5'-P-OP1	-5.78	100.50	105.70
1	X	2541	U	N3-C2-O2	-5.78	118.15	122.20
1	X	559	C	N1-C2-O2	5.78	122.37	118.90
1	X	2406	C	O4'-C1'-N1	5.78	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	952	A	P-O5'-C5'	5.78	130.15	120.90
1	X	1097	A	P-O3'-C3'	5.78	126.63	119.70
1	X	2616	U	O4'-C1'-N1	5.78	112.82	108.20
1	X	2619	G	N7-C8-N9	5.78	115.99	113.10
1	X	1546	C	O4'-C1'-N1	5.78	112.82	108.20
1	X	873	U	O4'-C1'-N1	5.77	112.82	108.20
1	X	648	A	C1'-O4'-C4'	-5.77	105.28	109.90
1	X	683	A	C2'-C3'-O3'	5.77	122.94	113.70
1	X	1086	C	C3'-C2'-C1'	5.77	106.12	101.50
1	X	327	C	O4'-C1'-N1	5.77	112.81	108.20
1	X	508	G	O4'-C1'-N9	5.77	112.82	108.20
1	X	1092	U	O4'-C1'-N1	5.77	112.82	108.20
1	X	2795	A	C3'-C2'-C1'	5.77	106.11	101.50
1	X	2697	G	P-O3'-C3'	-5.77	112.78	119.70
1	X	2371	A	N7-C8-N9	5.76	116.68	113.80
1	X	1191	G	P-O3'-C3'	5.76	126.61	119.70
1	X	199	A	P-O3'-C3'	5.75	126.61	119.70
1	X	2668	U	N3-C4-O4	-5.75	115.37	119.40
14	L	88	VAL	C-N-CA	5.75	136.08	121.70
1	X	1363	C	O4'-C1'-N1	5.75	112.80	108.20
1	X	1806	G	C8-N9-C4	-5.75	104.10	106.40
1	X	2370	G	O4'-C1'-N9	5.75	112.80	108.20
1	X	1964	A	O4'-C1'-N9	5.75	112.80	108.20
1	X	3	U	O4'-C4'-C3'	-5.74	98.26	104.00
1	X	1010	U	N3-C2-O2	-5.74	118.18	122.20
1	X	1145	C	P-O3'-C3'	5.74	126.59	119.70
1	X	1712	G	C6-C5-N7	-5.74	126.95	130.40
1	X	2587	G	C5-C6-O6	-5.74	125.15	128.60
1	X	2869	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	2256	G	O4'-C1'-N9	5.74	112.79	108.20
1	X	1265	G	P-O3'-C3'	5.74	126.58	119.70
1	X	1762	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	2811	G	O4'-C1'-N9	5.74	112.79	108.20
1	X	1561	A	O4'-C4'-C3'	-5.73	98.27	104.00
1	X	339	U	P-O3'-C3'	5.73	126.58	119.70
9	G	108	GLY	N-CA-C	-5.73	98.78	113.10
1	X	322	A	O4'-C1'-N9	5.73	112.78	108.20
1	X	2329	C	O4'-C1'-N1	5.73	112.78	108.20
1	X	467	U	C5-C4-O4	-5.73	122.46	125.90
1	X	767	G	O4'-C1'-N9	5.72	112.78	108.20
1	X	955	G	N3-C4-N9	5.72	129.43	126.00
1	X	1575	C	C4'-C3'-C2'	5.72	108.32	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1467	U	C5'-C4'-O4'	-5.71	102.24	109.10
1	X	480	G	C5-C6-N1	5.71	114.36	111.50
1	X	537	C	N3-C4-C5	5.71	124.19	121.90
1	X	2230	G	C5-C6-O6	-5.71	125.17	128.60
1	X	2535	C	C5'-C4'-C3'	-5.71	106.86	116.00
1	X	777	A	C4'-C3'-C2'	5.71	108.31	102.60
1	X	2694	G	C5'-C4'-O4'	-5.71	102.25	109.10
1	X	2086	U	O4'-C1'-N1	5.70	112.76	108.20
1	X	2668	U	C5-C6-N1	-5.70	119.85	122.70
1	X	322	A	N9-C1'-C2'	5.70	121.41	114.00
1	X	1662	G	N9-C1'-C2'	5.70	121.41	114.00
1	X	660	G	C3'-C2'-C1'	-5.70	96.94	101.50
1	X	519	C	C5'-C4'-O4'	-5.70	102.26	109.10
1	X	1795	C	O4'-C1'-N1	5.70	112.76	108.20
2	Y	32	C	C5-C6-N1	5.70	123.85	121.00
1	X	1141	U	P-O3'-C3'	5.69	126.53	119.70
1	X	1631	C	N1-C1'-C2'	5.69	121.40	114.00
1	X	1828	C	O4'-C1'-N1	5.69	112.75	108.20
2	Y	111	C	P-O3'-C3'	5.69	126.53	119.70
2	Y	50	U	C3'-C2'-C1'	-5.69	96.95	101.50
1	X	1253	C	P-O3'-C3'	-5.69	112.88	119.70
1	X	1831	G	O4'-C1'-N9	5.69	112.75	108.20
1	X	1091	C	O4'-C1'-N1	5.69	112.75	108.20
1	X	1281	A	P-O3'-C3'	5.68	126.52	119.70
1	X	2495	G	O4'-C1'-N9	5.68	112.75	108.20
1	X	889	C	O4'-C1'-N1	5.68	112.75	108.20
1	X	955	G	N1-C2-N2	-5.68	111.09	116.20
1	X	1531	C	C1'-O4'-C4'	-5.68	105.36	109.90
1	X	2463	G	C5'-C4'-O4'	5.68	115.92	109.10
1	X	2552	C	N1-C1'-C2'	5.68	121.38	114.00
1	X	1063	C	O4'-C1'-N1	5.67	112.74	108.20
1	X	1182	U	O4'-C1'-N1	5.67	112.74	108.20
1	X	1105	U	O4'-C1'-N1	5.67	112.73	108.20
1	X	2528	G	OP1-P-O3'	5.67	117.67	105.20
1	X	1663	C	N3-C2-O2	-5.67	117.93	121.90
1	X	1824	C	C3'-C2'-C1'	-5.67	96.97	101.50
1	X	2080	U	O4'-C1'-N1	5.67	112.73	108.20
1	X	827	C	O4'-C1'-N1	5.67	112.73	108.20
1	X	2591	C	N1-C2-O2	5.67	122.30	118.90
1	X	2444	C	O4'-C1'-N1	5.66	112.73	108.20
1	X	816	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	1076	U	O4'-C1'-N1	5.66	112.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2198	U	P-O3'-C3'	5.66	126.49	119.70
1	X	224	G	O4'-C1'-N9	5.66	112.72	108.20
1	X	975	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	1531	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	660	G	N3-C2-N2	-5.65	115.94	119.90
1	X	450	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	545	C	C3'-C2'-C1'	-5.65	96.98	101.50
1	X	2745	A	C2-N3-C4	5.65	113.42	110.60
1	X	483	A	C5'-C4'-O4'	5.65	115.88	109.10
1	X	675	C	C3'-C2'-C1'	-5.65	96.98	101.50
1	X	1820	G	C4'-C3'-C2'	5.65	108.25	102.60
1	X	1347	C	OP2-P-O3'	5.65	117.62	105.20
2	Y	34	C	O4'-C1'-N1	5.65	112.72	108.20
2	Y	75	A	P-O3'-C3'	5.64	126.47	119.70
1	X	534	U	O4'-C1'-N1	5.64	112.71	108.20
1	X	702	A	O3'-P-O5'	-5.64	93.29	104.00
1	X	2485	U	N3-C2-O2	-5.64	118.25	122.20
1	X	332	C	P-O3'-C3'	5.64	126.47	119.70
1	X	1487	C	O4'-C1'-N1	5.63	112.71	108.20
1	X	540	G	C8-N9-C1'	-5.63	119.68	127.00
1	X	858	G	C3'-C2'-C1'	5.63	106.00	101.50
1	X	2481	G	O3'-P-O5'	-5.63	93.30	104.00
1	X	750	C	O4'-C1'-N1	5.63	112.70	108.20
1	X	1415	C	O4'-C1'-N1	5.63	112.70	108.20
1	X	219	G	O4'-C1'-C2'	-5.62	100.17	105.80
1	X	455	A	P-O3'-C3'	5.62	126.45	119.70
1	X	2479	U	C4'-C3'-C2'	-5.62	96.98	102.60
1	X	1241	G	O4'-C1'-N9	5.62	112.69	108.20
1	X	1567	A	O4'-C1'-N9	5.62	112.69	108.20
1	X	33	C	C4'-C3'-C2'	5.62	108.22	102.60
1	X	648	A	N9-C1'-C2'	5.62	121.30	114.00
1	X	2609	G	N3-C4-C5	-5.61	125.79	128.60
1	X	2417	U	P-O3'-C3'	5.61	126.44	119.70
1	X	1277	G	N3-C4-C5	-5.61	125.80	128.60
1	X	1266	G	N9-C1'-C2'	5.61	121.29	114.00
1	X	1925	C	O4'-C1'-N1	5.61	112.69	108.20
1	X	1833	U	O4'-C1'-N1	5.61	112.69	108.20
1	X	553	C	N1-C2-O2	5.61	122.26	118.90
1	X	827	C	P-O5'-C5'	5.61	129.87	120.90
1	X	879	A	C5'-C4'-C3'	-5.61	107.03	116.00
1	X	1249	G	N1-C6-O6	-5.61	116.54	119.90
1	X	1689	U	P-O3'-C3'	5.61	126.43	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1983	G	C4'-C3'-C2'	-5.61	97.00	102.60
1	X	2398	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	1341	G	P-O5'-C5'	5.60	129.86	120.90
1	X	1547	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	1570	C	C2-N1-C1'	5.60	124.96	118.80
1	X	2049	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	623	G	O4'-C1'-N9	5.60	112.68	108.20
1	X	208	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	699	G	C8-N9-C4	-5.60	104.16	106.40
1	X	1298	G	OP2-P-O3'	5.60	117.52	105.20
1	X	1734	C	N1-C2-O2	5.60	122.26	118.90
1	X	995	A	N9-C1'-C2'	5.60	121.28	114.00
1	X	1031	C	N1-C2-O2	5.59	122.26	118.90
1	X	2237	C	P-O3'-C3'	5.59	126.41	119.70
1	X	36	G	C8-N9-C4	-5.59	104.16	106.40
1	X	1344	C	O4'-C4'-C3'	-5.59	98.41	104.00
1	X	1882	G	P-O5'-C5'	5.59	129.85	120.90
1	X	558	G	O4'-C1'-N9	5.59	112.67	108.20
12	J	88	LYS	C-N-CA	5.59	134.04	122.30
1	X	1224	A	P-O3'-C3'	5.59	126.40	119.70
1	X	1971	C	O4'-C1'-N1	5.59	112.67	108.20
1	X	81	C	O4'-C1'-N1	5.58	112.67	108.20
1	X	1570	C	C3'-C2'-C1'	-5.58	97.03	101.50
1	X	2018	G	C4-C5-C6	-5.58	115.45	118.80
1	X	1993	G	O4'-C1'-N9	5.58	112.67	108.20
1	X	2528	G	C8-N9-C4	-5.58	104.17	106.40
1	X	215	G	O4'-C1'-N9	5.58	112.66	108.20
1	X	1776	A	C2-N3-C4	5.58	113.39	110.60
1	X	2273	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	2046	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	753	U	C5'-C4'-O4'	-5.58	102.41	109.10
1	X	1333	G	C5-N7-C8	-5.57	101.51	104.30
1	X	2447	G	P-O3'-C3'	5.57	126.38	119.70
1	X	2675	U	N3-C2-O2	-5.57	118.30	122.20
1	X	337	G	C8-N9-C4	-5.57	104.17	106.40
1	X	820	U	P-O3'-C3'	-5.57	113.02	119.70
1	X	978	U	O4'-C1'-N1	5.57	112.65	108.20
1	X	607	C	O4'-C4'-C3'	-5.56	98.44	104.00
1	X	681	A	N7-C8-N9	5.56	116.58	113.80
1	X	479	G	C5-C6-O6	-5.56	125.27	128.60
1	X	770	U	C5-C4-O4	-5.56	122.56	125.90
1	X	1013	G	C8-N9-C4	-5.56	104.18	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1031	C	C4'-C3'-C2'	5.56	108.16	102.60
1	X	175	C	C6-N1-C2	-5.56	118.08	120.30
1	X	2314	A	P-O3'-C3'	5.56	126.37	119.70
1	X	838	A	C2-N3-C4	5.56	113.38	110.60
1	X	1033	G	C2'-C3'-O3'	5.56	122.59	113.70
1	X	1333	G	C4-C5-C6	-5.55	115.47	118.80
1	X	1	G	P-O3'-C3'	5.55	126.36	119.70
1	X	828	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	840	U	O5'-P-OP2	-5.55	100.70	105.70
1	X	418	C	C5'-C4'-C3'	5.55	124.88	116.00
1	X	876	A	O4'-C1'-N9	5.55	112.64	108.20
1	X	2504	G	O4'-C1'-N9	5.55	112.64	108.20
2	Y	72	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	359	G	O4'-C1'-N9	5.55	112.64	108.20
1	X	449	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	1623	C	N1-C2-O2	5.55	122.23	118.90
1	X	2759	U	P-O3'-C3'	5.55	126.36	119.70
1	X	647	G	P-O3'-C3'	5.54	126.35	119.70
1	X	1544	A	P-O3'-C3'	5.54	126.35	119.70
1	X	1700	C	P-O3'-C3'	-5.54	113.05	119.70
1	X	2575	U	C5-C4-O4	-5.54	122.57	125.90
1	X	2742	G	O4'-C1'-N9	5.54	112.64	108.20
1	X	2229	G	P-O5'-C5'	-5.54	112.03	120.90
19	Q	62	ARG	C-N-CA	5.54	135.55	121.70
1	X	1143	A	C1'-O4'-C4'	-5.54	105.47	109.90
1	X	1814	G	O4'-C1'-N9	5.54	112.63	108.20
1	X	1108	U	O4'-C1'-N1	5.54	112.63	108.20
1	X	1389	C	O4'-C1'-N1	5.54	112.63	108.20
1	X	1570	C	C6-N1-C1'	-5.54	114.16	120.80
1	X	168	A	O4'-C1'-N9	5.54	112.63	108.20
1	X	462	G	C4-C5-C6	5.54	122.12	118.80
1	X	985	G	C5-N7-C8	-5.53	101.53	104.30
1	X	1201	G	N3-C2-N2	-5.53	116.03	119.90
1	X	2591	C	C2-N3-C4	5.53	122.67	119.90
1	X	1016	C	O4'-C1'-N1	5.53	112.63	108.20
1	X	1469	U	O3'-P-O5'	5.53	114.51	104.00
1	X	99	U	C2-N1-C1'	5.53	124.34	117.70
1	X	211	U	O4'-C1'-N1	5.53	112.62	108.20
1	X	467	U	N3-C4-O4	5.53	123.27	119.40
1	X	1252	C	O4'-C1'-N1	5.53	112.62	108.20
1	X	972	C	C1'-O4'-C4'	-5.53	105.48	109.90
2	Y	6	C	O4'-C1'-N1	5.53	112.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2490	U	O4'-C1'-N1	5.53	112.62	108.20
1	X	990	A	O4'-C4'-C3'	-5.53	98.47	104.00
1	X	1963	G	C3'-C2'-C1'	5.53	105.92	101.50
1	X	2870	C	O4'-C1'-N1	5.52	112.62	108.20
1	X	22	C	O4'-C1'-N1	5.52	112.62	108.20
1	X	689	A	N1-C6-N6	5.52	121.91	118.60
1	X	796	A	C8-N9-C4	-5.52	103.59	105.80
1	X	823	U	C2'-C3'-O3'	5.52	122.53	113.70
1	X	2708	U	C5'-C4'-C3'	-5.52	107.16	116.00
17	O	97	GLY	N-CA-C	5.52	126.90	113.10
1	X	1699	A	C5-C6-N1	-5.52	114.94	117.70
1	X	2771	C	O4'-C1'-N1	5.52	112.61	108.20
1	X	447	U	P-O3'-C3'	5.52	126.32	119.70
1	X	1630	A	O3'-P-O5'	-5.52	93.52	104.00
1	X	2797	G	C6-C5-N7	-5.52	127.09	130.40
1	X	998	C	O4'-C1'-N1	5.51	112.61	108.20
1	X	2190	A	C5'-C4'-C3'	5.51	124.82	116.00
1	X	2199	C	N1-C1'-C2'	5.51	121.17	114.00
1	X	2560	G	C6-N1-C2	-5.51	121.79	125.10
1	X	652	C	P-O5'-C5'	-5.51	112.08	120.90
1	X	155	G	O4'-C1'-N9	5.51	112.61	108.20
1	X	448	C	N1-C2-O2	5.51	122.21	118.90
2	Y	19	C	N1-C2-O2	5.51	122.20	118.90
1	X	580	A	N9-C1'-C2'	5.51	121.16	114.00
1	X	2285	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	2646	C	C6-N1-C2	-5.51	118.10	120.30
1	X	186	C	N1-C2-O2	5.51	122.20	118.90
1	X	555	U	P-O3'-C3'	5.51	126.31	119.70
1	X	1089	C	P-O3'-C3'	5.51	126.31	119.70
1	X	2255	G	C5-C6-O6	-5.51	125.30	128.60
2	Y	9	G	C3'-C2'-C1'	-5.50	97.10	101.50
1	X	309	G	C8-N9-C4	-5.50	104.20	106.40
1	X	1250	A	C5'-C4'-O4'	5.50	115.70	109.10
1	X	1337	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	1442	C	C4'-C3'-C2'	5.50	108.10	102.60
1	X	303	C	O4'-C1'-N1	5.50	112.60	108.20
1	X	1280	U	C5-C6-N1	5.50	125.45	122.70
1	X	2772	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	942	U	N3-C2-O2	-5.50	118.35	122.20
2	Y	30	C	P-O5'-C5'	5.50	129.70	120.90
1	X	63	A	C2-N3-C4	5.50	113.35	110.60
1	X	2619	G	C5-N7-C8	-5.49	101.55	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	7	G	C5'-C4'-C3'	-5.49	107.22	116.00
1	X	2018	G	C8-N9-C4	-5.49	104.20	106.40
2	Y	79	U	O4'-C1'-N1	5.49	112.59	108.20
1	X	180	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1169	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1513	U	O4'-C1'-N1	5.49	112.59	108.20
1	X	2222	U	N3-C2-O2	-5.49	118.36	122.20
1	X	2485	U	N1-C2-O2	5.48	126.64	122.80
1	X	2769	C	C5'-C4'-C3'	-5.48	107.23	116.00
2	Y	31	A	O4'-C1'-N9	5.48	112.59	108.20
19	Q	60	GLY	N-CA-C	5.48	126.80	113.10
1	X	2540	A	O4'-C4'-C3'	-5.48	98.52	104.00
1	X	1422	C	O4'-C1'-N1	5.48	112.58	108.20
1	X	1629	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	X	2808	U	P-O5'-C5'	5.48	129.66	120.90
1	X	2867	G	C8-N9-C4	-5.48	104.21	106.40
1	X	1979	C	P-O3'-C3'	5.48	126.27	119.70
1	X	669	G	O4'-C4'-C3'	-5.47	98.53	104.00
1	X	2484	G	C2-N3-C4	5.47	114.64	111.90
1	X	103	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1009	C	N1-C2-O2	5.47	122.18	118.90
1	X	1055	A	O4'-C1'-N9	5.47	112.58	108.20
1	X	1410	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1977	C	O4'-C1'-N1	5.47	112.58	108.20
1	X	2409	A	N9-C1'-C2'	5.47	121.11	114.00
1	X	753	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1939	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	2533	U	C5-C6-N1	5.47	125.43	122.70
1	X	344	G	N9-C1'-C2'	5.46	121.10	114.00
1	X	761	G	P-O5'-C5'	-5.46	112.16	120.90
1	X	1713	G	P-O5'-C5'	5.46	129.64	120.90
1	X	126	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	2782	G	C3'-C2'-C1'	-5.46	97.13	101.50
1	X	1745	C	C6-N1-C2	-5.46	118.12	120.30
1	X	542	A	C1'-O4'-C4'	5.46	114.27	109.90
1	X	1132	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	112	U	N1-C1'-C2'	5.46	121.09	114.00
1	X	1870	U	O4'-C1'-N1	5.46	112.56	108.20
1	X	63	A	N1-C2-N3	-5.46	126.57	129.30
1	X	802	A	C4'-C3'-C2'	5.46	108.06	102.60
1	X	1943	A	C5'-C4'-C3'	-5.46	107.27	116.00
1	X	214	C	O4'-C1'-N1	5.45	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	773	G	OP1-P-O3'	5.45	117.20	105.20
1	X	1223	G	N3-C4-N9	5.45	129.27	126.00
1	X	615	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2709	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	545	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	11	G	N7-C8-N9	5.45	115.82	113.10
1	X	774	A	N9-C4-C5	-5.45	103.62	105.80
1	X	1678	G	P-O3'-C3'	-5.45	113.16	119.70
1	X	1164	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2440	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	398	C	O4'-C1'-N1	5.44	112.56	108.20
1	X	1412	C	O4'-C1'-N1	5.44	112.55	108.20
1	X	56	C	O4'-C1'-N1	5.44	112.55	108.20
1	X	1635	G	C8-N9-C4	-5.44	104.22	106.40
1	X	1938	U	P-O5'-C5'	5.44	129.60	120.90
1	X	1963	G	O4'-C1'-N9	5.44	112.55	108.20
2	Y	5	C	N1-C2-O2	5.44	122.16	118.90
1	X	1500	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1935	A	P-O5'-C5'	-5.44	112.20	120.90
1	X	1421	U	O4'-C1'-N1	5.43	112.55	108.20
2	Y	32	C	O4'-C1'-N1	5.43	112.55	108.20
1	X	1286	U	O4'-C1'-N1	5.43	112.54	108.20
1	X	1975	G	N9-C1'-C2'	5.43	121.06	114.00
1	X	851	C	O4'-C1'-N1	5.43	112.54	108.20
1	X	1660	G	C4'-C3'-C2'	-5.43	97.17	102.60
1	X	2659	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	242	A	C5'-C4'-C3'	5.42	124.68	116.00
1	X	1617	G	C5-C6-N1	5.42	114.21	111.50
1	X	2172	U	O4'-C1'-N1	5.42	112.54	108.20
1	X	1608	U	O4'-C1'-N1	5.42	112.54	108.20
1	X	2792	C	O4'-C1'-N1	5.42	112.54	108.20
2	Y	58	G	P-O3'-C3'	5.42	126.20	119.70
1	X	79	G	C8-N9-C4	-5.42	104.23	106.40
1	X	1821	A	O4'-C4'-C3'	-5.42	98.58	104.00
1	X	1695	U	O4'-C1'-N1	5.42	112.53	108.20
1	X	1927	U	P-O3'-C3'	5.42	126.20	119.70
1	X	2484	G	P-O5'-C5'	5.42	129.57	120.90
1	X	673	G	C4'-C3'-C2'	5.42	108.02	102.60
1	X	806	A	O4'-C1'-N9	-5.41	103.87	108.20
1	X	976	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	1043	A	O4'-C1'-N9	5.41	112.53	108.20
1	X	1937	G	P-O3'-C3'	5.41	126.19	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	798	G	P-O3'-C3'	5.41	126.19	119.70
1	X	959	C	P-O3'-C3'	-5.41	113.21	119.70
1	X	2499	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	11	G	C8-N9-C4	-5.41	104.24	106.40
1	X	923	A	N1-C6-N6	5.41	121.84	118.60
1	X	1077	U	P-O3'-C3'	5.41	126.19	119.70
1	X	2042	A	C4'-C3'-C2'	-5.41	97.19	102.60
2	Y	118	G	O4'-C1'-N9	5.41	112.53	108.20
1	X	1909	U	N1-C2-O2	5.40	126.58	122.80
1	X	2075	U	O4'-C1'-N1	5.40	112.52	108.20
1	X	2854	G	N7-C8-N9	5.40	115.80	113.10
1	X	479	G	N1-C6-O6	5.40	123.14	119.90
1	X	2323	U	P-O3'-C3'	5.40	126.18	119.70
1	X	2694	G	C5-C6-O6	-5.40	125.36	128.60
2	Y	17	A	P-O3'-C3'	5.39	126.17	119.70
1	X	157	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	X	749	C	O4'-C1'-N1	5.39	112.51	108.20
2	Y	90	C	N1-C2-O2	5.39	122.13	118.90
1	X	430	C	C6-N1-C2	-5.38	118.15	120.30
1	X	1712	G	C4-N9-C1'	5.38	133.50	126.50
1	X	1986	G	N3-C4-C5	-5.38	125.91	128.60
1	X	2570	C	O4'-C1'-N1	5.38	112.51	108.20
1	X	175	C	C5-C6-N1	5.38	123.69	121.00
1	X	246	C	N1-C2-O2	5.38	122.13	118.90
1	X	1014	G	N3-C4-C5	-5.38	125.91	128.60
1	X	1490	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	1385	C	N1-C2-O2	5.38	122.13	118.90
1	X	2015	G	N9-C1'-C2'	5.38	120.99	114.00
1	X	793	G	N1-C6-O6	-5.38	116.67	119.90
1	X	1036	G	P-O3'-C3'	5.38	126.15	119.70
1	X	2072	C	O4'-C1'-N1	5.38	112.50	108.20
1	X	2089	C	O4'-C1'-N1	5.38	112.50	108.20
1	X	941	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	2492	G	N3-C4-C5	-5.38	125.91	128.60
1	X	184	A	O4'-C1'-N9	5.37	112.50	108.20
1	X	542	A	P-O3'-C3'	5.37	126.15	119.70
1	X	1139	A	O4'-C1'-C2'	-5.37	100.43	105.80
1	X	1467	U	O4'-C4'-C3'	-5.37	98.63	104.00
1	X	1685	A	P-O5'-C5'	5.37	129.50	120.90
2	Y	92	G	C3'-C2'-C1'	-5.37	97.20	101.50
1	X	467	U	C5'-C4'-C3'	5.37	124.59	116.00
1	X	1858	C	N1-C2-O2	5.37	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2403	C	N1-C2-O2	5.37	122.12	118.90
1	X	2717	G	O4'-C1'-N9	5.37	112.50	108.20
2	Y	29	C	O4'-C1'-N1	5.37	112.49	108.20
1	X	751	G	O5'-P-OP2	-5.37	100.87	105.70
1	X	1339	U	OP2-P-O3'	5.37	117.01	105.20
1	X	1715	A	P-O3'-C3'	5.37	126.14	119.70
1	X	2658	A	O5'-P-OP2	-5.37	100.87	105.70
1	X	213	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	863	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	99	U	N3-C2-O2	-5.36	118.45	122.20
1	X	682	G	C3'-C2'-C1'	5.36	105.79	101.50
1	X	2232	G	C5-C6-O6	-5.36	125.38	128.60
1	X	2691	C	N3-C2-O2	-5.36	118.15	121.90
1	X	308	C	P-O3'-C3'	-5.36	113.27	119.70
1	X	1497	C	C6-N1-C2	-5.36	118.16	120.30
1	X	1840	A	O4'-C1'-N9	5.36	112.48	108.20
1	X	235	C	N1-C2-O2	5.36	122.11	118.90
1	X	513	A	C1'-O4'-C4'	-5.36	105.61	109.90
1	X	2666	U	C3'-C2'-C1'	5.36	105.78	101.50
1	X	472	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	1219	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	1222	G	P-O3'-C3'	5.35	126.12	119.70
1	X	1491	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	319	G	C5-C6-O6	-5.35	125.39	128.60
1	X	814	G	N9-C1'-C2'	5.35	120.95	114.00
1	X	1199	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	1390	G	N3-C4-C5	-5.35	125.93	128.60
1	X	2483	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	2870	C	C6-N1-C2	-5.35	118.16	120.30
1	X	1803	G	O4'-C1'-N9	5.34	112.48	108.20
1	X	1622	G	N3-C4-C5	-5.34	125.93	128.60
1	X	417	C	N1-C2-O2	5.34	122.10	118.90
1	X	2410	U	OP2-P-O3'	5.34	116.95	105.20
1	X	2688	G	P-O3'-C3'	-5.34	113.29	119.70
1	X	1172	U	O4'-C1'-N1	5.34	112.47	108.20
1	X	1496	G	O4'-C1'-N9	5.34	112.47	108.20
1	X	1753	A	C8-N9-C4	-5.34	103.67	105.80
1	X	2553	G	N7-C8-N9	5.34	115.77	113.10
1	X	2700	U	OP1-P-O3'	5.34	116.94	105.20
1	X	458	G	C3'-C2'-C1'	5.33	105.77	101.50
1	X	694	G	O4'-C1'-N9	5.33	112.47	108.20
1	X	1283	C	N3-C4-C5	-5.33	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1711	C	P-O3'-C3'	5.33	126.10	119.70
1	X	1278	A	C5-N7-C8	-5.33	101.23	103.90
1	X	1882	G	O4'-C1'-N9	5.33	112.47	108.20
1	X	2535	C	N1-C2-O2	5.33	122.10	118.90
2	Y	101	A	C3'-C2'-C1'	-5.33	97.24	101.50
1	X	70	A	P-O5'-C5'	-5.33	112.38	120.90
1	X	1790	G	C2'-C3'-O3'	5.33	122.22	113.70
1	X	2774	U	P-O3'-C3'	5.33	126.09	119.70
2	Y	10	U	O4'-C4'-C3'	-5.33	98.67	104.00
11	I	44	GLY	N-CA-C	5.33	126.42	113.10
1	X	757	U	P-O3'-C3'	5.33	126.09	119.70
1	X	1720	G	P-O3'-C3'	-5.33	113.31	119.70
1	X	1301	U	N3-C2-O2	-5.33	118.47	122.20
1	X	2429	A	P-O3'-C3'	-5.33	113.31	119.70
2	Y	12	C	O4'-C4'-C3'	-5.33	98.67	104.00
1	X	973	U	O3'-P-O5'	-5.32	93.89	104.00
1	X	1722	G	O4'-C1'-N9	5.32	112.46	108.20
1	X	61	U	C1'-O4'-C4'	-5.32	105.65	109.90
1	X	1225	G	N9-C1'-C2'	5.32	120.91	114.00
1	X	1785	A	O4'-C1'-N9	5.32	112.45	108.20
2	Y	55	C	P-O3'-C3'	5.32	126.08	119.70
1	X	858	G	P-O3'-C3'	5.32	126.08	119.70
1	X	1202	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2375	G	O4'-C4'-C3'	-5.32	98.69	104.00
1	X	2732	C	N1-C2-O2	5.32	122.09	118.90
23	U	32	ARG	N-CA-C	-5.31	96.65	111.00
1	X	1716	G	C1'-O4'-C4'	5.31	114.15	109.90
1	X	2015	G	C5-C6-N1	5.31	114.16	111.50
1	X	1238	A	O4'-C1'-N9	5.31	112.45	108.20
1	X	1725	C	P-O3'-C3'	5.31	126.07	119.70
1	X	524	A	O4'-C4'-C3'	-5.31	98.69	104.00
1	X	146	C	O4'-C1'-N1	5.30	112.44	108.20
1	X	2275	U	P-O5'-C5'	5.30	129.39	120.90
1	X	536	A	C3'-C2'-C1'	5.30	105.74	101.50
1	X	1056	U	P-O3'-C3'	5.30	126.06	119.70
1	X	1248	G	O3'-P-O5'	-5.30	93.93	104.00
1	X	876	A	P-O3'-C3'	5.30	126.06	119.70
1	X	1210	C	O4'-C1'-N1	5.30	112.44	108.20
1	X	2691	C	N1-C2-O2	5.30	122.08	118.90
1	X	418	C	P-O5'-C5'	5.30	129.37	120.90
1	X	1661	C	C4'-C3'-C2'	-5.30	97.30	102.60
1	X	2071	G	O4'-C1'-N9	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2568	A	O4'-C1'-N9	5.30	112.44	108.20
1	X	33	C	N1-C2-O2	5.29	122.08	118.90
1	X	1988	A	C5-N7-C8	-5.29	101.25	103.90
1	X	179	U	O4'-C1'-N1	5.29	112.44	108.20
1	X	723	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2256	G	N7-C8-N9	5.29	115.75	113.10
2	Y	90	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	817	A	O4'-C1'-N9	5.29	112.43	108.20
1	X	2321	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2551	A	OP1-P-O3'	5.29	116.84	105.20
1	X	851	C	C3'-C2'-C1'	-5.29	97.27	101.50
1	X	2567	G	N3-C4-C5	-5.29	125.96	128.60
