



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:57 PM GMT

PDB ID : 4IOC
Title : Crystal structure of compound 4f bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.60 Å(reported)

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

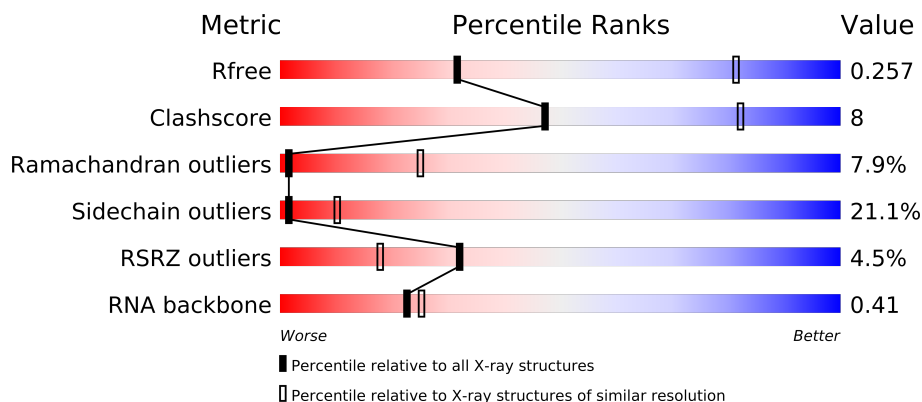
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
RNA backbone	1838	1012 (4.40-2.76)

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

Mol	Chain	Length	Quality of chain
1	X	2880	
2	Y	123	
3	A	274	
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Geometry	Electron density
31	MG	M	201	-	X
31	MG	X	2901	-	X
31	MG	X	2902	-	X
31	MG	X	2903	-	X
31	MG	X	2904	-	X
31	MG	X	2905	-	X
31	MG	X	2906	-	X
31	MG	X	2907	-	X
31	MG	X	2908	-	X
31	MG	X	2909	-	X
31	MG	X	2910	-	X
31	MG	X	2911	-	X
31	MG	X	2912	-	X
31	MG	X	2913	-	X
31	MG	X	2914	-	X
31	MG	X	2915	-	X
31	MG	X	2916	-	X
31	MG	X	2917	-	X
31	MG	X	2918	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
31	MG	X	2919	-	X
31	MG	X	2920	-	X
31	MG	X	2921	-	X
31	MG	X	2922	-	X
31	MG	X	2923	-	X
31	MG	X	2924	-	X
31	MG	X	2926	-	X
31	MG	X	2927	-	X
31	MG	X	2928	-	X
31	MG	Y	201	-	X
31	MG	Y	202	-	X
31	MG	Y	203	-	X
31	MG	Y	204	-	X
31	MG	Y	205	-	X
31	MG	Y	206	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83877 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	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

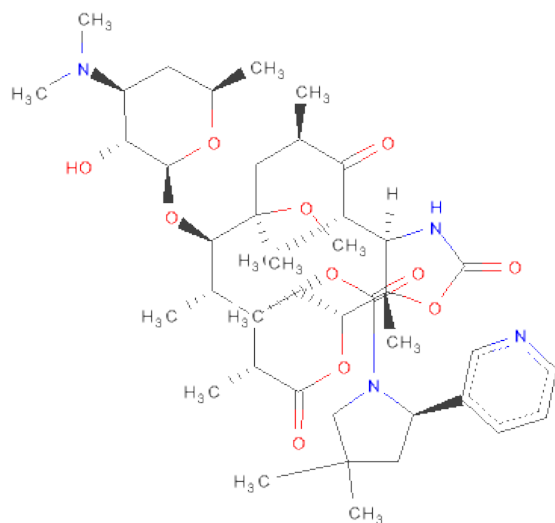
- Molecule 30 is a protein called 50S ribosomal protein L36.

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	28	Total Mg 28 28	0	0
31	Y	6	Total Mg 6 6	0	0
31	M	1	Total Mg 1 1	0	0

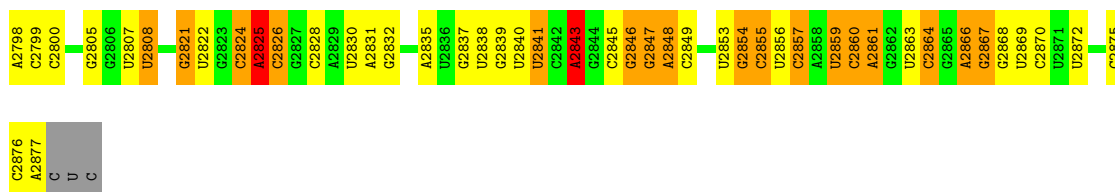
- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15S,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{[3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL]OXY}TETRADECAHYDRO-2H-OXACYCLO TETRADECINO[4,3-D][1,3]OXAZOL-8-YL(2R)-4,4-DIMETHYL-2-(PYRIDIN-3-YL)PYRROLIDINE-1-CARBOXYLATE (three-letter code: 1F4) (formula: C₄₃H₆₈N₄O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	X	1	58	43	4	11	0	0

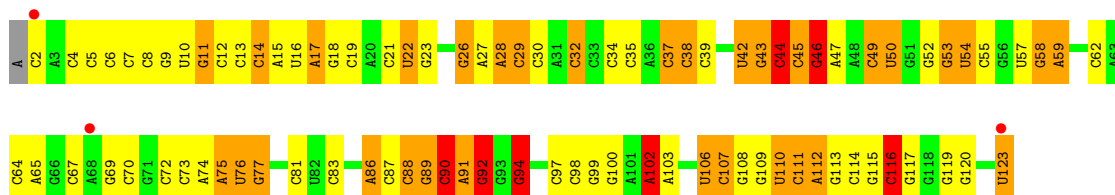
U1710	A1561	G1488	C1343	G1200	A1196	C1064	A994	U919	G854	G789	C723
C1711	G1562	C1489	C1344	G1201	C1127	G1067	A995	A922	G858	A790	C724
G1712	U1563	G1490	G1345	U1202	A1129	A1068	A996	A923	U859	G793	C725
A1713	A1567	G1491	C1346	A1203	U1130	G1069	C997	C924	U860	A794	G726
A1714	G1495	G1496	C1347	A1208	G1131	G1070	C998	U925	A795	A796	G727
G1716	C1496	C1497	A1348	G1209	C1132	U1071	A999	C926	C963	A797	G728
A1717	C1422	U1421	A1349	G1210	G1133	U1072	G1000	C927	C964	A798	G729
	U1426	G1427	A1353	G1211	C1134	G1073	A1001		A965	C799	C730
	G1428	C1429	A1354	U1217	C1135	G1074	C1002	G931	G867	C732	A731
	A1429	U1430	A1355	G1218	G1136	G1075	C1003	G932	U868	U800	G733
	G1431	C1432	A1356	C1219	A1137	U1076		G933	U869	A801	
	U1433	G1434	U1357	G1220	A1138	U1077	C1006	G934	C936	A802	G738
	G1436	U1437	C1358	G1221	A1139	A1078	A1007	C935	C870	A803	G739
	A1437	U1438	G1359	G1222	U1140	G1079	G1008	A936	U871	C804	A740
	U1439	G1440	A1360	G1223	A1141	A1080	C1009	C937	G872	G805	G741
	A1441	U1442	C1361	G1224	G1142	G1081	U1010	G938	U873	A806	G742
	G1443	G1443	U1362	A1224	A1143	G1082	C1019	C939	A874	A807	A743
			G1363	G1225	U1144	G1083	G1014	G940	G875	C808	G744
			A1364		C1145	A1084	U1015	U941	A876	C809	C745
			G1365		G1146	G1085	C1016	U942	G877	U810	G746
			A1366		G1147	A1086	C1017	U943	C878	G811	
			G1367		G1148	C1087	C1018	U944	A879	G812	
			A1368		G1149	A1088	U1019	G945	C880	A813	C749
			G1369		C1150	G1089	C1020	U946	U881	G814	G750
			U1370		U1151	C1090	A1021	C947	C882	A815	G751
			C1371		A1152	U1091	A1022		A883	U816	G752
			G1372		C1153	C1092	U1023		C884	A817	U753
			A1373		U1154	U1093	G1024		A885	G818	C755
			C1374		G1155	C1094	C1094		A886	C819	C756
			U1375		U1156	A1095	U954		C889	U822	U757
			G1376		C1160	A1096	G955		U823	U824	C758
			A1377		U1161	A1097	A956		U890	C825	U760
			G1378		A1162	G1098	C957		G	G	G761
			C1379		C1163	A1099	G958		G	U826	A762
			A1380		G1164	G1100	C1032		G	C827	A763
			G1381		A1167	U1101	U1034		G	C828	A764
			C1382		G1168	G1102	G1035		G	C829	C765
			A1383		C1169	C1103	G1036		C	C830	
			G1384		U1172	G1104	U1037		C	G831	U768
			C1385		G1173	A1105	U1038		U	A832	C769
			A1386		U1174	A1106	A1039		C	A833	U770
			G1387		C1181	U1107	A1040		A	A834	C771
			C1388		U1182	A1108	U1044		C		
			A1389		C1183	A1109	G1045		A	U837	A774
			G1390		U1257	G1110	G1049		G	U838	G775
			U1391		G1261	C1111	C1049		U	U839	G776
			C1392		U1262	C1112	U1051		C	U840	A777
			A1393		G1263	C1113	G1052		A	G841	G778
			G1394		C1264	C1114	C1053		C	A842	U779
			U1395		G1265	C1115	G1054		C	G843	U780
			C1396		U1266	C1116	C1055		C	G844	G781
			A1397		G1267	C1117	U1056			U845	U782
			G1398		C1268	C1118	U1057			G846	G783
			C1399		U1269	C1119	G1058			C850	U784
			U1400		C1270	C1120	A1059			C851	U785
			A1401		G1271	C1121	G1122			U852	A787
			C1402		U1342	C1122	G1123			C853	G788
			G1403		A1343	C1123	U1199				
			C1404		G1334	C1124					
			A1405		U1335	C1125					
			G1406		G1336	C1126					
			C1407		U1337	C1127					
			A1408		G1338	C1128					
			U1409		C1339	C1129					
			C1410		U1340	C1130					
			G1411		C1411	C1131					
			U1412		C1412	C1132					
			C1413		U1413	C1133					
			G1414		G1414	C1134					
			A1415		C1415	C1135					
			U1416		U1416	C1136					
			C1417		G1417	C1137					
			A1418		U1418	C1138					
			G1419		C1419	C1139					
			U1420		U1420	C1140					
			C1421		G1421	C1141					
			A1422		U1422	C1142					
			U1423		C1423	C1143					
			G1424		U1424	C1144					
			C1425		G1425	C1145					
			U1426		U1426	C1146					
			A1427		C1427	C1147					
			G1428		U1428	C1148					
			C1429		G1429	C1149					
			U1430		U1430	C1150					
			A1431		C1431	C1151					
			G1432		U1432	C1152					
			C1433		G1433	C1153					
			U1434		U1434	C1154					
			A1435		C1435	C1155					
			G1436		U1436	C1156					
			C1437		G1437	C1157					
			U1438		U1438	C1158					
			A1439		C1439	C1159					
			G1440		U1440	C1160					
			C1441		G1441	C1161					
			U1442		U1442	C1162					
			G1443		C1443	C1163					
			U1444		U1444	C1164					
			A1445		C1445	C1165					
			G1446		U1446	C1166					
			C1447		C1447	C1167					
			U1448		U1448	C1168					
			A1449		C1449	C1169					
			G1450		U1450	C1170					
			C1451		G1451	C1171					
			U1452		U1452	C1172					
			A1453		C1453	C1173					
			G1454		U1454	C1174					
			C1455		C1455	C1175					
			U1456		U1456	C1176					
			A1457		C1457	C1177					
			G1458		U1458	C1178					
			C1459		C1459	C1179					
			U1460		U1460	C1180					
			A1461		C1461	C1181					
			G1462		U1462	C1182					
			C1463		C1463	C1183					
			U1464		U1464	C1184					
			A1465		C1465	C1185					
			G1466		U1466	C1186					
			C1467		C1467	C1187					
			U1468		U1468	C1188					
			A1469		C1469	C1189					
			G1470		U1470	C1190					
			C1471		C1471	C1191					
			U1472		U1472	C1192					
			A1473		C1473	C1193					
			G1474		U1474	C1194					
			C1475		C1475	C1195					
			U1476		U1476	C1196					
			A1477		C1477	C1197					
			G1478		U1478	C1198					
			C1479		C1479	C1199					
			U1480		U1480	C1200					
			A1481		C1481	C1201					
			G1482		U1482	C1202					
			C1483		C1483	C1203					
			U1484		U1484	C1204					
			A1485		C1485	C1205					
			G1486		U1486	C1206					
			C1487		C1487	C1207					
			U1488		U1488	C1208					
			A1489		C1489	C1209					
			G1490		U1490	C1210					
			C1491		C1491	C1211					
			U1492		U1492	C1212					
			A1493		C1493	C1213					
			G1494		U1494	C1214					
			C1495		C1495	C1215					
			U1496		U1496	C1216					
			A1497		C1497	C1217					
			G1498		U1498	C1218					
			C1499		C1499	C1219					
			U1500		U1500	C1220					
			A1501		C1501	C1221					
			G1502		U1502	C1222					
			C1503		C1503	C1223					
			U1504		U1504	C1224					
			A1505		C1505	C1225					
			G1506		U1506	C1226					
			C1507		C1507	C1227					

A2720	A2654	G2587	G2593	C2459	G2388	G2320	A2252	C2184	A	G2053	C1991	U1922	U1856	C1786
G2685	G2655	U2588	G2524	G2460	G2389	C2321	A2253	U2185	C	A2054	G1992	U1923	G1857	U1787
G2656	G2657	C2589	U2525	C2461	G2392	U2322	C2254		G	G2055	G1993	C1924	C1858	C1788
U2726	U2590	U2526	G2526	G2462	G2392	U2323	G2255	A2188	U	G2056	U1994	C1925	C1859	U1789
G2658	G2591	G2527	G2463	G2463	G2393	G2324	G2256	A2189	G	A2060	G1995	U1926	A1861	G1790
G2727	G2592	G2528	G2464	G2464	G2394	A2325	A2257	A2190	C	G2061	A1996	U1927	G1862	C1791
A2728	A2593	G2529	G2465	G2465	G2395	C2326	G2258	A2191	C	U2062	A1997	G1928	C1863	G1792
A2729	G2661	G2530	G2466	G2466	G2396	C2329	G2261	U2192	U	U2063	A1998	U1929	U1863	A1793
C2730	C2662	U2531	A2467	G2468	C2397	G2330	C2262	C2193	U	U2064	U1999	C1930	G1795	A1794
G2731	G2663	G2532	G2469	G2469	A2401	A2333	C2263	C2194	U	U2065	G2001	G1932	G1865	A1796
C2732	G2664	U2533	U2470	U2470	A2402	A2334	C2264	C2195	G	U2066	A2002	G1933	G1866	
U2733	G2665	U2534	U2471	U2471	G2403	U2335	A2265	U2197	G	G2067	A2003	U1934	A1867	A1798
A2734	U2535	G2535	U2472	U2472	A2404	U2336	A2266	U2198	G	G2068	A2004	A1935	U1870	A1800
C2735	G2536	C2537	C2475	C2475	A2405	U2337	A2267	U2199	G	U2069	U2005	A1936	U1871	A1801
U2736	C2538	C2538	C2476	C2476	C2406	A2337	G2268	C2200	G	G2070	G2006	G1937	G1874	U1804
A2737	C2539	C2539	A2477	A2477	G2407	C2338	G2269	G2201	C	G2071		U1938	C1875	U1805
C2740	G2605	A2540	C2478	C2478	G2408	A2339	U2270		G	C2072	U2009	U1939	C1876	G1806
U2741	U2541	A2541	U2479	U2479	A2409	C2340	C2271	C2204	G	U2073	G2010	C1940	C1877	A1807
A2745	U2542	U2542	U2479	U2479	U2410			C2205	U	U2075	U2011	A1943	U1881	A1808
U2677	A2543	A2543	C2480	C2480		C2343	C2274	C2206	G	G2076	A2012		G1882	G1809
C2748	G2608	G2608	G2481	G2481	A2414	G2344	U2275	C2207	G	G2077	A2013	U1946	A1883	U1810
G2679	G2609	G2609	A2482	A2482	G2415	G2345	U2276	U2208	A	G2078	A2014	U1947	A1884	U1811
U2680	A2611	A2611	U2483	U2483	U2416	A2346	A2277	G2209	G	A2079	G2015	G1947	C1885	U1812
	G2546	G2546	U2484	U2484	U2417	C2347	A2278	C2210	G	U2080	A2016	A1948	G1886	A1813
C2683	G2547	G2547	U2485	U2485	A2418	U2348		U2211	C	U2081	U2017	A1949	G1887	
A2684	G2548	G2548	U2486	U2486	C2419	G2349	C2281	U2212	A	C2082	G2018	G1951	C1888	G1816
	U2549	U2549	C2487	C2487	C2420	G2350	G2282	G2213	C	U2083	C2019	A1952	G	U1817
G2687	C2550	C2550	G2488	G2488	C2421	G2351	U2283	G2214	G	C2084		A1953	C	U1818
U2688	A2551	A2551	G2489	G2489	C2422	G2352	U2284	C2215	G	U2085	C2022	A1954	C	G1819
C2689	G2552	G2552	U2490	U2490	G2423	G2353	U2285	G2216	G	U2086	C2023	A1955	C	U1810
A2690	C2554	C2554	C2491	C2491		A2357	G2286	G2217	U	U2087	A2025	G1956	C	U1811
G2691	G2555	G2555	U2492	U2492	G2426	C2358	G2287	G2218	G	U2088	C2026	A1957	C	G1820
U2692	A2556	A2556	U2493	U2493	A2427	U2359	U2288	U2219	A	C	A2027	G1958	C	A1821
G2693	G2557	G2557	C2494	C2494	U2428		A2289	G2221	A	U2089	C2028	A1963	A	C1824
G2694	G2495	G2495	U2495	U2495		G2362	A2290	G2222	U	C	C2029	G1964	C	C1825
C2767	U2559	U2559	C2496	C2496	C2431	G2363	U2291	U2223	A	U	U2030	U1965	U	G1828
G2768	G2560	G2560	A2497	A2497	A2432	C2364		U2224	C	A	A2031	U1966	A	C1829
U2774	G2561	G2561	U2498	U2498		U2365	U2294	U2225	C	G	G2032	C1971	U	C1830
U2775			C2499	C2499	C2435	U2366	U2295	A2226	A	U	C2033	G1972	A	G1831
A2776	U2564	U2564	C2500	C2500		A2367	U2296	G2227	C	G	A2034	G1973	A	G1832
G2769	C2565	C2565	G2503	G2503	A2438	G2368	G2297	C2228	C	U	G2035	G1974	C	U1833
U2770	A2566	A2566	G2504	G2504	U2439	U2369	U2298	U2229	C	A	C2036	G1975	G	G1834
C2771	G2567	G2567	G2505	G2505	G2440	G2370	A2299	G2229	C	U	A2037	U1976	U	C1835
G2772	A2568	A2568	G2506	G2506	U2441	A2371	G2300	G2230	U	G	G2038	C1977	C	C1836
U2773	G2634	G2634	C2507	C2507	C2442	C2372	A2301	G2235	G	U	C2039	U1978	C	A1839
U2776	U2635	U2635	U2572	U2572	C2443	C2373	G2302	U2236	G	G	A2041	C1979	U1909	A1840
A2777	A2636	A2636	C2508	C2508	C2444	C2374	G2303	G2237	G	U	A2042	A1980	A1910	G1841
G2778	G2640	G2640	A2509	A2509	G2447	G2375	C2304	C2238	C	U	G2043	A1981	A1911	G1842
U2779	A2641	A2641	G2510	G2510	A2448	G2376	C2305	C2239	U	G	A2044	C1982	G1912	U1843
C2780	G2642	G2642	G2511	G2511	G2449	U2377	A2306	G2240	G	A	G2045	A1983	U1914	A1845
U2781			G2514	G2514		U2380		U2241	C	U	C2046	A1984	G1913	A1846
G2782	G2643	G2643	G2515	G2515	U2452	A2381	U2311	G2242	C	U	C2047	G1985	C1917	
A2783	C2644	C2644	U2516	U2516	C2453	G2382	G2312	G2243	C	U	C2048	G1986	G1918	G1850
U2784	A2649	A2649	G2517	G2517	A2455	C2383	G2313	C2244	C	U	C2049	G1987	A1919	A1851
C2785	G2650	G2650	G2518	G2518	U2456	G2384	A2314	A2245	C	U	G2050	A1988	A1920	G1852
U2786	U2651	U2651	C2519	C2519	A2457	U2385	A2315	A2246	G	A	G2051	C1989	A1921	
G2787	G2652	G2652	U2457	U2457		U2386	U2318	A2247						
U2788	A2653	A2653	U2458	U2458		U2387	G2319							