1	X	2804	G	C5-C6-O6	-5.29	125.43	128.60
1	X	2229	G	C2-N3-C4	5.29	114.54	111.90
1	X	98	U	O4'-C1'-N1	5.29	112.43	108.20
1	X	427	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	1154	A	C4'-C3'-C2'	5.29	107.89	102.60
1	X	2667	C	N1-C2-O2	5.29	122.07	118.90
1	X	329	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	554	U	C3'-C2'-C1'	-5.28	97.27	101.50
1	X	1054	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	1496	G	C4'-C3'-O3'	5.28	123.57	113.00
1	X	2418	A	C3'-C2'-C1'	5.28	105.73	101.50
1	X	2854	G	C5-N7-C8	-5.28	101.66	104.30
1	X	969	U	C4'-C3'-C2'	5.28	107.88	102.60
1	X	1746	A	N1-C6-N6	-5.28	115.43	118.60
1	X	2464	G	C3'-C2'-C1'	-5.28	97.28	101.50
1	X	337	G	N7-C8-N9	5.28	115.74	113.10
1	X	4	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	664	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1741	G	C8-N9-C4	-5.28	104.29	106.40
1	X	1987	G	N3-C4-C5	-5.28	125.96	128.60
1	X	2276	C	O4'-C1'-N1	5.28	112.42	108.20
2	Y	86	A	N1-C6-N6	5.28	121.77	118.60
1	X	1863	U	O4'-C1'-N1	5.27	112.42	108.20
1	X	346	C	C2-N3-C4	5.27	122.54	119.90
1	X	1841	G	C8-N9-C4	-5.27	104.29	106.40
1	X	78	C	C6-N1-C2	-5.27	118.19	120.30
1	X	352	G	P-O5'-C5'	5.27	129.33	120.90
1	X	1326	U	C2-N1-C1'	5.27	124.02	117.70
1	X	1341	G	C5-C6-N1	5.27	114.14	111.50
1	X	746	G	N3-C4-N9	5.27	129.16	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1263	G	P-O3'-C3'	5.27	126.02	119.70
1	X	1873	A	O4'-C1'-N9	5.27	112.41	108.20
1	X	2568	A	O4'-C4'-C3'	-5.27	98.73	104.00
2	Y	107	C	N1-C2-O2	5.27	122.06	118.90
1	X	927	C	N1-C2-O2	5.26	122.06	118.90
1	X	1980	A	C4-C5-C6	5.26	119.63	117.00
2	Y	97	C	O4'-C1'-N1	5.26	112.41	108.20
1	X	358	C	C5-C6-N1	5.26	123.63	121.00
1	X	1478	U	N3-C2-O2	-5.26	118.52	122.20
1	X	1755	G	O5'-P-OP2	-5.26	100.97	105.70
1	X	2047	C	O4'-C1'-N1	5.26	112.41	108.20
1	X	1194	U	C2'-C3'-O3'	5.26	122.11	113.70
1	X	2479	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	2564	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	617	U	C2-N1-C1'	5.26	124.01	117.70
1	X	1657	A	C5'-C4'-O4'	-5.26	102.79	109.10
1	X	2000	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	765	C	N1-C2-O2	5.25	122.05	118.90
1	X	1703	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1923	U	P-O3'-C3'	5.25	126.00	119.70
1	X	2380	U	O4'-C1'-N1	5.25	112.40	108.20
1	X	940	G	O4'-C1'-N9	5.25	112.40	108.20
1	X	954	U	C5-C4-O4	-5.25	122.75	125.90
1	X	1687	C	P-O3'-C3'	5.25	126.00	119.70
1	X	2524	G	C8-N9-C4	-5.25	104.30	106.40
1	X	320	A	O4'-C1'-N9	5.25	112.40	108.20
1	X	1458	A	P-O3'-C3'	5.25	126.00	119.70
2	Y	41	A	P-O3'-C3'	5.25	126.00	119.70
13	K	11	ASN	C-N-CA	5.25	134.81	121.70
1	X	949	G	C3'-C2'-C1'	-5.24	97.31	101.50
1	X	1432	G	C1'-O4'-C4'	-5.24	105.70	109.90
1	X	2826	C	P-O3'-C3'	5.24	125.99	119.70
1	X	133	C	N1-C2-O2	5.24	122.05	118.90
1	X	2481	G	P-O3'-C3'	5.24	125.99	119.70
1	X	1201	G	P-O3'-C3'	5.24	125.99	119.70
1	X	2422	C	N3-C4-C5	5.24	124.00	121.90
1	X	1830	C	N1-C1'-C2'	5.24	120.81	114.00
1	X	2773	G	P-O3'-C3'	5.24	125.98	119.70
1	X	884	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1765	C	N3-C2-O2	-5.24	118.23	121.90
15	M	29	PRO	N-CA-C	5.24	125.72	112.10
1	X	1231	A	O4'-C1'-N9	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1273	G	C5-C6-O6	-5.24	125.46	128.60
1	X	1278	A	N7-C8-N9	5.24	116.42	113.80
1	X	1663	C	O3'-P-O5'	-5.24	94.05	104.00
1	X	2014	A	C4'-C3'-C2'	5.24	107.84	102.60
1	X	2848	A	C1'-O4'-C4'	-5.24	105.71	109.90
1	X	1811	A	C4'-C3'-C2'	5.23	107.83	102.60
1	X	2039	G	N3-C2-N2	-5.23	116.24	119.90
1	X	169	C	O5'-P-OP2	-5.23	100.99	105.70
1	X	1338	G	C2-N3-C4	5.23	114.51	111.90
1	X	1326	U	N1-C2-O2	5.22	126.46	122.80
1	X	2662	C	N1-C2-O2	5.22	122.03	118.90
2	Y	63	A	O4'-C1'-N9	5.22	112.38	108.20
4	B	162	MET	CB-CA-C	5.22	120.84	110.40
1	X	985	G	N7-C8-N9	5.22	115.71	113.10
1	X	542	A	N1-C6-N6	5.22	121.73	118.60
1	X	967	G	P-O5'-C5'	5.22	129.25	120.90
1	X	1446	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	1764	A	C5-C6-N6	-5.22	119.53	123.70
1	X	2209	G	C8-N9-C4	-5.22	104.31	106.40
1	X	1235	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2619	G	C8-N9-C4	-5.22	104.31	106.40
1	X	245	C	N1-C2-O2	5.21	122.03	118.90
1	X	480	G	C6-C5-N7	-5.21	127.27	130.40
1	X	559	C	C5'-C4'-O4'	5.21	115.36	109.10
1	X	825	C	C5'-C4'-O4'	5.21	115.36	109.10
1	X	2190	A	C4'-C3'-C2'	-5.21	97.39	102.60
1	X	2488	G	C5-C6-N1	5.21	114.11	111.50
1	X	468	A	P-O3'-C3'	5.21	125.95	119.70
1	X	617	U	N1-C2-O2	5.21	126.45	122.80
1	X	2243	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	483	A	O5'-C5'-C4'	5.21	121.60	111.70
1	X	1637	U	O4'-C1'-N1	5.21	112.37	108.20
1	X	2473	G	N3-C4-C5	-5.21	125.99	128.60
1	X	2605	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	1885	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	542	A	C5-C6-N6	-5.21	119.53	123.70
1	X	799	C	P-O3'-C3'	5.21	125.95	119.70
1	X	1877	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	2284	U	O4'-C1'-N1	5.21	112.36	108.20
1	X	2448	A	O4'-C1'-N9	5.21	112.37	108.20
2	Y	41	A	O4'-C1'-N9	5.21	112.36	108.20
1	X	1729	C	O4'-C1'-N1	5.21	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2349	G	C3'-C2'-C1'	-5.21	97.34	101.50
1	X	945	G	C8-N9-C4	-5.20	104.32	106.40
1	X	1631	C	C4'-C3'-C2'	-5.20	97.40	102.60
1	X	593	C	P-O5'-C5'	5.20	129.22	120.90
1	X	1629	G	P-O3'-C3'	5.20	125.94	119.70
2	Y	53	G	C8-N9-C4	-5.20	104.32	106.40
1	X	542	A	C5'-C4'-O4'	5.20	115.34	109.10
1	X	560	G	P-O3'-C3'	-5.20	113.46	119.70
1	X	2441	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2697	G	C5-C6-O6	-5.20	125.48	128.60
1	X	2018	G	O4'-C1'-C2'	-5.20	100.60	105.80
1	X	2408	G	C2'-C3'-O3'	5.20	122.02	113.70
1	X	2013	A	C1'-O4'-C4'	-5.20	105.74	109.90
1	X	349	G	P-O5'-C5'	5.20	129.21	120.90
1	X	1142	G	C5-C6-O6	-5.20	125.48	128.60
1	X	1336	G	N9-C4-C5	-5.20	103.32	105.40
1	X	1699	A	O4'-C1'-N9	-5.20	104.04	108.20
1	X	1747	G	N9-C1'-C2'	5.20	120.75	114.00
1	X	1963	G	C8-N9-C4	-5.20	104.32	106.40
1	X	2471	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2573	C	O4'-C1'-N1	5.20	112.36	108.20
1	X	2854	G	P-O5'-C5'	5.20	129.21	120.90
1	X	596	C	P-O3'-C3'	5.19	125.93	119.70
1	X	2810	A	C1'-O4'-C4'	-5.19	105.74	109.90
1	X	1613	G	O4'-C1'-N9	5.19	112.35	108.20
2	Y	54	U	C5'-C4'-O4'	5.19	115.33	109.10
1	X	874	A	O4'-C1'-N9	5.19	112.35	108.20
1	X	2560	G	C8-N9-C4	-5.19	104.32	106.40
1	X	499	G	O4'-C1'-N9	5.19	112.35	108.20
1	X	956	A	C5'-C4'-O4'	5.19	115.33	109.10
1	X	1626	A	N1-C2-N3	-5.19	126.71	129.30
1	X	2377	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	18	U	P-O3'-C3'	-5.19	113.48	119.70
1	X	786	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	97	U	C5'-C4'-C3'	-5.18	107.70	116.00
1	X	2489	C	P-O3'-C3'	-5.18	113.48	119.70
1	X	2799	C	N3-C4-C5	5.18	123.97	121.90
1	X	78	C	C5-C6-N1	5.18	123.59	121.00
1	X	422	C	C6-N1-C2	-5.18	118.23	120.30
1	X	1496	G	C8-N9-C4	-5.18	104.33	106.40
11	I	35	LYS	N-CA-C	-5.18	97.02	111.00
1	X	2858	A	P-O5'-C5'	5.18	129.19	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	646	C	C6-N1-C2	-5.18	118.23	120.30
1	X	751	G	C3'-C2'-C1'	-5.18	97.36	101.50
11	I	64	GLY	N-CA-C	5.18	126.04	113.10
1	X	230	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	1396	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	246	C	N3-C2-O2	-5.17	118.28	121.90
1	X	309	G	C5-C6-O6	-5.17	125.50	128.60
1	X	330	C	N1-C2-O2	5.17	122.00	118.90
1	X	2543	A	O4'-C1'-N9	5.17	112.34	108.20
1	X	341	A	C3'-C2'-C1'	5.17	105.64	101.50
1	X	1170	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	2790	C	O4'-C1'-N1	5.17	112.33	108.20
1	X	1038	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	1112	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	1150	C	O4'-C1'-N1	5.17	112.33	108.20
1	X	1825	C	C3'-C2'-C1'	-5.17	97.37	101.50
1	X	351	A	C3'-C2'-C1'	-5.16	97.37	101.50
1	X	1717	A	C5-C6-N1	5.16	120.28	117.70
1	X	2237	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	2385	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2493	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2705	A	C4'-C3'-O3'	5.16	123.33	113.00
1	X	2855	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	454	G	P-O3'-C3'	5.16	125.89	119.70
1	X	1711	C	P-O5'-C5'	5.16	129.16	120.90
1	X	2776	U	P-O3'-C3'	5.16	125.89	119.70
1	X	200	A	P-O3'-C3'	5.16	125.89	119.70
1	X	1014	G	C2-N3-C4	5.16	114.48	111.90
1	X	1281	A	OP2-P-O3'	5.16	116.55	105.20
1	X	823	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2650	G	C4'-C3'-C2'	5.16	107.76	102.60
1	X	2766	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2786	G	O4'-C1'-N9	5.16	112.32	108.20
1	X	951	G	O4'-C4'-C3'	-5.15	98.85	104.00
1	X	1124	U	O4'-C1'-N1	5.15	112.32	108.20
1	X	1623	C	P-O3'-C3'	5.15	125.88	119.70
1	X	2593	A	O3'-P-O5'	-5.15	94.21	104.00
1	X	730	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	1469	U	N1-C2-N3	5.15	117.99	114.90
1	X	1265	G	O5'-P-OP1	5.15	116.88	110.70
3	A	248	THR	CB-CA-C	5.15	125.50	111.60
1	X	72	A	O4'-C1'-N9	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1390	G	C8-N9-C4	-5.15	104.34	106.40
1	X	1987	G	C8-N9-C4	-5.15	104.34	106.40
1	X	1250	A	P-O3'-C3'	5.14	125.87	119.70
1	X	1622	G	P-O3'-C3'	5.14	125.87	119.70
1	X	1940	C	O4'-C1'-N1	5.14	112.32	108.20
1	X	1429	A	N9-C1'-C2'	5.14	120.68	114.00
1	X	1912	G	P-O3'-C3'	5.14	125.87	119.70
1	X	2039	G	N7-C8-N9	5.14	115.67	113.10
2	Y	53	G	N3-C4-C5	-5.14	126.03	128.60
1	X	70	A	C5'-C4'-C3'	-5.14	107.77	116.00
1	X	2561	G	C5-C6-O6	-5.14	125.52	128.60
1	X	1648	C	N1-C2-O2	5.14	121.98	118.90
1	X	2274	C	C6-N1-C2	-5.14	118.24	120.30
1	X	1790	G	C4'-C3'-C2'	5.14	107.74	102.60
1	X	2663	U	P-O3'-C3'	-5.14	113.53	119.70
1	X	1014	G	C8-N9-C4	-5.14	104.35	106.40
1	X	1167	A	O4'-C1'-N9	-5.14	104.09	108.20
9	G	106	TYR	CA-C-N	-5.14	105.90	117.20
1	X	582	G	P-O3'-C3'	5.13	125.86	119.70
1	X	771	C	N1-C2-O2	5.13	121.98	118.90
1	X	955	G	C4-N9-C1'	5.13	133.18	126.50
1	X	1248	G	OP1-P-O3'	5.13	116.49	105.20
11	I	32	ARG	N-CA-C	-5.13	97.14	111.00
1	X	626	A	P-O3'-C3'	5.13	125.86	119.70
1	X	2298	U	C4'-C3'-C2'	5.13	107.73	102.60
1	X	1975	G	C2-N3-C4	5.13	114.47	111.90
1	X	2697	G	N3-C4-C5	-5.13	126.04	128.60
1	X	2855	C	C6-N1-C2	-5.13	118.25	120.30
1	X	2176	U	O4'-C1'-N1	5.13	112.30	108.20
1	X	2279	G	C8-N9-C4	-5.13	104.35	106.40
2	Y	10	U	O4'-C1'-N1	5.12	112.30	108.20
1	X	1432	G	P-O3'-C3'	5.12	125.85	119.70
1	X	240	U	O4'-C4'-C3'	-5.12	98.88	104.00
1	X	984	A	P-O3'-C3'	5.12	125.84	119.70
1	X	2681	A	C4'-C3'-C2'	-5.12	97.48	102.60
1	X	820	U	O4'-C1'-N1	5.12	112.30	108.20
1	X	1409	U	C1'-O4'-C4'	-5.12	105.81	109.90
1	X	2011	U	C5-C4-O4	-5.12	122.83	125.90
1	X	2619	G	C5'-C4'-C3'	-5.12	107.81	116.00
1	X	2846	G	O5'-P-OP2	-5.12	101.09	105.70
1	X	2296	U	O4'-C1'-N1	5.12	112.29	108.20
1	X	2804	G	C6-N1-C2	-5.12	122.03	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1279	G	C1'-O4'-C4'	-5.12	105.81	109.90
1	X	577	U	C2-N3-C4	5.11	130.07	127.00
1	X	2867	G	C3'-C2'-C1'	5.11	105.59	101.50
2	Y	8	C	O4'-C1'-N1	5.11	112.29	108.20
1	X	1351	G	C3'-C2'-C1'	5.11	105.59	101.50
1	X	660	G	C8-N9-C4	-5.11	104.36	106.40
1	X	2006	G	C5'-C4'-O4'	5.11	115.23	109.10
10	H	26	ASN	C-N-CA	5.11	134.47	121.70
12	J	88	LYS	N-CA-C	5.11	124.80	111.00
1	X	1559	G	P-O3'-C3'	5.11	125.83	119.70
1	X	1712	G	C8-N9-C1'	-5.11	120.36	127.00
1	X	225	G	O4'-C1'-N9	5.11	112.28	108.20
1	X	1407	G	C4-N9-C1'	5.11	133.14	126.50
1	X	1627	C	O4'-C1'-N1	5.11	112.28	108.20
1	X	1853	C	O4'-C1'-N1	5.11	112.28	108.20
4	B	132	LYS	C-N-CA	5.11	134.46	121.70
1	X	1244	U	C5-C6-N1	5.10	125.25	122.70
1	X	1218	C	O4'-C1'-N1	5.10	112.28	108.20
1	X	1468	A	N1-C6-N6	-5.10	115.54	118.60
1	X	327	C	N1-C2-O2	5.10	121.96	118.90
1	X	334	G	C2-N3-C4	5.10	114.45	111.90
1	X	519	C	C5-C6-N1	5.10	123.55	121.00
1	X	1142	G	P-O3'-C3'	5.10	125.82	119.70
1	X	1245	G	O4'-C1'-N9	5.10	112.28	108.20
1	X	1733	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	1679	U	N1-C2-N3	5.10	117.96	114.90
1	X	2196	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	579	G	C5-N7-C8	5.10	106.85	104.30
1	X	1340	C	O3'-P-O5'	-5.10	94.32	104.00
1	X	561	U	C3'-C2'-C1'	-5.09	97.42	101.50
1	X	1120	C	C3'-C2'-C1'	5.09	105.58	101.50
1	X	2659	C	P-O5'-C5'	5.09	129.05	120.90
1	X	132	U	O4'-C1'-N1	5.09	112.28	108.20
1	X	34	U	C5'-C4'-O4'	5.09	115.21	109.10
1	X	485	G	P-O5'-C5'	5.09	129.04	120.90
1	X	523	A	N9-C1'-C2'	5.09	120.62	114.00
1	X	1237	G	O4'-C1'-N9	5.09	112.27	108.20
1	X	2396	C	P-O5'-C5'	-5.09	112.76	120.90
1	X	2476	A	P-O3'-C3'	5.09	125.81	119.70
1	X	2650	G	N3-C4-C5	-5.09	126.06	128.60
1	X	345	U	P-O5'-C5'	5.09	129.04	120.90
1	X	206	U	N1-C2-O2	5.09	126.36	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	759	C	O5'-C5'-C4'	5.09	121.37	111.70
1	X	993	C	P-O3'-C3'	-5.09	113.60	119.70
1	X	1497	C	C5-C6-N1	5.09	123.54	121.00
1	X	2680	U	O4'-C1'-N1	5.09	112.27	108.20
1	X	2784	A	O4'-C1'-N9	-5.08	104.13	108.20
1	X	2794	G	P-O5'-C5'	-5.08	112.76	120.90
3	A	242	ALA	N-CA-C	5.08	124.73	111.00
1	X	2416	U	C3'-C2'-C1'	-5.08	97.43	101.50
1	X	2827	G	N3-C4-C5	-5.08	126.06	128.60
1	X	2867	G	C5'-C4'-O4'	5.08	115.20	109.10
2	Y	28	A	C2-N3-C4	5.08	113.14	110.60
1	X	1944	C	N1-C2-O2	5.08	121.95	118.90
1	X	1994	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	2487	G	C8-N9-C4	-5.08	104.37	106.40
1	X	2620	G	C5-C6-O6	-5.08	125.55	128.60
1	X	551	A	C3'-C2'-C1'	-5.08	97.44	101.50
1	X	639	G	C5-C6-O6	-5.08	125.55	128.60
1	X	811	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	2299	A	N9-C1'-C2'	5.08	120.60	114.00
1	X	2314	A	P-O5'-C5'	5.08	129.03	120.90
1	X	2632	U	P-O3'-C3'	5.08	125.79	119.70
1	X	1994	U	OP1-P-O3'	5.08	116.36	105.20
1	X	71	A	P-O5'-C5'	5.07	129.02	120.90
1	X	812	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1695	U	N3-C2-O2	-5.07	118.65	122.20
1	X	2229	G	N9-C4-C5	5.07	107.43	105.40
1	X	70	A	P-O3'-C3'	5.07	125.78	119.70
1	X	777	A	C5'-C4'-C3'	-5.07	107.89	116.00
1	X	773	G	O4'-C1'-N9	5.07	112.25	108.20
1	X	1753	A	N7-C8-N9	5.07	116.33	113.80
1	X	1264	C	N1-C2-O2	5.07	121.94	118.90
1	X	1509	A	P-O5'-C5'	5.07	129.01	120.90
1	X	69	G	O4'-C1'-N9	5.07	112.25	108.20
1	X	1973	C	O4'-C1'-N1	5.07	112.25	108.20
1	X	2681	A	C6-N1-C2	-5.07	115.56	118.60
1	X	1099	A	C3'-C2'-C1'	5.06	105.55	101.50
1	X	1528	C	C5-C6-N1	5.06	123.53	121.00
1	X	1223	G	C5-C6-O6	-5.06	125.56	128.60
1	X	2251	U	P-O3'-C3'	5.06	125.77	119.70
1	X	2487	G	C5-C6-N1	5.06	114.03	111.50
1	X	1524	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	1928	G	P-O5'-C5'	5.06	128.99	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2324	G	N3-C4-C5	-5.06	126.07	128.60
5	C	163	ASN	C-N-CA	5.06	134.34	121.70
1	X	664	C	N1-C2-O2	5.06	121.93	118.90
1	X	2485	U	P-O3'-C3'	5.06	125.77	119.70
1	X	2731	G	O4'-C1'-N9	5.06	112.25	108.20
1	X	26	G	C5-C6-O6	-5.05	125.57	128.60
1	X	559	C	N3-C2-O2	-5.05	118.36	121.90
1	X	1451	C	C5'-C4'-O4'	5.05	115.16	109.10
1	X	1674	C	C5'-C4'-O4'	-5.05	103.04	109.10
1	X	1796	A	C2-N3-C4	5.05	113.13	110.60
1	X	1799	A	C5'-C4'-O4'	5.05	115.16	109.10
1	X	2744	A	P-O3'-C3'	5.05	125.76	119.70
1	X	624	A	O4'-C1'-N9	5.05	112.24	108.20
1	X	1250	A	O4'-C1'-N9	-5.05	104.16	108.20
1	X	1666	G	O4'-C4'-C3'	-5.05	98.95	104.00
1	X	2064	U	O4'-C1'-N1	5.05	112.24	108.20
1	X	2288	A	P-O3'-C3'	5.05	125.76	119.70
1	X	2426	G	C1'-O4'-C4'	-5.05	105.86	109.90
1	X	461	A	C2-N3-C4	5.05	113.12	110.60
1	X	536	A	N1-C6-N6	5.05	121.63	118.60
1	X	635	C	C6-N1-C2	-5.05	118.28	120.30
1	X	1986	G	N1-C6-O6	-5.05	116.87	119.90
1	X	1665	C	O5'-P-OP2	-5.05	101.16	105.70
1	X	2507	U	P-O3'-C3'	5.05	125.75	119.70
1	X	1426	U	O4'-C1'-N1	5.04	112.24	108.20
1	X	1497	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1535	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1282	A	C5'-C4'-C3'	-5.04	107.93	116.00
1	X	1980	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	2729	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	1284	G	N7-C8-N9	5.04	115.62	113.10
1	X	769	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1199	U	OP2-P-O3'	5.04	116.28	105.20
1	X	1467	U	C1'-O4'-C4'	5.04	113.93	109.90
1	X	1838	G	P-O3'-C3'	5.04	125.75	119.70
1	X	337	G	C5-C6-O6	-5.04	125.58	128.60
1	X	407	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	753	U	P-O3'-C3'	5.04	125.74	119.70
1	X	2745	A	N1-C2-N3	-5.04	126.78	129.30
1	X	107	G	C5'-C4'-C3'	-5.04	107.94	116.00
1	X	1872	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	X	349	G	N3-C4-C5	-5.03	126.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	964	A	C5'-C4'-O4'	5.03	115.14	109.10
1	X	1291	G	O4'-C4'-C3'	-5.03	98.97	104.00
1	X	465	C	P-O5'-C5'	-5.03	112.85	120.90
1	X	1229	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	2691	C	O3'-P-O5'	-5.03	94.44	104.00
1	X	17	G	P-O3'-C3'	-5.03	113.67	119.70
1	X	467	U	C5'-C4'-O4'	5.03	115.14	109.10
1	X	2228	U	N3-C4-O4	5.03	122.92	119.40
1	X	228	A	OP1-P-O3'	5.03	116.26	105.20
1	X	616	U	C5'-C4'-C3'	-5.03	107.96	116.00
1	X	1000	G	O4'-C1'-N9	5.03	112.22	108.20
1	X	1033	G	C5'-C4'-O4'	-5.03	103.07	109.10
1	X	1669	A	C3'-C2'-C1'	-5.03	97.48	101.50
1	X	1766	U	C5-C4-O4	-5.03	122.88	125.90
1	X	190	A	C1'-O4'-C4'	-5.03	105.88	109.90
1	X	560	G	C4'-C3'-C2'	5.03	107.63	102.60
1	X	633	G	P-O5'-C5'	5.03	128.94	120.90
1	X	1174	G	O4'-C1'-N9	5.03	112.22	108.20
1	X	1812	U	P-O5'-C5'	5.03	128.94	120.90
1	X	2503	G	C5-C6-N1	5.03	114.01	111.50
1	X	2567	G	C6-N1-C2	-5.03	122.08	125.10
1	X	2598	C	N3-C4-C5	5.03	123.91	121.90
1	X	2620	G	C4'-C3'-C2'	-5.03	97.57	102.60
1	X	767	G	P-O5'-C5'	5.02	128.94	120.90
1	X	1541	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	2701	A	P-O3'-C3'	-5.02	113.67	119.70
1	X	2727	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	1222	G	N3-C4-N9	5.02	129.01	126.00
1	X	1777	A	C1'-O4'-C4'	-5.02	105.88	109.90
1	X	2737	A	C5'-C4'-C3'	-5.02	107.97	116.00
2	Y	35	C	O4'-C1'-N1	5.02	112.22	108.20
1	X	232	A	P-O5'-C5'	5.02	128.93	120.90
1	X	344	G	C8-N9-C4	-5.02	104.39	106.40
1	X	480	G	N1-C6-O6	5.02	122.91	119.90
1	X	537	C	C3'-C2'-C1'	-5.01	97.49	101.50
1	X	573	C	N1-C2-O2	5.01	121.91	118.90
1	X	1049	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	1669	A	C1'-O4'-C4'	-5.01	105.89	109.90
2	Y	54	U	C1'-O4'-C4'	-5.01	105.89	109.90
1	X	845	U	N3-C2-O2	-5.01	118.69	122.20
1	X	2261	G	C4'-C3'-C2'	5.01	107.61	102.60
1	X	73	A	N9-C1'-C2'	5.01	120.51	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	610	G	O3'-P-O5'	-5.01	94.48	104.00
1	X	1234	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	1770	U	C4-C5-C6	5.01	122.71	119.70
1	X	1418	C	N1-C2-O2	5.01	121.91	118.90
1	X	497	C	C3'-C2'-C1'	-5.01	97.50	101.50
1	X	2340	C	OP1-P-OP2	5.01	127.11	119.60
1	X	1280	U	N1-C1'-C2'	5.00	120.51	114.00
1	X	1812	U	C2-N1-C1'	5.00	123.71	117.70
1	X	2347	C	C3'-C2'-C1'	-5.00	97.50	101.50
2	Y	45	C	N3-C2-O2	-5.00	118.40	121.90
1	X	1075	C	C3'-C2'-C1'	5.00	105.50	101.50
1	X	1671	A	OP1-P-OP2	5.00	127.10	119.60
1	X	1822	C	C3'-C2'-C1'	-5.00	97.50	101.50
1	X	2292	C	O4'-C1'-N1	5.00	112.20	108.20
1	X	2298	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1288	A	Sidechain
1	X	1684	G	Sidechain
1	X	219	G	Sidechain
1	X	474	G	Sidechain
1	X	683	A	Sidechain
1	X	739	G	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	431	0
2	Y	2598	0	1328	17	0
3	A	1826	0	1885	62	0
4	B	1539	0	1600	62	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	1286	0	1336	9	0
8	F	503	0	520	3	0
9	G	1114	0	1144	63	0
10	H	997	0	1046	24	0
11	I	1067	0	1103	48	0
12	J	1090	0	1125	32	0
13	K	878	0	930	28	0
14	L	779	0	820	17	0
15	M	871	0	894	29	0
16	N	978	0	1020	25	0
17	O	741	0	756	30	0
18	P	1014	0	1096	20	0
19	Q	726	0	753	23	0
20	R	825	0	881	28	0
21	S	1345	0	1372	21	0
22	T	625	0	655	11	0
23	U	552	0	604	28	0
24	V	533	0	558	4	0
25	W	424	0	470	9	0
26	Z	457	0	462	16	0
27	1	53	0	0	0	0
28	2	46	0	0	2	0
29	3	63	0	0	2	0
30	4	297	0	330	5	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
32	X	60	0	66	2	0
All	All	83879	0	54809	969	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (969) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.93	1.47
11:I:62:LYS:NZ	11:I:64:GLY:HA2	1.60	1.15
1:X:1333:G:N2	1:X:1344:C:H41	1.44	1.12
15:M:79:ARG:HH11	15:M:79:ARG:HG3	1.03	1.10
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.35	1.09
1:X:759:C:H6	1:X:759:C:H5"	1.07	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:542:A:C2	1:X:2004:U:H2'	1.93	1.03
11:I:62:LYS:HZ1	11:I:64:GLY:HA2	1.24	1.02
1:X:542:A:H2	1:X:2004:U:H2'	1.24	1.00
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.39	1.00
1:X:759:C:H5''	1:X:759:C:C6	1.98	0.98
1:X:617:U:H5	1:X:632:A:C2	1.82	0.96
1:X:1919:A:H2	1:X:1926:U:H3	0.99	0.95
1:X:1333:G:H22	1:X:1344:C:N4	1.62	0.95
1:X:1448:A:H61	1:X:1574:A:H61	0.97	0.94
1:X:1466:C:H2'	1:X:1467:U:O4'	1.69	0.91
16:N:93:LYS:HE3	17:O:5:ILE:HD13	1.52	0.91
1:X:2042:A:H5''	5:C:65:GLY:HA2	1.53	0.91
1:X:1333:G:H22	1:X:1344:C:H41	0.94	0.91
1:X:2371:A:H2	1:X:2403:C:H42	1.15	0.91
15:M:79:ARG:HG3	15:M:79:ARG:NH1	1.80	0.91
1:X:787:A:H2	1:X:800:U:HO2'	1.16	0.90
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.53	0.89
1:X:617:U:H5	1:X:632:A:H2	1.16	0.89
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.04	0.89
17:O:5:ILE:HD12	17:O:6:GLN:H	1.35	0.88
1:X:1468:A:H5'	1:X:1472:C:N4	1.87	0.88
1:X:1919:A:H2	1:X:1926:U:N3	1.70	0.88
1:X:1542:G:H22	1:X:1562:G:H1	1.15	0.88
1:X:1770:U:H5	1:X:1775:A:N7	1.73	0.87
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.56	0.86
1:X:617:U:C5	1:X:632:A:C2	2.64	0.86
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.07	0.85
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.56	0.85
1:X:542:A:H2	1:X:2004:U:C2'	1.88	0.85
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.59	0.83
23:U:48:LYS:HG2	23:U:49:LYS:H	1.42	0.82
1:X:1882:G:N2	1:X:1885:C:H41	1.77	0.82
4:B:131:SER:O	4:B:132:LYS:HG3	1.78	0.81
4:B:54:LYS:HB2	4:B:75:THR:O	1.81	0.81
1:X:971:A:H61	12:J:83:ARG:HH22	1.27	0.81
1:X:1266:G:N7	11:I:32:ARG:NH1	2.29	0.81
1:X:1811:A:H4'	1:X:1812:U:H5''	1.62	0.80
11:I:62:LYS:HZ3	11:I:64:GLY:HA2	1.45	0.80
1:X:1173:G:H21	17:O:88:GLN:HE22	1.29	0.80
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.16	0.80
1:X:70:A:H5'	1:X:71:A:H3'	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.63	0.79
11:I:58:ALA:O	11:I:59:ARG:HB2	1.80	0.79
1:X:689:A:H8	1:X:2052:G:H21	1.31	0.79
1:X:482:A:H2'	1:X:483:A:O4'	1.83	0.78
1:X:320:A:N3	1:X:340:G:O2'	2.15	0.78
9:G:33:ILE:HB	9:G:34:PRO:CD	2.13	0.78
1:X:215:G:H21	1:X:632:A:H8	1.33	0.77
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.66	0.77
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.50	0.77
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.99	0.77
1:X:1448:A:N6	1:X:1574:A:H61	1.79	0.76
1:X:1673:C:H5''	4:B:136:ARG:CD	2.15	0.76
1:X:1333:G:N2	1:X:1344:C:N4	2.25	0.76
1:X:463:C:H42	1:X:467:U:H5	1.30	0.76
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.50	0.76
1:X:1963:G:O2'	1:X:1965:U:OP2	2.03	0.76
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.67	0.75
16:N:66:ASN:ND2	16:N:70:ARG:HH12	1.84	0.75
15:M:79:ARG:HH11	15:M:79:ARG:CG	1.92	0.75
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.69	0.75
1:X:2617:G:P	4:B:82:ARG:HH22	2.10	0.74
2:Y:46:G:H5'	6:D:92:ARG:HH12	1.53	0.74
13:K:17:ARG:NH1	13:K:20:LEU:HD23	2.01	0.74
1:X:2551:A:N7	4:B:145:LYS:HB2	2.04	0.73
1:X:1054:C:H42	1:X:1123:G:H1	1.37	0.73
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.70	0.72
1:X:1811:A:H5''	3:A:161:THR:HG21	1.71	0.72
3:A:231:HIS:HD2	3:A:233:HIS:H	1.35	0.72
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.71	0.72
1:X:759:C:C5'	1:X:759:C:H6	1.95	0.71
1:X:2042:A:H5''	5:C:65:GLY:CA	2.19	0.71
1:X:1673:C:C5'	4:B:136:ARG:HD2	2.19	0.71
1:X:2266:A:H2	1:X:2325:A:H62	1.38	0.71
25:W:12:ARG:CG	25:W:12:ARG:HH11	2.02	0.71
25:W:12:ARG:HG2	25:W:12:ARG:HH11	1.56	0.71
3:A:231:HIS:CD2	3:A:233:HIS:H	2.08	0.71
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.24	0.71
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.24	0.71
4:B:116:VAL:HG22	4:B:136:ARG:NE	2.05	0.70
1:X:304:A:H2'	1:X:305:A:H5''	1.71	0.70
18:P:92:VAL:HG13	18:P:126:ILE:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:17:SER:HB2	23:U:44:ALA:HA	1.74	0.70
23:U:48:LYS:CG	23:U:49:LYS:H	2.04	0.70
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.74	0.70
1:X:640:C:H4'	1:X:660:G:H21	1.54	0.70
1:X:1030:U:H3	1:X:1153:A:H62	1.38	0.70
1:X:2772:U:H3	1:X:2780:A:H61	1.39	0.70
5:C:38:ARG:HH12	5:C:176:ASN:HD21	1.40	0.69
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.73	0.69
3:A:36:ALA:HB1	3:A:62:TYR:O	1.91	0.69
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.58	0.69
1:X:1673:C:H5''	4:B:136:ARG:HD2	1.75	0.69
17:O:66:GLY:O	17:O:87:ARG:NH1	2.26	0.69
23:U:32:ARG:HE	23:U:32:ARG:H	1.41	0.69
1:X:2779:C:H2'	1:X:2780:A:C8	2.28	0.69
1:X:797:A:C5	3:A:229:VAL:HG21	2.28	0.68
4:B:7:THR:HG21	15:M:5:ILE:HD11	1.75	0.68
1:X:415:A:H61	1:X:436:A:H61	1.41	0.68
13:K:11:ASN:OD1	13:K:11:ASN:N	2.26	0.68
1:X:1753:A:O5'	1:X:1753:A:H8	1.76	0.68
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.47	0.68
1:X:1238:A:H4'	17:O:83:ARG:HG2	1.76	0.68
15:M:34:ARG:NH2	15:M:88:VAL:HG13	2.09	0.68
1:X:797:A:N7	3:A:229:VAL:HG21	2.08	0.67
1:X:2501:U:H5''	1:X:2501:U:H6	1.59	0.67
15:M:27:PHE:HA	15:M:96:ARG:HH21	1.59	0.67
10:H:98:ILE:HG22	10:H:106:ARG:HG3	1.76	0.67
11:I:76:LYS:HB2	11:I:79:GLN:HG2	1.76	0.67
16:N:83:LEU:HD12	16:N:113:SER:HB2	1.77	0.67
16:N:88:ILE:HG13	17:O:49:GLU:HB2	1.76	0.67
23:U:47:HIS:CD2	23:U:48:LYS:H	2.13	0.66
1:X:841:G:H2'	1:X:842:A:C8	2.30	0.66
23:U:48:LYS:HG2	23:U:49:LYS:N	2.10	0.66
1:X:38:G:H1	1:X:453:U:H3	1.43	0.66
1:X:652:C:H42	1:X:657:A:H61	1.42	0.66
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.76	0.66
1:X:1816:G:O2'	3:A:252:LYS:HG2	1.95	0.66
1:X:1468:A:H5'	1:X:1472:C:H41	1.56	0.66
3:A:89:SER:HB2	3:A:201:HIS:CE1	2.30	0.66
12:J:14:PHE:HE1	12:J:90:ALA:HA	1.59	0.65
1:X:219:G:N2	1:X:231:G:H2'	2.12	0.65
1:X:1467:U:H2'	1:X:1468:A:OP1	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.24	0.65
1:X:1770:U:C5	1:X:1775:A:N7	2.61	0.65
9:G:70:PHE:CB	16:N:64:ARG:HG2	2.27	0.65
1:X:2266:A:H62	1:X:2323:U:H3	1.43	0.65
1:X:1466:C:C2'	1:X:1467:U:O4'	2.44	0.65
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.78	0.65
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.78	0.65
11:I:28:LYS:HE3	11:I:36:GLY:HA3	1.79	0.65
19:Q:60:GLY:H	19:Q:72:ARG:HD3	1.62	0.64
20:R:92:THR:HB	20:R:95:ARG:HH22	1.60	0.64
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.27	0.64
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.12	0.64
3:A:183:ARG:HH11	3:A:183:ARG:HB3	1.62	0.64
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.32	0.64
3:A:96:HIS:HE1	3:A:100:GLY:HA2	1.62	0.64
1:X:1584:G:H4'	3:A:59:LYS:HB3	1.80	0.64
1:X:2222:U:H2'	1:X:2223:U:C6	2.32	0.64
3:A:172:TYR:HA	3:A:186:HIS:HA	1.80	0.64
1:X:1033:G:N2	1:X:1153:A:C2	2.66	0.63
20:R:105:ARG:HH12	20:R:112:LYS:HA	1.63	0.63
13:K:17:ARG:HH11	13:K:20:LEU:HD23	1.60	0.63
9:G:61:ARG:HH11	9:G:66:HIS:H	1.44	0.63
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.79	0.63
1:X:2545:A:H61	10:H:40:GLY:HA3	1.63	0.63
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.81	0.63
11:I:28:LYS:HZ1	11:I:37:GLN:H	1.47	0.63
15:M:25:PRO:HD2	15:M:91:VAL:HG12	1.81	0.63
1:X:203:G:H1'	1:X:205:A:H61	1.64	0.63
1:X:1803:G:H21	3:A:46:ARG:HD2	1.64	0.63
9:G:161:GLN:HG2	9:G:165:VAL:HG11	1.80	0.62
5:C:133:PHE:HB2	5:C:160:ALA:HB1	1.81	0.62
3:A:244:ARG:HB3	3:A:252:LYS:NZ	2.13	0.62
1:X:564:U:H2'	1:X:565:A:C8	2.33	0.62
4:B:55:ALA:HB3	4:B:58:LYS:HG3	1.81	0.62
11:I:73:GLU:OE1	11:I:101:ARG:HB2	1.98	0.62
1:X:2790:C:O2'	26:Z:43:HIS:HD2	1.82	0.62
1:X:1007:A:H4'	16:N:93:LYS:HB3	1.81	0.62
16:N:66:ASN:HB3	16:N:76:TYR:H	1.64	0.62
13:K:24:GLN:HB3	13:K:44:LEU:HD22	1.82	0.62
1:X:82:G:H1	1:X:100:G:H2'	1.64	0.62
20:R:22:VAL:HG11	20:R:80:LYS:HZ3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1033:G:H4'	1:X:1034:U:H5'	1.82	0.62
32:X:2931:1F3:H61	32:X:2931:1F3:H20	1.81	0.61
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.15	0.61
20:R:46:VAL:HG11	20:R:80:LYS:HD3	1.81	0.61
1:X:617:U:C5	1:X:632:A:H2	2.06	0.61
20:R:92:THR:HB	20:R:95:ARG:NH2	2.16	0.61
5:C:164:VAL:C	5:C:166:TRP:H	2.04	0.61
1:X:346:C:H2'	1:X:347:C:C6	2.36	0.61
1:X:224:G:OP2	1:X:226:C:N4	2.31	0.60
1:X:2037:A:H2'	26:Z:8:LYS:HE3	1.82	0.60
1:X:971:A:N6	12:J:83:ARG:HH22	1.99	0.60
1:X:774:A:H8	1:X:774:A:O5'	1.85	0.60
4:B:116:VAL:H	4:B:136:ARG:HE	1.49	0.60
1:X:649:G:H1	1:X:660:G:H1	1.49	0.60
1:X:2197:U:H2'	1:X:2198:U:C6	2.37	0.60
1:X:540:G:O6	1:X:2006:G:OP1	2.18	0.60
10:H:85:ASP:HB3	15:M:87:LEU:HD12	1.83	0.60
9:G:67:ARG:CG	9:G:70:PHE:HA	2.29	0.60
16:N:66:ASN:HD22	16:N:70:ARG:HH12	1.49	0.60
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.33	0.60
9:G:62:ILE:HG22	9:G:135:LEU:HD21	1.84	0.60
17:O:5:ILE:HD12	17:O:6:GLN:N	2.12	0.60
1:X:2334:C:H1'	22:T:39:ARG:HH21	1.65	0.60
1:X:2551:A:C8	4:B:144:ARG:HD3	2.37	0.60
1:X:946:U:H2'	1:X:947:C:H6	1.67	0.59
17:O:11:GLN:HE22	17:O:38:LEU:HB3	1.65	0.59
1:X:2362:G:H2'	1:X:2363:G:C8	2.37	0.59
16:N:66:ASN:HB3	16:N:76:TYR:N	2.18	0.59
1:X:2597:G:H21	4:B:150:VAL:HG11	1.66	0.59
5:C:3:GLN:HG2	5:C:116:LYS:HD2	1.84	0.59
20:R:10:HIS:O	20:R:11:ASN:HB2	2.02	0.59
1:X:2713:A:H61	4:B:203:LYS:HG2	1.68	0.59
1:X:504:G:H21	18:P:78:ASN:HD21	1.51	0.59
1:X:760:U:C6	26:Z:3:LYS:HG3	2.38	0.59
4:B:152:LYS:HD2	9:G:106:TYR:H	1.68	0.59
1:X:512:A:H4'	18:P:15:LYS:HB3	1.84	0.59
12:J:92:GLU:HG3	12:J:93:TYR:HD2	1.67	0.58
1:X:827:C:H2'	1:X:828:C:H6	1.68	0.58
25:W:4:LYS:HG2	25:W:52:GLU:HB3	1.85	0.58
1:X:597:U:O4	1:X:683:A:H1'	2.03	0.58
1:X:946:U:H2'	1:X:947:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:78:SER:HA	10:H:91:PHE:O	2.04	0.58
1:X:2371:A:H8	11:I:59:ARG:HG3	1.69	0.58
11:I:81:GLN:HG2	11:I:114:ILE:HG22	1.86	0.58
18:P:13:GLN:O	18:P:16:GLN:HG2	2.02	0.58
29:3:10:ALA:CA	29:3:12:ARG:CA	2.82	0.58
1:X:2617:G:P	4:B:82:ARG:NH2	2.76	0.58
1:X:1050:G:H1	1:X:1127:C:H42	1.51	0.58
1:X:1468:A:H5'	1:X:1472:C:H42	1.68	0.58
9:G:61:ARG:NH1	9:G:66:HIS:H	2.02	0.58
1:X:451:A:H2'	1:X:452:G:C8	2.39	0.58
3:A:91:ARG:HG3	3:A:198:ASN:H	1.69	0.58
3:A:39:LYS:HB2	3:A:62:TYR:HB2	1.86	0.58
20:R:16:PHE:HZ	20:R:46:VAL:HG22	1.69	0.58
4:B:120:TRP:HB3	4:B:155:ARG:HH11	1.69	0.58
5:C:43:ALA:CB	5:C:86:PRO:HB2	2.32	0.57
1:X:1962:C:H2'	1:X:1963:G:H5'	1.85	0.57
5:C:48:ARG:C	5:C:50:GLN:H	2.07	0.57
1:X:623:G:H3'	1:X:624:A:H5''	1.86	0.57
1:X:1773:C:H1'	1:X:2588:U:H5''	1.85	0.57
15:M:32:THR:CG2	15:M:91:VAL:HG22	2.34	0.57
5:C:27:LEU:O	5:C:31:VAL:HG23	2.05	0.57
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.86	0.57
1:X:759:C:C5'	1:X:759:C:C6	2.78	0.57
12:J:99:LYS:HG3	12:J:100:PRO:HD2	1.87	0.57
1:X:1287:A:H2'	1:X:1288:A:H5''	1.86	0.57
16:N:88:ILE:HG23	17:O:48:GLY:HA3	1.86	0.57
1:X:1918:G:H1'	1:X:1947:G:N2	2.20	0.57
11:I:17:LYS:O	11:I:18:ARG:HB2	2.03	0.57
9:G:102:ARG:HB3	9:G:102:ARG:HH11	1.70	0.57
1:X:787:A:H2	1:X:800:U:O2'	1.84	0.57
4:B:131:SER:O	4:B:132:LYS:CG	2.52	0.57
1:X:1811:A:H4'	1:X:1812:U:C5'	2.32	0.57
1:X:558:G:O3'	1:X:559:C:H4'	2.03	0.57
1:X:504:G:H4'	18:P:27:VAL:HG13	1.87	0.57
1:X:1882:G:H22	1:X:1885:C:H41	1.49	0.57
18:P:105:ARG:HD3	18:P:119:LYS:HE3	1.86	0.57
9:G:69:ASP:H	9:G:76:GLN:HE21	1.51	0.56
13:K:10:LEU:HA	13:K:17:ARG:HG2	1.86	0.56
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.69	0.56
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.35	0.56
1:X:670:U:H2'	1:X:671:A:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:954:U:OP2	11:I:38:LYS:HG2	2.04	0.56
13:K:3:HIS:CG	13:K:5:LYS:HZ3	2.23	0.56
15:M:31:ASP:N	15:M:31:ASP:OD2	2.31	0.56
6:D:47:SER:HA	6:D:50:ILE:HD12	1.87	0.56
1:X:673:G:H5'	5:C:93:TYR:CD1	2.41	0.56
1:X:1030:U:HO2'	1:X:1032:A:H2	1.52	0.56
1:X:1033:G:H22	1:X:1153:A:H2	1.49	0.56
17:O:36:LYS:HZ1	17:O:54:TYR:HB3	1.70	0.56
9:G:105:GLY:O	9:G:106:TYR:C	2.42	0.56
17:O:10:LYS:HD2	17:O:37:ALA:HB3	1.88	0.56
1:X:1113:C:H2'	1:X:1114:A:H8	1.70	0.56
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.87	0.56
5:C:48:ARG:C	5:C:50:GLN:N	2.58	0.56
5:C:176:ASN:HD22	5:C:179:ASP:H	1.54	0.56
1:X:760:U:O2	1:X:1997:A:H1'	2.06	0.56
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.70	0.56
1:X:172:A:H61	1:X:175:C:H3'	1.71	0.56
1:X:334:G:H3'	5:C:162:ARG:HE	1.70	0.56
21:S:149:ALA:HA	21:S:152:ILE:HD12	1.87	0.55
5:C:30:VAL:HG11	5:C:177:VAL:HG21	1.88	0.55
4:B:134:TRP:H	4:B:134:TRP:HD1	1.53	0.55
9:G:116:ARG:HD2	9:G:119:LEU:HD12	1.89	0.55
11:I:75:VAL:HG22	11:I:99:VAL:HG11	1.88	0.55
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.54	0.55
1:X:1032:A:H8	1:X:1033:G:H5''	1.71	0.55
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.88	0.55
23:U:48:LYS:CG	23:U:49:LYS:N	2.70	0.55
1:X:1673:C:H5'	4:B:136:ARG:HD2	1.88	0.55
13:K:33:ARG:HD3	13:K:112:LEU:HD22	1.89	0.55
13:K:7:GLY:O	13:K:8:ARG:HG2	2.06	0.55
11:I:94:GLU:HA	11:I:97:ARG:HE	1.71	0.55
20:R:90:LYS:HB2	20:R:108:VAL:HG11	1.88	0.55
1:X:1278:A:H2	1:X:1997:A:H62	1.54	0.55
7:E:164:PHE:HB2	7:E:167:GLU:HB2	1.88	0.55
1:X:2387:U:H2'	1:X:2388:G:H8	1.71	0.55
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.89	0.55
12:J:44:LYS:HD3	12:J:47:GLN:HE22	1.71	0.55
1:X:1448:A:H61	1:X:1574:A:N6	1.82	0.55
1:X:1373:G:H22	1:X:2192:U:H3	1.54	0.55
1:X:746:G:N7	1:X:774:A:C6	2.75	0.54
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:38:ILE:O	19:Q:42:ILE:HG22	2.07	0.54
9:G:104:THR:OG1	9:G:110:LEU:HB3	2.07	0.54
3:A:89:SER:HB2	3:A:201:HIS:HE1	1.72	0.54
3:A:96:HIS:HE1	3:A:100:GLY:CA	2.20	0.54
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.40	0.54
21:S:25:ASN:HB3	21:S:85:MET:HB2	1.88	0.54
1:X:1473:U:H6	1:X:1473:U:OP2	1.90	0.54
1:X:2617:G:OP2	4:B:82:ARG:NH2	2.40	0.54
18:P:57:LEU:HA	18:P:60:ILE:HD12	1.89	0.54
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.90	0.54
12:J:12:LYS:O	12:J:13:GLN:HB2	2.08	0.54
2:Y:62:C:H2'	2:Y:63:A:C8	2.42	0.54
16:N:81:ASN:HD22	16:N:117:ARG:HH21	1.56	0.54
1:X:1790:G:H5'	1:X:1811:A:H61	1.73	0.54
5:C:146:GLU:HG3	5:C:185:ARG:HH11	1.72	0.54
1:X:2371:A:C8	11:I:59:ARG:HG3	2.41	0.54
11:I:10:PRO:HA	11:I:14:LYS:HB2	1.89	0.54
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.90	0.54
4:B:147:PRO:C	4:B:149:ARG:H	2.11	0.53
6:D:92:ARG:HB2	6:D:92:ARG:HH21	1.72	0.53
1:X:2790:C:O2'	26:Z:43:HIS:CD2	2.61	0.53
13:K:3:HIS:HB3	13:K:5:LYS:CE	2.39	0.53
1:X:346:C:H2'	1:X:347:C:H6	1.73	0.53
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.91	0.53
11:I:117:ALA:HA	11:I:137:GLY:O	2.08	0.53
1:X:2196:U:H2'	1:X:2197:U:O4'	2.08	0.53
1:X:748:A:H3'	1:X:749:C:H6	1.73	0.53
10:H:116:ARG:HG3	15:M:38:LYS:HZ3	1.73	0.53
2:Y:42:U:H1'	2:Y:47:A:H61	1.73	0.53
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.90	0.53
15:M:28:ARG:H	15:M:96:ARG:NH2	2.06	0.53
10:H:116:ARG:HG3	15:M:38:LYS:NZ	2.22	0.53
1:X:1976:U:H4'	4:B:128:SER:OG	2.08	0.53
2:Y:9:G:O2'	14:L:41:GLN:NE2	2.41	0.53
5:C:98:GLN:HA	5:C:101:GLN:HG3	1.90	0.53
1:X:2306:A:H2'	1:X:2307:A:C8	2.43	0.53
1:X:1467:U:H3'	1:X:1467:U:H6	1.74	0.53
9:G:158:HIS:HA	9:G:161:GLN:CD	2.29	0.53
6:D:75:SER:HB2	6:D:79:LEU:HD13	1.90	0.53
23:U:49:LYS:HB2	23:U:61:TRP:HA	1.91	0.53
1:X:77:C:H42	1:X:106:G:H1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:206:LEU:HA	3:A:211:ARG:HG2	1.90	0.53
1:X:490:A:N3	1:X:492:G:H5''	2.24	0.53
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.91	0.53
1:X:2766:U:OP1	4:B:69:LYS:HE2	2.09	0.53
2:Y:83:C:N4	2:Y:98:C:N3	2.57	0.53
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.22	0.53
9:G:67:ARG:NE	9:G:70:PHE:O	2.40	0.53
15:M:27:PHE:HB3	15:M:93:ILE:HD12	1.89	0.53
9:G:61:ARG:HH11	9:G:65:LYS:HB3	1.73	0.53
1:X:172:A:H5''	1:X:173:A:OP2	2.09	0.53
7:E:89:LEU:HD23	7:E:162:VAL:HG22	1.91	0.53
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.91	0.53
20:R:22:VAL:HG11	20:R:80:LYS:HD2	1.91	0.52
1:X:2272:A:H5''	14:L:15:ARG:HH21	1.73	0.52
13:K:32:GLY:HA2	13:K:115:LEU:HD12	1.91	0.52
1:X:1519:G:H2'	1:X:1520:G:H8	1.73	0.52
1:X:870:C:H4'	22:T:23:VAL:HG21	1.90	0.52
5:C:14:THR:HG22	5:C:15:ILE:H	1.74	0.52
1:X:1943:A:H5''	1:X:1943:A:H8	1.74	0.52
1:X:2811:G:H2'	1:X:2812:A:C8	2.45	0.52
9:G:67:ARG:HB3	9:G:70:PHE:HA	1.90	0.52
3:A:145:LEU:HD23	3:A:155:LEU:HD12	1.92	0.52
1:X:2241:U:H5	22:T:17:ASN:OD1	1.92	0.52
1:X:2659:C:H5'	4:B:189:PRO:HA	1.91	0.52
9:G:103:TYR:CE2	9:G:111:LYS:HB2	2.44	0.52
1:X:823:U:OP1	11:I:32:ARG:NH1	2.42	0.52
1:X:793:G:H21	1:X:796:A:H62	1.57	0.52
20:R:16:PHE:CE2	20:R:80:LYS:HE2	2.43	0.52
10:H:41:ASN:H	10:H:41:ASN:ND2	2.07	0.52
1:X:2505:G:H1'	30:4:1:MET:HB2	1.91	0.52
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.92	0.52
12:J:62:GLY:H	21:S:175:ARG:H	1.57	0.52
21:S:3:LEU:HD11	21:S:33:ALA:H	1.75	0.52
1:X:2484:G:C2	32:X:2931:1F3:H7	2.45	0.52
19:Q:66:GLY:C	19:Q:68:PHE:H	2.13	0.52
21:S:3:LEU:HD22	21:S:34:LEU:HB3	1.92	0.52
19:Q:68:PHE:O	19:Q:70:GLY:N	2.42	0.52
20:R:60:PRO:HD2	20:R:62:MET:HB2	1.91	0.52
1:X:760:U:C5	26:Z:3:LYS:HG3	2.44	0.52
1:X:666:U:O2'	1:X:667:U:H5''	2.10	0.52
3:A:226:MET:HG2	3:A:230:ASP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:553:C:H42	1:X:559:C:N4	2.08	0.52
1:X:1909:U:H5'	1:X:1911:A:OP2	2.09	0.52
1:X:1850:G:H1'	1:X:1867:A:N6	2.25	0.52
11:I:97:ARG:O	11:I:98:LEU:HB2	2.10	0.51
3:A:108:PRO:HB3	3:A:143:HIS:CE1	2.45	0.51
23:U:41:VAL:HG23	23:U:42:GLN:H	1.74	0.51
15:M:34:ARG:HB2	15:M:91:VAL:HG23	1.91	0.51
12:J:79:PRO:HD2	12:J:88:LYS:HD2	1.90	0.51
11:I:28:LYS:CE	11:I:36:GLY:HA3	2.40	0.51
1:X:2387:U:H2'	1:X:2388:G:C8	2.46	0.51
26:Z:16:ARG:HD3	26:Z:20:ARG:CZ	2.40	0.51
1:X:1805:G:H1'	3:A:50:THR:HG21	1.92	0.51
1:X:1673:C:C5'	4:B:136:ARG:CD	2.80	0.51
23:U:49:LYS:HB3	23:U:61:TRP:CE3	2.46	0.51
1:X:1071:U:H4'	1:X:1072:U:H3'	1.92	0.51
4:B:46:ALA:HB2	4:B:82:ARG:HG2	1.92	0.51
3:A:244:ARG:HB3	3:A:252:LYS:HZ1	1.76	0.51
4:B:110:GLY:O	13:K:3:HIS:CD2	2.64	0.51
19:Q:31:PRO:HA	19:Q:76:LYS:HD2	1.92	0.51
19:Q:12:ILE:HG12	19:Q:13:SER:H	1.74	0.51
7:E:6:LYS:HB3	7:E:69:ARG:HD2	1.92	0.51
1:X:168:A:H2'	1:X:169:C:C6	2.45	0.51
14:L:76:ALA:HB2	14:L:107:ALA:HA	1.91	0.51
1:X:2867:G:H8	1:X:2867:G:O5'	1.93	0.51
11:I:108:LEU:HD23	11:I:129:ALA:HB1	1.93	0.51
9:G:100:TYR:CB	9:G:116:ARG:NH1	2.72	0.51
1:X:686:C:H5''	5:C:74:VAL:HB	1.93	0.51
13:K:45:ARG:HB3	13:K:46:PRO:HD3	1.91	0.51
1:X:2725:C:H1'	7:E:143:GLN:HG3	1.91	0.51
21:S:3:LEU:HD21	21:S:32:PHE:HB3	1.93	0.50
17:O:57:GLN:H	17:O:97:GLY:CA	2.25	0.50
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.92	0.50
1:X:1134:C:H2'	1:X:1135:C:H6	1.76	0.50
12:J:78:LYS:HA	12:J:88:LYS:NZ	2.26	0.50
1:X:553:C:H42	1:X:559:C:H42	1.58	0.50
24:V:23:LYS:O	24:V:27:GLU:HG2	2.10	0.50
13:K:49:GLU:O	13:K:52:ILE:HG12	2.12	0.50
1:X:2542:U:O2	1:X:2544:A:H8	1.95	0.50
1:X:2406:C:H5''	1:X:2408:G:OP1	2.11	0.50
9:G:103:TYR:CG	9:G:111:LYS:HA	2.46	0.50
1:X:1142:G:H5''	9:G:111:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2543:A:H5'	1:X:2627:G:H4'	1.93	0.50
1:X:2355:A:H61	14:L:91:ARG:CZ	2.25	0.50
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.76	0.50
13:K:10:LEU:CD2	13:K:17:ARG:HB2	2.42	0.50
3:A:79:VAL:HG21	3:A:111:LEU:HD22	1.94	0.50
1:X:1699:A:H61	1:X:1723:U:H3	1.58	0.50
1:X:1467:U:C2'	1:X:1468:A:OP1	2.58	0.50
4:B:116:VAL:HG13	4:B:136:ARG:HH21	1.75	0.50
5:C:96:PRO:HB2	5:C:99:VAL:HG23	1.93	0.50
2:Y:62:C:H2'	2:Y:63:A:H8	1.76	0.50
1:X:1827:G:H1'	1:X:1914:U:C2	2.47	0.50
5:C:151:VAL:HG11	5:C:175:VAL:HG22	1.93	0.50
10:H:75:VAL:HG12	10:H:118:LEU:HD11	1.94	0.50
4:B:147:PRO:C	4:B:149:ARG:N	2.65	0.50
1:X:2006:G:H5'	1:X:2596:C:H4'	1.93	0.50
9:G:154:GLU:O	9:G:157:PRO:HD2	2.11	0.50
9:G:104:THR:OG1	9:G:105:GLY:N	2.44	0.50
1:X:1032:A:C8	1:X:1033:G:H5''	2.47	0.50
9:G:103:TYR:CZ	9:G:111:LYS:HB2	2.46	0.50
1:X:1006:C:O2	16:N:61:TRP:HZ2	1.95	0.50
1:X:347:C:H4'	20:R:15:HIS:CD2	2.48	0.49
11:I:108:LEU:HD13	11:I:120:VAL:HG11	1.94	0.49
1:X:2423:G:P	5:C:62:LYS:HD2	2.52	0.49
11:I:77:LEU:HB2	11:I:111:SER:H	1.77	0.49
1:X:1033:G:H5'	9:G:93:LYS:NZ	2.26	0.49
1:X:341:A:H2	1:X:1223:G:H2'	1.77	0.49
6:D:33:LYS:HB3	6:D:92:ARG:HG2	1.94	0.49
18:P:103:LEU:HB2	18:P:119:LYS:HB2	1.95	0.49
1:X:1805:G:H1'	3:A:50:THR:CG2	2.43	0.49
12:J:15:ARG:HB3	12:J:73:LYS:HZ2	1.78	0.49
1:X:2657:G:H2'	1:X:2658:A:O4'	2.13	0.49
1:X:1443:G:H2'	1:X:1444:C:C6	2.47	0.49
18:P:49:SER:O	18:P:51:GLN:N	2.45	0.49
1:X:494:A:C8	20:R:56:LYS:HD2	2.48	0.49
9:G:106:TYR:O	9:G:110:LEU:HD12	2.12	0.49
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.95	0.49
26:Z:16:ARG:HD3	26:Z:20:ARG:NH1	2.28	0.49
11:I:47:ALA:O	11:I:49:PHE:N	2.41	0.49
1:X:2490:U:H2'	1:X:2491:C:O4'	2.13	0.49
16:N:17:VAL:HG11	16:N:36:PHE:HB2	1.94	0.49
1:X:1219:C:H5''	11:I:7:LYS:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:22:VAL:HG13	5:C:106:MET:HG2	1.93	0.49
11:I:62:LYS:HZ3	11:I:64:GLY:CA	2.21	0.49
1:X:746:G:N7	1:X:774:A:C5	2.81	0.49
13:K:3:HIS:CG	13:K:5:LYS:NZ	2.80	0.49
16:N:75:ASN:ND2	16:N:78:THR:H	2.10	0.49
1:X:2178:U:H2'	1:X:2179:C:C6	2.48	0.49
1:X:418:C:H4'	1:X:418:C:OP2	2.13	0.49
3:A:161:THR:O	3:A:196:VAL:HG23	2.13	0.49
19:Q:71:GLN:HG2	19:Q:72:ARG:N	2.27	0.49
13:K:10:LEU:HD23	13:K:17:ARG:HB2	1.95	0.49
1:X:1674:C:H2'	1:X:1675:C:H6	1.78	0.49
10:H:83:ARG:NE	10:H:89:ILE:HD11	2.28	0.49
3:A:150:GLY:O	3:A:152:GLY:N	2.46	0.49
18:P:38:VAL:HG12	18:P:97:VAL:HG21	1.95	0.49
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.94	0.48
1:X:827:C:H2'	1:X:828:C:C6	2.48	0.48
4:B:2:LYS:HB2	4:B:200:SER:HB3	1.95	0.48
1:X:969:U:C4	12:J:17:ARG:HB2	2.48	0.48
1:X:2212:U:H2'	1:X:2213:G:C8	2.48	0.48
14:L:27:LEU:HD23	14:L:44:ASP:HA	1.95	0.48
1:X:224:G:H4'	1:X:399:G:C5	2.48	0.48
14:L:8:ARG:HG3	14:L:9:ARG:H	1.77	0.48
14:L:68:ALA:HB1	14:L:102:ALA:HB3	1.95	0.48
16:N:49:ASP:HA	16:N:52:ASN:HB2	1.95	0.48
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.95	0.48
1:X:609:U:H5'	11:I:18:ARG:HD3	1.94	0.48
1:X:1329:U:H2'	1:X:1330:G:C8	2.48	0.48
21:S:132:GLN:HE21	21:S:132:GLN:H	1.61	0.48
15:M:5:ILE:HB	15:M:7:ILE:HG12	1.95	0.48
1:X:791:G:H5'	3:A:48:ARG:HH21	1.77	0.48
10:H:110:VAL:HG23	10:H:129:LEU:HD12	1.94	0.48
1:X:2362:G:H2'	1:X:2363:G:H8	1.77	0.48
7:E:9:ILE:HD11	7:E:69:ARG:HG2	1.95	0.48
14:L:30:SER:HB2	14:L:43:ILE:HD11	1.96	0.48
14:L:30:SER:O	14:L:40:ALA:HA	2.13	0.48
1:X:1833:U:H2'	1:X:1834:G:C8	2.48	0.48
1:X:517:A:H5''	1:X:518:A:H5'	1.96	0.48
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.96	0.48
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.94	0.48
9:G:96:ASP:O	9:G:98:LYS:N	2.46	0.48
14:L:8:ARG:HG3	14:L:9:ARG:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:13:ARG:HE	11:I:13:ARG:H	1.62	0.48
1:X:2209:G:H4'	23:U:46:LEU:HB2	1.96	0.48
20:R:95:ARG:HH12	20:R:107:ALA:H	1.61	0.48
1:X:1922:U:OP1	1:X:2583:U:O2'	2.29	0.48
1:X:879:A:H2'	1:X:879:A:N3	2.29	0.48
1:X:2307:A:H2'	1:X:2308:A:C8	2.49	0.48
1:X:1753:A:O5'	1:X:1753:A:C8	2.63	0.48
1:X:572:G:N3	16:N:37:GLN:NE2	2.60	0.48