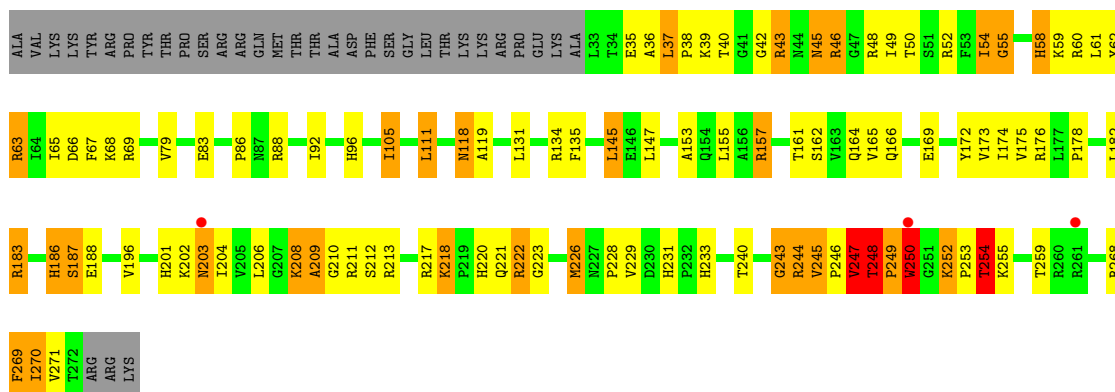
- Molecule 2: 5S ribosomal RNA

Chain Y:



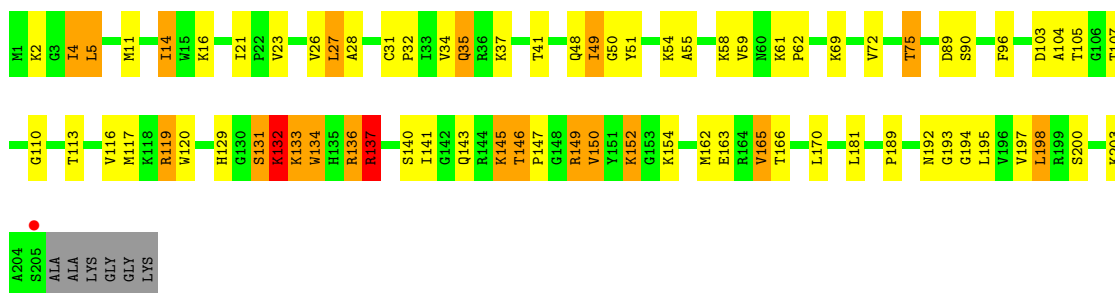
- Molecule 3: 50S ribosomal protein L2

Chain A: 



- Molecule 4: 50S ribosomal protein L3

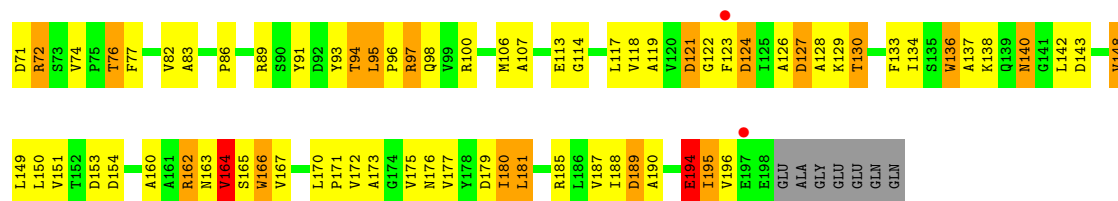
Chain B:



- Molecule 5: 50S ribosomal protein L4

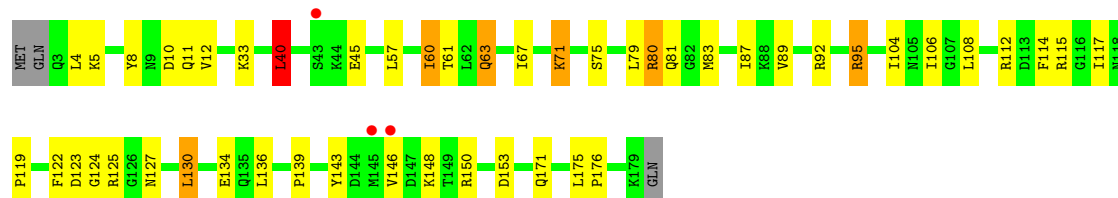
Chain C:





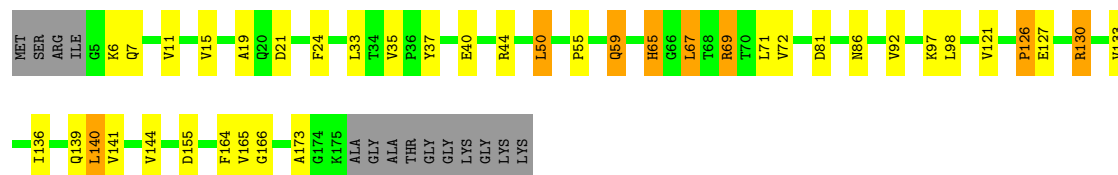
• Molecule 6: 50S ribosomal protein L5

Chain D:



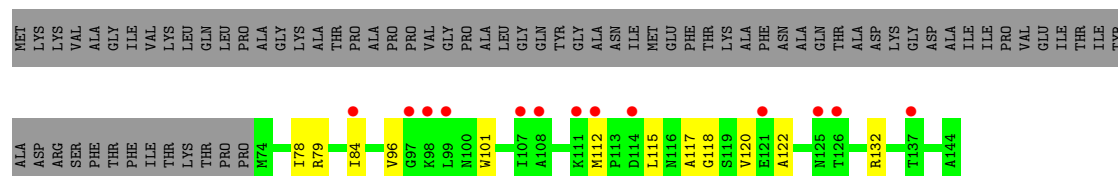
• Molecule 7: 50S ribosomal protein L6

Chain E:



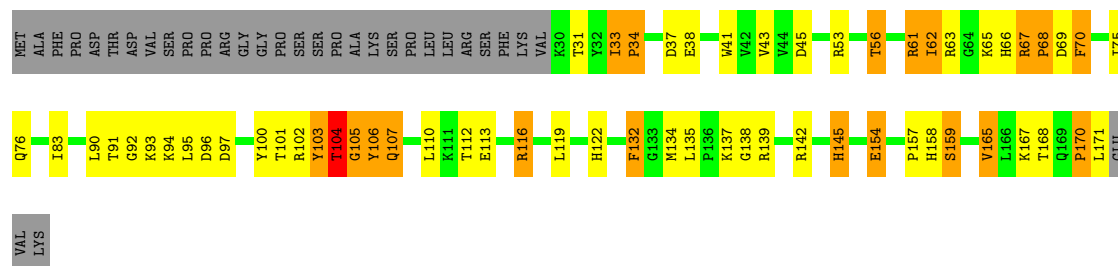
• Molecule 8: 50S ribosomal protein L11

Chain F:



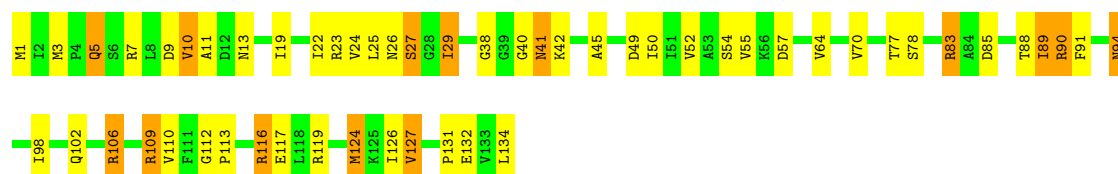
• Molecule 9: 50S ribosomal protein L13

Chain G:



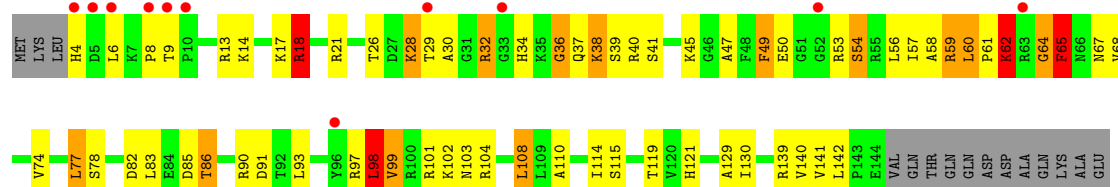
• Molecule 10: 50S ribosomal protein L14

Chain H:



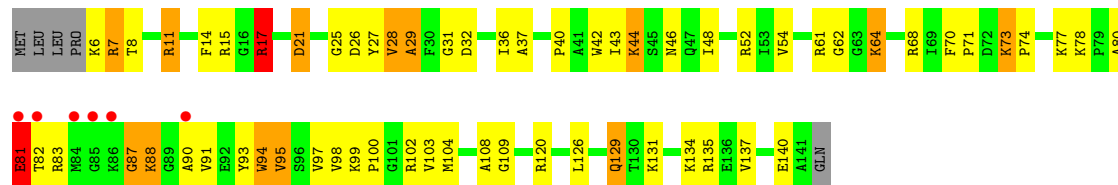
• Molecule 11: 50S ribosomal protein L15

Chain I:



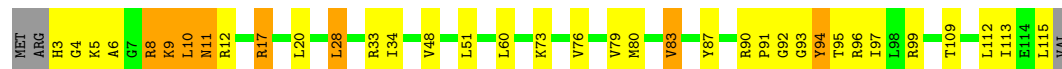
• Molecule 12: 50S ribosomal protein L16

Chain J:



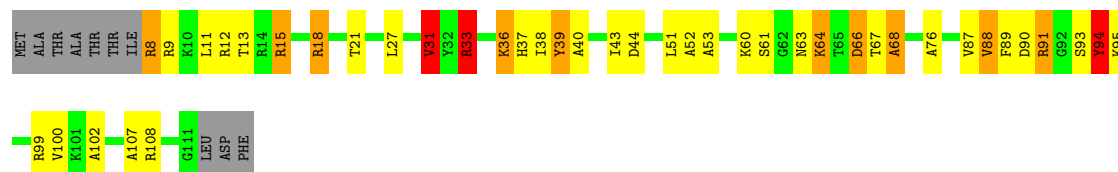
• Molecule 13: 50S ribosomal protein L17

Chain K:



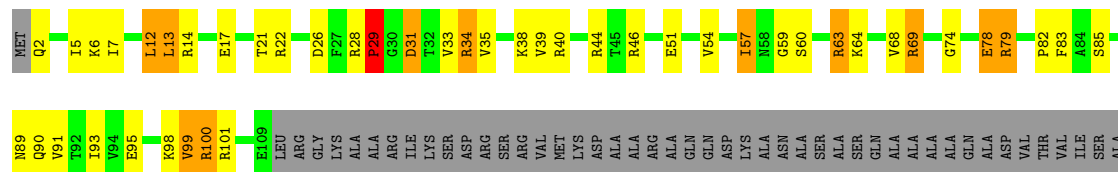
• Molecule 14: 50S ribosomal protein L18

Chain L:



• Molecule 15: 50S ribosomal protein L19

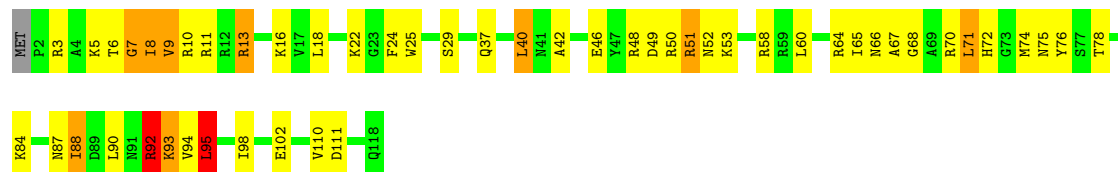
Chain M:



ALA
PRO
GLU
VAL
ALA
GLU
PRO
THR
GLN
GLY
GLU

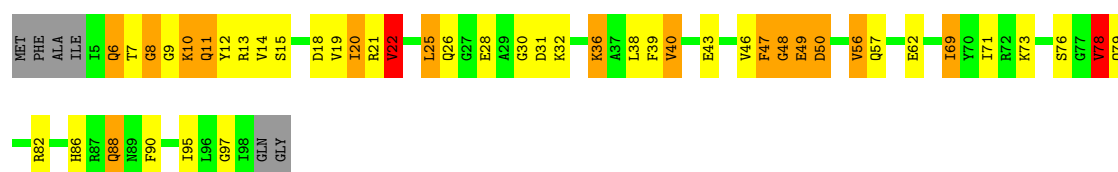
- Molecule 16: 50S ribosomal protein L20

Chain N:



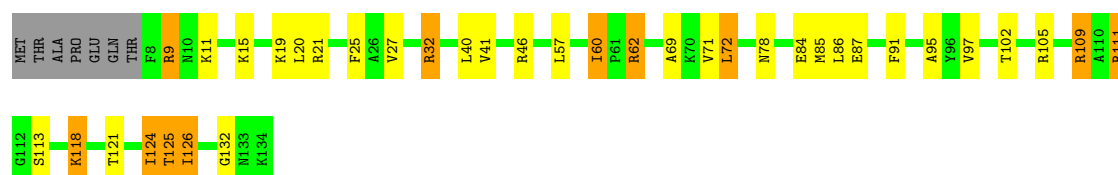
- Molecule 17: 50S ribosomal protein L21

Chain O:



- Molecule 18: 50S ribosomal protein L22

Chain P:



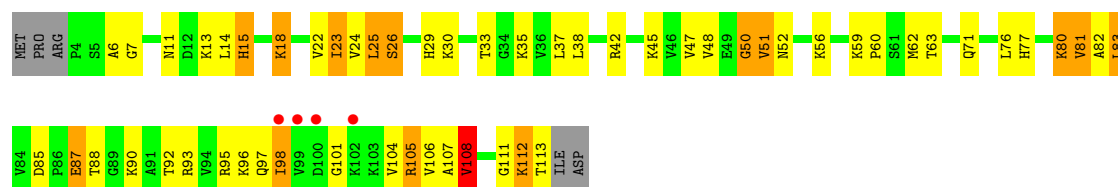
- Molecule 19: 50S ribosomal protein L23

Chain Q:



- Molecule 20: 50S ribosomal protein L24

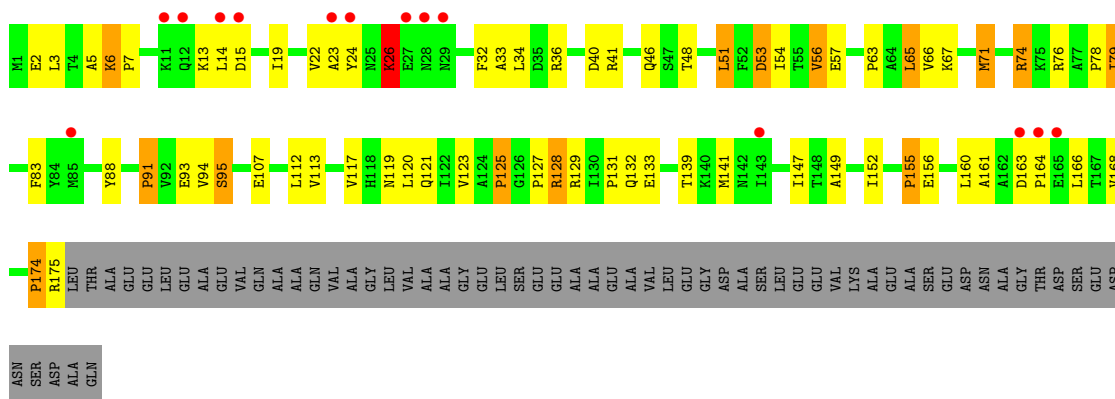
Chain R:



- Molecule 21: 50S ribosomal protein L25

Chain S:





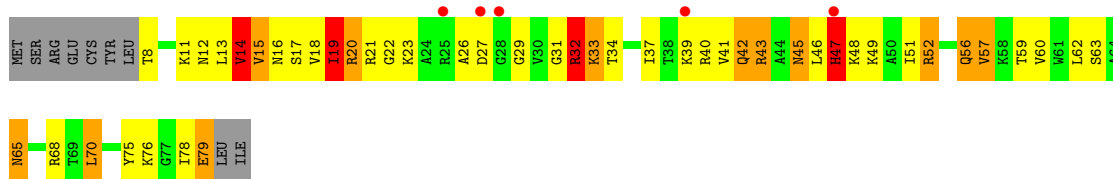
- Molecule 22: 50S ribosomal protein L27

Chain T:



- Molecule 23: 50S ribosomal protein L28

Chain U:



- Molecule 24: 50S ribosomal protein L29

Chain V:



- Molecule 25: 50S ribosomal protein L30

Chain W:



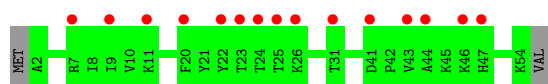
- Molecule 26: 50S ribosomal protein L32

Chain Z:



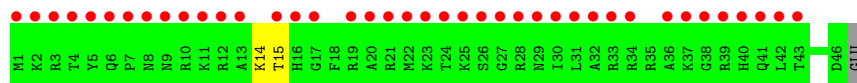
- Molecule 27: 50S ribosomal protein L33

Chain 1:



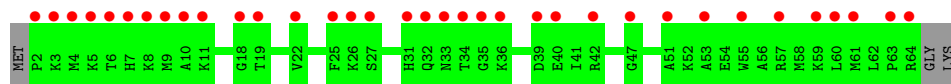
- Molecule 28: 50S ribosomal protein L34

Chain 2:



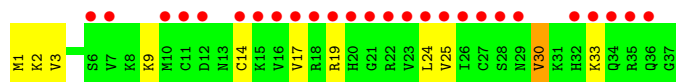
- Molecule 29: 50S ribosomal protein L35

Chain 3:



- Molecule 30: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.11 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.5 (30.11-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.65Å)	Xtriage
Refinement program	autobuster	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.257	Depositor DCC
R_{free} test set	12232 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 242941 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1F4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	1.02	36/64561 (0.1%)	1.86	1991/100708 (2.0%)
2	Y	1.22	2/2904 (0.1%)	1.83	99/4525 (2.2%)
3	A	0.58	0/1862	0.93	4/2510 (0.2%)
4	B	0.55	0/1567	0.88	1/2105 (0.0%)
5	C	0.62	0/1529	0.96	0/2070
6	D	0.46	0/1419	0.68	0/1903
7	E	0.47	0/1308	0.71	0/1771
8	F	0.50	0/508	0.67	0/683
9	G	0.58	0/1138	0.92	2/1539 (0.1%)
10	H	0.53	0/1007	0.84	0/1352
11	I	0.67	0/1081	1.06	2/1448 (0.1%)
12	J	0.86	0/1113	0.96	1/1486 (0.1%)
13	K	0.66	0/886	0.92	0/1188
14	L	0.52	0/785	0.93	0/1048
15	M	0.59	0/884	1.00	2/1186 (0.2%)
16	N	0.53	0/994	0.79	0/1323
17	O	0.52	0/750	0.96	1/1000 (0.1%)
18	P	0.57	0/1027	0.88	0/1373
19	Q	0.56	0/737	0.99	2/988 (0.2%)
20	R	0.59	0/835	1.02	0/1121
21	S	0.61	0/1370	0.76	0/1862
22	T	0.54	0/633	0.88	0/838
23	U	0.71	0/556	1.08	2/741 (0.3%)
24	V	0.52	0/537	0.73	0/714
25	W	0.51	0/426	0.81	0/568
26	Z	0.62	0/469	0.98	0/629
30	4	0.49	0/298	0.73	0/390
All	All	0.94	38/91184 (0.0%)	1.68	2107/137069 (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	3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	559	C	C3'-O3'	8.19	1.53	1.42
1	X	655	A	C3'-O3'	7.84	1.53	1.42
1	X	774	A	C5-C4	7.25	1.43	1.38
1	X	699	G	N9-C4	-6.97	1.32	1.38
1	X	1688	U	C2-N3	6.58	1.42	1.37
1	X	1674	C	C3'-O3'	-6.46	1.33	1.42
1	X	393	U	C1'-N1	6.43	1.58	1.48
1	X	1468	A	N7-C5	-6.24	1.35	1.39
1	X	2189	A	C3'-O3'	6.22	1.50	1.42
1	X	343	A	N9-C4	6.22	1.41	1.37
1	X	759	C	N3-C4	6.21	1.38	1.33
1	X	236	C	C1'-N1	6.10	1.57	1.48
1	X	540	G	C2-N3	5.99	1.37	1.32
1	X	346	C	C1'-N1	5.97	1.57	1.48
1	X	774	A	C6-N1	5.88	1.39	1.35
1	X	646	C	C1'-N1	5.79	1.57	1.48
1	X	2018	G	C3'-O3'	5.78	1.50	1.42
1	X	927	C	C1'-N1	5.72	1.57	1.48
1	X	868	U	C1'-N1	5.65	1.57	1.48
1	X	917	U	C1'-N1	5.60	1.57	1.48
1	X	1522	C	C1'-N1	5.52	1.57	1.48
1	X	1946	U	C1'-N1	5.45	1.56	1.48
2	Y	87	C	C3'-O3'	5.44	1.49	1.42
1	X	774	A	N3-C4	5.37	1.38	1.34
1	X	434	C	C1'-N1	5.35	1.56	1.48
1	X	31	C	C1'-N1	5.30	1.56	1.48
2	Y	32	C	C1'-N1	5.27	1.56	1.48
1	X	1688	U	N3-C4	5.25	1.43	1.38
1	X	422	C	C1'-N1	5.18	1.56	1.48
1	X	327	C	C1'-N1	5.15	1.56	1.48
1	X	2072	C	C1'-N1	5.14	1.56	1.48
1	X	1182	U	C1'-N1	5.14	1.56	1.48
1	X	2321	C	C1'-N1	5.14	1.56	1.48
1	X	1825	C	C1'-N1	5.11	1.56	1.48
1	X	358	C	C1'-N1	5.08	1.56	1.48
1	X	558	G	C3'-O3'	5.08	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	430	C	C1'-N1	5.06	1.56	1.48
1	X	774	A	N1-C2	5.03	1.38	1.34