1:X:1777:A:H1'	1:X:1921:A:N6	2.29	0.48
1:X:2522:G:H2'	1:X:2523:G:C8	2.49	0.48
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.96	0.48
1:X:1468:A:H8	1:X:1468:A:O5'	1.97	0.47
20:R:25:LEU:HD12	20:R:81:VAL:HB	1.96	0.47
13:K:3:HIS:HB3	13:K:5:LYS:HE2	1.96	0.47
1:X:2774:U:O2'	1:X:2775:U:H5''	2.14	0.47
1:X:1169:C:H4'	25:W:28:ILE:O	2.14	0.47
21:S:117:VAL:HB	21:S:168:VAL:HG13	1.97	0.47
1:X:88:G:OP2	1:X:89:A:H3'	2.14	0.47
14:L:12:ARG:HA	14:L:92:GLY:O	2.14	0.47
1:X:1257:U:H5''	11:I:17:LYS:HG3	1.95	0.47
1:X:1582:A:OP1	3:A:211:ARG:NE	2.43	0.47
21:S:3:LEU:HD13	21:S:4:THR:H	1.78	0.47
1:X:1685:A:N6	1:X:1693:A:H61	2.12	0.47
1:X:2516:U:H2'	1:X:2517:C:C6	2.49	0.47
23:U:43:ARG:HG2	23:U:44:ALA:N	2.30	0.47
1:X:2779:C:H2'	1:X:2780:A:H8	1.79	0.47
1:X:1998:A:N3	26:Z:6:VAL:HG23	2.29	0.47
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.49	0.47
17:O:11:GLN:NE2	17:O:38:LEU:HB3	2.30	0.47
3:A:43:ARG:HH21	3:A:54:ILE:HG13	1.80	0.47
5:C:186:LEU:HG	5:C:188:ILE:HG12	1.95	0.47
5:C:3:GLN:O	5:C:12:GLY:HA3	2.15	0.47
1:X:503:G:H2'	1:X:504:G:O4'	2.15	0.47
11:I:78:SER:HB3	11:I:112:GLY:HA3	1.96	0.47
1:X:681:A:H8	1:X:681:A:H5''	1.79	0.47
1:X:1173:G:H1'	17:O:21:ARG:HD2	1.97	0.47
3:A:244:ARG:HB3	3:A:252:LYS:HZ2	1.80	0.47
20:R:105:ARG:HH22	20:R:112:LYS:CA	2.28	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
2:Y:64:C:H2'	2:Y:65:A:H8	1.79	0.47
13:K:11:ASN:ND2	13:K:12:ARG:HE	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:922:A:H2'	1:X:923:A:C8	2.50	0.47
26:Z:16:ARG:O	26:Z:20:ARG:HD2	2.14	0.47
1:X:2498:U:H4'	1:X:2499:C:OP1	2.14	0.47
1:X:1662:G:H5''	1:X:1663:C:H5'	1.96	0.47
1:X:1854:G:H1	1:X:1863:U:H3	1.62	0.47
1:X:1787:U:H2'	1:X:1788:C:C6	2.50	0.47
1:X:203:G:H5'	1:X:234:C:H4'	1.97	0.47
20:R:22:VAL:HG13	20:R:81:VAL:O	2.14	0.47
5:C:112:GLN:HA	5:C:116:LYS:HD3	1.96	0.47
1:X:1287:A:C2'	1:X:1288:A:H5''	2.45	0.47
17:O:57:GLN:H	17:O:97:GLY:HA2	1.79	0.47
1:X:241:C:H2'	1:X:242:A:H5''	1.96	0.47
22:T:14:ARG:HG3	22:T:15:ASP:H	1.80	0.47
1:X:2343:C:H2'	1:X:2344:G:O4'	2.15	0.47
30:4:2:LYS:HA	30:4:2:LYS:HE2	1.97	0.47
1:X:1342:U:H5''	1:X:1343:C:H5	1.80	0.47
9:G:75:ILE:HG13	9:G:75:ILE:H	1.58	0.47
1:X:341:A:C2	1:X:1223:G:H2'	2.50	0.46
1:X:1788:C:H2'	1:X:1789:U:H6	1.81	0.46
1:X:1367:A:H2'	1:X:1368:G:O4'	2.16	0.46
7:E:17:VAL:HG13	7:E:26:VAL:HG22	1.97	0.46
8:F:77:LEU:HD13	8:F:107:ILE:HG23	1.96	0.46
1:X:1509:A:H8	1:X:1510:A:C8	2.33	0.46
4:B:195:LEU:H	15:M:2:GLN:HG2	1.79	0.46
23:U:47:HIS:HD2	23:U:48:LYS:O	1.97	0.46
12:J:69:ILE:HG23	12:J:104:MET:HA	1.97	0.46
5:C:158:ARG:HA	5:C:169:VAL:HG21	1.96	0.46
3:A:67:PHE:HD2	3:A:153:ALA:HB3	1.79	0.46
20:R:15:HIS:O	20:R:16:PHE:HB3	2.15	0.46
4:B:120:TRP:O	4:B:121:ASN:HB2	2.14	0.46
1:X:341:A:HO2'	1:X:342:G:H8	1.63	0.46
1:X:651:C:H2'	1:X:652:C:H5''	1.98	0.46
3:A:243:GLY:C	3:A:244:ARG:HD3	2.36	0.46
1:X:1278:A:H61	1:X:1996:A:H5''	1.80	0.46
14:L:10:LYS:O	14:L:14:ARG:HB2	2.16	0.46
1:X:2661:G:O6	1:X:2708:U:H1'	2.16	0.46
9:G:108:GLY:H	9:G:110:LEU:HG	1.79	0.46
4:B:131:SER:O	4:B:132:LYS:CB	2.64	0.46
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.96	0.46
1:X:240:U:H2'	1:X:241:C:O4'	2.15	0.46
3:A:43:ARG:HD2	3:A:43:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:19:ARG:HB2	30:4:24:LEU:HD13	1.98	0.46
1:X:956:A:C4	1:X:2427:A:C2	3.03	0.46
26:Z:33:CYS:SG	26:Z:46:CYS:SG	3.11	0.46
7:E:124:ALA:HB3	7:E:132:ASP:HB2	1.97	0.46
4:B:133:LYS:HE2	4:B:133:LYS:HB3	1.61	0.46
15:M:27:PHE:HB3	15:M:93:ILE:CD1	2.45	0.46
3:A:252:LYS:H	3:A:252:LYS:HE3	1.80	0.46
21:S:87:THR:O	21:S:88:TYR:HB3	2.16	0.46
9:G:36:ASN:O	9:G:38:GLU:N	2.34	0.46
1:X:590:C:H2'	1:X:591:G:C8	2.51	0.46
5:C:5:ASN:HB2	5:C:10:ASN:HA	1.98	0.46
1:X:2266:A:N6	1:X:2323:U:H3	2.13	0.46
16:N:74:MET:HB3	16:N:75:ASN:H	1.63	0.46
14:L:66:ASP:C	14:L:68:ALA:H	2.19	0.46
1:X:1845:A:N1	1:X:2070:G:H1'	2.30	0.46
9:G:90:LEU:HD23	9:G:94:LYS:HA	1.98	0.46
1:X:1882:G:H21	1:X:1885:C:H41	1.62	0.46
20:R:25:LEU:H	20:R:80:LYS:HA	1.81	0.46
12:J:73:LYS:HB3	12:J:95:VAL:HG12	1.97	0.46
3:A:67:PHE:HB3	3:A:153:ALA:H	1.81	0.46
1:X:627:A:H2'	1:X:628:A:C8	2.50	0.46
9:G:162:LYS:N	9:G:163:PRO:HD2	2.31	0.46
10:H:27:SER:HB2	10:H:121:ARG:HH22	1.81	0.46
23:U:10:LYS:HD3	23:U:60:VAL:HG21	1.97	0.46
10:H:24:VAL:HA	10:H:51:ILE:HG22	1.98	0.46
1:X:331:U:H1'	5:C:162:ARG:NH1	2.31	0.46
1:X:1630:A:C2	18:P:114:ALA:HB2	2.51	0.46
1:X:2167:A:H2'	1:X:2168:A:H8	1.80	0.46
11:I:57:ILE:HA	11:I:57:ILE:HD13	1.93	0.46
11:I:30:ALA:HB3	11:I:34:HIS:HE1	1.78	0.46
30:4:19:ARG:HD2	30:4:24:LEU:HD22	1.98	0.46
4:B:181:LEU:HD11	15:M:12:LEU:HD23	1.98	0.46
21:S:127:PRO:C	21:S:129:ARG:H	2.19	0.46
5:C:45:THR:HB	5:C:86:PRO:O	2.15	0.45
12:J:14:PHE:CE1	12:J:90:ALA:HA	2.46	0.45
1:X:2795:A:H4'	13:K:5:LYS:HG2	1.97	0.45
9:G:57:LEU:HD22	9:G:170:PRO:HA	1.98	0.45
5:C:119:ALA:H	5:C:189:ASP:HA	1.81	0.45
3:A:108:PRO:HB3	3:A:143:HIS:HE1	1.81	0.45
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.45
1:X:2324:G:N3	1:X:2360:C:H2'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:95:LEU:HD12	3:A:105:ILE:HD13	1.98	0.45
10:H:26:ASN:HD22	10:H:26:ASN:HA	1.41	0.45
1:X:1142:G:OP1	9:G:107:GLN:HB3	2.16	0.45
1:X:1466:C:H2'	1:X:1467:U:C1'	2.46	0.45
9:G:67:ARG:CB	9:G:70:PHE:HA	2.47	0.45
1:X:1817:U:O4'	3:A:252:LYS:HD3	2.16	0.45
5:C:164:VAL:HB	5:C:165:SER:H	1.57	0.45
9:G:157:PRO:C	9:G:159:SER:H	2.20	0.45
18:P:94:GLU:HG3	18:P:127:ILE:HB	1.99	0.45
1:X:2477:C:H5'	1:X:2477:C:H6	1.81	0.45
12:J:28:VAL:HG21	12:J:135:ARG:HA	1.98	0.45
2:Y:54:U:H4'	2:Y:54:U:OP1	2.17	0.45
1:X:1468:A:O5'	1:X:1468:A:C8	2.70	0.45
1:X:2772:U:H2'	1:X:2773:G:C8	2.52	0.45
4:B:14:ILE:HG13	15:M:20:HIS:CE1	2.52	0.45
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.98	0.45
11:I:108:LEU:HB2	11:I:122:VAL:HG11	1.98	0.45
5:C:102:LEU:O	5:C:106:MET:HB2	2.17	0.45
1:X:2397:A:H2'	1:X:2398:U:O4'	2.17	0.45
1:X:29:U:H6	1:X:29:U:O5'	2.00	0.45
19:Q:11:VAL:HB	19:Q:26:SER:HB2	1.99	0.45
1:X:1467:U:C5'	1:X:1467:U:C6	3.00	0.45
1:X:2074:U:H1'	23:U:48:LYS:HE3	1.97	0.45
20:R:48:VAL:HG12	20:R:50:GLY:H	1.80	0.45
1:X:336:A:H2'	1:X:337:G:C8	2.52	0.45
1:X:227:G:H2'	1:X:228:A:C8	2.52	0.45
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.51	0.45
1:X:1268:U:C2	5:C:66:ASN:HA	2.52	0.45
1:X:1187:A:H2'	1:X:1188:A:C8	2.52	0.45
1:X:1467:U:H5	1:X:1468:A:O4'	2.00	0.45
5:C:43:ALA:HB1	5:C:86:PRO:CB	2.41	0.45
13:K:17:ARG:NH1	13:K:20:LEU:CD2	2.77	0.45
1:X:1218:C:O4'	11:I:13:ARG:HD3	2.16	0.45
6:D:136:LEU:HD11	6:D:143:TYR:HB2	1.99	0.45
8:F:93:LYS:HA	21:S:109:GLN:HG3	1.98	0.45
10:H:2:ILE:HB	10:H:45:ALA:HB3	1.99	0.45
17:O:69:ILE:HG22	17:O:86:HIS:HB3	1.98	0.45
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.17	0.45
5:C:45:THR:HG22	5:C:47:THR:OG1	2.17	0.45
1:X:231:G:H4'	1:X:397:U:H5"	1.98	0.45
1:X:2797:G:OP2	13:K:3:HIS:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1373:G:H1	1:X:2192:U:H3	1.64	0.45
3:A:250:TRP:HB3	3:A:251:GLY:H	1.54	0.45
23:U:29:GLY:C	23:U:31:GLY:H	2.16	0.45
1:X:1919:A:C2	1:X:1926:U:N3	2.62	0.45
1:X:1467:U:C5	1:X:1468:A:O4'	2.70	0.45
25:W:3:ILE:HD12	25:W:51:LEU:HD13	1.99	0.44
1:X:1022:A:H5''	16:N:77:SER:HB2	2.00	0.44
1:X:1234:C:H2'	1:X:1235:C:H6	1.82	0.44
1:X:1437:A:H2'	1:X:1438:G:H8	1.82	0.44
5:C:146:GLU:HG3	5:C:185:ARG:NH1	2.32	0.44
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.99	0.44
19:Q:29:VAL:HG21	19:Q:38:ILE:HG13	1.98	0.44
1:X:800:U:H5''	1:X:801:A:H5'	1.99	0.44
23:U:22:GLY:N	23:U:39:LYS:HB2	2.32	0.44
1:X:814:G:OP1	5:C:50:GLN:HB2	2.18	0.44
1:X:1675:C:OP1	4:B:134:TRP:CD1	2.69	0.44
3:A:147:LEU:HD22	3:A:183:ARG:HH22	1.81	0.44
10:H:116:ARG:HG3	15:M:38:LYS:CE	2.47	0.44
1:X:424:G:H4'	1:X:425:A:O5'	2.18	0.44
9:G:132:PHE:CE1	9:G:145:HIS:HB2	2.52	0.44
15:M:28:ARG:O	15:M:96:ARG:NH2	2.50	0.44
20:R:45:LYS:HA	20:R:76:LEU:O	2.16	0.44
1:X:2545:A:N6	10:H:40:GLY:HA3	2.31	0.44
13:K:3:HIS:CE1	13:K:5:LYS:HZ3	2.34	0.44
12:J:61:ARG:HG2	21:S:175:ARG:HG3	2.00	0.44
7:E:103:LEU:HD11	7:E:131:ILE:HG12	1.99	0.44
12:J:92:GLU:HG3	12:J:93:TYR:CD2	2.51	0.44
1:X:553:C:H4'	1:X:554:U:OP1	2.17	0.44
5:C:74:VAL:HG23	5:C:76:THR:H	1.83	0.44
13:K:46:PRO:O	13:K:50:GLN:HG3	2.18	0.44
1:X:341:A:O2'	1:X:342:G:H8	2.01	0.44
3:A:248:THR:HB	3:A:249:PRO:HD2	2.00	0.44
1:X:1190:C:H2'	1:X:1191:G:H8	1.82	0.44
12:J:11:ARG:HH12	12:J:72:ASP:HB2	1.83	0.44
1:X:689:A:H8	1:X:2052:G:N2	2.06	0.44
1:X:1030:U:O2'	1:X:1032:A:H2	1.99	0.44
19:Q:60:GLY:H	19:Q:72:ARG:HH11	1.66	0.44
17:O:72:ARG:HD2	17:O:83:ARG:HH11	1.82	0.44
1:X:673:G:H5'	5:C:93:TYR:CE1	2.52	0.44
1:X:712:A:H2'	1:X:713:G:O4'	2.18	0.44
17:O:23:GLU:HB2	17:O:91:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1012:A:H2'	1:X:1013:G:O4'	2.17	0.44
1:X:585:U:H2'	1:X:586:G:C8	2.52	0.44
28:2:26:SER:CA	28:2:27:GLY:CA	2.95	0.44
1:X:1255:A:H2'	1:X:1256:C:C6	2.53	0.44
1:X:649:G:H22	1:X:660:G:N2	2.16	0.44
1:X:1273:G:H2'	1:X:1274:C:O4'	2.18	0.44
1:X:2339:A:H4'	11:I:56:LEU:HD21	2.00	0.44
1:X:1405:A:N6	19:Q:14:GLU:HG2	2.32	0.44
11:I:45:LYS:H	11:I:45:LYS:HD3	1.82	0.44
1:X:1674:C:H2'	1:X:1675:C:C6	2.53	0.43
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.18	0.43
16:N:17:VAL:HG13	16:N:39:LEU:HD12	1.98	0.43
1:X:1547:U:H2'	1:X:1548:U:C6	2.53	0.43
1:X:1421:U:H2'	1:X:1422:C:O4'	2.18	0.43
15:M:41:GLU:HG3	15:M:46:ARG:HD2	2.00	0.43
1:X:1979:C:H4'	1:X:1980:A:OP1	2.18	0.43
24:V:21:ARG:HG3	24:V:46:LEU:HD22	2.00	0.43
23:U:25:ARG:O	23:U:32:ARG:HD2	2.18	0.43
1:X:38:G:H21	5:C:42:THR:HG21	1.83	0.43
2:Y:39:C:H2'	14:L:97:HIS:HE1	1.83	0.43
1:X:116:A:C8	1:X:117:A:C8	3.06	0.43
15:M:33:VAL:HG22	15:M:51:GLU:HB2	2.00	0.43
1:X:875:G:O2'	2:Y:80:A:N3	2.44	0.43
3:A:97:TYR:HE2	3:A:103:ARG:HB2	1.83	0.43
1:X:748:A:H5'	1:X:749:C:OP2	2.19	0.43
1:X:748:A:H5''	1:X:749:C:H5	1.84	0.43
6:D:35:VAL:HG22	6:D:90:THR:HG23	1.99	0.43
22:T:25:LYS:HB2	22:T:37:LEU:HB3	2.00	0.43
1:X:2485:U:O2	1:X:2485:U:H2'	2.17	0.43
1:X:1307:U:H5''	1:X:1307:U:H6	1.83	0.43
5:C:6:VAL:HG12	5:C:7:ILE:HG12	1.99	0.43
18:P:39:ARG:HG3	18:P:97:VAL:HB	2.00	0.43
1:X:2310:G:H4'	22:T:43:THR:H	1.83	0.43
23:U:64:ALA:C	23:U:66:ALA:H	2.21	0.43
9:G:103:TYR:O	9:G:107:GLN:NE2	2.51	0.43
5:C:118:VAL:HG22	5:C:188:ILE:HD12	2.00	0.43
3:A:188:GLU:HG2	3:A:188:GLU:H	1.54	0.43
1:X:336:A:H2'	1:X:337:G:H8	1.83	0.43
6:D:60:ILE:HB	6:D:99:PHE:HE1	1.83	0.43
1:X:1765:C:O5'	1:X:1765:C:H6	2.01	0.43
19:Q:35:LYS:HA	19:Q:38:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1574:A:O2'	1:X:1575:C:H3'	2.18	0.43
11:I:28:LYS:NZ	11:I:36:GLY:CA	2.81	0.43
1:X:577:U:O5'	1:X:956:A:N6	2.52	0.43
1:X:2186:G:H2'	1:X:2187:A:C8	2.54	0.43
1:X:2556:A:H5''	1:X:2557:G:H5'	2.00	0.43
1:X:517:A:C5'	1:X:518:A:H5'	2.48	0.43
28:2:40:HIS:CA	28:2:41:GLN:CA	2.97	0.43
6:D:65:PRO:HA	6:D:89:VAL:HG13	2.01	0.43
1:X:2270:U:H2'	1:X:2271:C:C6	2.53	0.43
2:Y:30:C:H2'	2:Y:31:A:H8	1.84	0.43
1:X:1859:A:H2'	1:X:1860:A:C8	2.54	0.43
19:Q:28:TRP:CZ3	19:Q:77:LYS:HB2	2.53	0.43
4:B:77:ILE:HD13	15:M:3:THR:HG22	2.00	0.43
10:H:116:ARG:HG3	15:M:38:LYS:HE2	2.01	0.43
1:X:1329:U:H2'	1:X:1330:G:H8	1.84	0.43
21:S:51:LEU:HD13	21:S:86:VAL:HG21	2.00	0.43
4:B:105:THR:HB	4:B:166:THR:HA	2.01	0.43
1:X:890:U:H2'	1:X:891:A:H3'	2.00	0.43
20:R:9:HIS:H	20:R:9:HIS:CD2	2.37	0.43
1:X:651:C:C2'	1:X:652:C:H5''	2.49	0.43
3:A:108:PRO:HD2	3:A:111:LEU:HB2	2.01	0.43
10:H:113:PRO:HB3	10:H:132:GLU:HB3	2.01	0.43
23:U:51:ILE:HG12	23:U:59:THR:HB	2.00	0.43
1:X:460:U:O4	1:X:592:G:H1'	2.18	0.43
11:I:102:LYS:O	11:I:104:ARG:N	2.52	0.43
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.84	0.42
1:X:614:G:C8	11:I:98:LEU:HD21	2.53	0.42
1:X:590:C:H2'	1:X:591:G:H8	1.84	0.42
1:X:719:A:H2'	1:X:720:A:O4'	2.18	0.42
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.84	0.42
9:G:102:ARG:O	9:G:102:ARG:HG2	2.19	0.42
1:X:748:A:H3'	1:X:749:C:C6	2.53	0.42
6:D:73:SER:O	6:D:79:LEU:HB3	2.19	0.42
23:U:78:ILE:HG12	23:U:79:GLU:H	1.85	0.42
1:X:1583:A:H3'	3:A:86:PRO:HG3	2.01	0.42
17:O:36:LYS:NZ	17:O:54:TYR:HB3	2.35	0.42
12:J:78:LYS:HA	12:J:88:LYS:HZ3	1.84	0.42
1:X:533:C:H1'	1:X:563:U:O2'	2.19	0.42
11:I:83:LEU:HD23	11:I:84:GLU:H	1.84	0.42
1:X:1193:G:H2'	1:X:1194:U:C6	2.54	0.42
1:X:333:A:O4'	1:X:351:A:H1'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:873:U:H1'	1:X:2247:A:H5''	2.00	0.42
1:X:216:U:H2'	1:X:217:U:C6	2.55	0.42
12:J:26:ASP:HB3	12:J:27:TYR:H	1.61	0.42
1:X:1790:G:H5'	1:X:1811:A:N6	2.34	0.42
3:A:231:HIS:HD2	3:A:233:HIS:N	2.11	0.42
1:X:1336:G:OP1	18:P:105:ARG:HD2	2.20	0.42
19:Q:66:GLY:O	19:Q:68:PHE:N	2.52	0.42
19:Q:68:PHE:C	19:Q:70:GLY:H	2.21	0.42
1:X:103:U:H2'	1:X:104:C:H6	1.82	0.42
1:X:1483:G:N2	1:X:1541:G:H1'	2.35	0.42
1:X:394:U:H2'	1:X:395:G:C8	2.54	0.42
1:X:1779:C:OP1	3:A:222:ARG:NH1	2.52	0.42
1:X:771:C:O2	1:X:1964:A:H2	2.03	0.42
2:Y:78:A:H2'	2:Y:79:U:O4'	2.18	0.42
1:X:1974:U:H2'	1:X:1975:G:H5''	2.00	0.42
1:X:2015:G:O2'	4:B:145:LYS:HE2	2.20	0.42
22:T:23:VAL:HA	22:T:38:VAL:HG23	2.01	0.42
9:G:107:GLN:C	9:G:109:GLY:N	2.72	0.42
1:X:1493:A:H2'	1:X:1494:G:O4'	2.19	0.42
10:H:77:THR:HA	10:H:94:ASN:HB3	2.00	0.42
1:X:409:G:H1'	23:U:45:ASN:HD22	1.83	0.42
1:X:1339:U:H5''	1:X:1994:U:H1'	2.01	0.42
1:X:2784:A:C6	1:X:2866:A:C8	3.07	0.42
1:X:1384:G:N2	1:X:1385:C:H41	2.17	0.42
3:A:182:LEU:HB2	3:A:268:ARG:O	2.19	0.42
1:X:1687:C:H6	1:X:1687:C:O5'	2.01	0.42
9:G:98:LYS:HB3	9:G:116:ARG:HB2	2.01	0.42
1:X:954:U:P	11:I:38:LYS:HG2	2.59	0.42
9:G:107:GLN:C	9:G:109:GLY:H	2.23	0.42
15:M:33:VAL:HA	15:M:51:GLU:HB2	2.01	0.42
18:P:89:ARG:CZ	18:P:132:GLY:H	2.32	0.42
19:Q:53:ILE:HD13	19:Q:80:VAL:HG13	2.01	0.42
1:X:542:A:H2	1:X:2004:U:O2'	2.01	0.42
16:N:88:ILE:CG1	17:O:49:GLU:HB2	2.48	0.42
3:A:96:HIS:CE1	3:A:100:GLY:HA2	2.47	0.42
10:H:85:ASP:OD2	10:H:87:SER:HB3	2.20	0.42
21:S:3:LEU:HB3	21:S:56:VAL:HA	2.02	0.42
1:X:2238:G:O4'	1:X:2406:C:H2'	2.20	0.42
1:X:1736:C:H2'	1:X:1737:G:H8	1.84	0.42
21:S:23:ALA:HA	21:S:83:PHE:O	2.19	0.42
1:X:1563:U:H2'	1:X:1564:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:852:U:H2'	1:X:853:C:C6	2.55	0.42
1:X:520:C:H2'	1:X:520:C:O2	2.18	0.42
1:X:616:U:H5'	1:X:617:U:OP2	2.20	0.42
1:X:689:A:H2	1:X:815:A:H61	1.64	0.42
1:X:347:C:H2'	1:X:348:U:C6	2.54	0.42
1:X:2237:C:O2'	1:X:2406:C:OP2	2.37	0.42
1:X:830:C:O2'	1:X:852:U:H5''	2.19	0.42
1:X:1441:A:H4'	1:X:1442:C:O5'	2.20	0.42
1:X:56:C:H2'	1:X:57:G:O4'	2.19	0.42
1:X:693:A:H2'	1:X:694:G:C8	2.54	0.42
23:U:52:ARG:HD3	23:U:62:LEU:HD22	2.01	0.42
12:J:48:ILE:HD12	12:J:71:PRO:HG3	2.01	0.42
19:Q:35:LYS:O	19:Q:38:ILE:HG22	2.20	0.42
9:G:33:ILE:O	9:G:69:ASP:OD1	2.38	0.42
12:J:82:THR:HB	12:J:83:ARG:H	1.76	0.42
1:X:1033:G:N2	1:X:1153:A:H2	2.10	0.42
1:X:101:A:H5''	1:X:102:C:H5	1.85	0.42
1:X:487:G:H4'	1:X:512:A:N1	2.34	0.42
12:J:88:LYS:HB3	12:J:89:GLY:H	1.59	0.42
3:A:43:ARG:N	3:A:43:ARG:CD	2.83	0.42
4:B:177:ALA:C	4:B:179:GLU:H	2.24	0.42
1:X:1128:G:H3'	1:X:1129:A:H5''	2.01	0.42
9:G:106:TYR:O	9:G:108:GLY:N	2.48	0.41
1:X:2621:G:OP1	9:G:110:LEU:HD22	2.20	0.41
1:X:649:G:N2	1:X:660:G:N2	2.68	0.41
1:X:1219:C:H2'	1:X:1220:G:O4'	2.20	0.41
4:B:85:ALA:H	4:B:86:PRO:HD2	1.85	0.41
1:X:1644:G:H2'	1:X:1645:U:H6	1.85	0.41
10:H:25:LEU:HD11	10:H:52:VAL:HG23	2.01	0.41
1:X:339:U:O4	1:X:343:A:C8	2.73	0.41
1:X:2445:C:H5''	30:4:6:SER:HB3	2.01	0.41
3:A:88:ARG:O	3:A:89:SER:CB	2.68	0.41
1:X:534:U:H4'	1:X:564:U:H4'	2.01	0.41
20:R:10:HIS:O	20:R:11:ASN:CB	2.68	0.41
5:C:33:TRP:CD1	5:C:95:LEU:HB2	2.55	0.41
6:D:40:LEU:HB2	6:D:41:GLY:H	1.70	0.41
4:B:5:LEU:HG	4:B:195:LEU:HD11	2.02	0.41
1:X:679:C:H2'	1:X:680:U:C6	2.55	0.41
21:S:25:ASN:O	21:S:26:LYS:HB3	2.20	0.41
29:3:31:HIS:CA	29:3:32:GLN:CA	2.98	0.41
1:X:1276:U:H1'	26:Z:10:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2226:A:H2'	1:X:2227:C:C6	2.55	0.41
6:D:34:ILE:HG12	6:D:96:MET:HG3	2.02	0.41
1:X:2851:G:H4'	15:M:8:ASN:ND2	2.35	0.41
1:X:1542:G:N2	1:X:1562:G:H1	1.99	0.41
1:X:2796:A:H2'	1:X:2797:G:C8	2.55	0.41
17:O:56:VAL:HG12	17:O:97:GLY:HA3	2.02	0.41
3:A:67:PHE:CD2	3:A:153:ALA:HB3	2.56	0.41
1:X:1437:A:H2'	1:X:1438:G:C8	2.55	0.41
25:W:45:LYS:O	25:W:48:LYS:HB2	2.19	0.41
1:X:85:C:H5''	20:R:42:ARG:HH21	1.85	0.41
1:X:1117:G:H2'	1:X:1118:G:H8	1.85	0.41
15:M:55:ILE:O	15:M:103:LYS:O	2.38	0.41
11:I:62:LYS:CE	11:I:64:GLY:HA2	2.45	0.41
16:N:93:LYS:CE	17:O:5:ILE:HD13	2.37	0.41
1:X:71:A:C5	24:V:54:ASN:HB3	2.55	0.41
1:X:1672:A:H3'	1:X:1673:C:C6	2.55	0.41
1:X:2266:A:C2	1:X:2325:A:N6	2.81	0.41
5:C:164:VAL:C	5:C:166:TRP:N	2.72	0.41
1:X:922:A:N1	1:X:2256:G:H1'	2.34	0.41
14:L:26:ARG:HG2	14:L:86:GLN:HB3	2.02	0.41
17:O:73:LYS:HB2	17:O:82:ARG:HB2	2.03	0.41
6:D:114:PHE:HZ	6:D:176:PRO:HG2	1.84	0.41
1:X:1658:A:H2'	1:X:1659:G:O4'	2.21	0.41
9:G:50:PRO:HG2	9:G:53:ARG:HG3	2.02	0.41
1:X:2736:U:H1'	1:X:2737:A:H5''	2.02	0.41
12:J:42:TRP:CD1	12:J:97:VAL:HG12	2.56	0.41
4:B:149:ARG:CZ	9:G:106:TYR:CD1	3.02	0.41
1:X:203:G:H1'	1:X:205:A:N6	2.32	0.41
1:X:572:G:H22	1:X:587:A:H2	1.68	0.41
1:X:2292:C:H5''	6:D:88:LYS:HD3	2.01	0.41
4:B:4:ILE:HD13	4:B:28:ALA:HB1	2.02	0.41
17:O:5:ILE:CD1	17:O:6:GLN:H	2.19	0.41
1:X:829:C:H2'	1:X:830:C:H6	1.86	0.41
1:X:2035:G:N2	4:B:148:GLY:O	2.48	0.41
3:A:169:GLU:HB3	3:A:170:SER:H	1.63	0.41
12:J:36:ILE:HD12	12:J:133:VAL:HG21	2.02	0.41
6:D:92:ARG:HB2	6:D:92:ARG:NH2	2.36	0.41
25:W:12:ARG:HG3	25:W:50:LEU:HD21	2.03	0.41
12:J:14:PHE:HE1	12:J:90:ALA:CA	2.28	0.41
1:X:2508:G:H5''	1:X:2509:A:H5''	2.01	0.41
20:R:110:SER:OG	20:R:111:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:59:LEU:HD12	22:T:79:ILE:HD12	2.02	0.41
20:R:84:VAL:HG23	20:R:88:THR:O	2.20	0.41
3:A:134:ARG:HG3	3:A:135:PHE:HD2	1.86	0.41
4:B:149:ARG:NH1	9:G:106:TYR:HB2	2.36	0.41
23:U:22:GLY:H	23:U:39:LYS:HB2	1.85	0.41
11:I:28:LYS:HZ2	11:I:36:GLY:HA2	1.86	0.41
19:Q:12:ILE:O	19:Q:16:ALA:HB3	2.20	0.41
22:T:14:ARG:HG3	22:T:15:ASP:N	2.36	0.41
4:B:5:LEU:HD22	4:B:49:ILE:HG22	2.02	0.41
20:R:7:GLY:HA3	20:R:42:ARG:O	2.20	0.41
21:S:13:LYS:HB2	21:S:18:MET:HB2	2.03	0.41
22:T:48:GLY:H	22:T:51:VAL:HB	1.86	0.41
18:P:25:PHE:C	18:P:25:PHE:CD2	2.94	0.41
7:E:48:ASP:HB3	7:E:49:GLN:HE21	1.86	0.41
1:X:2206:C:H1'	3:A:262:LYS:HE3	2.02	0.41
1:X:2552:C:H5''	1:X:2553:G:H5''	2.03	0.41
1:X:1378:A:H2'	1:X:1378:A:N3	2.36	0.41
4:B:67:PHE:CE1	4:B:75:THR:HG22	2.56	0.41
5:C:3:GLN:CG	5:C:116:LYS:HD2	2.51	0.41
1:X:1997:A:H2'	1:X:1998:A:C8	2.56	0.41
5:C:146:GLU:HB3	5:C:184:ASP:HB2	2.03	0.41
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.48	0.41
1:X:2407:G:H5''	1:X:2408:G:OP1	2.21	0.41
1:X:1443:G:H2'	1:X:1444:C:H6	1.86	0.41
10:H:27:SER:HA	10:H:50:ILE:HD12	2.02	0.41
1:X:2869:U:H2'	1:X:2870:C:C6	2.56	0.41
1:X:986:A:O3'	16:N:48:ARG:NH1	2.54	0.41
4:B:14:ILE:HG22	4:B:21:ILE:HB	2.04	0.40
26:Z:51:TYR:HA	26:Z:55:ARG:HA	2.03	0.40
1:X:654:A:H2'	1:X:654:A:N3	2.36	0.40
5:C:166:TRP:HB3	5:C:167:VAL:H	1.63	0.40
1:X:88:G:H3'	1:X:89:A:H5''	2.04	0.40
22:T:14:ARG:CG	22:T:15:ASP:H	2.34	0.40
1:X:1623:C:H4'	1:X:1624:A:O5'	2.21	0.40
23:U:14:VAL:O	23:U:15:VAL:HG22	2.21	0.40
1:X:2561:G:H8	1:X:2561:G:H5'	1.86	0.40
1:X:70:A:H5'	1:X:71:A:C3'	2.44	0.40
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.54	0.40
20:R:108:VAL:HB	20:R:109:ALA:H	1.49	0.40
19:Q:68:PHE:C	19:Q:70:GLY:N	2.75	0.40
12:J:79:PRO:CD	12:J:88:LYS:HD2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:64:C:H2'	2:Y:65:A:C8	2.56	0.40
9:G:162:LYS:N	9:G:163:PRO:CD	2.85	0.40
2:Y:58:G:H4'	2:Y:59:A:H5"	2.04	0.40
19:Q:89:GLU:HB3	19:Q:90:ALA:H	1.51	0.40
21:S:95:SER:HB3	21:S:119:ASN:HD22	1.86	0.40
23:U:21:ARG:HG2	23:U:40:ARG:HG2	2.04	0.40
1:X:10:A:H2'	1:X:11:G:C8	2.56	0.40
1:X:463:C:N4	1:X:467:U:H5	2.08	0.40
1:X:923:A:C5	12:J:12:LYS:HE3	2.57	0.40
5:C:188:ILE:H	5:C:188:ILE:HG13	1.42	0.40
1:X:1467:U:H3'	1:X:1467:U:C6	2.54	0.40
14:L:15:ARG:HA	14:L:15:ARG:HD3	1.93	0.40
25:W:3:ILE:O	25:W:31:SER:HA	2.22	0.40
1:X:811:G:OP2	5:C:56:ARG:HG3	2.21	0.40
1:X:1004:A:H5'	17:O:71:ILE:HD11	2.04	0.40
12:J:54:VAL:CG1	12:J:121:LEU:HB3	2.52	0.40
14:L:67:THR:O	14:L:70:ALA:HB3	2.22	0.40
1:X:1016:C:O2'	9:G:56:THR:HG21	2.21	0.40
1:X:682:G:C2'	1:X:682:G:N3	2.83	0.40
11:I:72:TYR:CE2	11:I:105:PRO:HB2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	238/274 (87%)	170 (71%)	39 (16%)	29 (12%)	0	2
4	B	203/211 (96%)	172 (85%)	17 (8%)	14 (7%)	1	10
5	C	195/205 (95%)	131 (67%)	37 (19%)	27 (14%)	0	1
6	D	175/180 (97%)	136 (78%)	26 (15%)	13 (7%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	E	169/185 (91%)	132 (78%)	29 (17%)	8 (5%)	3	22
8	F	69/144 (48%)	59 (86%)	8 (12%)	2 (3%)	6	36
9	G	140/174 (80%)	103 (74%)	23 (16%)	14 (10%)	1	4
10	H	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	3	24
11	I	139/156 (89%)	79 (57%)	34 (24%)	26 (19%)	0	0
12	J	134/141 (95%)	97 (72%)	26 (19%)	11 (8%)	1	7
13	K	111/116 (96%)	96 (86%)	7 (6%)	8 (7%)	1	10
14	L	102/114 (90%)	72 (71%)	20 (20%)	10 (10%)	1	4
15	M	106/166 (64%)	95 (90%)	7 (7%)	4 (4%)	4	28
16	N	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	4	31
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	1
18	P	125/134 (93%)	114 (91%)	5 (4%)	6 (5%)	3	22
19	Q	91/95 (96%)	59 (65%)	19 (21%)	13 (14%)	0	1
20	R	108/115 (94%)	66 (61%)	23 (21%)	19 (18%)	0	0
21	S	173/237 (73%)	145 (84%)	20 (12%)	8 (5%)	3	23
22	T	82/91 (90%)	64 (78%)	9 (11%)	9 (11%)	0	3
23	U	70/81 (86%)	39 (56%)	17 (24%)	14 (20%)	0	0
24	V	64/67 (96%)	57 (89%)	3 (5%)	4 (6%)	2	13
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
26	Z	56/60 (93%)	47 (84%)	5 (9%)	4 (7%)	1	10
30	4	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	17
All	All	2977/3390 (88%)	2294 (77%)	415 (14%)	268 (9%)	1	5