All (2107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-30.77	85.29	109.90
1	X	1019	U	P-O3'-C3'	19.01	142.51	119.70
1	X	1288	A	C5'-C4'-O4'	18.79	131.64	109.10
1	X	774	A	N1-C6-N6	17.73	129.24	118.60
1	X	559	C	O4'-C1'-N1	17.43	122.14	108.20
1	X	2808	U	O4'-C1'-N1	16.51	121.41	108.20
1	X	1288	A	O4'-C1'-N9	16.46	121.37	108.20
1	X	2564	U	P-O3'-C3'	16.04	138.95	119.70
1	X	176	A	P-O3'-C3'	15.97	138.86	119.70
1	X	655	A	P-O3'-C3'	15.78	138.64	119.70
1	X	558	G	P-O3'-C3'	15.40	138.18	119.70
1	X	1775	A	P-O3'-C3'	15.14	137.87	119.70
1	X	1278	A	O4'-C1'-N9	14.65	119.92	108.20
1	X	1473	U	P-O3'-C3'	14.53	137.13	119.70
1	X	204	A	P-O3'-C3'	14.46	137.05	119.70
1	X	33	C	P-O3'-C3'	14.32	136.88	119.70
1	X	1634	A	P-O3'-C3'	14.15	136.69	119.70
1	X	100	G	P-O3'-C3'	14.14	136.66	119.70
1	X	559	C	C4'-C3'-C2'	-14.06	88.54	102.60
1	X	2497	A	P-O3'-C3'	13.90	136.38	119.70
1	X	2736	U	P-O3'-C3'	13.74	136.19	119.70
1	X	2018	G	P-O3'-C3'	13.71	136.16	119.70
1	X	814	G	P-O3'-C3'	13.68	136.11	119.70
1	X	1790	G	P-O3'-C3'	13.67	136.11	119.70
1	X	342	G	P-O3'-C3'	13.52	135.92	119.70
1	X	2312	A	P-O3'-C3'	13.31	135.68	119.70
1	X	994	A	P-O3'-C3'	13.30	135.66	119.70
1	X	774	A	N7-C8-N9	13.21	120.41	113.80
1	X	334	G	P-O3'-C3'	13.15	135.48	119.70
1	X	788	G	P-O3'-C3'	13.06	135.38	119.70
1	X	1475	U	P-O3'-C3'	12.98	135.28	119.70
1	X	181	A	P-O3'-C3'	12.91	135.19	119.70
1	X	1574	A	O4'-C1'-N9	12.86	118.49	108.20
1	X	343	A	O4'-C1'-N9	12.82	118.46	108.20
1	X	664	C	P-O3'-C3'	12.82	135.08	119.70
1	X	1468	A	C8-N9-C4	-12.70	100.72	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	48	A	P-O3'-C3'	12.66	134.89	119.70
1	X	683	A	P-O3'-C3'	12.61	134.82	119.70
1	X	1036	G	P-O3'-C3'	12.58	134.79	119.70
1	X	1938	U	P-O3'-C3'	12.51	134.71	119.70
1	X	469	G	P-O3'-C3'	12.51	134.71	119.70
1	X	2323	U	P-O3'-C3'	12.48	134.68	119.70
1	X	774	A	C5-N7-C8	-12.45	97.68	103.90
1	X	559	C	P-O3'-C3'	12.37	134.54	119.70
1	X	2854	G	C1'-O4'-C4'	-12.31	100.05	109.90
1	X	774	A	C6-C5-N7	-12.29	123.70	132.30
1	X	2691	C	P-O3'-C3'	12.27	134.42	119.70
1	X	399	G	P-O3'-C3'	12.25	134.40	119.70
1	X	1249	G	P-O3'-C3'	12.20	134.34	119.70
1	X	822	G	P-O3'-C3'	12.20	134.34	119.70
1	X	2261	G	P-O3'-C3'	12.06	134.17	119.70
1	X	537	C	N1-C2-O2	11.88	126.03	118.90
1	X	218	A	P-O3'-C3'	11.84	133.91	119.70
1	X	73	A	P-O3'-C3'	11.83	133.90	119.70
1	X	1442	C	P-O3'-C3'	11.82	133.88	119.70
1	X	33	C	O4'-C1'-N1	11.81	117.65	108.20
1	X	454	G	P-O3'-C3'	11.81	133.87	119.70
1	X	514	G	P-O3'-C3'	11.70	133.74	119.70
1	X	1441	A	P-O3'-C3'	11.69	133.72	119.70
2	Y	58	G	P-O3'-C3'	11.69	133.72	119.70
1	X	2854	G	N9-C1'-C2'	11.57	129.04	114.00
1	X	540	G	N1-C6-O6	-11.44	113.04	119.90
1	X	2298	U	P-O3'-C3'	11.43	133.41	119.70
1	X	774	A	C4-C5-N7	11.39	116.39	110.70
1	X	2189	A	P-O3'-C3'	11.34	133.30	119.70
1	X	98	U	P-O3'-C3'	11.30	133.26	119.70
1	X	1096	A	P-O3'-C3'	11.30	133.26	119.70
1	X	490	A	P-O3'-C3'	11.30	133.26	119.70
1	X	1391	A	P-O3'-C3'	11.28	133.24	119.70
1	X	2426	G	P-O3'-C3'	11.26	133.21	119.70
1	X	1122	A	P-O3'-C3'	11.22	133.16	119.70
1	X	1288	A	C4'-C3'-C2'	-11.03	91.57	102.60
2	Y	16	U	P-O3'-C3'	11.01	132.91	119.70
1	X	841	G	O4'-C4'-C3'	-11.00	93.00	104.00
1	X	1746	A	O4'-C1'-N9	10.89	116.91	108.20
1	X	1923	U	P-O3'-C3'	10.88	132.76	119.70
1	X	554	U	P-O3'-C3'	10.87	132.74	119.70
1	X	522	G	O4'-C1'-N9	10.80	116.84	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	691	C	O4'-C1'-N1	10.80	116.84	108.20
1	X	1468	A	O4'-C1'-C2'	-10.79	95.00	105.80
1	X	1261	G	P-O3'-C3'	10.78	132.64	119.70
1	X	699	G	N3-C4-N9	-10.76	119.54	126.00
1	X	2491	C	O4'-C1'-N1	10.75	116.80	108.20
1	X	71	A	P-O3'-C3'	10.72	132.57	119.70
1	X	2770	A	P-O3'-C3'	10.71	132.55	119.70
1	X	1186	G	P-O3'-C3'	10.64	132.47	119.70
1	X	2371	A	O4'-C1'-N9	10.63	116.71	108.20
1	X	242	A	C1'-O4'-C4'	-10.63	101.40	109.90
1	X	1632	A	O4'-C1'-N9	-10.53	99.78	108.20
1	X	333	A	P-O3'-C3'	10.48	132.27	119.70
1	X	2634	G	O4'-C1'-N9	10.44	116.55	108.20
1	X	1820	G	P-O3'-C3'	10.44	132.22	119.70
1	X	1732	U	P-O3'-C3'	10.42	132.21	119.70
1	X	1053	G	P-O3'-C3'	10.38	132.16	119.70
1	X	1333	G	N3-C4-N9	-10.31	119.81	126.00
1	X	1280	U	P-O3'-C3'	10.29	132.04	119.70
1	X	699	G	N3-C4-C5	10.28	133.74	128.60
1	X	1055	A	P-O3'-C3'	10.26	132.01	119.70
1	X	805	G	O4'-C1'-N9	-10.22	100.02	108.20
1	X	809	C	O4'-C1'-N1	10.21	116.37	108.20
1	X	1684	G	P-O3'-C3'	10.16	131.90	119.70
1	X	2731	G	P-O3'-C3'	10.16	131.89	119.70
1	X	1403	U	P-O3'-C3'	10.15	131.88	119.70
1	X	1409	U	P-O3'-C3'	10.14	131.87	119.70
1	X	341	A	P-O3'-C3'	10.14	131.87	119.70
1	X	2593	A	P-O3'-C3'	10.11	131.83	119.70
1	X	321	A	P-O3'-C3'	10.11	131.83	119.70
1	X	1474	A	P-O3'-C3'	10.10	131.82	119.70
1	X	2018	G	C1'-O4'-C4'	-10.01	101.89	109.90
1	X	434	C	P-O3'-C3'	9.91	131.60	119.70
1	X	666	U	O4'-C1'-N1	9.91	116.13	108.20
1	X	89	A	P-O3'-C3'	9.91	131.59	119.70
1	X	813	A	P-O3'-C3'	9.89	131.57	119.70
1	X	651	C	P-O3'-C3'	9.83	131.50	119.70
1	X	2228	U	P-O3'-C3'	9.83	131.50	119.70
1	X	1278	A	C1'-O4'-C4'	-9.83	102.03	109.90
1	X	655	A	O4'-C1'-N9	9.83	116.06	108.20
1	X	1799	A	C1'-O4'-C4'	-9.77	102.09	109.90
1	X	2229	G	P-O3'-C3'	9.77	131.42	119.70
1	X	540	G	P-O3'-C3'	9.76	131.41	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	467	U	P-O3'-C3'	9.73	131.38	119.70
1	X	2730	A	P-O3'-C3'	9.73	131.37	119.70
1	X	1601	U	P-O3'-C3'	9.68	131.32	119.70
1	X	1770	U	C1'-O4'-C4'	-9.68	102.16	109.90
1	X	1086	C	P-O3'-C3'	9.66	131.29	119.70
1	X	1976	U	O4'-C1'-N1	9.66	115.92	108.20
1	X	1353	A	P-O3'-C3'	9.65	131.28	119.70
1	X	2689	C	P-O3'-C3'	9.58	131.20	119.70
1	X	638	A	P-O3'-C3'	9.57	131.19	119.70
1	X	1975	G	P-O3'-C3'	9.56	131.17	119.70
1	X	632	A	O4'-C1'-N9	9.53	115.83	108.20
1	X	343	A	C8-N9-C4	-9.53	101.99	105.80
1	X	2330	G	N9-C1'-C2'	9.53	126.38	114.00
1	X	731	A	P-O3'-C3'	9.52	131.12	119.70
1	X	483	A	P-O3'-C3'	-9.50	108.30	119.70
1	X	1278	A	C3'-C2'-C1'	-9.50	93.90	101.50
1	X	1811	A	P-O3'-C3'	9.49	131.09	119.70
1	X	172	A	P-O3'-C3'	9.48	131.08	119.70
1	X	242	A	O4'-C1'-N9	9.46	115.77	108.20
1	X	557	U	C1'-O4'-C4'	-9.45	102.34	109.90
1	X	803	C	P-O3'-C3'	9.45	131.04	119.70
1	X	939	C	P-O3'-C3'	9.43	131.01	119.70
1	X	1575	C	P-O3'-C3'	9.43	131.01	119.70
1	X	1489	C	O4'-C1'-N1	9.39	115.71	108.20
1	X	646	C	O4'-C1'-N1	9.36	115.69	108.20
1	X	2190	A	O4'-C1'-N9	9.36	115.69	108.20
1	X	2591	C	N1-C2-O2	9.34	124.50	118.90
1	X	1574	A	C1'-O4'-C4'	-9.32	102.44	109.90
2	Y	90	C	P-O3'-C3'	-9.30	108.53	119.70
1	X	1313	U	O4'-C1'-N1	9.29	115.64	108.20
1	X	1459	U	P-O3'-C3'	9.29	130.85	119.70
1	X	1338	G	P-O3'-C3'	9.28	130.84	119.70
1	X	34	U	O4'-C1'-N1	9.27	115.62	108.20
1	X	841	G	O4'-C1'-N9	9.25	115.60	108.20
1	X	1439	G	P-O3'-C3'	9.23	130.78	119.70
1	X	941	U	O4'-C1'-N1	9.21	115.57	108.20
1	X	2222	U	O4'-C1'-N1	9.21	115.57	108.20
1	X	2324	G	P-O3'-C3'	9.17	130.71	119.70
1	X	2566	A	P-O3'-C3'	9.13	130.65	119.70
1	X	1663	C	N1-C2-O2	9.12	124.37	118.90
1	X	2634	G	C3'-C2'-C1'	-9.12	94.21	101.50
1	X	2039	G	C8-N9-C4	-9.11	102.75	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	247	A	C1'-O4'-C4'	-9.11	102.61	109.90
2	Y	81	C	O4'-C1'-N1	9.11	115.48	108.20
1	X	2472	U	P-O3'-C3'	-9.09	108.79	119.70
1	X	494	A	P-O3'-C3'	9.08	130.60	119.70
1	X	883	A	C5'-C4'-O4'	9.07	119.99	109.10
1	X	1790	G	O4'-C1'-N9	9.05	115.44	108.20
1	X	416	U	O4'-C1'-N1	9.01	115.41	108.20
1	X	2270	U	O4'-C1'-N1	9.01	115.41	108.20
1	X	312	G	C1'-O4'-C4'	-8.99	102.71	109.90
1	X	841	G	N9-C1'-C2'	8.97	125.66	114.00
1	X	656	U	P-O3'-C3'	8.95	130.44	119.70
1	X	1333	G	C8-N9-C4	-8.95	102.82	106.40
1	X	1984	A	C3'-C2'-C1'	-8.95	94.34	101.50
1	X	2018	G	C5-N7-C8	-8.95	99.83	104.30
1	X	2626	U	O4'-C1'-N1	8.95	115.36	108.20
1	X	1688	U	N3-C4-O4	8.93	125.65	119.40
1	X	817	A	C1'-O4'-C4'	-8.91	102.77	109.90
1	X	774	A	C5-C6-N1	-8.91	113.25	117.70
1	X	2018	G	C4-C5-N7	8.91	114.36	110.80
1	X	332	C	O4'-C1'-N1	8.84	115.27	108.20
1	X	755	C	P-O3'-C3'	-8.82	109.11	119.70
1	X	1268	U	P-O3'-C3'	8.77	130.22	119.70
1	X	825	C	P-O3'-C3'	-8.73	109.22	119.70
1	X	938	G	P-O3'-C3'	8.73	130.18	119.70
1	X	774	A	N9-C4-C5	-8.73	102.31	105.80
1	X	2228	U	N3-C4-C5	-8.73	109.36	114.60
1	X	976	C	O4'-C1'-N1	8.73	115.18	108.20
1	X	666	U	C1'-O4'-C4'	-8.71	102.94	109.90
1	X	845	U	O4'-C1'-N1	8.70	115.16	108.20
1	X	320	A	O4'-C1'-N9	8.68	115.15	108.20
1	X	2034	A	P-O3'-C3'	8.68	130.12	119.70
1	X	1496	G	P-O3'-C3'	8.67	130.11	119.70
1	X	173	A	C1'-O4'-C4'	-8.67	102.97	109.90
1	X	1574	A	C4'-C3'-C2'	-8.67	93.93	102.60
1	X	1790	G	C1'-O4'-C4'	-8.64	102.99	109.90
1	X	2204	A	P-O3'-C3'	8.60	130.02	119.70
1	X	1288	A	C3'-C2'-C1'	-8.60	94.62	101.50
1	X	99	U	P-O3'-C3'	8.58	130.00	119.70
1	X	1161	U	O4'-C1'-N1	8.58	115.06	108.20
1	X	817	A	O4'-C4'-C3'	-8.57	95.43	104.00
1	X	2824	C	P-O3'-C3'	8.57	129.98	119.70
1	X	2039	G	N9-C4-C5	8.56	108.83	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1710	U	P-O3'-C3'	8.56	129.97	119.70
1	X	236	C	O4'-C1'-N1	8.56	115.05	108.20
1	X	1468	A	O4'-C1'-N9	8.55	115.04	108.20
1	X	841	G	C8-N9-C4	-8.54	102.99	106.40
1	X	358	C	O4'-C1'-N1	8.53	115.02	108.20
2	Y	86	A	O4'-C1'-N9	8.49	115.00	108.20
1	X	2414	A	P-O3'-C3'	8.49	129.89	119.70
1	X	2051	U	O4'-C1'-N1	8.47	114.98	108.20
1	X	1072	U	P-O3'-C3'	8.46	129.85	119.70
1	X	761	G	C1'-O4'-C4'	-8.45	103.14	109.90
1	X	216	U	O4'-C1'-N1	8.45	114.96	108.20
1	X	432	C	O4'-C1'-N1	8.44	114.95	108.20
1	X	2452	U	P-O3'-C3'	8.44	129.83	119.70
1	X	2481	G	P-O3'-C3'	8.44	129.82	119.70
1	X	2497	A	C1'-O4'-C4'	-8.43	103.15	109.90
1	X	1468	A	P-O3'-C3'	8.43	129.82	119.70
1	X	346	C	N1-C1'-C2'	8.43	124.96	114.00
1	X	2018	G	N9-C1'-C2'	8.43	124.96	114.00
1	X	774	A	C5-C6-N6	-8.42	116.96	123.70
1	X	577	U	O4'-C1'-N1	8.41	114.93	108.20
1	X	2703	C	O4'-C1'-N1	8.41	114.93	108.20
1	X	515	A	P-O3'-C3'	8.41	129.79	119.70
1	X	117	A	P-O3'-C3'	8.40	129.78	119.70
1	X	577	U	C4'-C3'-C2'	-8.39	94.21	102.60
1	X	1333	G	O4'-C1'-N9	8.39	114.91	108.20
1	X	1705	U	O4'-C1'-N1	8.39	114.91	108.20
1	X	2025	A	O4'-C1'-N9	8.39	114.91	108.20
1	X	1466	C	C6-N1-C2	-8.36	116.96	120.30
1	X	1966	C	O4'-C1'-N1	8.34	114.88	108.20
1	X	518	A	P-O3'-C3'	8.34	129.70	119.70
1	X	1731	C	O4'-C1'-N1	8.33	114.86	108.20
2	Y	88	C	O4'-C1'-N1	8.32	114.85	108.20
1	X	2853	U	O4'-C1'-N1	8.31	114.85	108.20
1	X	1467	U	N1-C2-O2	8.30	128.61	122.80
1	X	940	G	P-O5'-C5'	8.29	134.17	120.90
1	X	1524	C	P-O3'-C3'	8.29	129.65	119.70
1	X	2196	U	P-O3'-C3'	8.29	129.64	119.70
1	X	579	G	C4-C5-N7	-8.28	107.49	110.80
1	X	2439	U	O4'-C1'-N1	8.28	114.82	108.20
1	X	387	A	C5'-C4'-O4'	8.27	119.03	109.10
1	X	2370	G	O4'-C1'-N9	8.26	114.81	108.20
1	X	2228	U	N3-C4-O4	8.26	125.18	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2778	U	P-O3'-C3'	8.26	129.61	119.70
1	X	2237	C	P-O3'-C3'	8.24	129.59	119.70
1	X	2198	U	P-O3'-C3'	8.23	129.58	119.70
1	X	582	G	P-O3'-C3'	8.22	129.57	119.70
1	X	2669	C	N1-C2-O2	8.21	123.83	118.90
1	X	184	A	O4'-C1'-N9	8.21	114.77	108.20
1	X	192	G	P-O3'-C3'	8.19	129.53	119.70
1	X	190	A	O4'-C1'-N9	8.19	114.75	108.20
1	X	650	U	O4'-C1'-N1	8.19	114.75	108.20
1	X	1223	G	C3'-C2'-C1'	8.19	108.05	101.50
1	X	2859	U	O4'-C1'-N1	8.19	114.75	108.20
1	X	1975	G	C2'-C3'-O3'	8.18	127.50	109.50
1	X	1917	C	O4'-C1'-N1	8.17	114.73	108.20
1	X	2409	A	C1'-O4'-C4'	-8.16	103.38	109.90
1	X	394	U	O4'-C1'-N1	8.15	114.72	108.20
1	X	1468	A	C3'-C2'-C1'	-8.14	94.99	101.50
1	X	1468	A	N7-C8-N9	8.13	117.87	113.80
1	X	1991	C	P-O3'-C3'	-8.13	109.94	119.70
1	X	969	U	P-O3'-C3'	8.13	129.45	119.70
1	X	2291	U	O4'-C1'-N1	8.13	114.70	108.20
1	X	1467	U	N1-C1'-C2'	8.12	124.56	114.00
1	X	1285	A	P-O3'-C3'	8.11	129.43	119.70
1	X	1315	A	P-O3'-C3'	8.10	129.42	119.70
1	X	2795	A	P-O3'-C3'	8.10	129.42	119.70
1	X	338	G	C8-N9-C4	-8.09	103.16	106.40
1	X	2758	A	C1'-O4'-C4'	-8.08	103.43	109.90
1	X	1749	G	C1'-O4'-C4'	-8.08	103.43	109.90
1	X	2726	U	O4'-C1'-N1	8.05	114.64	108.20
2	Y	90	C	O4'-C1'-N1	8.05	114.64	108.20
1	X	1313	U	C1'-O4'-C4'	-8.05	103.46	109.90
1	X	841	G	C1'-O4'-C4'	-8.02	103.48	109.90
1	X	1412	C	P-O3'-C3'	8.02	129.32	119.70
1	X	843	G	P-O3'-C3'	8.02	129.32	119.70
1	X	2531	U	N3-C2-O2	-7.99	116.61	122.20
1	X	2693	U	C1'-O4'-C4'	-7.99	103.51	109.90
1	X	2258	G	C4'-C3'-C2'	-7.98	94.62	102.60
1	X	2432	A	O4'-C1'-N9	7.97	114.58	108.20
1	X	1345	G	C5'-C4'-O4'	7.97	118.66	109.10
1	X	242	A	C4'-C3'-C2'	-7.96	94.64	102.60
1	X	1656	U	P-O3'-C3'	7.95	129.24	119.70
1	X	1288	A	O4'-C4'-C3'	-7.95	96.05	104.00
1	X	499	G	O4'-C1'-N9	7.94	114.55	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1523	A	P-O3'-C3'	7.93	129.22	119.70
1	X	1217	U	O4'-C1'-N1	7.92	114.54	108.20
2	Y	54	U	O4'-C1'-N1	7.92	114.53	108.20
1	X	1850	G	P-O3'-C3'	7.90	129.18	119.70
1	X	938	G	O4'-C1'-N9	7.89	114.51	108.20
1	X	458	G	P-O3'-C3'	7.87	129.14	119.70
1	X	346	C	C6-N1-C2	-7.87	117.15	120.30
1	X	882	C	O4'-C1'-N1	7.87	114.49	108.20
1	X	1188	A	P-O3'-C3'	7.85	129.12	119.70
1	X	509	U	O4'-C1'-N1	7.85	114.48	108.20
1	X	1339	U	P-O3'-C3'	7.84	129.11	119.70
1	X	2507	U	P-O3'-C3'	7.84	129.11	119.70
1	X	1830	C	P-O3'-C3'	7.84	129.10	119.70
1	X	1467	U	P-O3'-C3'	-7.83	110.30	119.70
1	X	1469	U	N3-C2-O2	-7.82	116.72	122.20
1	X	1152	C	P-O3'-C3'	7.82	129.08	119.70
1	X	593	C	O4'-C1'-N1	7.80	114.44	108.20
1	X	2702	G	C5-C6-O6	-7.78	123.93	128.60
1	X	2049	C	O4'-C1'-N1	7.76	114.41	108.20
1	X	696	U	O4'-C1'-N1	7.76	114.41	108.20
1	X	2485	U	O4'-C1'-N1	-7.75	102.00	108.20
1	X	1791	C	O4'-C1'-N1	7.74	114.39	108.20
1	X	816	U	O4'-C1'-N1	7.74	114.39	108.20
1	X	2872	U	O4'-C1'-N1	7.73	114.38	108.20
1	X	2860	C	O4'-C1'-N1	7.73	114.38	108.20
1	X	1496	G	C3'-C2'-C1'	-7.71	95.33	101.50
1	X	223	C	O4'-C1'-N1	7.71	114.36	108.20
1	X	1777	A	C1'-O4'-C4'	-7.71	103.73	109.90
1	X	2664	G	N1-C6-O6	7.70	124.52	119.90
1	X	357	A	P-O3'-C3'	7.69	128.93	119.70
1	X	1172	U	O4'-C1'-N1	7.69	114.36	108.20
1	X	2651	U	O4'-C1'-N1	7.68	114.35	108.20
1	X	2788	C	O4'-C1'-N1	7.68	114.34	108.20
1	X	2288	A	P-O3'-C3'	7.68	128.91	119.70
1	X	2039	G	O4'-C1'-N9	7.68	114.34	108.20
1	X	868	U	O4'-C1'-N1	7.67	114.34	108.20
1	X	1268	U	O4'-C1'-N1	7.67	114.34	108.20
1	X	2481	G	C5-C6-O6	-7.67	124.00	128.60
1	X	2018	G	C3'-C2'-C1'	-7.66	95.37	101.50
1	X	2530	C	P-O3'-C3'	7.66	128.90	119.70
1	X	2664	G	C6-C5-N7	-7.66	125.80	130.40
1	X	198	A	P-O3'-C3'	7.66	128.89	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	742	G	P-O3'-C3'	7.66	128.89	119.70
1	X	1071	U	P-O3'-C3'	7.66	128.89	119.70
1	X	1618	U	P-O3'-C3'	7.65	128.88	119.70
1	X	2274	C	O4'-C1'-N1	7.65	114.32	108.20
1	X	18	U	O4'-C1'-N1	7.65	114.32	108.20
1	X	308	C	O4'-C1'-N1	7.63	114.30	108.20
1	X	690	A	C4'-C3'-C2'	-7.63	94.97	102.60
1	X	788	G	C1'-O4'-C4'	-7.61	103.81	109.90
1	X	636	G	C8-N9-C4	-7.61	103.36	106.40
1	X	1302	C	O4'-C1'-N1	7.59	114.28	108.20
1	X	1935	A	N9-C1'-C2'	7.59	123.87	114.00
1	X	2005	U	O4'-C1'-N1	7.58	114.27	108.20
1	X	926	C	O4'-C1'-N1	7.58	114.27	108.20
1	X	1654	A	C3'-C2'-C1'	-7.58	95.44	101.50
1	X	774	A	P-O5'-C5'	7.56	133.00	120.90
1	X	937	C	O4'-C1'-N1	7.55	114.24	108.20
1	X	2841	U	O4'-C1'-N1	7.55	114.24	108.20
1	X	1327	C	C5-C6-N1	7.54	124.77	121.00
1	X	1001	A	P-O3'-C3'	7.54	128.75	119.70
1	X	2671	C	O4'-C1'-N1	7.54	114.23	108.20
1	X	2460	G	P-O5'-C5'	7.54	132.97	120.90
1	X	2460	G	O4'-C1'-N9	7.53	114.23	108.20
1	X	2190	A	C1'-O4'-C4'	-7.53	103.88	109.90
1	X	247	A	O4'-C1'-N9	7.52	114.22	108.20
1	X	1211	G	P-O3'-C3'	-7.52	110.68	119.70
1	X	242	A	P-O3'-C3'	7.51	128.71	119.70
2	Y	29	C	O4'-C1'-N1	7.51	114.21	108.20
1	X	1357	U	P-O3'-C3'	7.51	128.71	119.70
1	X	1433	A	O4'-C1'-N9	7.51	114.20	108.20
1	X	307	C	O4'-C1'-N1	7.50	114.20	108.20
1	X	2015	G	P-O3'-C3'	7.49	128.69	119.70
1	X	925	U	P-O3'-C3'	7.49	128.69	119.70
1	X	2431	C	O4'-C1'-N1	7.49	114.19	108.20
1	X	626	A	P-O3'-C3'	7.48	128.68	119.70
1	X	2694	G	P-O3'-C3'	7.48	128.68	119.70
2	Y	30	C	O4'-C1'-N1	7.48	114.18	108.20
1	X	1283	C	P-O3'-C3'	7.47	128.67	119.70
1	X	2710	C	O4'-C1'-N1	7.47	114.17	108.20
1	X	1221	C	O4'-C1'-N1	7.47	114.17	108.20
1	X	1223	G	P-O3'-C3'	7.47	128.66	119.70
1	X	2056	C	P-O3'-C3'	7.46	128.66	119.70
1	X	2477	C	P-O5'-C5'	7.46	132.84	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1985	G	O4'-C1'-N9	7.46	114.17	108.20
1	X	2384	G	P-O3'-C3'	7.46	128.65	119.70
1	X	94	C	O4'-C1'-N1	7.46	114.17	108.20
2	Y	26	G	P-O3'-C3'	7.45	128.64	119.70
1	X	2830	U	O4'-C1'-N1	7.45	114.16	108.20
1	X	2660	C	O4'-C1'-N1	7.44	114.15	108.20
1	X	2088	U	P-O3'-C3'	7.44	128.63	119.70
1	X	837	U	O4'-C1'-N1	7.44	114.15	108.20
1	X	177	U	O4'-C1'-N1	7.43	114.14	108.20
1	X	1664	G	O5'-P-OP2	7.43	119.61	110.70
1	X	2580	C	P-O3'-C3'	7.43	128.61	119.70
1	X	841	G	N7-C8-N9	7.42	116.81	113.10
1	X	117	A	O4'-C1'-N9	7.41	114.13	108.20
1	X	1607	A	P-O3'-C3'	7.41	128.59	119.70
1	X	2033	C	P-O3'-C3'	7.40	128.58	119.70
1	X	2799	C	O4'-C1'-N1	7.40	114.12	108.20
1	X	1681	A	P-O3'-C3'	7.40	128.58	119.70
1	X	2633	A	P-O3'-C3'	7.40	128.58	119.70
1	X	2564	U	C1'-O4'-C4'	-7.40	103.98	109.90
1	X	1412	C	O4'-C1'-N1	7.39	114.12	108.20
1	X	1142	G	P-O3'-C3'	7.39	128.57	119.70
1	X	2258	G	O4'-C1'-N9	7.39	114.11	108.20
1	X	1469	U	P-O5'-C5'	7.38	132.70	120.90
1	X	1412	C	C3'-C2'-C1'	-7.36	95.61	101.50
1	X	2662	C	C4'-C3'-C2'	-7.36	95.24	102.60
1	X	1559	G	P-O3'-C3'	7.35	128.52	119.70
1	X	31	C	O4'-C1'-N1	7.34	114.07	108.20
1	X	788	G	N9-C1'-C2'	7.34	123.54	114.00
1	X	796	A	C4'-C3'-C2'	-7.33	95.27	102.60
1	X	1909	U	O4'-C1'-N1	7.33	114.06	108.20
1	X	815	A	P-O3'-C3'	7.33	128.49	119.70
1	X	1688	U	N3-C4-C5	-7.32	110.21	114.60
1	X	92	U	O4'-C1'-N1	7.32	114.06	108.20
1	X	2298	U	O4'-C1'-N1	7.31	114.05	108.20
1	X	1143	A	C5'-C4'-O4'	7.30	117.86	109.10
1	X	1051	U	O4'-C1'-N1	7.30	114.04	108.20
1	X	2006	G	O4'-C1'-N9	7.30	114.04	108.20
1	X	1000	G	O4'-C1'-N9	7.29	114.03	108.20
1	X	2239	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	2290	A	P-O3'-C3'	7.28	128.44	119.70
1	X	567	G	O4'-C1'-N9	7.28	114.02	108.20
1	X	742	G	C1'-O4'-C4'	-7.28	104.08	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	539	A	C1'-O4'-C4'	-7.27	104.09	109.90
1	X	1439	G	C3'-C2'-C1'	-7.27	95.69	101.50
1	X	180	C	O4'-C1'-N1	7.26	114.01	108.20
1	X	2702	G	N1-C6-O6	7.24	124.25	119.90
1	X	972	C	C1'-O4'-C4'	-7.24	104.11	109.90
1	X	2561	G	C5-C6-O6	-7.24	124.26	128.60
1	X	1333	G	N9-C4-C5	7.24	108.30	105.40
1	X	2870	C	O4'-C1'-N1	7.23	113.99	108.20
1	X	875	G	O4'-C1'-N9	7.23	113.99	108.20
1	X	2267	A	P-O3'-C3'	7.23	128.38	119.70
1	X	2560	G	C8-N9-C4	-7.23	103.51	106.40
1	X	2634	G	C1'-O4'-C4'	-7.23	104.12	109.90
1	X	564	U	O4'-C1'-N1	7.23	113.98	108.20
1	X	1776	A	P-O3'-C3'	7.23	128.37	119.70
1	X	1865	C	O4'-C1'-N1	7.23	113.98	108.20
1	X	1080	A	C1'-O4'-C4'	-7.22	104.12	109.90
1	X	1920	A	P-O3'-C3'	7.22	128.37	119.70
1	X	520	C	P-O3'-C3'	7.22	128.36	119.70
1	X	1513	U	O4'-C1'-N1	7.22	113.97	108.20
1	X	61	U	C1'-O4'-C4'	-7.21	104.13	109.90
1	X	631	G	O4'-C1'-N9	7.21	113.97	108.20
1	X	2608	A	C1'-O4'-C4'	-7.21	104.13	109.90
2	Y	19	C	N1-C2-O2	7.21	123.22	118.90
1	X	174	A	P-O3'-C3'	7.20	128.34	119.70
1	X	430	C	O4'-C1'-N1	7.20	113.96	108.20
1	X	802	A	O4'-C1'-N9	-7.19	102.45	108.20
1	X	1467	U	C4-C5-C6	-7.19	115.39	119.70
2	Y	106	U	O4'-C1'-N1	7.19	113.95	108.20
1	X	465	C	P-O5'-C5'	-7.19	109.40	120.90
1	X	810	U	P-O3'-C3'	-7.19	111.08	119.70
1	X	1289	A	O4'-C1'-N9	-7.18	102.45	108.20
1	X	1461	C	O4'-C1'-N1	7.18	113.95	108.20
1	X	1218	C	O4'-C1'-N1	7.18	113.94	108.20
1	X	1310	C	O4'-C1'-N1	7.18	113.94	108.20
1	X	331	U	O4'-C1'-N1	7.17	113.94	108.20
1	X	2284	U	O4'-C1'-N1	7.17	113.93	108.20
1	X	81	C	O4'-C1'-N1	7.16	113.93	108.20
1	X	531	G	P-O3'-C3'	-7.16	111.11	119.70
1	X	518	A	N9-C1'-C2'	7.15	123.29	114.00
1	X	2509	A	P-O3'-C3'	7.13	128.26	119.70
1	X	2026	C	N3-C2-O2	-7.13	116.91	121.90
1	X	117	A	C1'-O4'-C4'	-7.13	104.20	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2039	G	N3-C2-N2	-7.12	114.91	119.90
1	X	2449	G	O4'-C1'-N9	7.12	113.90	108.20
1	X	758	G	O4'-C1'-N9	7.12	113.90	108.20
1	X	514	G	N9-C1'-C2'	7.12	123.25	114.00
1	X	526	C	C3'-C2'-C1'	-7.11	95.81	101.50
1	X	1788	C	O4'-C1'-N1	7.11	113.89	108.20
1	X	943	U	O4'-C1'-N1	7.11	113.88	108.20
1	X	1938	U	N1-C1'-C2'	7.11	123.24	114.00
1	X	2338	C	P-O3'-C3'	7.11	128.23	119.70
1	X	455	A	P-O3'-C3'	7.10	128.22	119.70
1	X	2705	A	P-O3'-C3'	7.10	128.22	119.70
1	X	59	G	P-O3'-C3'	7.10	128.22	119.70
1	X	1652	G	P-O3'-C3'	7.09	128.21	119.70
2	Y	92	G	P-O3'-C3'	-7.09	111.19	119.70
1	X	1364	C	O4'-C1'-N1	7.09	113.87	108.20
1	X	2620	G	C4'-C3'-C2'	-7.09	95.51	102.60
2	Y	6	C	O4'-C1'-N1	7.08	113.87	108.20
1	X	2691	C	O4'-C1'-N1	7.07	113.86	108.20
1	X	2699	G	P-O3'-C3'	7.07	128.18	119.70
1	X	2243	C	O4'-C1'-N1	7.07	113.85	108.20
1	X	1950	C	O4'-C1'-N1	7.06	113.85	108.20
1	X	2498	U	P-O3'-C3'	7.06	128.17	119.70
1	X	558	G	N9-C1'-C2'	7.05	123.17	114.00
1	X	343	A	N7-C8-N9	7.04	117.32	113.80
1	X	1772	C	O4'-C1'-N1	7.04	113.84	108.20
1	X	1966	C	P-O3'-C3'	-7.04	111.25	119.70
1	X	2403	C	N1-C2-O2	7.04	123.13	118.90
1	X	2567	G	C8-N9-C4	-7.04	103.58	106.40
1	X	822	G	C4'-C3'-C2'	-7.04	95.56	102.60
1	X	1975	G	O4'-C1'-N9	-7.04	102.57	108.20
1	X	2782	G	O4'-C1'-N9	7.04	113.83	108.20
1	X	1723	U	O4'-C1'-N1	7.03	113.82	108.20
1	X	1470	G	P-O5'-C5'	-7.03	109.66	120.90
1	X	2845	C	O4'-C1'-N1	7.03	113.82	108.20
1	X	1201	G	P-O3'-C3'	7.02	128.13	119.70
1	X	2238	G	O4'-C1'-N9	7.02	113.82	108.20
1	X	190	A	C1'-O4'-C4'	-7.02	104.28	109.90
1	X	756	C	N1-C2-O2	7.02	123.11	118.90
1	X	2795	A	C3'-C2'-C1'	7.02	107.11	101.50
1	X	2593	A	O3'-P-O5'	-7.00	90.69	104.00
1	X	2080	U	O4'-C1'-N1	7.00	113.80	108.20
1	X	1403	U	O4'-C1'-N1	7.00	113.80	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	801	A	P-O3'-C3'	6.99	128.09	119.70
1	X	1754	G	P-O3'-C3'	6.99	128.08	119.70
1	X	113	C	O4'-C1'-N1	6.98	113.79	108.20
1	X	2550	C	O4'-C1'-N1	6.97	113.78	108.20
1	X	1711	C	C1'-O4'-C4'	-6.97	104.32	109.90
1	X	2406	C	P-O3'-C3'	6.96	128.06	119.70
1	X	399	G	C4'-C3'-C2'	6.96	109.56	102.60
1	X	946	U	O4'-C1'-N1	6.95	113.76	108.20
1	X	2662	C	N1-C2-O2	6.95	123.07	118.90
1	X	1458	A	P-O3'-C3'	6.94	128.03	119.70
1	X	796	A	N1-C6-N6	6.94	122.76	118.60
1	X	74	G	O4'-C4'-C3'	-6.93	97.07	104.00
1	X	2072	C	O4'-C1'-N1	6.93	113.74	108.20
1	X	814	G	N9-C1'-C2'	6.93	123.01	114.00
1	X	1308	C	C3'-C2'-C1'	-6.92	95.96	101.50
1	X	2551	A	P-O3'-C3'	6.92	128.01	119.70
1	X	1801	C	P-O3'-C3'	6.92	128.01	119.70
1	X	2782	G	C1'-O4'-C4'	-6.92	104.36	109.90
1	X	1139	A	N9-C1'-C2'	6.92	122.99	114.00
1	X	2794	G	P-O3'-C3'	6.91	127.99	119.70
2	Y	107	C	P-O3'-C3'	6.91	127.99	119.70
1	X	2488	G	P-O3'-C3'	-6.90	111.42	119.70
1	X	83	A	C1'-O4'-C4'	-6.90	104.38	109.90
1	X	95	G	P-O3'-C3'	6.90	127.98	119.70
1	X	1409	U	C1'-O4'-C4'	-6.90	104.38	109.90
1	X	2667	C	N1-C2-O2	6.90	123.04	118.90
1	X	1108	U	O4'-C1'-N1	6.89	113.71	108.20
1	X	2030	U	P-O3'-C3'	-6.89	111.43	119.70
1	X	560	G	P-O3'-C3'	-6.89	111.44	119.70
1	X	2533	U	O4'-C1'-N1	6.88	113.71	108.20
1	X	1313	U	C3'-C2'-C1'	-6.88	96.00	101.50
1	X	483	A	N9-C1'-C2'	6.88	122.94	114.00
1	X	826	U	O4'-C1'-N1	6.88	113.70	108.20
1	X	636	G	N7-C8-N9	6.87	116.54	113.10
2	Y	32	C	C6-N1-C2	-6.87	117.55	120.30
1	X	247	A	P-O3'-C3'	6.87	127.94	119.70
2	Y	74	A	P-O3'-C3'	6.87	127.94	119.70
1	X	2217	G	C1'-O4'-C4'	-6.87	104.41	109.90
1	X	796	A	C5-N7-C8	-6.87	100.47	103.90
1	X	1487	C	O4'-C1'-N1	6.87	113.69	108.20
1	X	2691	C	C1'-O4'-C4'	-6.86	104.41	109.90
1	X	1422	C	O4'-C1'-N1	6.86	113.69	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2018	G	O4'-C1'-C2'	-6.85	98.95	105.80
1	X	774	A	C8-N9-C4	-6.85	103.06	105.80
1	X	1086	C	O4'-C1'-N1	6.85	113.68	108.20
1	X	1522	C	C3'-C2'-C1'	-6.85	96.02	101.50
1	X	1602	G	P-O3'-C3'	6.84	127.91	119.70
1	X	2418	A	P-O3'-C3'	6.84	127.91	119.70
1	X	1200	G	O4'-C1'-N9	6.83	113.67	108.20
1	X	1465	G	P-O3'-C3'	-6.83	111.50	119.70
1	X	927	C	C6-N1-C2	-6.83	117.57	120.30
1	X	2245	A	P-O3'-C3'	6.82	127.89	119.70
1	X	617	U	N3-C2-O2	-6.82	117.42	122.20
2	Y	90	C	C3'-C2'-C1'	-6.82	96.05	101.50
1	X	1433	A	C1'-O4'-C4'	-6.82	104.45	109.90
2	Y	37	C	O4'-C1'-N1	6.81	113.65	108.20
1	X	1469	U	P-O3'-C3'	6.81	127.88	119.70
1	X	1963	G	P-O3'-C3'	6.81	127.87	119.70
1	X	527	C	C5-C6-N1	6.81	124.41	121.00
1	X	170	U	N3-C2-O2	-6.81	117.43	122.20
1	X	567	G	P-O3'-C3'	-6.81	111.53	119.70
1	X	1410	U	O4'-C1'-N1	6.80	113.64	108.20
1	X	580	A	N9-C1'-C2'	6.80	122.83	114.00
1	X	1686	A	C1'-O4'-C4'	-6.80	104.46	109.90
1	X	1466	C	N3-C2-O2	-6.79	117.14	121.90
1	X	1656	U	O4'-C1'-N1	6.79	113.64	108.20
1	X	1745	C	O4'-C1'-N1	6.79	113.63	108.20
1	X	2339	A	O4'-C1'-N9	6.79	113.63	108.20
2	Y	123	U	C2-N1-C1'	6.79	125.85	117.70
1	X	2554	C	O4'-C1'-N1	6.78	113.63	108.20
1	X	699	G	O4'-C1'-N9	6.78	113.62	108.20
1	X	1164	C	O4'-C1'-N1	6.78	113.62	108.20
1	X	39	C	O4'-C1'-N1	6.78	113.62	108.20
2	Y	44	C	O4'-C1'-N1	6.77	113.62	108.20
1	X	542	A	C5-N7-C8	-6.77	100.52	103.90
1	X	514	G	O4'-C1'-N9	-6.76	102.79	108.20
1	X	559	C	C5'-C4'-O4'	6.76	117.22	109.10
1	X	582	G	N3-C4-C5	-6.76	125.22	128.60
2	Y	17	A	P-O3'-C3'	6.75	127.80	119.70
1	X	1526	U	O4'-C1'-N1	6.75	113.60	108.20
1	X	2672	U	N1-C2-O2	6.75	127.52	122.80
1	X	477	A	O5'-P-OP2	-6.74	99.63	105.70
1	X	1652	G	C6-C5-N7	-6.74	126.36	130.40
1	X	886	A	C3'-C2'-C1'	-6.74	96.11	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2347	C	O4'-C1'-N1	6.74	113.59	108.20
1	X	2590	U	P-O5'-C5'	6.73	131.67	120.90
1	X	1608	U	O4'-C1'-N1	6.73	113.58	108.20
1	X	2479	U	C5-C6-N1	6.73	126.06	122.70
1	X	2579	A	C3'-C2'-C1'	6.72	106.88	101.50
1	X	870	C	O4'-C1'-N1	6.72	113.58	108.20
1	X	2855	C	P-O3'-C3'	-6.72	111.64	119.70
1	X	2022	C	O4'-C1'-N1	6.72	113.57	108.20
1	X	501	G	O4'-C1'-N9	6.71	113.57	108.20
1	X	697	G	O4'-C1'-N9	6.71	113.57	108.20
1	X	1958	G	O4'-C4'-C3'	-6.71	97.29	104.00
1	X	575	U	P-O3'-C3'	6.71	127.75	119.70
2	Y	53	G	N3-C4-C5	-6.71	125.25	128.60
1	X	739	G	O4'-C1'-N9	6.70	113.56	108.20
1	X	1632	A	P-O3'-C3'	6.70	127.75	119.70
1	X	1792	C	P-O3'-C3'	6.70	127.75	119.70
1	X	1833	U	O4'-C1'-N1	6.70	113.56	108.20
1	X	1184	G	P-O3'-C3'	6.70	127.74	119.70
1	X	208	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	1308	C	P-O5'-C5'	-6.69	110.19	120.90
1	X	133	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	699	G	P-O3'-C3'	6.69	127.73	119.70
1	X	1163	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	2838	U	O4'-C1'-N1	6.69	113.55	108.20
2	Y	8	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1468	A	N9-C1'-C2'	6.69	122.70	114.00
1	X	2392	G	O4'-C1'-N9	6.69	113.55	108.20
1	X	864	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1663	C	P-O3'-C3'	6.69	127.73	119.70
1	X	1743	C	P-O3'-C3'	-6.69	111.67	119.70
1	X	1979	C	P-O3'-C3'	6.69	127.73	119.70
1	X	624	A	O4'-C1'-N9	6.69	113.55	108.20
1	X	823	U	O4'-C1'-N1	6.69	113.55	108.20
2	Y	87	C	O4'-C1'-N1	6.68	113.55	108.20
1	X	2538	C	N1-C2-O2	6.68	122.91	118.90
1	X	1744	G	C4'-C3'-C2'	-6.68	95.92	102.60
1	X	234	C	N1-C2-O2	6.68	122.91	118.90
1	X	2483	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	2574	G	O4'-C1'-N9	6.67	113.54	108.20
1	X	2256	G	C8-N9-C4	-6.67	103.73	106.40
1	X	2190	A	P-O3'-C3'	6.66	127.70	119.70
1	X	83	A	P-O3'-C3'	6.66	127.69	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1068	A	P-O3'-C3'	6.66	127.69	119.70
1	X	2459	C	N1-C2-O2	6.66	122.90	118.90
1	X	649	G	O4'-C1'-N9	6.66	113.53	108.20
1	X	1404	C	O4'-C1'-N1	6.66	113.53	108.20
1	X	2854	G	P-O3'-C3'	6.66	127.69	119.70
1	X	1343	C	O4'-C1'-N1	6.65	113.52	108.20
1	X	559	C	C1'-O4'-C4'	-6.64	104.58	109.90
1	X	1232	U	O4'-C1'-N1	6.64	113.52	108.20
1	X	1927	U	P-O3'-C3'	6.64	127.67	119.70
1	X	346	C	C2-N1-C1'	6.64	126.11	118.80
1	X	1716	G	O3'-P-O5'	-6.64	91.38	104.00
1	X	559	C	C3'-C2'-C1'	6.64	106.81	101.50
1	X	996	C	N1-C2-O2	6.64	122.88	118.90
1	X	2487	G	O4'-C1'-N9	6.64	113.51	108.20
1	X	689	A	C1'-O4'-C4'	-6.63	104.59	109.90
1	X	343	A	O4'-C1'-C2'	-6.63	99.17	105.80
1	X	578	U	O4'-C1'-N1	6.63	113.51	108.20
1	X	2622	G	C5-C6-O6	-6.62	124.63	128.60
1	X	2481	G	N1-C6-O6	6.62	123.87	119.90
2	Y	62	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	1749	G	C3'-C2'-C1'	-6.61	96.21	101.50
1	X	2585	C	C3'-C2'-C1'	-6.61	96.21	101.50
1	X	2208	U	O4'-C1'-N1	6.61	113.49	108.20
1	X	2276	C	O4'-C1'-N1	6.60	113.48	108.20
1	X	2199	C	P-O5'-C5'	6.60	131.45	120.90