All (268) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	151	LYS
3	A	170	SER
3	A	187	SER
3	A	199	ALA
3	A	248	THR
3	A	250	TRP
3	A	271	VAL
4	B	76	ARG

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Mol	Chain	Res	Type
4	B	86	PRO
4	B	122	PHE
5	C	20	PRO
5	C	64	THR
5	C	67	ALA
5	C	129	LYS
5	C	163	ASN
5	C	164	VAL
5	C	172	VAL
7	E	126	PRO
9	G	33	ILE
9	G	37	ASP
9	G	67	ARG
9	G	91	THR
9	G	97	ASP
9	G	104	THR
9	G	107	GLN
9	G	158	HIS
9	G	170	PRO
10	H	27	SER
10	H	29	ILE
11	I	17	LYS
11	I	18	ARG
11	I	37	GLN
11	I	39	SER
11	I	48	PHE
11	I	56	LEU
11	I	59	ARG
11	I	62	LYS
11	I	86	THR
11	I	98	LEU
11	I	103	ASN
12	J	13	GLN
12	J	26	ASP
12	J	83	ARG
12	J	89	GLY
12	J	136	GLU
13	K	6	ALA
13	K	8	ARG
13	K	95	THR
14	L	21	THR
14	L	40	ALA

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Mol	Chain	Res	Type
14	L	68	ALA
14	L	95	LYS
15	M	27	PHE
15	M	29	PRO
16	N	7	GLY
16	N	8	ILE
16	N	92	ARG
17	O	10	LYS
17	O	31	ASP
17	O	97	GLY
18	P	9	ARG
18	P	50	VAL
19	Q	12	ILE
19	Q	13	SER
19	Q	67	ARG
19	Q	69	ILE
19	Q	84	GLU
20	R	11	ASN
20	R	62	MET
20	R	66	GLN
20	R	82	ALA
20	R	98	ILE
20	R	108	VAL
21	S	26	LYS
21	S	156	GLU
22	T	15	ASP
22	T	19	LYS
23	U	15	VAL
23	U	27	ASP
23	U	47	HIS
23	U	48	LYS
23	U	60	VAL
24	V	2	LYS
26	Z	4	HIS
3	A	54	ILE
3	A	98	ALA
3	A	197	GLY
3	A	198	ASN
3	A	220	HIS
4	B	121	ASN
4	B	123	ALA
4	B	132	LYS

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Mol	Chain	Res	Type
4	B	135	HIS
4	B	146	THR
5	C	9	GLN
5	C	22	VAL
5	C	55	GLY
5	C	60	GLY
5	C	121	ASP
5	C	125	ILE
5	C	127	ASP
5	C	165	SER
5	C	195	ILE
6	D	4	LEU
6	D	9	ASN
6	D	121	ALA
6	D	124	GLY
7	E	19	ALA
10	H	31	GLY
11	I	19	VAL
11	I	47	ALA
11	I	49	PHE
12	J	17	ARG
12	J	21	ASP
12	J	60	ARG
12	J	80	ALA
13	K	14	SER
13	K	92	GLY
14	L	45	ASP
14	L	92	GLY
15	M	41	GLU
16	N	87	ASN
17	O	30	GLY
17	O	48	GLY
19	Q	6	ILE
19	Q	63	LYS
20	R	5	SER
20	R	6	ALA
20	R	7	GLY
20	R	60	PRO
21	S	57	GLU
21	S	88	TYR
21	S	91	PRO
22	T	5	LYS

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Mol	Chain	Res	Type
22	T	14	ARG
23	U	19	ILE
23	U	30	VAL
23	U	41	VAL
23	U	55	GLY
23	U	78	ILE
26	Z	36	CYS
26	Z	37	HIS
30	4	20	HIS
3	A	109	GLU
3	A	206	LEU
3	A	219	PRO
3	A	249	PRO
3	A	263	ARG
4	B	73	ALA
4	B	74	PRO
5	C	15	ILE
5	C	173	ALA
5	C	189	ASP
5	C	190	ALA
6	D	5	LYS
6	D	122	PHE
7	E	55	PRO
7	E	119	ALA
7	E	173	ALA
9	G	34	PRO
9	G	68	PRO
10	H	41	ASN
11	I	54	SER
11	I	65	PHE
11	I	82	ASP
13	K	93	GLY
14	L	52	ALA
14	L	96	TYR
17	O	43	GLU
18	P	20	LEU
18	P	80	LEU
18	P	131	LYS
19	Q	61	LYS
19	Q	86	GLN
19	Q	87	SER
20	R	49	GLU

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Mol	Chain	Res	Type
20	R	85	ASP
20	R	87	GLU
20	R	110	SER
24	V	3	PRO
24	V	10	GLN
26	Z	53	ASP
3	A	35	GLU
3	A	45	ASN
3	A	89	SER
3	A	127	LEU
3	A	254	THR
3	A	269	PHE
4	B	85	ALA
4	B	137	ARG
5	C	13	ARG
6	D	10	ASP
6	D	40	LEU
6	D	52	LYS
7	E	7	GLN
7	E	13	SER
10	H	5	GLN
11	I	28	LYS
11	I	88	PHE
11	I	115	SER
13	K	4	GLY
14	L	53	ALA
17	O	9	GLY
17	O	28	GLU
17	O	29	ALA
17	O	49	GLU
19	Q	3	HIS
19	Q	4	TYR
20	R	16	PHE
20	R	63	THR
21	S	58	GLY
21	S	125	PRO
22	T	74	LYS
23	U	34	THR
23	U	42	GLN
23	U	76	LYS
3	A	55	GLY
3	A	244	ARG

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Mol	Chain	Res	Type
3	A	270	ILE
5	C	196	VAL
6	D	21	GLY
6	D	42	SER
6	D	71	LYS
6	D	81	GLN
7	E	59	GLN
9	G	165	VAL
10	H	42	LYS
11	I	8	PRO
11	I	9	THR
11	I	131	LYS
12	J	11	ARG
12	J	84	MET
13	K	10	LEU
14	L	33	ARG
17	O	7	THR
17	O	36	LYS
19	Q	5	ASP
20	R	31	GLY
20	R	111	GLY
22	T	7	VAL
23	U	12	ASN
4	B	17	ASN
4	B	75	THR
5	C	11	GLY
5	C	126	ALA
8	F	143	ASN
11	I	29	THR
17	O	11	GLN
21	S	6	LYS
30	4	5	SER
9	G	163	PRO
11	I	68	VAL
24	V	64	GLY
3	A	47	GLY
3	A	252	LYS
5	C	41	GLY
5	C	103	GLY
8	F	118	GLY
18	P	132	GLY
20	R	64	ASN