1	X	1115	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	537	C	N1-C2-N3	-6.59	114.58	119.20
1	X	2782	G	N9-C1'-C2'	-6.59	104.75	112.00
1	X	355	G	O4'-C1'-N9	6.59	113.47	108.20
1	X	2875	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	1092	U	O4'-C1'-N1	6.58	113.47	108.20
1	X	1247	U	O4'-C1'-N1	6.58	113.46	108.20
1	X	42	G	C8-N9-C4	-6.58	103.77	106.40
1	X	131	C	O4'-C1'-N1	6.58	113.46	108.20
2	Y	75	A	P-O5'-C5'	6.57	131.42	120.90
1	X	2857	C	O4'-C1'-N1	6.57	113.46	108.20
1	X	1223	G	C4-C5-N7	6.57	113.43	110.80
1	X	1664	G	O5'-P-OP1	-6.57	99.79	105.70
1	X	1685	A	P-O3'-C3'	6.56	127.57	119.70
1	X	2475	C	O4'-C1'-N1	6.56	113.44	108.20
1	X	2492	G	O4'-C1'-N9	6.55	113.44	108.20
1	X	2596	C	O4'-C1'-N1	6.55	113.44	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	824	U	C1'-O4'-C4'	-6.54	104.67	109.90
1	X	1812	U	P-O3'-C3'	6.54	127.55	119.70
1	X	1333	G	N3-C4-C5	6.54	131.87	128.60
2	Y	123	U	N1-C1'-C2'	6.54	122.50	114.00
1	X	1090	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2056	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2037	A	O4'-C1'-N9	6.53	113.43	108.20
1	X	2206	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	1319	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	2864	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	866	U	O4'-C1'-N1	6.53	113.42	108.20
1	X	1415	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	1468	A	P-O5'-C5'	6.53	131.34	120.90
1	X	1939	U	N3-C2-O2	-6.53	117.63	122.20
1	X	332	C	P-O3'-C3'	6.52	127.53	119.70
1	X	2808	U	C1'-O4'-C4'	-6.52	104.68	109.90
1	X	1770	U	C5-C6-N1	-6.52	119.44	122.70
1	X	12	U	C2-N1-C1'	6.51	125.52	117.70
1	X	562	G	C3'-C2'-C1'	-6.51	96.29	101.50
1	X	1745	C	P-O3'-C3'	-6.51	111.89	119.70
1	X	2731	G	O4'-C1'-N9	6.51	113.41	108.20
1	X	1567	A	O4'-C1'-N9	6.51	113.41	108.20
1	X	1706	A	P-O5'-C5'	-6.51	110.48	120.90
1	X	2228	U	C3'-C2'-C1'	6.51	106.71	101.50
1	X	1830	C	C1'-O4'-C4'	-6.51	104.69	109.90
1	X	193	A	O4'-C1'-N9	6.50	113.40	108.20
1	X	1467	U	C5-C6-N1	6.50	125.95	122.70
2	Y	55	C	O4'-C1'-N1	6.50	113.40	108.20
1	X	1067	G	P-O3'-C3'	6.50	127.49	119.70
1	X	1009	C	N1-C2-O2	6.48	122.79	118.90
1	X	2625	U	C5-C4-O4	-6.48	122.01	125.90
1	X	2700	U	P-O3'-C3'	-6.48	111.92	119.70
1	X	182	G	P-O3'-C3'	6.48	127.47	119.70
1	X	418	C	C1'-O4'-C4'	-6.48	104.72	109.90
1	X	1764	A	C3'-C2'-C1'	-6.48	96.32	101.50
1	X	393	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	1598	C	O4'-C1'-N1	6.47	113.38	108.20
2	Y	110	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	689	A	C5-N7-C8	-6.47	100.67	103.90
1	X	2009	U	O4'-C1'-N1	6.47	113.37	108.20
1	X	2663	U	P-O3'-C3'	-6.47	111.94	119.70
1	X	460	U	P-O3'-C3'	6.46	127.46	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2306	A	O4'-C1'-N9	6.46	113.37	108.20
1	X	408	U	P-O3'-C3'	6.46	127.45	119.70
1	X	2671	C	N1-C2-O2	6.46	122.78	118.90
1	X	1318	A	P-O3'-C3'	6.46	127.45	119.70
1	X	1862	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	1947	G	O4'-C1'-N9	-6.46	103.03	108.20
1	X	2281	C	O4'-C1'-N1	6.46	113.36	108.20
1	X	22	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	2038	C	O4'-C1'-N1	6.45	113.36	108.20
2	Y	50	U	O4'-C1'-N1	6.45	113.36	108.20
1	X	873	U	O4'-C1'-N1	6.45	113.36	108.20
1	X	1223	G	C6-C5-N7	-6.45	126.53	130.40
1	X	349	G	N3-C4-C5	-6.43	125.39	128.60
1	X	1574	A	C5'-C4'-O4'	6.43	116.82	109.10
1	X	422	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	1291	G	O4'-C1'-N9	6.43	113.34	108.20
1	X	1317	G	O4'-C1'-N9	6.42	113.34	108.20
1	X	1496	G	C2'-C3'-O3'	6.42	123.98	113.70
1	X	431	G	O4'-C1'-N9	6.42	113.34	108.20
1	X	446	C	N1-C2-O2	6.42	122.75	118.90
1	X	1692	C	C3'-C2'-C1'	6.42	106.64	101.50
1	X	1940	C	P-O3'-C3'	-6.42	111.99	119.70
1	X	424	G	P-O3'-C3'	6.42	127.40	119.70
1	X	2488	G	C5-C6-N1	6.42	114.71	111.50
1	X	619	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1208	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1552	C	P-O3'-C3'	6.41	127.39	119.70
1	X	559	C	C5'-C4'-C3'	6.41	126.25	116.00
1	X	1152	C	C1'-O4'-C4'	-6.41	104.78	109.90
1	X	1222	G	P-O3'-C3'	6.41	127.39	119.70
1	X	1333	G	C8-N9-C1'	6.41	135.33	127.00
1	X	244	C	O4'-C1'-N1	6.40	113.32	108.20
1	X	527	C	P-O3'-C3'	6.40	127.38	119.70
1	X	630	G	O4'-C1'-N9	6.40	113.32	108.20
2	Y	57	U	O4'-C1'-N1	6.40	113.32	108.20
1	X	956	A	P-O5'-C5'	6.39	131.13	120.90
1	X	1999	U	P-O3'-C3'	-6.39	112.03	119.70
1	X	2185	U	O4'-C1'-N1	6.39	113.32	108.20
1	X	1241	G	P-O3'-C3'	-6.39	112.03	119.70
1	X	322	A	P-O3'-C3'	6.38	127.36	119.70
1	X	429	C	O4'-C1'-N1	6.38	113.31	108.20
1	X	40	U	O4'-C1'-N1	6.38	113.31	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1229	C	N1-C2-O2	6.38	122.73	118.90
1	X	2082	C	O4'-C1'-N1	6.38	113.30	108.20
1	X	1446	U	O4'-C1'-N1	6.38	113.30	108.20
1	X	1796	A	C2-N3-C4	6.38	113.79	110.60
2	Y	17	A	O4'-C1'-N9	6.38	113.30	108.20
1	X	2032	G	C5-C6-O6	-6.38	124.78	128.60
1	X	2719	U	O4'-C1'-N1	6.38	113.30	108.20
1	X	169	C	O4'-C1'-N1	6.37	113.30	108.20
1	X	338	G	N7-C8-N9	6.37	116.29	113.10
1	X	2582	G	P-O5'-C5'	6.37	131.09	120.90
23	U	18	VAL	C-N-CA	6.37	137.63	121.70
1	X	1291	G	O4'-C4'-C3'	-6.37	97.63	104.00
1	X	1454	U	O4'-C1'-N1	6.37	113.29	108.20
1	X	1647	U	N3-C4-C5	-6.37	110.78	114.60
1	X	2032	G	O4'-C4'-C3'	-6.36	97.64	104.00
1	X	2494	C	O4'-C1'-N1	6.36	113.29	108.20
1	X	1829	C	O4'-C1'-N1	6.36	113.29	108.20
1	X	1338	G	O4'-C1'-N9	6.36	113.29	108.20
1	X	2661	G	C5-C6-O6	-6.36	124.79	128.60
1	X	2578	G	P-O5'-C5'	6.35	131.07	120.90
1	X	2653	A	O4'-C1'-N9	6.35	113.28	108.20
2	Y	86	A	C1'-O4'-C4'	-6.35	104.82	109.90
1	X	757	U	N3-C2-O2	-6.35	117.76	122.20
1	X	1670	G	O4'-C1'-N9	-6.35	103.12	108.20
1	X	1036	G	C4'-C3'-C2'	6.35	108.95	102.60
1	X	981	C	O4'-C1'-N1	6.34	113.28	108.20
1	X	1732	U	O4'-C1'-N1	6.34	113.27	108.20
1	X	309	G	C8-N9-C4	-6.34	103.86	106.40
1	X	1988	A	P-O3'-C3'	6.34	127.31	119.70
1	X	520	C	C4'-C3'-C2'	-6.34	96.26	102.60
1	X	975	C	O4'-C1'-N1	6.33	113.27	108.20
1	X	1306	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	1914	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	838	A	OP1-P-O3'	6.33	119.13	105.20
1	X	2772	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	633	G	O4'-C1'-N9	6.33	113.26	108.20
1	X	650	U	P-O5'-C5'	6.33	131.02	120.90
1	X	967	G	P-O3'-C3'	6.32	127.29	119.70
1	X	2408	G	N3-C4-C5	-6.32	125.44	128.60
2	Y	70	C	O4'-C1'-N1	6.32	113.25	108.20
1	X	1509	A	P-O3'-C3'	6.32	127.28	119.70
1	X	1986	G	O4'-C1'-N9	6.32	113.25	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2544	A	O3'-P-O5'	-6.32	92.00	104.00
1	X	1044	U	P-O3'-C3'	6.31	127.28	119.70
1	X	774	A	C6-N1-C2	6.31	122.39	118.60
1	X	1392	U	P-O3'-C3'	6.31	127.27	119.70
1	X	2670	C	O4'-C1'-N1	6.31	113.25	108.20
1	X	2409	A	N9-C1'-C2'	6.31	122.20	114.00
1	X	1749	G	O4'-C1'-C2'	-6.30	99.50	105.80
1	X	2482	A	C2-N3-C4	6.30	113.75	110.60
2	Y	88	C	C1'-O4'-C4'	-6.30	104.86	109.90
1	X	1333	G	N7-C8-N9	6.30	116.25	113.10
1	X	90	G	P-O3'-C3'	6.30	127.26	119.70
1	X	98	U	O4'-C1'-N1	6.29	113.23	108.20
1	X	1017	C	O4'-C1'-N1	6.29	113.23	108.20
1	X	730	C	P-O3'-C3'	6.29	127.25	119.70
1	X	1407	G	N9-C1'-C2'	6.29	122.17	114.00
1	X	789	G	P-O3'-C3'	6.29	127.24	119.70
1	X	1236	G	C8-N9-C4	-6.29	103.89	106.40
1	X	779	U	O4'-C1'-N1	6.28	113.23	108.20
1	X	2808	U	P-O5'-C5'	6.28	130.95	120.90
2	Y	4	C	O4'-C1'-N1	6.28	113.23	108.20
1	X	343	A	N9-C1'-C2'	6.28	122.16	114.00
1	X	430	C	C6-N1-C2	-6.28	117.79	120.30
1	X	607	C	C3'-C2'-C1'	-6.28	96.48	101.50
1	X	805	G	N9-C1'-C2'	6.28	122.16	114.00
1	X	1792	C	N1-C1'-C2'	6.28	122.16	114.00
1	X	2375	G	O4'-C4'-C3'	-6.28	97.72	104.00
1	X	1982	C	O4'-C4'-C3'	-6.28	97.72	104.00
1	X	2043	A	P-O3'-C3'	6.28	127.23	119.70
19	Q	62	ARG	C-N-CA	6.27	137.38	121.70
1	X	1112	U	O4'-C1'-N1	6.27	113.22	108.20
1	X	1261	G	O4'-C1'-N9	-6.27	103.18	108.20
1	X	1689	U	P-O3'-C3'	6.27	127.23	119.70
1	X	1669	A	O4'-C4'-C3'	-6.27	97.73	104.00
1	X	1783	G	N9-C1'-C2'	-6.27	105.10	112.00
1	X	1882	G	C3'-C2'-C1'	6.27	106.52	101.50
1	X	968	C	C5'-C4'-O4'	6.26	116.61	109.10
1	X	1359	G	C5'-C4'-C3'	-6.26	105.98	116.00
1	X	1825	C	O4'-C1'-N1	6.26	113.21	108.20
1	X	2572	U	N3-C4-O4	6.26	123.78	119.40
1	X	672	C	O4'-C4'-C3'	-6.25	97.75	104.00
1	X	1522	C	N1-C2-O2	6.25	122.65	118.90
1	X	1938	U	C4'-C3'-C2'	6.25	108.85	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	456	C	O4'-C1'-N1	6.25	113.20	108.20
1	X	540	G	C5-C6-N1	6.25	114.62	111.50
1	X	655	A	C1'-O4'-C4'	-6.25	104.90	109.90
2	Y	42	U	O4'-C1'-N1	6.25	113.20	108.20
1	X	2081	U	O4'-C1'-N1	6.25	113.20	108.20
1	X	2666	U	P-O3'-C3'	6.25	127.19	119.70
1	X	1288	A	C5'-C4'-C3'	6.24	125.99	116.00
1	X	49	U	P-O3'-C3'	6.24	127.19	119.70
1	X	2258	G	O4'-C4'-C3'	-6.24	97.76	104.00
1	X	485	G	P-O3'-C3'	6.24	127.18	119.70
1	X	480	G	C5-C6-O6	-6.24	124.86	128.60
1	X	968	C	C5-C6-N1	6.24	124.12	121.00
1	X	2867	G	N7-C8-N9	6.23	116.22	113.10
1	X	517	A	P-O3'-C3'	6.23	127.17	119.70
1	X	1983	G	C3'-C2'-C1'	-6.23	96.52	101.50
1	X	2012	A	O4'-C1'-N9	6.23	113.18	108.20
1	X	2366	U	O4'-C1'-N1	6.23	113.18	108.20
1	X	2698	G	C5'-C4'-O4'	6.23	116.57	109.10
1	X	750	C	O4'-C1'-N1	6.23	113.18	108.20
1	X	79	G	C8-N9-C4	-6.22	103.91	106.40
1	X	1473	U	C4'-C3'-C2'	6.22	108.82	102.60
1	X	2667	C	C4'-C3'-C2'	-6.22	96.38	102.60
1	X	2680	U	O4'-C1'-N1	6.22	113.18	108.20
1	X	684	C	N3-C4-C5	-6.22	119.41	121.90
2	Y	90	C	C4'-C3'-C2'	6.22	108.82	102.60
1	X	1744	G	C5-C6-N1	6.21	114.61	111.50
1	X	2847	G	C8-N9-C4	-6.21	103.92	106.40
1	X	2677	U	O4'-C1'-N1	6.21	113.17	108.20
1	X	160	C	O4'-C1'-N1	6.21	113.17	108.20
1	X	699	G	C4-N9-C1'	-6.21	118.43	126.50
1	X	1190	C	O4'-C1'-N1	6.20	113.16	108.20
1	X	1230	C	O4'-C1'-N1	6.20	113.16	108.20
1	X	2717	G	O4'-C1'-N9	6.20	113.16	108.20
1	X	82	G	P-O3'-C3'	6.20	127.14	119.70
1	X	559	C	N1-C2-O2	6.20	122.62	118.90
1	X	1544	A	P-O3'-C3'	6.19	127.13	119.70
1	X	302	U	O4'-C1'-N1	6.19	113.15	108.20
1	X	2695	C	O4'-C1'-N1	6.19	113.15	108.20
1	X	725	C	O4'-C1'-N1	6.18	113.15	108.20
1	X	1819	U	O4'-C1'-N1	6.18	113.15	108.20
1	X	1412	C	C2'-C3'-O3'	6.18	123.59	113.70
1	X	699	G	C8-N9-C1'	6.18	135.03	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1947	G	P-O3'-C3'	6.18	127.12	119.70
1	X	2553	G	O4'-C1'-N9	6.18	113.14	108.20
1	X	2653	A	C3'-C2'-C1'	-6.18	96.56	101.50
1	X	1599	G	P-O3'-C3'	6.17	127.11	119.70
1	X	2500	C	O4'-C1'-N1	6.17	113.14	108.20
1	X	2507	U	O4'-C1'-N1	6.17	113.14	108.20
1	X	579	G	C5-C6-O6	6.17	132.30	128.60
1	X	942	U	N3-C2-O2	-6.17	117.88	122.20
1	X	1270	C	N3-C4-C5	-6.17	119.43	121.90
1	X	2344	G	P-O3'-C3'	6.17	127.11	119.70
2	Y	22	U	O4'-C1'-N1	6.17	113.14	108.20
2	Y	53	G	C8-N9-C4	-6.16	103.94	106.40
1	X	1056	U	P-O3'-C3'	6.16	127.09	119.70
1	X	2764	U	O4'-C1'-N1	6.16	113.13	108.20
1	X	607	C	N1-C2-O2	6.16	122.59	118.90
1	X	1570	C	P-O3'-C3'	6.16	127.09	119.70
1	X	2393	G	P-O3'-C3'	-6.15	112.32	119.70
1	X	1472	C	N1-C2-O2	6.15	122.59	118.90
2	Y	87	C	N1-C2-O2	6.15	122.59	118.90
1	X	729	A	P-O3'-C3'	6.15	127.08	119.70
1	X	940	G	C5'-C4'-O4'	6.15	116.48	109.10
1	X	2416	U	O4'-C1'-N1	6.14	113.11	108.20
1	X	631	G	P-O3'-C3'	6.14	127.07	119.70
1	X	1169	C	N1-C2-O2	6.14	122.58	118.90
1	X	1001	A	C8-N9-C4	-6.14	103.34	105.80
1	X	1128	G	P-O3'-C3'	6.13	127.06	119.70
1	X	2735	C	O4'-C1'-N1	6.13	113.11	108.20
1	X	2790	C	N1-C2-O2	6.13	122.58	118.90
2	Y	46	G	C3'-C2'-C1'	6.13	106.40	101.50
2	Y	54	U	P-O3'-C3'	6.13	127.05	119.70
1	X	539	A	N9-C1'-C2'	6.13	121.97	114.00
1	X	594	G	P-O3'-C3'	6.13	127.05	119.70
1	X	859	U	N1-C1'-C2'	6.12	121.96	114.00
1	X	933	G	P-O3'-C3'	-6.12	112.35	119.70
1	X	199	A	P-O3'-C3'	6.12	127.05	119.70
1	X	917	U	O4'-C1'-N1	6.12	113.10	108.20
1	X	2791	C	N1-C2-O2	6.12	122.57	118.90
1	X	35	G	O4'-C1'-N9	6.12	113.10	108.20
1	X	540	G	C8-N9-C4	-6.12	103.95	106.40
1	X	1824	C	N1-C2-O2	6.12	122.57	118.90
1	X	536	A	O4'-C1'-N9	6.11	113.09	108.20
1	X	1375	C	N1-C2-O2	6.11	122.57	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	19	C	O4'-C1'-N1	6.11	113.08	108.20
2	Y	45	C	N1-C2-O2	6.11	122.56	118.90
1	X	566	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1185	C	P-O5'-C5'	6.10	130.66	120.90
1	X	1325	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1647	U	N3-C4-O4	6.10	123.67	119.40
1	X	2465	G	O4'-C1'-N9	6.10	113.08	108.20
2	Y	13	C	O4'-C1'-N1	6.10	113.08	108.20
1	X	1469	U	N1-C1'-C2'	6.10	121.93	114.00
1	X	2223	U	P-O3'-C3'	-6.10	112.38	119.70
1	X	2275	U	P-O3'-C3'	6.10	127.02	119.70
1	X	2808	U	C5'-C4'-O4'	6.10	116.42	109.10
1	X	2240	C	N1-C2-O2	6.09	122.56	118.90
1	X	2415	G	P-O3'-C3'	6.09	127.01	119.70
1	X	476	G	N3-C4-C5	-6.09	125.56	128.60
1	X	875	G	C8-N9-C4	-6.09	103.97	106.40
2	Y	34	C	O4'-C1'-N1	6.08	113.07	108.20
1	X	1953	A	P-O5'-C5'	-6.08	111.17	120.90
1	X	2014	A	P-O3'-C3'	6.08	127.00	119.70
1	X	2609	G	O4'-C1'-N9	6.08	113.06	108.20
1	X	757	U	P-O3'-C3'	6.08	126.99	119.70
1	X	2315	A	O4'-C1'-N9	-6.08	103.34	108.20
1	X	1692	C	O4'-C1'-N1	6.08	113.06	108.20
1	X	1409	U	N1-C1'-C2'	6.07	121.89	114.00
1	X	2224	U	O4'-C1'-N1	6.07	113.06	108.20
1	X	2337	A	O4'-C1'-N9	6.07	113.06	108.20
2	Y	114	C	O4'-C1'-N1	6.07	113.06	108.20
1	X	955	G	P-O3'-C3'	6.07	126.98	119.70
1	X	246	C	N1-C2-O2	6.07	122.54	118.90
1	X	784	U	O4'-C1'-N1	6.07	113.05	108.20
1	X	2758	A	O4'-C1'-N9	6.07	113.05	108.20
1	X	56	C	O4'-C1'-N1	6.07	113.05	108.20
1	X	1249	G	N9-C1'-C2'	6.07	121.89	114.00
1	X	1183	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2329	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2869	U	O4'-C1'-N1	6.06	113.05	108.20
1	X	236	C	C6-N1-C2	-6.06	117.88	120.30
1	X	242	A	C5'-C4'-O4'	6.06	116.37	109.10
1	X	632	A	P-O3'-C3'	6.06	126.97	119.70
1	X	1986	G	P-O3'-C3'	-6.06	112.43	119.70
1	X	1773	C	N1-C2-O2	6.06	122.53	118.90
1	X	2782	G	N1-C6-O6	6.05	123.53	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	483	A	C4'-C3'-C2'	6.05	108.65	102.60
1	X	610	G	O3'-P-O5'	-6.05	92.51	104.00
1	X	2554	C	N1-C2-O2	6.04	122.53	118.90
1	X	423	G	C8-N9-C4	-6.04	103.98	106.40
1	X	794	A	N9-C1'-C2'	6.04	121.86	114.00
1	X	2795	A	C2-N3-C4	6.04	113.62	110.60
2	Y	97	C	N1-C2-O2	6.04	122.53	118.90
1	X	103	U	O4'-C1'-N1	6.04	113.03	108.20
1	X	1306	U	N3-C2-O2	-6.04	117.97	122.20