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Mol	Chain	Res	Type
22	T	13	GLY
22	T	73	GLY
5	C	171	PRO
9	G	157	PRO
11	I	57	ILE
15	M	74	GLY
22	T	27	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	185/215 (86%)	144 (78%)	41 (22%)	1	5
4	B	155/157 (99%)	135 (87%)	20 (13%)	5	24
5	C	157/163 (96%)	125 (80%)	32 (20%)	1	7
6	D	153/156 (98%)	129 (84%)	24 (16%)	3	15
7	E	136/144 (94%)	117 (86%)	19 (14%)	4	20
8	F	51/107 (48%)	46 (90%)	5 (10%)	10	38
9	G	118/146 (81%)	95 (80%)	23 (20%)	2	9
10	H	103/103 (100%)	81 (79%)	22 (21%)	1	6
11	I	108/121 (89%)	72 (67%)	36 (33%)	0	0
12	J	110/115 (96%)	93 (84%)	17 (16%)	3	15
13	K	90/93 (97%)	73 (81%)	17 (19%)	2	10
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	2
15	M	94/134 (70%)	75 (80%)	19 (20%)	1	7
16	N	96/97 (99%)	81 (84%)	15 (16%)	3	15
17	O	75/79 (95%)	60 (80%)	15 (20%)	1	8
18	P	109/115 (95%)	94 (86%)	15 (14%)	4	21
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	8
20	R	91/96 (95%)	71 (78%)	20 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	149/192 (78%)	126 (85%)	23 (15%)	3	16
22	T	62/67 (92%)	53 (86%)	9 (14%)	4	19
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	0
24	V	54/55 (98%)	44 (82%)	10 (18%)	2	10
25	W	48/48 (100%)	38 (79%)	10 (21%)	1	7
26	Z	51/53 (96%)	37 (72%)	14 (28%)	0	1
30	4	35/35 (100%)	31 (89%)	4 (11%)	7	31
All	All	2436/2715 (90%)	1967 (81%)	469 (19%)	2	9

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	33	LEU
3	A	34	THR
3	A	35	GLU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	44	ASN
3	A	46	ARG
3	A	48	ARG
3	A	49	ILE
3	A	50	THR
3	A	52	ARG
3	A	54	ILE
3	A	61	LEU
3	A	68	LYS
3	A	69	ARG
3	A	92	ILE
3	A	105	ILE
3	A	108	PRO
3	A	111	LEU
3	A	131	LEU
3	A	133	LEU
3	A	151	LYS
3	A	157	ARG
3	A	164	GLN
3	A	175	VAL
3	A	183	ARG
3	A	203	ASN

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Mol	Chain	Res	Type
3	A	208	LYS
3	A	214	TRP
3	A	215	LEU
3	A	217	ARG
3	A	218	LYS
3	A	226	MET
3	A	240	THR
3	A	244	ARG
3	A	248	THR
3	A	252	LYS
3	A	259	THR
3	A	260	ARG
3	A	270	ILE
4	B	5	LEU
4	B	14	ILE
4	B	37	LYS
4	B	49	ILE
4	B	69	LYS
4	B	82	ARG
4	B	87	ASP
4	B	105	THR
4	B	111	LYS
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	137	ARG
4	B	149	ARG
4	B	150	VAL
4	B	168	GLN
4	B	179	GLU
4	B	184	VAL
4	B	203	LYS
5	C	5	ASN
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	31	VAL
5	C	40	ARG
5	C	45	THR
5	C	48	ARG

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Mol	Chain	Res	Type
5	C	51	VAL
5	C	53	LYS
5	C	74	VAL
5	C	90	SER
5	C	95	LEU
5	C	101	GLN
5	C	102	LEU
5	C	104	LEU
5	C	117	LEU
5	C	124	ASP
5	C	134	ILE
5	C	138	LYS
5	C	143	ASP
5	C	148	VAL
5	C	150	LEU
5	C	153	ASP
5	C	154	ASP
5	C	155	GLU
5	C	164	VAL
5	C	166	TRP
5	C	175	VAL
5	C	180	ILE
5	C	188	ILE
6	D	40	LEU
6	D	45	GLU
6	D	57	LEU
6	D	67	ILE
6	D	74	ILE
6	D	80	ARG
6	D	89	VAL
6	D	92	ARG
6	D	106	ILE
6	D	112	ARG
6	D	115	ARG
6	D	117	ILE
6	D	125	ARG
6	D	129	ASN
6	D	130	LEU
6	D	135	GLN
6	D	136	LEU
6	D	140	GLU
6	D	142	THR

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Mol	Chain	Res	Type
6	D	145	MET
6	D	147	ASP
6	D	150	ARG
6	D	163	ASP
6	D	175	LEU
7	E	11	VAL
7	E	33	LEU
7	E	35	VAL
7	E	38	ASN
7	E	44	ARG
7	E	49	GLN
7	E	50	LEU
7	E	57	ASP
7	E	64	LEU
7	E	67	LEU
7	E	68	THR
7	E	69	ARG
7	E	90	ARG
7	E	92	VAL
7	E	113	VAL
7	E	116	GLU
7	E	132	ASP
7	E	140	LEU
7	E	152	ARG
8	F	76	TYR
8	F	100	ASN
8	F	101	TRP
8	F	111	LYS
8	F	115	LEU
9	G	31	THR
9	G	37	ASP
9	G	38	GLU
9	G	41	TRP
9	G	53	ARG
9	G	62	ILE
9	G	71	THR
9	G	75	ILE
9	G	93	LYS
9	G	95	LEU
9	G	102	ARG
9	G	104	THR
9	G	113	GLU

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Mol	Chain	Res	Type
9	G	116	ARG
9	G	126	VAL
9	G	132	PHE
9	G	145	HIS
9	G	146	THR
9	G	154	GLU
9	G	165	VAL
9	G	166	LEU
9	G	168	THR
9	G	169	GLN
10	H	3	MET
10	H	8	LEU
10	H	18	GLU
10	H	20	MET
10	H	25	LEU
10	H	26	ASN
10	H	27	SER
10	H	32	LYS
10	H	36	THR
10	H	41	ASN
10	H	47	VAL
10	H	81	ILE
10	H	83	ARG
10	H	87	SER
10	H	89	ILE
10	H	94	ASN
10	H	106	ARG
10	H	116	ARG
10	H	117	GLU
10	H	120	ASP
10	H	122	ARG
10	H	129	LEU
11	I	7	LYS
11	I	12	SER
11	I	13	ARG
11	I	19	VAL
11	I	27	ASP
11	I	29	THR
11	I	32	ARG
11	I	34	HIS
11	I	35	LYS
11	I	37	GLN

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Mol	Chain	Res	Type
11	I	38	LYS
11	I	39	SER
11	I	40	ARG
11	I	45	LYS
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	59	ARG
11	I	60	LEU
11	I	65	PHE
11	I	78	SER
11	I	83	LEU
11	I	84	GLU
11	I	85	ASP
11	I	88	PHE
11	I	96	TYR
11	I	98	LEU
11	I	101	ARG
11	I	103	ASN
11	I	106	VAL
11	I	107	LYS
11	I	113	GLU
11	I	114	ILE
11	I	120	VAL
11	I	123	ASP
11	I	142	LEU
12	J	8	THR
12	J	10	PHE
12	J	11	ARG
12	J	19	THR
12	J	21	ASP
12	J	26	ASP
12	J	27	TYR
12	J	49	GLU
12	J	61	ARG
12	J	64	LYS
12	J	81	GLU
12	J	91	VAL
12	J	94	TRP
12	J	113	GLU
12	J	132	MET
12	J	133	VAL

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Mol	Chain	Res	Type
12	J	134	LYS
13	K	5	LYS
13	K	8	ARG
13	K	10	LEU
13	K	11	ASN
13	K	12	ARG
13	K	17	ARG
13	K	28	LEU
13	K	35	GLN
13	K	45	ARG
13	K	51	LEU
13	K	53	THR
13	K	83	VAL
13	K	94	TYR
13	K	95	THR
13	K	99	ARG
13	K	102	THR
13	K	109	THR
14	L	8	ARG
14	L	11	LEU
14	L	12	ARG
14	L	13	THR
14	L	18	ARG
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS
14	L	37	HIS
14	L	38	ILE
14	L	43	ILE
14	L	45	ASP
14	L	47	ARG
14	L	64	LYS
14	L	66	ASP
14	L	71	VAL
14	L	89	PHE
14	L	91	ARG
14	L	93	SER
14	L	108	ARG
15	M	2	GLN
15	M	5	ILE
15	M	6	LYS
15	M	11	GLU

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Mol	Chain	Res	Type
15	M	12	LEU
15	M	13	LEU
15	M	19	ASP
15	M	22	ARG
15	M	31	ASP
15	M	34	ARG
15	M	37	THR
15	M	51	GLU
15	M	63	ARG
15	M	79	ARG
15	M	91	VAL
15	M	92	THR
15	M	96	ARG
15	M	99	VAL
15	M	101	ARG
16	N	8	ILE
16	N	16	LYS
16	N	18	LEU
16	N	19	LYS
16	N	22	LYS
16	N	30	LYS
16	N	51	ARG
16	N	71	LEU
16	N	78	THR
16	N	88	ILE
16	N	90	LEU
16	N	91	ASN
16	N	93	LYS
16	N	97	ASP
16	N	104	GLU
17	O	7	THR
17	O	14	VAL
17	O	18	ASP
17	O	22	VAL
17	O	26	GLN
17	O	28	GLU
17	O	39	PHE
17	O	40	VAL
17	O	55	THR
17	O	56	VAL
17	O	65	ARG
17	O	69	ILE

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Mol	Chain	Res	Type
17	O	81	ARG
17	O	88	GLN
17	O	96	LEU
18	P	16	GLN
18	P	17	GLN
18	P	25	PHE
18	P	32	ARG
18	P	37	LYS
18	P	45	ILE
18	P	50	VAL
18	P	89	ARG
18	P	116	ILE
18	P	118	LYS
18	P	120	ARG
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
18	P	133	ASN
19	Q	7	LEU
19	Q	8	GLN
19	Q	12	ILE
19	Q	14	GLU
19	Q	26	SER
19	Q	37	GLU
19	Q	38	ILE
19	Q	42	ILE
19	Q	61	LYS
19	Q	63	LYS
19	Q	65	VAL
19	Q	69	ILE
19	Q	71	GLN
19	Q	79	ILE
19	Q	84	GLU
20	R	11	ASN
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU
20	R	26	SER
20	R	32	GLN
20	R	37	LEU
20	R	38	LEU
20	R	42	ARG

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Mol	Chain	Res	Type
20	R	44	GLN
20	R	71	GLN
20	R	73	GLU
20	R	79	SER
20	R	80	LYS
20	R	95	ARG
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
21	S	3	LEU
21	S	13	LYS
21	S	18	MET
21	S	22	VAL
21	S	26	LYS
21	S	29	ASN
21	S	51	LEU
21	S	65	LEU
21	S	67	LYS
21	S	71	MET
21	S	82	ASP
21	S	88	TYR
21	S	100	THR
21	S	120	LEU
21	S	123	VAL
21	S	128	ARG
21	S	132	GLN
21	S	134	LEU
21	S	159	THR
21	S	160	LEU
21	S	166	LEU
21	S	169	VAL
21	S	175	ARG
22	T	5	LYS
22	T	16	SER
22	T	17	ASN
22	T	37	LEU
22	T	38	VAL
22	T	62	LEU
22	T	63	SER
22	T	64	ASP

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Mol	Chain	Res	Type
22	T	85	GLN
23	U	8	THR
23	U	10	LYS
23	U	11	LYS
23	U	13	LEU
23	U	14	VAL
23	U	17	SER
23	U	19	ILE
23	U	20	ARG
23	U	21	ARG
23	U	23	LYS
23	U	32	ARG
23	U	35	THR
23	U	37	ILE
23	U	42	GLN
23	U	43	ARG
23	U	46	LEU
23	U	49	LYS
23	U	54	ASN
23	U	56	GLN
23	U	63	SER
23	U	65	ASN
23	U	67	LEU
23	U	69	THR
23	U	76	LYS
24	V	1	MET
24	V	7	ARG
24	V	13	ASP
24	V	14	PHE
24	V	19	ASP
24	V	21	ARG
24	V	25	LEU
24	V	41	HIS
24	V	49	GLU
24	V	65	GLU
25	W	2	LYS
25	W	4	LYS
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	15	ASN
25	W	30	ASP

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Mol	Chain	Res	Type
25	W	32	ARG
25	W	34	VAL
25	W	36	ASP
26	Z	3	LYS
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	18	MET
26	Z	19	ARG
26	Z	31	THR
26	Z	35	GLN
26	Z	40	LYS
26	Z	41	LEU
26	Z	53	ASP
26	Z	55	ARG
26	Z	57	VAL
26	Z	58	LEU
30	4	2	LYS
30	4	9	LYS
30	4	14	CYS
30	4	30	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	96	HIS
3	A	201	HIS
3	A	231	HIS
4	B	129	HIS
4	B	180	ASN
5	C	5	ASN
5	C	61	GLN
5	C	66	ASN
5	C	176	ASN
6	D	9	ASN
7	E	38	ASN
7	E	49	GLN
7	E	106	ASN
7	E	143	GLN
9	G	76	GLN
10	H	26	ASN
10	H	41	ASN

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Mol	Chain	Res	Type
11	I	37	GLN
14	L	41	GLN
14	L	49	GLN
14	L	97	HIS
15	M	20	HIS
15	M	48	GLN
16	N	31	GLN
16	N	66	ASN
16	N	75	ASN
16	N	81	ASN
16	N	91	ASN
17	O	11	GLN
17	O	79	GLN
17	O	88	GLN
18	P	13	GLN
18	P	16	GLN
18	P	17	GLN
18	P	78	ASN
18	P	81	HIS
18	P	115	ASN
19	Q	71	GLN
20	R	15	HIS
20	R	69	GLN
21	S	80	HIS
21	S	119	ASN
21	S	132	GLN
22	T	17	ASN
22	T	35	ASN
23	U	42	GLN
23	U	47	HIS
24	V	41	HIS
25	W	49	HIS
26	Z	43	HIS
26	Z	44	HIS
30	4	36	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2681/2880 (93%)	638 (23%)	238 (8%)
2	Y	121/123 (98%)	28 (23%)	5 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2802/3003 (93%)	666 (23%)	243 (8%)

All (666) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	3	U
1	X	4	C
1	X	13	A
1	X	14	A
1	X	33	C
1	X	34	U
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	51	A
1	X	54	G
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	87	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	95	G
1	X	97	U
1	X	98	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	105	G
1	X	107	G
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A

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Mol	Chain	Res	Type
1	X	124	A
1	X	125	A
1	X	127	C
1	X	129	A
1	X	136	A
1	X	138	G
1	X	143	A
1	X	147	G
1	X	149	A
1	X	154	U
1	X	155	G
1	X	157	G
1	X	158	A
1	X	173	A
1	X	176	A
1	X	177	U
1	X	192	G
1	X	193	A
1	X	194	G
1	X	199	A
1	X	204	A
1	X	206	U
1	X	207	U
1	X	210	A
1	X	222	G
1	X	225	G
1	X	229	G
1	X	242	A
1	X	243	G
1	X	245	C
1	X	246	C
1	X	248	A
1	X	304	A
1	X	305	A
1	X	306	G
1	X	310	A
1	X	312	G
1	X	313	U
1	X	321	A
1	X	322	A
1	X	323	G
1	X	328	A

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Mol	Chain	Res	Type
1	X	333	A
1	X	335	A
1	X	340	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	344	G
1	X	358	C
1	X	388	G
1	X	393	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	409	G
1	X	414	A
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	441	A
1	X	456	C
1	X	459	A
1	X	461	A
1	X	463	C
1	X	466	A
1	X	467	U
1	X	468	A
1	X	469	G
1	X	486	U
1	X	491	A
1	X	492	G
1	X	504	G
1	X	513	A
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	520	C
1	X	523	A
1	X	539	A
1	X	540	G
1	X	541	C

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Mol	Chain	Res	Type
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	558	G
1	X	559	C
1	X	560	G
1	X	572	G
1	X	577	U
1	X	580	A
1	X	581	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	595	A
1	X	600	G
1	X	613	A
1	X	614	G
1	X	617	U
1	X	623	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	628	A
1	X	633	G
1	X	638	A
1	X	645	G
1	X	648	A
1	X	649	G
1	X	651	C
1	X	652	C
1	X	654	A
1	X	655	A
1	X	656	U
1	X	657	A
1	X	664	C
1	X	665	A
1	X	667	U
1	X	669	G
1	X	682	G

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Mol	Chain	Res	Type
1	X	683	A
1	X	684	C
1	X	698	A
1	X	699	G
1	X	700	C
1	X	728	G
1	X	729	A
1	X	730	C
1	X	731	A
1	X	732	G
1	X	736	G
1	X	743	A
1	X	747	A
1	X	751	G
1	X	752	G
1	X	753	U
1	X	758	G
1	X	759	C
1	X	760	U
1	X	777	A
1	X	778	G
1	X	780	U
1	X	781	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	814	G
1	X	815	A
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	858	G

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Mol	Chain	Res	Type
1	X	859	U
1	X	872	G
1	X	879	A
1	X	880	C
1	X	922	A
1	X	926	C
1	X	931	G
1	X	938	G
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	973	U
1	X	985	G
1	X	994	A
1	X	995	A
1	X	1000	G
1	X	1001	A
1	X	1006	C
1	X	1007	A
1	X	1014	G
1	X	1016	C
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1028	G
1	X	1031	C
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1038	U
1	X	1044	U
1	X	1051	U
1	X	1053	G

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Mol	Chain	Res	Type
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1060	C
1	X	1068	A
1	X	1073	G
1	X	1077	U
1	X	1078	A
1	X	1081	A
1	X	1082	G
1	X	1086	C
1	X	1087	C
1	X	1090	C
1	X	1094	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1100	G
1	X	1108	U
1	X	1115	C
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1139	A
1	X	1140	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	1154	A
1	X	1155	G
1	X	1161	U
1	X	1183	C
1	X	1185	C

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Mol	Chain	Res	Type
1	X	1187	A
1	X	1188	A
1	X	1189	G
1	X	1191	G
1	X	1192	A
1	X	1194	U
1	X	1195	U
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1234	C
1	X	1240	G
1	X	1250	A
1	X	1251	G
1	X	1265	G
1	X	1266	G
1	X	1269	G
1	X	1275	A
1	X	1281	A
1	X	1284	G
1	X	1285	A
1	X	1286	U
1	X	1288	A
1	X	1289	A
1	X	1297	A
1	X	1299	A
1	X	1300	A
1	X	1302	C
1	X	1307	U
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1319	C
1	X	1334	A
1	X	1339	U
1	X	1341	G
1	X	1342	U
1	X	1358	C
1	X	1365	U
1	X	1378	A
1	X	1381	G
1	X	1392	U

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Mol	Chain	Res	Type
1	X	1399	C
1	X	1404	C
1	X	1410	U
1	X	1412	C
1	X	1413	U
1	X	1428	G
1	X	1429	A
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1441	A
1	X	1442	C
1	X	1443	G
1	X	1451	C
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1473	U
1	X	1474	A
1	X	1475	U
1	X	1476	G
1	X	1482	U
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C
1	X	1508	G
1	X	1509	A
1	X	1513	U
1	X	1514	C
1	X	1523	A
1	X	1524	C
1	X	1525	A
1	X	1528	C
1	X	1531	C
1	X	1532	A
1	X	1533	G

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Mol	Chain	Res	Type
1	X	1545	G
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	1571	G
1	X	1574	A
1	X	1575	C
1	X	1576	G
1	X	1583	A
1	X	1584	G
1	X	1585	A
1	X	1594	U
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1608	U
1	X	1613	G
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1648	C
1	X	1657	A
1	X	1665	C
1	X	1669	A
1	X	1691	G
1	X	1710	U
1	X	1711	C
1	X	1712	G
1	X	1713	G
1	X	1716	G
1	X	1717	A
1	X	1732	U
1	X	1733	U
1	X	1734	C
1	X	1747	G

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Mol	Chain	Res	Type
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1773	C
1	X	1776	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1806	G
1	X	1807	A
1	X	1808	C
1	X	1812	U
1	X	1813	A
1	X	1820	G
1	X	1821	A
1	X	1825	C
1	X	1831	G
1	X	1840	A
1	X	1850	G
1	X	1861	G
1	X	1863	U
1	X	1867	A
1	X	1874	G
1	X	1882	G
1	X	1883	A
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1913	G
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1939	U
1	X	1943	A
1	X	1947	G
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	1958	G
1	X	1963	G
1	X	1964	A
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1980	A
1	X	2006	G
1	X	2010	G
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2035	G
1	X	2038	C
1	X	2039	G
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2076	G
1	X	2079	A
1	X	2088	U
1	X	2089	C
1	X	2171	U
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2218	G
1	X	2222	U
1	X	2247	A

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Mol	Chain	Res	Type
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2283	G
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2291	U
1	X	2294	U
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2306	A
1	X	2313	G
1	X	2314	A
1	X	2315	A
1	X	2324	G
1	X	2325	A
1	X	2326	C
1	X	2329	C
1	X	2339	A
1	X	2351	G
1	X	2355	A
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2371	A
1	X	2375	G
1	X	2381	A
1	X	2382	C
1	X	2385	U
1	X	2389	G
1	X	2396	C
1	X	2401	A
1	X	2402	U
1	X	2404	A

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Mol	Chain	Res	Type
1	X	2405	A
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2448	A
1	X	2449	G
1	X	2452	U
1	X	2455	A
1	X	2463	G
1	X	2470	U
1	X	2475	C
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2498	U
1	X	2499	C
1	X	2501	U
1	X	2504	G
1	X	2508	G
1	X	2514	G
1	X	2543	A
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2552	C
1	X	2553	G
1	X	2557	G
1	X	2561	G
1	X	2565	C
1	X	2580	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2589	C
1	X	2591	C

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Mol	Chain	Res	Type
1	X	2594	U
1	X	2600	A
1	X	2609	G
1	X	2611	A
1	X	2613	A
1	X	2615	U
1	X	2620	G
1	X	2633	A
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2668	U
1	X	2692	A
1	X	2693	U
1	X	2694	G
1	X	2705	A
1	X	2706	U
1	X	2707	G
1	X	2713	A
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2736	U
1	X	2737	A
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2758	A
1	X	2759	U
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2775	U
1	X	2776	U
1	X	2777	A
1	X	2778	U
1	X	2779	C
1	X	2780	A
1	X	2782	G
1	X	2795	A
1	X	2796	A
1	X	2808	U

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Mol	Chain	Res	Type
1	X	2810	A
1	X	2811	G
1	X	2824	C
1	X	2825	A
1	X	2843	A
1	X	2846	G
1	X	2847	G
1	X	2848	A
1	X	2849	C
1	X	2854	G
1	X	2855	C
1	X	2859	U
1	X	2868	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	37	C
2	Y	39	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	53	G
2	Y	54	U
2	Y	56	G
2	Y	58	G
2	Y	59	A
2	Y	69	G
2	Y	75	A
2	Y	76	U
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	112	A
2	Y	115	G
2	Y	123	U

All (243) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	3	U
1	X	13	A
1	X	33	C
1	X	48	A
1	X	50	G
1	X	62	U
1	X	70	A
1	X	71	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	89	A
1	X	98	U
1	X	99	U
1	X	100	G
1	X	117	A
1	X	124	A
1	X	154	U
1	X	176	A
1	X	190	A
1	X	198	A
1	X	199	A
1	X	242	A
1	X	312	G
1	X	321	A
1	X	322	A
1	X	328	A
1	X	332	C
1	X	334	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	396	U
1	X	399	G
1	X	416	U
1	X	417	C
1	X	418	C
1	X	458	G
1	X	466	A
1	X	467	U
1	X	469	G
1	X	490	A
1	X	504	G