1	X	1989	C	O4'-C4'-C3'	-6.03	97.97	104.00
1	X	1388	C	O4'-C1'-N1	6.03	113.02	108.20
1	X	408	U	O4'-C1'-N1	6.03	113.02	108.20
1	X	1543	G	P-O3'-C3'	6.03	126.93	119.70
1	X	2459	C	N3-C2-O2	-6.03	117.68	121.90
1	X	1482	U	N1-C1'-C2'	6.03	121.83	114.00
1	X	2303	C	P-O3'-C3'	6.02	126.92	119.70
1	X	804	C	O4'-C1'-N1	6.02	113.01	108.20
1	X	1629	G	N9-C1'-C2'	-6.02	105.38	112.00
1	X	330	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	796	A	N7-C8-N9	6.01	116.81	113.80
1	X	1594	U	O4'-C1'-N1	6.01	113.01	108.20
1	X	2178	U	O4'-C1'-N1	6.01	113.01	108.20
1	X	2840	U	P-O3'-C3'	6.01	126.92	119.70
1	X	1985	G	C3'-C2'-C1'	-6.01	96.69	101.50
1	X	2482	A	O4'-C1'-N9	6.01	113.01	108.20
1	X	2659	C	P-O3'-C3'	-6.01	112.49	119.70
1	X	343	A	P-O5'-C5'	6.00	130.51	120.90
1	X	2782	G	C5-C6-O6	-6.00	125.00	128.60
1	X	2590	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	699	G	C5-N7-C8	-6.00	101.30	104.30
1	X	1217	U	C3'-C2'-C1'	-6.00	96.70	101.50
1	X	1016	C	C6-N1-C2	-5.99	117.90	120.30
2	Y	98	C	N1-C2-O2	5.99	122.50	118.90
1	X	248	A	P-O5'-C5'	5.99	130.49	120.90
1	X	1034	U	O4'-C1'-N1	5.99	112.99	108.20
1	X	2467	A	N1-C6-N6	-5.99	115.01	118.60
1	X	1407	G	C5-C6-O6	-5.99	125.01	128.60
1	X	1933	G	O4'-C1'-N9	5.99	112.99	108.20
1	X	2228	U	C6-N1-C2	-5.99	117.41	121.00
1	X	2229	G	P-O5'-C5'	-5.98	111.33	120.90
1	X	2680	U	C3'-C2'-C1'	-5.98	96.72	101.50
1	X	2688	G	O4'-C1'-N9	-5.98	103.42	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	32	C	C5-C6-N1	5.98	123.99	121.00
1	X	1030	U	O4'-C1'-N1	5.98	112.98	108.20
1	X	1284	G	N7-C8-N9	5.98	116.09	113.10
1	X	1335	A	P-O3'-C3'	-5.98	112.53	119.70
1	X	2586	G	C4'-C3'-C2'	-5.98	96.62	102.60
1	X	2808	U	C3'-C2'-C1'	-5.98	96.72	101.50
1	X	786	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	1306	U	N1-C2-O2	5.97	126.98	122.80
1	X	1333	G	C5-N7-C8	-5.97	101.31	104.30
1	X	2380	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	111	G	P-O5'-C5'	5.97	130.45	120.90
1	X	2724	G	O5'-C5'-C4'	-5.97	100.36	111.70
1	X	1753	A	O4'-C1'-N9	5.97	112.97	108.20
1	X	1057	A	P-O3'-C3'	5.97	126.86	119.70
1	X	1181	C	O4'-C1'-N1	5.97	112.97	108.20
1	X	1816	G	O4'-C1'-N9	5.97	112.97	108.20
1	X	675	C	C3'-C2'-C1'	-5.96	96.73	101.50
1	X	1526	U	P-O5'-C5'	5.96	130.44	120.90
1	X	1076	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	1339	U	OP2-P-O3'	5.96	118.31	105.20
1	X	1249	G	C2'-C3'-O3'	5.96	123.23	113.70
1	X	1338	G	N3-C4-N9	5.96	129.57	126.00
1	X	2598	C	N1-C2-O2	5.96	122.47	118.90
1	X	1978	U	C5-C4-O4	-5.96	122.33	125.90
1	X	2672	U	N3-C2-O2	-5.96	118.03	122.20
1	X	1744	G	N3-C4-N9	5.96	129.57	126.00
1	X	2867	G	C5-N7-C8	-5.96	101.32	104.30
1	X	560	G	N9-C1'-C2'	5.95	121.74	114.00
1	X	1111	C	O4'-C1'-N1	5.95	112.96	108.20
1	X	2561	G	C6-C5-N7	-5.95	126.83	130.40
1	X	2708	U	O4'-C1'-N1	5.95	112.96	108.20
1	X	2649	A	C5'-C4'-C3'	-5.94	106.49	116.00
1	X	1142	G	O4'-C1'-C2'	-5.94	99.86	105.80
2	Y	35	C	O4'-C1'-N1	5.94	112.95	108.20
1	X	1582	A	C5'-C4'-O4'	5.94	116.23	109.10
1	X	1647	U	O4'-C1'-N1	5.94	112.95	108.20
1	X	2837	G	P-O3'-C3'	-5.94	112.57	119.70
1	X	852	U	P-O5'-C5'	-5.93	111.41	120.90
1	X	2616	U	O4'-C1'-N1	5.93	112.95	108.20
1	X	1439	G	C2'-C3'-O3'	5.93	123.19	113.70
1	X	2835	A	N1-C6-N6	5.93	122.16	118.60
1	X	580	A	C1'-O4'-C4'	-5.93	105.16	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1708	C	O4'-C1'-N1	5.93	112.94	108.20
1	X	2769	C	P-O3'-C3'	5.93	126.81	119.70
1	X	957	G	C5-C6-N1	5.93	114.46	111.50
1	X	2523	G	O4'-C1'-N9	5.93	112.94	108.20
1	X	1939	U	N1-C2-O2	5.93	126.95	122.80
1	X	2839	G	C5-C6-N1	5.93	114.46	111.50
1	X	1099	A	P-O3'-C3'	5.92	126.81	119.70
1	X	2201	G	C5'-C4'-O4'	5.92	116.21	109.10
1	X	1245	G	O4'-C1'-N9	5.92	112.94	108.20
1	X	2338	C	O4'-C1'-N1	5.92	112.93	108.20
2	Y	7	C	O4'-C1'-N1	5.92	112.93	108.20
1	X	938	G	C3'-C2'-C1'	5.91	106.23	101.50
1	X	2013	A	C5'-C4'-O4'	5.91	116.20	109.10
1	X	827	C	O4'-C1'-N1	5.91	112.93	108.20
1	X	26	G	C8-N9-C4	-5.91	104.03	106.40
1	X	334	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	468	A	P-O3'-C3'	5.91	126.79	119.70
1	X	2493	U	O4'-C1'-N1	5.91	112.93	108.20
2	Y	49	C	C5'-C4'-O4'	5.90	116.18	109.10
1	X	2359	U	O4'-C1'-N1	5.90	112.92	108.20
1	X	540	G	C5-C6-O6	5.90	132.14	128.60
1	X	1744	G	N3-C4-C5	-5.90	125.65	128.60
1	X	2599	U	P-O5'-C5'	-5.90	111.47	120.90
1	X	1678	G	C5-C6-O6	-5.90	125.06	128.60
1	X	2015	G	N9-C1'-C2'	5.90	121.67	114.00
1	X	2444	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	2636	A	O4'-C1'-N9	5.89	112.92	108.20
1	X	884	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	1529	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	657	A	C3'-C2'-C1'	-5.89	96.79	101.50
1	X	2017	U	O4'-C1'-N1	5.89	112.91	108.20
15	M	29	PRO	N-CA-C	5.89	127.41	112.10
1	X	1454	U	N3-C4-O4	5.88	123.52	119.40
1	X	2441	U	O4'-C1'-N1	5.88	112.90	108.20
1	X	1089	C	P-O3'-C3'	5.88	126.75	119.70
1	X	1244	U	C5-C6-N1	5.87	125.64	122.70
1	X	2572	U	O4'-C1'-N1	5.87	112.90	108.20
1	X	882	C	N1-C2-O2	5.87	122.42	118.90
1	X	1736	C	O4'-C1'-N1	5.87	112.90	108.20
1	X	155	G	O4'-C1'-N9	5.87	112.90	108.20
1	X	1429	A	P-O3'-C3'	5.87	126.74	119.70
1	X	237	G	O4'-C1'-N9	5.87	112.89	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	559	C	N3-C2-O2	-5.87	117.79	121.90
1	X	999	A	O4'-C1'-N9	5.87	112.89	108.20
1	X	2619	G	C5-C6-O6	-5.87	125.08	128.60
1	X	1678	G	O4'-C4'-C3'	-5.86	98.14	104.00
1	X	1023	U	P-O3'-C3'	5.86	126.73	119.70
1	X	2225	G	O4'-C1'-N9	5.86	112.89	108.20
1	X	2560	G	C3'-C2'-C1'	5.86	106.19	101.50
1	X	2745	A	P-O3'-C3'	5.86	126.73	119.70
1	X	2370	G	C1'-O4'-C4'	-5.86	105.21	109.90
1	X	1627	C	O4'-C1'-N1	5.86	112.89	108.20
1	X	939	C	C3'-C2'-C1'	5.85	106.18	101.50
1	X	998	C	O4'-C1'-N1	5.85	112.88	108.20
2	Y	2	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	234	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	771	C	C4'-C3'-C2'	-5.85	96.75	102.60
1	X	1353	A	O4'-C1'-N9	5.85	112.88	108.20
1	X	1667	A	N1-C6-N6	5.85	122.11	118.60
1	X	2797	G	P-O3'-C3'	5.85	126.72	119.70
2	Y	76	U	O4'-C1'-N1	5.85	112.88	108.20
1	X	577	U	C1'-O4'-C4'	-5.85	105.22	109.90
1	X	2797	G	N3-C4-N9	5.85	129.51	126.00
1	X	1389	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	1975	G	N1-C6-O6	-5.84	116.39	119.90
1	X	2635	U	O4'-C1'-N1	5.84	112.88	108.20
1	X	2303	C	N1-C2-O2	5.84	122.41	118.90
1	X	2376	G	P-O5'-C5'	5.84	130.24	120.90
1	X	2009	U	P-O3'-C3'	-5.84	112.69	119.70
9	G	106	TYR	N-CA-CB	5.84	121.11	110.60
2	Y	116	C	O4'-C1'-N1	5.84	112.87	108.20
1	X	68	C	N1-C2-O2	5.83	122.40	118.90
1	X	422	C	C6-N1-C2	-5.83	117.97	120.30
1	X	741	G	P-O3'-C3'	5.83	126.70	119.70
1	X	1888	C	C3'-C2'-C1'	5.83	106.16	101.50
1	X	770	U	C3'-C2'-C1'	-5.83	96.84	101.50
1	X	1223	G	C5-C6-O6	-5.83	125.11	128.60
1	X	2645	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	434	C	O4'-C1'-N1	5.82	112.86	108.20
1	X	522	G	N9-C1'-C2'	5.82	121.57	114.00
1	X	1993	G	C8-N9-C4	-5.82	104.07	106.40
1	X	2627	G	C5-C6-O6	-5.82	125.11	128.60
1	X	1032	A	C3'-C2'-C1'	-5.82	96.84	101.50
1	X	575	U	O4'-C1'-N1	5.82	112.86	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1682	A	C5-C6-N6	-5.82	119.05	123.70
1	X	2567	G	N7-C8-N9	5.82	116.01	113.10
1	X	533	C	O4'-C1'-N1	5.81	112.85	108.20
1	X	1778	U	O4'-C1'-N1	5.81	112.85	108.20
1	X	2797	G	C6-C5-N7	-5.81	126.92	130.40
1	X	797	A	P-O3'-C3'	5.80	126.67	119.70
1	X	220	U	O4'-C1'-N1	5.80	112.84	108.20
1	X	689	A	N7-C8-N9	5.80	116.70	113.80
1	X	582	G	C8-N9-C4	-5.80	104.08	106.40
1	X	339	U	C3'-C2'-C1'	5.80	106.14	101.50
1	X	1831	G	C8-N9-C4	-5.80	104.08	106.40
1	X	661	C	N1-C2-O2	5.79	122.38	118.90
1	X	2460	G	C8-N9-C4	-5.79	104.08	106.40
1	X	1407	G	C8-N9-C4	-5.79	104.08	106.40
1	X	1276	U	O4'-C1'-N1	5.79	112.83	108.20
1	X	466	A	P-O3'-C3'	5.79	126.64	119.70
1	X	1058	G	O4'-C1'-N9	5.79	112.83	108.20
1	X	1466	C	C4'-C3'-C2'	-5.79	96.81	102.60
1	X	1920	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	X	2230	G	C5'-C4'-O4'	-5.79	102.16	109.10
1	X	2778	U	C3'-C2'-C1'	5.79	106.13	101.50
1	X	541	C	P-O3'-C3'	5.78	126.64	119.70
1	X	1987	G	C5-C6-O6	-5.78	125.13	128.60
1	X	556	A	P-O3'-C3'	5.78	126.64	119.70
1	X	461	A	C2-N3-C4	5.78	113.49	110.60
1	X	774	A	C4-C5-C6	5.78	119.89	117.00
1	X	1286	U	P-O3'-C3'	5.78	126.63	119.70
1	X	2527	G	C8-N9-C4	-5.78	104.09	106.40
1	X	467	U	N3-C2-O2	-5.78	118.16	122.20
1	X	1122	A	N9-C1'-C2'	5.78	121.51	114.00
1	X	1288	A	P-O3'-C3'	-5.77	112.77	119.70
1	X	1958	G	C5-C6-N1	5.77	114.39	111.50
1	X	1753	A	P-O5'-C5'	5.77	130.13	120.90
1	X	2487	G	C5-C6-N1	5.77	114.39	111.50
1	X	2604	G	C5-C6-N1	5.77	114.39	111.50
2	Y	64	C	O4'-C1'-N1	5.77	112.82	108.20
1	X	2571	G	C3'-C2'-C1'	-5.77	96.89	101.50
1	X	1224	A	P-O3'-C3'	5.76	126.62	119.70
1	X	202	A	O4'-C1'-N9	5.76	112.81	108.20
1	X	1058	G	C1'-O4'-C4'	-5.76	105.29	109.90
1	X	1841	G	O4'-C1'-N9	5.76	112.81	108.20
1	X	673	G	C2'-C3'-O3'	5.76	122.92	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1811	A	C2'-C3'-O3'	5.76	122.92	113.70
2	Y	76	U	N3-C2-O2	-5.76	118.17	122.20
1	X	29	U	O4'-C1'-N1	5.76	112.81	108.20
1	X	396	U	C1'-O4'-C4'	-5.76	105.30	109.90
1	X	764	A	O5'-P-OP2	-5.76	100.52	105.70
1	X	2840	U	O4'-C1'-N1	5.75	112.80	108.20
1	X	1311	C	N1-C2-O2	5.75	122.35	118.90
1	X	1251	G	N9-C1'-C2'	-5.75	105.68	112.00
2	Y	5	C	O4'-C1'-N1	5.75	112.80	108.20
1	X	352	G	P-O5'-C5'	5.74	130.09	120.90
1	X	603	C	N1-C2-O2	5.74	122.34	118.90
1	X	2458	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	223	C	P-O3'-C3'	-5.74	112.81	119.70
1	X	1843	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	2427	A	P-O3'-C3'	5.74	126.58	119.70
1	X	1081	A	P-O3'-C3'	5.74	126.58	119.70
1	X	420	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	447	U	P-O3'-C3'	5.74	126.58	119.70
1	X	1729	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	2572	U	C3'-C2'-C1'	-5.73	96.91	101.50
1	X	2735	C	C6-N1-C2	-5.73	118.01	120.30
1	X	67	G	O4'-C1'-N9	5.73	112.78	108.20
1	X	1442	C	N1-C2-O2	5.73	122.34	118.90
1	X	2364	C	O4'-C1'-N1	5.73	112.78	108.20
1	X	799	C	P-O5'-C5'	-5.72	111.74	120.90
1	X	860	U	C5'-C4'-O4'	5.72	115.97	109.10
1	X	2048	C	P-O5'-C5'	-5.72	111.75	120.90
1	X	2559	U	N1-C2-O2	5.72	126.80	122.80
1	X	2573	C	O4'-C1'-N1	5.72	112.78	108.20
1	X	574	C	P-O3'-C3'	-5.71	112.84	119.70
1	X	1394	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	12	U	N3-C2-O2	-5.71	118.20	122.20
1	X	1093	U	O4'-C1'-N1	5.71	112.77	108.20
1	X	2018	G	C5'-C4'-C3'	-5.71	106.86	116.00
1	X	2724	G	P-O5'-C5'	5.71	130.04	120.90
2	Y	109	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	421	G	P-O5'-C5'	5.71	130.03	120.90
1	X	474	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	536	A	P-O3'-C3'	5.71	126.55	119.70
1	X	724	C	O4'-C1'-N1	5.71	112.77	108.20
1	X	2876	C	O4'-C1'-N1	5.71	112.77	108.20
1	X	1635	G	P-O3'-C3'	-5.70	112.86	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	924	C	N1-C2-O2	5.70	122.32	118.90
1	X	2277	A	O4'-C1'-N9	5.70	112.76	108.20
1	X	2075	U	P-O3'-C3'	5.70	126.54	119.70
1	X	464	G	C3'-C2'-C1'	5.70	106.06	101.50
1	X	1490	U	O4'-C1'-N1	5.70	112.76	108.20
1	X	2258	G	C1'-O4'-C4'	-5.70	105.34	109.90
1	X	2235	G	C3'-C2'-C1'	-5.69	96.94	101.50
2	Y	83	C	N1-C2-O2	5.69	122.32	118.90
1	X	1570	C	N1-C2-O2	5.69	122.31	118.90
1	X	2552	C	O3'-P-O5'	-5.69	93.19	104.00
1	X	516	G	C5-C6-O6	-5.69	125.19	128.60
1	X	656	U	P-O5'-C5'	5.69	130.00	120.90
1	X	2015	G	N7-C8-N9	5.69	115.94	113.10
1	X	1518	C	O4'-C1'-N1	5.68	112.75	108.20
2	Y	120	G	O4'-C1'-N9	5.68	112.75	108.20
1	X	1668	G	P-O5'-C5'	5.68	129.99	120.90
1	X	2702	G	C6-C5-N7	-5.68	126.99	130.40
1	X	156	G	C3'-C2'-C1'	-5.68	96.96	101.50
1	X	889	C	O4'-C1'-N1	5.68	112.74	108.20
1	X	689	A	N1-C6-N6	5.67	122.00	118.60
1	X	2715	C	O4'-C1'-N1	5.67	112.74	108.20
1	X	34	U	C2-N1-C1'	5.67	124.51	117.70
1	X	1341	G	C4'-C3'-C2'	5.67	108.27	102.60
1	X	2846	G	O4'-C1'-N9	5.67	112.74	108.20
15	M	28	ARG	N-CA-C	-5.67	95.69	111.00
1	X	490	A	C5'-C4'-O4'	5.67	115.90	109.10
1	X	2245	A	C5'-C4'-O4'	5.67	115.90	109.10
1	X	467	U	N1-C2-O2	5.67	126.77	122.80
1	X	1075	C	O4'-C1'-N1	5.67	112.73	108.20
1	X	225	G	O4'-C1'-N9	5.67	112.73	108.20
1	X	1222	G	N3-C4-C5	-5.67	125.77	128.60
1	X	1500	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	2285	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	1237	G	O4'-C1'-N9	5.66	112.73	108.20
1	X	1415	C	N1-C2-O2	5.66	122.30	118.90
1	X	1570	C	N3-C2-O2	-5.66	117.94	121.90
1	X	2013	A	C1'-O4'-C4'	-5.66	105.37	109.90
1	X	1324	G	O4'-C1'-C2'	-5.66	100.14	105.80
1	X	2671	C	C4'-C3'-C2'	-5.66	96.94	102.60
1	X	454	G	C4'-C3'-C2'	5.66	108.26	102.60
1	X	478	G	P-O3'-C3'	-5.65	112.92	119.70
1	X	1252	C	C5-C6-N1	5.65	123.83	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2300	G	O4'-C1'-N9	5.65	112.72	108.20
1	X	413	G	O4'-C1'-N9	5.65	112.72	108.20
1	X	459	A	P-O3'-C3'	5.65	126.48	119.70
1	X	1159	U	O4'-C1'-N1	5.65	112.72	108.20
1	X	1281	A	OP2-P-O3'	5.65	117.63	105.20
1	X	516	G	P-O3'-C3'	5.65	126.48	119.70
1	X	1277	G	N3-C4-C5	-5.65	125.78	128.60
1	X	915	C	O4'-C1'-N1	5.64	112.72	108.20
1	X	1421	U	O4'-C1'-N1	5.64	112.72	108.20
1	X	1700	C	P-O3'-C3'	-5.64	112.93	119.70
1	X	175	C	C5-C6-N1	5.64	123.82	121.00
1	X	2018	G	N3-C4-C5	5.64	131.42	128.60
1	X	2552	C	O4'-C1'-N1	5.64	112.71	108.20
1	X	21	A	P-O3'-C3'	-5.64	112.93	119.70
1	X	1337	G	C3'-C2'-C1'	-5.64	96.99	101.50
1	X	2791	C	N3-C2-O2	-5.64	117.95	121.90
1	X	2545	A	P-O3'-C3'	5.64	126.46	119.70
1	X	219	G	O4'-C1'-N9	-5.63	103.69	108.20
1	X	2296	U	O4'-C1'-N1	5.63	112.71	108.20
1	X	42	G	N7-C8-N9	5.63	115.92	113.10
1	X	742	G	C5'-C4'-O4'	5.63	115.86	109.10
1	X	2075	U	O4'-C1'-N1	5.63	112.71	108.20
1	X	2353	G	N3-C4-C5	-5.63	125.78	128.60
1	X	1683	G	O4'-C1'-N9	5.63	112.70	108.20
1	X	1753	A	N7-C8-N9	5.63	116.61	113.80
1	X	806	A	P-O3'-C3'	5.62	126.45	119.70
1	X	426	C	O4'-C1'-N1	5.62	112.70	108.20
1	X	2559	U	P-O3'-C3'	5.62	126.44	119.70
1	X	12	U	N1-C2-O2	5.62	126.73	122.80
1	X	1229	C	O4'-C1'-N1	5.62	112.69	108.20
1	X	75	C	O4'-C1'-N1	5.62	112.69	108.20
1	X	168	A	O4'-C1'-N9	5.62	112.69	108.20
1	X	746	G	N3-C4-C5	-5.62	125.79	128.60