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Mol	Chain	Res	Type
1	X	513	A
1	X	522	G
1	X	537	C
1	X	539	A
1	X	542	A
1	X	553	C
1	X	554	U
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	583	C
1	X	648	A
1	X	655	A
1	X	664	C
1	X	668	A
1	X	672	C
1	X	682	G
1	X	683	A
1	X	698	A
1	X	751	G
1	X	758	G
1	X	759	C
1	X	761	G
1	X	777	A
1	X	780	U
1	X	788	G
1	X	789	G
1	X	796	A
1	X	802	A
1	X	803	C
1	X	806	A
1	X	813	A
1	X	814	G
1	X	824	U
1	X	841	G
1	X	842	A
1	X	858	G
1	X	859	U
1	X	872	G
1	X	878	C
1	X	879	A

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Mol	Chain	Res	Type
1	X	939	C
1	X	940	G
1	X	955	G
1	X	969	U
1	X	972	C
1	X	994	A
1	X	1000	G
1	X	1031	C
1	X	1033	G
1	X	1037	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1072	U
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A
1	X	1120	C
1	X	1121	G
1	X	1139	A
1	X	1141	U
1	X	1152	C
1	X	1154	A
1	X	1182	U
1	X	1186	G
1	X	1191	G
1	X	1194	U
1	X	1223	G
1	X	1233	A
1	X	1249	G
1	X	1288	A
1	X	1299	A
1	X	1313	U
1	X	1314	A
1	X	1353	A
1	X	1357	U
1	X	1378	A
1	X	1409	U
1	X	1410	U
1	X	1412	C
1	X	1432	G

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Mol	Chain	Res	Type
1	X	1433	A
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1473	U
1	X	1475	U
1	X	1496	G
1	X	1505	U
1	X	1513	U
1	X	1531	C
1	X	1541	G
1	X	1552	C
1	X	1561	A
1	X	1562	G
1	X	1574	A
1	X	1575	C
1	X	1581	C
1	X	1583	A
1	X	1601	U
1	X	1607	A
1	X	1618	U
1	X	1624	A
1	X	1625	A
1	X	1631	C
1	X	1680	U
1	X	1710	U
1	X	1711	C
1	X	1716	G
1	X	1732	U
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1791	C
1	X	1799	A
1	X	1800	A
1	X	1807	A
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1820	G
1	X	1865	C
1	X	1872	A

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Mol	Chain	Res	Type
1	X	1882	G
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1921	A
1	X	1938	U
1	X	1953	A
1	X	1963	G
1	X	1975	G
1	X	1980	A
1	X	2014	A
1	X	2018	G
1	X	2075	U
1	X	2083	G
1	X	2088	U
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2198	U
1	X	2204	A
1	X	2217	G
1	X	2228	U
1	X	2254	C
1	X	2258	G
1	X	2261	G
1	X	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A
1	X	2314	A
1	X	2324	G
1	X	2354	G
1	X	2361	G
1	X	2370	G
1	X	2381	A
1	X	2401	A
1	X	2404	A
1	X	2409	A
1	X	2447	G
1	X	2477	C
1	X	2482	A
1	X	2497	A

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Mol	Chain	Res	Type
1	X	2498	U
1	X	2560	G
1	X	2564	U
1	X	2580	C
1	X	2608	A
1	X	2615	U
1	X	2624	G
1	X	2660	C
1	X	2669	C
1	X	2691	C
1	X	2705	A
1	X	2706	U
1	X	2731	G
1	X	2736	U
1	X	2744	A
1	X	2758	A
1	X	2769	C
1	X	2770	A
1	X	2778	U
1	X	2807	U
1	X	2808	U
1	X	2810	A
1	X	2824	C
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
2	Y	26	G
2	Y	46	G
2	Y	54	U
2	Y	58	G
2	Y	86	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
32	1F3	X	2931	-	60,64,64	1.10	5 (8%)	82,96,96	1.83	18 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F3	X	2931	-	-	0/78/119/119	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2931	1F3	C48-C47	-3.82	1.51	1.54
32	X	2931	1F3	O17-C5	-2.86	1.43	1.47
32	X	2931	1F3	C51-C47	-2.09	1.48	1.51
32	X	2931	1F3	C41-N40	2.31	1.37	1.33
32	X	2931	1F3	C50-N45	2.74	1.44	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2931	1F3	C59-C58-N57	-5.79	106.72	114.97
32	X	2931	1F3	C28-O20-C8	-4.72	107.83	116.30
32	X	2931	1F3	C23-C6-C5	-4.63	108.42	115.25
32	X	2931	1F3	C5-O17-C41	-4.35	105.67	109.28
32	X	2931	1F3	C27-C12-C13	-3.01	106.28	112.97
32	X	2931	1F3	C4-N40-C41	-3.00	108.91	112.55
32	X	2931	1F3	O29-C30-C38	-2.97	100.49	106.78
32	X	2931	1F3	C48-C47-C51	-2.90	108.03	114.00
32	X	2931	1F3	C30-C31-C32	-2.39	105.99	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2931	1F3	C54-N57-C58	-2.37	124.36	128.03
32	X	2931	1F3	C52-C51-C47	-2.33	116.42	120.76
32	X	2931	1F3	C16-C1-C3	-2.08	104.41	108.21
32	X	2931	1F3	O10-C11-O26	2.01	128.02	123.89
32	X	2931	1F3	C47-C48-C49	2.19	107.55	102.70
32	X	2931	1F3	C9-C7-C2	2.25	119.85	116.09
32	X	2931	1F3	C13-C14-C8	2.28	115.08	110.85
32	X	2931	1F3	O10-C6-C23	2.35	111.63	107.36
32	X	2931	1F3	O60-C58-N57	4.34	128.31	123.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2931	1F3	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 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	2686/2880 (93%)	-0.19	77 (2%) 55 41	43, 87, 194, 279	0
2	Y	122/123 (99%)	-0.12	2 (1%) 74 62	82, 129, 165, 187	0
3	A	240/274 (87%)	0.06	6 (2%) 61 47	63, 107, 137, 156	0
4	B	205/211 (97%)	-0.33	3 (1%) 76 63	38, 68, 99, 145	0
5	C	197/205 (96%)	0.15	14 (7%) 19 10	55, 107, 150, 178	0
6	D	177/180 (98%)	0.47	16 (9%) 12 6	148, 178, 210, 216	0
7	E	171/185 (92%)	-0.14	4 (2%) 64 49	98, 139, 178, 188	0
8	F	71/144 (49%)	2.76	38 (53%) 0 0	221, 234, 251, 259	0
9	G	142/174 (81%)	0.08	8 (5%) 28 16	65, 89, 137, 149	0
10	H	134/134 (100%)	-0.50	0 100 100	49, 62, 88, 110	0
11	I	141/156 (90%)	0.79	23 (16%) 2 1	54, 120, 171, 195	0
12	J	136/141 (96%)	0.05	7 (5%) 32 18	83, 106, 147, 172	0
13	K	113/116 (97%)	-0.50	0 100 100	37, 53, 71, 99	0
14	L	104/114 (91%)	0.29	5 (4%) 34 21	91, 122, 149, 166	0
15	M	108/166 (65%)	-0.51	0 100 100	44, 64, 106, 128	0
16	N	117/118 (99%)	-0.28	2 (1%) 73 60	54, 86, 124, 152	0
17	O	94/100 (94%)	-0.14	3 (3%) 51 36	67, 106, 146, 160	0
18	P	127/134 (94%)	-0.48	0 100 100	48, 64, 103, 143	0
19	Q	93/95 (97%)	0.10	6 (6%) 22 12	69, 101, 156, 193	0
20	R	110/115 (95%)	0.41	12 (10%) 7 4	84, 113, 170, 173	0
21	S	175/237 (73%)	0.31	13 (7%) 17 10	119, 154, 178, 190	0
22	T	84/91 (92%)	0.81	16 (19%) 2 1	72, 103, 176, 195	0
23	U	72/81 (88%)	0.57	5 (6%) 20 11	86, 122, 146, 182	0
24	V	66/67 (98%)	0.79	8 (12%) 6 3	88, 128, 213, 230	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
25	W	55/55 (100%)	-0.29	0	100 100	76, 96, 123, 161	0
26	Z	58/60 (96%)	-0.25	2 (3%)	49 34	47, 64, 96, 108	0
27	1	53/55 (96%)	0.89	9 (16%)	2 1	6, 28, 62, 73	0
28	2	46/47 (97%)	2.89	32 (69%)	0 0	3, 10, 27, 42	0
29	3	63/66 (95%)	2.14	27 (42%)	0 0	3, 18, 41, 84	0
30	4	37/37 (100%)	8.19	36 (97%)	0 0	191, 239, 247, 252	0
All	All	5997/6561 (91%)	0.07	374 (6%)	24 13	3, 96, 193, 279	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	25	VAL	20.6
30	4	16	VAL	17.9
24	V	1	MET	17.0
8	F	114	ASP	16.1
30	4	29	ASN	15.8
30	4	17	VAL	14.5
30	4	24	LEU	13.8
30	4	6	SER	12.7
22	T	9	SER	12.7
30	4	28	SER	12.4
30	4	11	CYS	12.1
1	X	731	A	11.3
30	4	34	GLN	10.9
27	1	4	ASP	10.8
23	U	27	ASP	10.5
24	V	3	PRO	10.4
30	4	32	HIS	10.3
8	F	137	THR	10.3
30	4	7	VAL	10.2
30	4	23	VAL	10.0
30	4	10	MET	9.2
11	I	8	PRO	8.9
29	3	33	ASN	8.7
30	4	20	HIS	8.6
30	4	36	GLN	8.2
2	Y	123	U	8.2
30	4	21	GLY	7.9
30	4	35	ARG	7.9
1	X	1089	C	7.8

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Mol	Chain	Res	Type	RSRZ
30	4	14	CYS	7.8
1	X	1086	C	7.8
19	Q	64	ARG	7.7
3	A	203	ASN	7.7
24	V	2	LYS	7.6
22	T	6	GLY	7.5
22	T	10	SER	7.4
8	F	113	PRO	7.4
23	U	28	GLY	7.4
30	4	27	CYS	7.3
11	I	9	THR	7.3
29	3	60	LEU	7.2
8	F	136	VAL	7.2
6	D	43	SER	7.0
1	X	1085	G	6.9
11	I	5	ASP	6.9
30	4	15	LYS	6.8
11	I	4	HIS	6.8
30	4	22	ARG	6.7
12	J	84	MET	6.6
30	4	19	ARG	6.6
24	V	4	SER	6.5
8	F	97	GLY	6.4
30	4	5	SER	6.4
30	4	26	ILE	6.3
28	2	9	ASN	6.3
8	F	98	LYS	6.3
5	C	165	SER	6.3
9	G	155	THR	6.2
26	Z	2	ALA	6.2
9	G	156	HIS	6.2
29	3	11	LYS	6.2
22	T	8	GLY	6.2
27	1	7	ARG	6.1
20	R	100	ASP	6.0
20	R	99	VAL	5.9
11	I	6	LEU	5.8
5	C	47	THR	5.8
1	X	1079	G	5.8
1	X	1069	G	5.7
30	4	13	ASN	5.7
28	2	27	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
22	T	7	VAL	5.7
29	3	27	SER	5.6
1	X	1524	C	5.6
29	3	31	HIS	5.5
3	A	250	TRP	5.5
1	X	1186	G	5.5
30	4	12	ASP	5.5
1	X	1095	A	5.5
28	2	4	THR	5.4
11	I	52	GLY	5.3
20	R	94	VAL	5.3
1	X	248	A	5.3
11	I	29	THR	5.2
27	1	24	THR	5.2
11	I	63	ARG	5.2
1	X	730	C	5.2
30	4	4	ARG	5.2
8	F	125	ASN	5.1
8	F	84	ILE	5.1
30	4	33	LYS	5.0
30	4	30	VAL	5.0
28	2	36	ALA	4.9
28	2	8	ASN	4.9
29	3	30	ARG	4.9
28	2	7	PRO	4.9
20	R	102	LYS	4.9
30	4	1	MET	4.9
1	X	1091	C	4.8
2	Y	2	C	4.8
6	D	42	SER	4.7
6	D	23	SER	4.7
22	T	4	LYS	4.7
28	2	24	THR	4.7
8	F	131	ALA	4.7
28	2	34	ARG	4.6
9	G	97	ASP	4.5
1	X	1114	A	4.5
1	X	1080	A	4.5
28	2	32	ALA	4.5
24	V	6	MET	4.5
28	2	11	LYS	4.4
5	C	19	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
30	4	9	LYS	4.4
8	F	123	ALA	4.4
27	1	41	ASP	4.4
29	3	42	ARG	4.3
1	X	2088	U	4.3
1	X	1068	A	4.2
8	F	121	GLU	4.2
22	T	15	ASP	4.2
22	T	3	HIS	4.2
1	X	1078	A	4.2
1	X	1104	G	4.2
1	X	1077	U	4.2
29	3	39	ASP	4.2
1	X	1090	C	4.2
1	X	1523	A	4.1
21	S	124	ALA	4.1
8	F	144	ALA	4.1
24	V	11	ALA	4.1
5	C	123	PHE	4.1
22	T	5	LYS	4.1
1	X	2089	C	4.1
8	F	126	THR	4.1
1	X	1106	A	4.1
28	2	6	GLN	4.0
28	2	29	ASN	4.0
1	X	2776	U	4.0
1	X	1187	A	3.9
1	X	1525	A	3.9
27	1	43	VAL	3.9
8	F	119	SER	3.9
11	I	7	LYS	3.9
12	J	140	GLU	3.9
28	2	30	ILE	3.9
8	F	111	LYS	3.8
1	X	891	A	3.8
8	F	92	ASN	3.8
29	3	34	THR	3.8
6	D	145	MET	3.8
29	3	7	HIS	3.8
21	S	91	PRO	3.8
8	F	96	VAL	3.7
8	F	133	SER	3.7

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Mol	Chain	Res	Type	RSRZ
21	S	15	ASP	3.7
1	X	2778	U	3.7
5	C	21	GLU	3.7
6	D	134	GLU	3.7
1	X	728	G	3.7
1	X	361	G	3.7
8	F	107	ILE	3.7
8	F	112	MET	3.7
1	X	1084	A	3.7
23	U	16	ASN	3.7
1	X	1188	A	3.6
19	Q	69	ILE	3.6
11	I	30	ALA	3.6
30	4	8	LYS	3.6
7	E	5	GLY	3.6
23	U	47	HIS	3.6
29	3	10	ALA	3.6
30	4	3	VAL	3.5
4	B	205	SER	3.5
4	B	94	ASP	3.5
17	O	39	PHE	3.5
29	3	28	GLY	3.5
11	I	10	PRO	3.5
28	2	5	TYR	3.5
1	X	1067	G	3.5
21	S	12	GLN	3.4
1	X	729	A	3.4
29	3	6	THR	3.4
8	F	110	THR	3.4
5	C	44	SER	3.4
8	F	115	LEU	3.4
28	2	23	LYS	3.4
6	D	147	ASP	3.4
20	R	101	GLY	3.3
22	T	17	ASN	3.3
5	C	20	PRO	3.3
3	A	249	PRO	3.3
28	2	2	LYS	3.3
28	2	22	MET	3.3
21	S	24	TYR	3.3
1	X	2280	A	3.3
6	D	94	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
6	D	76	ASN	3.3
1	X	2777	A	3.2
28	2	21	ARG	3.2
8	F	122	ALA	3.2
1	X	1189	G	3.2
3	A	219	PRO	3.2
6	D	144	ASP	3.2
14	L	34	SER	3.2
20	R	58	VAL	3.2
29	3	5	LYS	3.1
28	2	1	MET	3.1
17	O	41	GLY	3.1
8	F	93	LYS	3.1
29	3	40	GLU	3.1
11	I	48	PHE	3.1
24	V	36	GLN	3.1
8	F	127	VAL	3.1
21	S	14	LEU	3.1
11	I	50	GLU	3.0
5	C	91	TYR	3.0
28	2	25	LYS	3.0
6	D	146	VAL	3.0
14	L	64	LYS	3.0
1	X	1098	G	3.0
27	1	25	THR	3.0
29	3	36	LYS	3.0
29	3	2	PRO	2.9
9	G	103	TYR	2.9
11	I	54	SER	2.9
29	3	37	SER	2.9
1	X	665	A	2.9
8	F	129	GLY	2.9
8	F	94	ALA	2.9
30	4	37	GLY	2.9
21	S	60	GLU	2.9
11	I	82	ASP	2.9
6	D	11	GLN	2.8
1	X	1088	A	2.8
1	X	1093	U	2.8
29	3	8	LYS	2.8
11	I	33	GLY	2.8
8	F	128	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
11	I	36	GLY	2.8
1	X	1734	C	2.8
28	2	10	ARG	2.8
8	F	99	LEU	2.8
6	D	37	ASN	2.8
4	B	135	HIS	2.7
22	T	85	GLN	2.8
8	F	108	ALA	2.7
8	F	143	ASN	2.7
1	X	1913	G	2.7
27	1	3	LYS	2.7
1	X	1072	U	2.7
8	F	120	VAL	2.7
12	J	85	GLY	2.7
28	2	41	GLN	2.7
20	R	82	ALA	2.7
8	F	118	GLY	2.7
26	Z	3	LYS	2.7
9	G	37	ASP	2.7
20	R	103	LYS	2.6
8	F	83	GLY	2.6
6	D	113	ASP	2.6
1	X	1115	C	2.6
28	2	26	SER	2.6
1	X	1551	U	2.6
29	3	17	THR	2.6
9	G	162	LYS	2.6
24	V	12	THR	2.6
29	3	32	GLN	2.6
1	X	1094	C	2.6
9	G	106	TYR	2.5
1	X	1076	U	2.5
7	E	46	ASP	2.5
30	4	2	LYS	2.5
29	3	47	GLY	2.5
11	I	53	ARG	2.5
17	O	5	ILE	2.5
1	X	1109	A	2.5
1	X	2172	U	2.5
5	C	48	ARG	2.5
9	G	129	HIS	2.5
1	X	1102	G	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	4	18	ARG	2.4
22	T	11	LYS	2.4
1	X	727	U	2.4
1	X	2775	U	2.4
8	F	102	ASP	2.4
12	J	90	ALA	2.4
20	R	93	ARG	2.4
1	X	435	A	2.4
29	3	18	GLY	2.4
14	L	97	HIS	2.4
1	X	1037	U	2.4
28	2	20	ALA	2.4
28	2	3	ARG	2.4
5	C	189	ASP	2.4
21	S	123	VAL	2.4
1	X	1120	C	2.4
1	X	1841	G	2.4
21	S	93	GLU	2.4
1	X	732	G	2.4
5	C	198	GLU	2.4
19	Q	72	ARG	2.3
29	3	4	MET	2.3
5	C	172	VAL	2.3
11	I	100	ARG	2.3
1	X	1057	A	2.3
1	X	2581	A	2.3
5	C	193	LEU	2.3
28	2	31	LEU	2.3
11	I	67	ASN	2.3
27	1	27	ASN	2.3
1	X	304	A	2.3
20	R	61	SER	2.3
8	F	91	PRO	2.3
3	A	85	ASP	2.3
1	X	1553	G	2.3
20	R	77	HIS	2.3
1	X	1092	U	2.3
19	Q	65	VAL	2.2
23	U	26	ALA	2.2
7	E	58	ALA	2.2
27	1	44	ALA	2.2
29	3	61	MET	2.2

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Mol	Chain	Res	Type	RSRZ
28	2	28	ARG	2.2
22	T	71	ASN	2.2
1	X	1070	G	2.2
22	T	84	ALA	2.2
1	X	1087	C	2.2
1	X	2170	C	2.2
6	D	153	ASP	2.2
28	2	16	HIS	2.2
1	X	2174	G	2.2
16	N	94	VAL	2.2
14	L	36	LYS	2.2
19	Q	63	LYS	2.2
22	T	2	ALA	2.2
1	X	358	C	2.1
20	R	63	THR	2.1
5	C	197	GLU	2.1
7	E	29	PRO	2.1
1	X	1101	U	2.1
21	S	92	VAL	2.1
12	J	7	ARG	2.1
16	N	92	ARG	2.1
28	2	19	ARG	2.1
14	L	53	ALA	2.1
29	3	38	GLY	2.1
11	I	56	LEU	2.1
11	I	60	LEU	2.1
21	S	10	PRO	2.1
3	A	254	THR	2.1
12	J	14	PHE	2.1
8	F	109	LYS	2.1
21	S	86	VAL	2.1
28	2	45	SER	2.1
1	X	1051	U	2.1
1	X	1066	G	2.1
1	X	1110	G	2.1
6	D	81	GLN	2.0
12	J	21	ASP	2.0
28	2	33	ARG	2.0
28	2	43	THR	2.0
21	S	11	LYS	2.0
1	X	1065	A	2.0
1	X	1099	A	2.0

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Mol	Chain	Res	Type	RSRZ
11	I	87	THR	2.0
6	D	46	ASP	2.0
22	T	12	ASN	2.0
1	X	2169	A	2.0
19	Q	67	ARG	2.0
1	X	1911	A	2.0
8	F	135	GLY	2.0
1	X	1074	G	2.0
29	3	25	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	X	2928	1/1	0.98	0.89	43.39	42,42,42,42	0
31	MG	X	2916	1/1	0.91	0.56	25.04	53,53,53,53	0
31	MG	X	2908	1/1	0.89	0.51	23.90	49,49,49,49	0
31	MG	X	2926	1/1	0.93	0.99	23.35	56,56,56,56	0
31	MG	X	2924	1/1	0.97	0.64	20.57	39,39,39,39	0
31	MG	Y	201	1/1	0.84	0.50	17.67	82,82,82,82	0
31	MG	X	2902	1/1	0.97	0.42	16.65	45,45,45,45	0
31	MG	X	2919	1/1	0.95	0.57	14.56	56,56,56,56	0
31	MG	X	2915	1/1	0.99	0.28	0.71	24,24,24,24	0
32	1F3	X	2931	60/60	0.97	0.23	0.04	38,60,90,99	0
31	MG	X	2907	1/1	0.98	0.42	-	53,53,53,53	0
31	MG	X	2906	1/1	0.87	0.40	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	2909	1/1	0.95	1.00	-	37,37,37,37	0
31	MG	X	2927	1/1	0.84	0.49	-	106,106,106,106	0
31	MG	X	2929	1/1	0.80	0.36	-	77,77,77,77	0
31	MG	X	2901	1/1	0.83	0.39	-	110,110,110,110	0
31	MG	X	2921	1/1	0.97	0.47	-	18,18,18,18	0
31	MG	X	2913	1/1	0.80	0.56	-	66,66,66,66	0
31	MG	Y	202	1/1	0.94	0.48	-	54,54,54,54	0
31	MG	X	2920	1/1	0.97	0.62	-	38,38,38,38	0
31	MG	X	2904	1/1	0.55	0.55	-	90,90,90,90	0
31	MG	X	2911	1/1	0.99	0.43	-	35,35,35,35	0
31	MG	Y	204	1/1	0.95	0.19	-	67,67,67,67	0
31	MG	X	2903	1/1	0.96	0.12	-	82,82,82,82	0
31	MG	X	2925	1/1	0.94	0.46	-	39,39,39,39	0
31	MG	X	2917	1/1	0.98	0.85	-	37,37,37,37	0
31	MG	X	2910	1/1	0.78	0.18	-	85,85,85,85	0
31	MG	X	2914	1/1	0.96	0.59	-	51,51,51,51	0
31	MG	Y	203	1/1	0.75	0.49	-	87,87,87,87	0
31	MG	X	2930	1/1	0.86	0.98	-	71,71,71,71	0
31	MG	X	2922	1/1	0.64	0.87	-	81,81,81,81	0
31	MG	X	2912	1/1	0.90	0.29	-	60,60,60,60	0
31	MG	Y	205	1/1	0.79	0.33	-	77,77,77,77	0
31	MG	X	2918	1/1	0.98	0.60	-	32,32,32,32	0
31	MG	X	2905	1/1	0.70	0.54	-	104,104,104,104	0
31	MG	X	2923	1/1	0.98	0.81	-	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.