1	X	749	C	C5-C6-N1	5.62	123.81	121.00
1	X	190	A	O4'-C4'-C3'	-5.61	98.39	104.00
1	X	540	G	N9-C1'-C2'	5.61	121.30	114.00
1	X	2294	U	P-O3'-C3'	5.61	126.43	119.70
1	X	2782	G	C6-C5-N7	-5.61	127.03	130.40
1	X	1201	G	C8-N9-C4	-5.61	104.16	106.40
1	X	1249	G	N1-C6-O6	-5.61	116.54	119.90
1	X	2652	G	N3-C4-C5	-5.61	125.80	128.60
1	X	2541	U	N3-C2-O2	-5.60	118.28	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	690	A	P-O3'-C3'	5.60	126.42	119.70
1	X	1037	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	2033	C	N1-C2-O2	5.60	122.26	118.90
1	X	1086	C	C3'-C2'-C1'	5.60	105.98	101.50
1	X	1314	A	O4'-C1'-C2'	-5.60	100.20	105.80
1	X	746	G	N3-C4-N9	5.60	129.36	126.00
1	X	982	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1399	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1341	G	C5-C6-N1	5.60	114.30	111.50
1	X	1411	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1660	G	O4'-C1'-N9	5.60	112.68	108.20
1	X	441	A	P-O3'-C3'	5.60	126.42	119.70
1	X	1607	A	C2'-C3'-O3'	5.59	122.65	113.70
1	X	169	C	N1-C2-O2	5.59	122.25	118.90
1	X	392	G	P-O3'-C3'	-5.59	112.99	119.70
1	X	1257	U	O4'-C1'-N1	5.59	112.67	108.20
1	X	534	U	O4'-C1'-N1	5.59	112.67	108.20
1	X	555	U	C1'-O4'-C4'	-5.59	105.43	109.90
1	X	927	C	N3-C2-O2	-5.59	117.99	121.90
1	X	13	A	P-O3'-C3'	5.59	126.41	119.70
1	X	1986	G	O5'-P-OP2	-5.59	100.67	105.70
12	J	87	GLY	C-N-CA	5.59	135.67	121.70
1	X	327	C	N1-C2-O2	5.59	122.25	118.90
1	X	1528	C	O4'-C1'-N1	5.59	112.67	108.20
1	X	1439	G	C8-N9-C4	-5.58	104.17	106.40
1	X	1922	U	P-O3'-C3'	5.58	126.40	119.70
2	Y	14	C	N1-C2-O2	5.58	122.25	118.90
1	X	165	G	O4'-C1'-N9	5.58	112.67	108.20
1	X	719	A	P-O3'-C3'	5.58	126.40	119.70
1	X	1304	U	O4'-C1'-N1	5.58	112.66	108.20
1	X	204	A	C2'-C3'-O3'	5.58	122.63	113.70
1	X	1636	G	O4'-C1'-N9	5.58	112.66	108.20
1	X	1087	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	2338	C	N1-C2-O2	5.58	122.25	118.90
1	X	2403	C	N3-C2-O2	-5.58	118.00	121.90
1	X	327	C	P-O3'-C3'	-5.58	113.01	119.70
1	X	2421	C	O4'-C1'-N1	5.57	112.66	108.20
1	X	2527	G	C2-N3-C4	5.57	114.69	111.90
1	X	1010	U	C5'-C4'-O4'	5.57	115.79	109.10
1	X	2228	U	C4-C5-C6	5.57	123.04	119.70
1	X	878	C	O4'-C1'-N1	5.57	112.66	108.20
2	Y	54	U	C3'-C2'-C1'	5.57	105.96	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2015	G	C8-N9-C4	-5.57	104.17	106.40
1	X	2321	C	O4'-C1'-N1	5.57	112.66	108.20
1	X	2435	C	P-O3'-C3'	-5.57	113.02	119.70
1	X	2470	U	P-O3'-C3'	5.57	126.38	119.70
2	Y	32	C	O4'-C1'-N1	5.57	112.65	108.20
1	X	687	G	C3'-C2'-C1'	-5.57	97.05	101.50
1	X	541	C	N1-C1'-C2'	5.56	121.23	114.00
1	X	842	A	C1'-O4'-C4'	-5.56	105.45	109.90
1	X	70	A	P-O3'-C3'	5.56	126.38	119.70
1	X	162	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	617	U	C2-N1-C1'	5.56	124.38	117.70
1	X	2047	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2791	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2748	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2821	G	O4'-C1'-N9	5.56	112.65	108.20
1	X	1630	A	C8-N9-C4	-5.56	103.58	105.80
1	X	1771	A	N1-C6-N6	5.56	121.94	118.60
1	X	2444	C	N1-C2-O2	5.56	122.23	118.90
1	X	2702	G	N7-C8-N9	5.56	115.88	113.10
1	X	2459	C	O4'-C1'-N1	5.56	112.64	108.20
1	X	2668	U	C5-C4-O4	5.56	129.23	125.90
1	X	1593	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	2016	A	N1-C2-N3	-5.55	126.52	129.30
1	X	2422	C	N3-C2-O2	-5.55	118.01	121.90
1	X	1858	C	N1-C2-O2	5.55	122.23	118.90
1	X	86	U	C3'-C2'-C1'	-5.55	97.06	101.50
1	X	1182	U	O4'-C1'-N1	5.55	112.64	108.20
1	X	1251	G	O4'-C1'-N9	5.55	112.64	108.20
1	X	1506	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	467	U	O4'-C1'-N1	5.54	112.64	108.20
1	X	957	G	N3-C4-C5	-5.54	125.83	128.60
1	X	398	C	P-O5'-C5'	5.54	129.76	120.90
1	X	1850	G	O4'-C1'-N9	5.54	112.63	108.20
1	X	2367	A	O4'-C1'-N9	5.54	112.63	108.20
1	X	562	G	O4'-C4'-C3'	-5.54	98.46	104.00
1	X	956	A	C5'-C4'-O4'	5.54	115.74	109.10
1	X	537	C	C6-N1-C1'	-5.54	114.16	120.80
1	X	1275	A	P-O5'-C5'	5.54	129.76	120.90
1	X	1533	G	C5-C6-O6	-5.54	125.28	128.60
1	X	2321	C	C6-N1-C2	-5.54	118.09	120.30
1	X	2775	U	P-O3'-C3'	5.54	126.34	119.70
1	X	224	G	C3'-C2'-C1'	5.53	105.92	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	236	C	N1-C2-O2	5.53	122.22	118.90
1	X	2204	A	C5'-C4'-O4'	5.53	115.74	109.10
1	X	156	G	P-O3'-C3'	-5.53	113.07	119.70
1	X	640	C	O4'-C1'-N1	5.53	112.62	108.20
1	X	1142	G	N3-C4-N9	5.53	129.31	126.00
1	X	1630	A	P-O3'-C3'	-5.53	113.07	119.70
1	X	1829	C	P-O3'-C3'	-5.53	113.07	119.70
1	X	2315	A	P-O3'-C3'	5.53	126.33	119.70
1	X	612	G	O4'-C1'-N9	5.52	112.62	108.20
1	X	632	A	C4'-C3'-C2'	-5.52	97.08	102.60
1	X	1233	A	P-O3'-C3'	5.52	126.32	119.70
1	X	1539	U	O4'-C1'-N1	5.52	112.61	108.20
1	X	2496	C	O4'-C1'-N1	5.52	112.61	108.20
1	X	919	U	N1-C2-O2	5.52	126.66	122.80
1	X	1280	U	N3-C2-O2	-5.52	118.34	122.20
1	X	1707	A	P-O3'-C3'	5.52	126.32	119.70
1	X	682	G	C5-C6-N1	5.51	114.26	111.50
1	X	1626	A	N1-C2-N3	-5.51	126.54	129.30
1	X	1840	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	1912	G	P-O3'-C3'	5.51	126.32	119.70
1	X	2222	U	P-O5'-C5'	5.51	129.72	120.90
1	X	440	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	1447	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	455	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	2591	C	N1-C2-N3	-5.51	115.34	119.20
2	Y	10	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	632	A	C1'-O4'-C4'	-5.51	105.49	109.90
1	X	689	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	565	A	P-O3'-C3'	-5.51	113.09	119.70
1	X	2863	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	1167	A	O4'-C1'-N9	-5.50	103.80	108.20
1	X	2620	G	C5-C6-O6	-5.50	125.30	128.60
1	X	2782	G	O4'-C4'-C3'	-5.50	98.50	104.00
1	X	770	U	P-O3'-C3'	-5.50	113.10	119.70
1	X	1225	G	N3-C4-C5	-5.50	125.85	128.60
1	X	1289	A	O4'-C4'-C3'	-5.50	98.50	104.00
1	X	1936	A	N1-C2-N3	-5.50	126.55	129.30
2	Y	55	C	P-O3'-C3'	5.50	126.30	119.70
1	X	1337	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	1743	C	O4'-C1'-N1	5.50	112.60	108.20
1	X	1976	U	C3'-C2'-C1'	5.50	105.90	101.50
1	X	738	G	C8-N9-C4	-5.50	104.20	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2088	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	2589	C	N1-C1'-C2'	5.50	121.14	114.00
1	X	476	G	O4'-C1'-N9	5.49	112.59	108.20
1	X	859	U	C5'-C4'-O4'	5.49	115.69	109.10
1	X	1294	G	C4'-C3'-C2'	-5.49	97.11	102.60
1	X	2628	C	C3'-C2'-C1'	-5.49	97.11	101.50
1	X	1162	A	O4'-C1'-N9	5.49	112.59	108.20
1	X	521	U	C2-N1-C1'	5.49	124.29	117.70
1	X	2382	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1782	A	P-O5'-C5'	5.49	129.68	120.90
1	X	2528	G	OP1-P-O3'	5.49	117.27	105.20
1	X	1831	G	O4'-C1'-N9	5.48	112.59	108.20
1	X	2184	C	O4'-C1'-N1	5.48	112.58	108.20
1	X	2496	C	O3'-P-O5'	-5.48	93.58	104.00
1	X	2528	G	N3-C4-C5	-5.48	125.86	128.60
1	X	796	A	C4-C5-N7	5.48	113.44	110.70
2	Y	112	A	O4'-C1'-N9	5.48	112.58	108.20
23	U	33	LYS	C-N-CA	5.48	135.40	121.70
1	X	322	A	O4'-C1'-N9	5.48	112.58	108.20
1	X	540	G	N9-C4-C5	5.48	107.59	105.40
1	X	698	A	C1'-O4'-C4'	-5.48	105.52	109.90
1	X	940	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	X	1456	C	O4'-C1'-N1	5.48	112.58	108.20
2	Y	76	U	N1-C2-O2	5.48	126.63	122.80
1	X	973	U	O3'-P-O5'	-5.48	93.59	104.00
1	X	2196	U	O4'-C1'-N1	5.48	112.58	108.20
1	X	707	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1469	U	C5'-C4'-O4'	5.47	115.67	109.10
1	X	1672	A	C3'-C2'-C1'	-5.47	97.12	101.50
1	X	2552	C	OP1-P-O3'	5.47	117.24	105.20
1	X	613	A	P-O3'-C3'	5.47	126.27	119.70
1	X	1308	C	C4'-C3'-C2'	-5.47	97.13	102.60
1	X	1808	C	N1-C2-O2	5.47	122.18	118.90
1	X	2330	G	C8-N9-C4	-5.47	104.21	106.40
1	X	2494	C	N3-C2-O2	-5.47	118.07	121.90
1	X	1965	U	N1-C2-O2	5.47	126.63	122.80
1	X	467	U	C2-N1-C1'	5.47	124.26	117.70
1	X	557	U	N1-C1'-C2'	5.47	121.11	114.00
1	X	1550	C	O4'-C1'-N1	5.47	112.58	108.20
1	X	1688	U	C5-C6-N1	5.47	125.43	122.70
1	X	165	G	C8-N9-C4	-5.46	104.21	106.40
1	X	1473	U	O4'-C1'-C2'	5.46	112.52	107.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2876	C	P-O3'-C3'	5.46	126.26	119.70
1	X	1142	G	N3-C4-C5	-5.46	125.87	128.60
1	X	535	U	O4'-C1'-N1	5.46	112.57	108.20
1	X	1664	G	P-O5'-C5'	5.46	129.64	120.90
1	X	1767	G	O4'-C1'-N9	5.46	112.57	108.20
1	X	2443	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	241	C	N1-C2-O2	5.46	122.17	118.90
1	X	1381	G	C8-N9-C4	-5.46	104.22	106.40
1	X	1663	C	OP1-P-O3'	5.46	117.21	105.20
1	X	2587	G	O4'-C1'-N9	5.46	112.57	108.20
1	X	358	C	C6-N1-C2	-5.46	118.12	120.30
1	X	979	A	O4'-C1'-N9	5.46	112.56	108.20
1	X	1235	C	C5-C6-N1	5.46	123.73	121.00
1	X	1439	G	N7-C8-N9	5.46	115.83	113.10
1	X	1715	A	P-O3'-C3'	5.46	126.25	119.70
1	X	2540	A	N9-C1'-C2'	-5.46	106.00	112.00
1	X	520	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	1882	G	P-O5'-C5'	5.45	129.62	120.90
1	X	2539	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2330	G	P-O3'-C3'	5.45	126.24	119.70
2	Y	30	C	P-O5'-C5'	5.45	129.62	120.90
1	X	429	C	N1-C2-O2	5.45	122.17	118.90
1	X	1146	G	P-O3'-C3'	-5.44	113.17	119.70
1	X	11	G	C8-N9-C4	-5.44	104.22	106.40
1	X	144	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1766	U	P-O5'-C5'	-5.44	112.19	120.90
1	X	2268	G	O4'-C1'-N9	5.44	112.55	108.20
1	X	1924	C	N1-C2-O2	5.44	122.17	118.90
1	X	2734	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1254	G	C8-N9-C4	-5.44	104.22	106.40
1	X	227	G	P-O3'-C3'	5.44	126.22	119.70
1	X	2668	U	C5-C6-N1	-5.44	119.98	122.70
1	X	1219	C	C5-C6-N1	5.44	123.72	121.00
1	X	1466	C	N1-C2-O2	5.43	122.16	118.90
1	X	2608	A	N9-C1'-C2'	5.43	121.06	114.00
1	X	2854	G	O4'-C1'-C2'	-5.43	100.36	105.80
1	X	191	G	C8-N9-C4	-5.43	104.23	106.40
1	X	458	G	C3'-C2'-C1'	5.43	105.85	101.50
1	X	579	G	N9-C4-C5	5.43	107.57	105.40
1	X	1680	U	P-O3'-C3'	5.43	126.22	119.70
1	X	1003	C	O4'-C1'-N1	5.43	112.54	108.20
1	X	1626	A	P-O3'-C3'	5.43	126.21	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	413	G	C8-N9-C4	-5.43	104.23	106.40
1	X	692	C	C6-N1-C2	-5.43	118.13	120.30
1	X	1690	U	O4'-C1'-N1	5.42	112.54	108.20
2	Y	123	U	N1-C2-O2	5.42	126.60	122.80
1	X	417	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	1627	C	N1-C2-O2	5.42	122.15	118.90
1	X	2039	G	N1-C2-N2	5.42	121.08	116.20
1	X	731	A	C3'-C2'-C1'	5.42	105.84	101.50
1	X	924	C	P-O3'-C3'	5.42	126.21	119.70
1	X	1753	A	C8-N9-C4	-5.42	103.63	105.80
1	X	1850	G	C8-N9-C4	-5.42	104.23	106.40
1	X	1514	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	2039	G	O4'-C1'-C2'	-5.42	100.38	105.80
1	X	2405	A	N9-C1'-C2'	5.42	121.04	114.00
1	X	342	G	N7-C8-N9	5.42	115.81	113.10
19	Q	60	GLY	C-N-CA	5.42	135.24	121.70
1	X	2295	C	O4'-C1'-N1	5.41	112.53	108.20
4	B	132	LYS	C-N-CA	5.41	135.23	121.70
1	X	1380	C	O4'-C1'-N1	5.41	112.53	108.20
2	Y	88	C	P-O5'-C5'	5.41	129.56	120.90
1	X	1877	C	N1-C2-O2	5.41	122.15	118.90
1	X	2694	G	C4'-C3'-C2'	-5.41	97.19	102.60
1	X	926	C	N1-C1'-C2'	-5.41	106.05	112.00
1	X	2845	C	C6-N1-C2	-5.41	118.14	120.30
1	X	1141	U	C3'-C2'-C1'	-5.41	97.17	101.50
1	X	329	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	731	A	O4'-C1'-N9	5.41	112.52	108.20
1	X	1454	U	N3-C4-C5	-5.41	111.36	114.60
1	X	2256	G	N7-C8-N9	5.41	115.80	113.10
1	X	2539	C	C6-N1-C2	-5.40	118.14	120.30
1	X	2656	G	P-O5'-C5'	-5.40	112.26	120.90
1	X	1225	G	N1-C6-O6	-5.40	116.66	119.90
1	X	1995	G	N3-C4-N9	5.40	129.24	126.00
1	X	549	G	O4'-C1'-N9	5.40	112.52	108.20
1	X	851	C	O4'-C1'-N1	5.40	112.52	108.20
1	X	1828	C	N1-C2-O2	5.40	122.14	118.90
1	X	2627	G	N1-C6-O6	5.40	123.14	119.90
2	Y	90	C	P-O5'-C5'	5.40	129.54	120.90
1	X	65	C	O4'-C1'-N1	5.39	112.52	108.20
1	X	583	C	O4'-C1'-N1	5.39	112.52	108.20
1	X	2043	A	C3'-C2'-C1'	-5.39	97.19	101.50
1	X	560	G	C4'-C3'-C2'	5.39	107.99	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	113	G	O4'-C1'-N9	5.39	112.51	108.20
1	X	1001	A	O4'-C1'-N9	5.39	112.51	108.20
1	X	1099	A	C3'-C2'-C1'	5.39	105.81	101.50
1	X	508	G	C8-N9-C4	-5.39	104.25	106.40
1	X	2335	U	O4'-C1'-N1	5.39	112.51	108.20
1	X	235	C	N1-C2-O2	5.39	122.13	118.90
1	X	647	G	O4'-C1'-N9	5.39	112.51	108.20
1	X	1255	A	O4'-C1'-N9	5.39	112.51	108.20
2	Y	45	C	O4'-C1'-N1	5.39	112.51	108.20
1	X	863	C	O4'-C1'-N1	5.38	112.51	108.20
1	X	985	G	N9-C1'-C2'	5.38	121.00	114.00
1	X	990	A	N1-C6-N6	-5.38	115.37	118.60
1	X	1632	A	N7-C8-N9	5.38	116.49	113.80
1	X	2043	A	O4'-C1'-N9	5.38	112.51	108.20
1	X	2347	C	C3'-C2'-C1'	-5.38	97.19	101.50
1	X	2659	C	O4'-C1'-N1	5.38	112.51	108.20
2	Y	44	C	N1-C2-O2	5.38	122.13	118.90
1	X	135	U	O4'-C1'-N1	5.38	112.51	108.20
1	X	2047	C	C5-C6-N1	5.38	123.69	121.00
1	X	2199	C	C5'-C4'-O4'	5.38	115.56	109.10
1	X	558	G	C8-N9-C4	-5.38	104.25	106.40
1	X	683	A	C2'-C3'-O3'	5.38	122.31	113.70
1	X	1669	A	P-O3'-C3'	5.38	126.16	119.70
1	X	1946	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	2010	G	C4'-C3'-C2'	-5.38	97.22	102.60
1	X	651	C	C3'-C2'-C1'	5.38	105.80	101.50
1	X	1648	C	C5'-C4'-O4'	-5.38	102.64	109.10
1	X	306	G	P-O3'-C3'	5.38	126.16	119.70
1	X	1563	U	C5'-C4'-O4'	5.38	115.56	109.10
1	X	1979	C	O4'-C1'-N1	-5.38	103.90	108.20
1	X	2393	G	C8-N9-C4	-5.38	104.25	106.40
1	X	1825	C	C3'-C2'-C1'	-5.38	97.20	101.50
1	X	2032	G	N3-C4-N9	5.38	129.23	126.00
1	X	1694	A	O4'-C1'-N9	5.37	112.50	108.20
1	X	1811	A	C4'-C3'-C2'	5.37	107.97	102.60
1	X	2463	G	C5'-C4'-O4'	5.37	115.54	109.10
1	X	82	G	O3'-P-O5'	-5.37	93.80	104.00
1	X	1385	C	N1-C2-O2	5.37	122.12	118.90
1	X	2367	A	C5'-C4'-C3'	-5.37	107.41	116.00
1	X	2754	C	O4'-C1'-N1	5.37	112.50	108.20
1	X	1407	G	N7-C8-N9	5.37	115.78	113.10
1	X	206	U	O4'-C1'-N1	5.37	112.49	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	758	G	C5-C6-N1	5.37	114.18	111.50
3	A	203	ASN	CA-CB-CG	5.37	125.20	113.40
1	X	1761	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	1975	G	C5-C6-N1	5.36	114.18	111.50
1	X	2703	C	C5'-C4'-O4'	5.36	115.54	109.10
1	X	655	A	C3'-C2'-C1'	5.36	105.79	101.50
1	X	934	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	1018	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	2004	U	P-O5'-C5'	-5.36	112.32	120.90
1	X	2299	A	P-O3'-C3'	5.36	126.13	119.70
1	X	90	G	N3-C4-C5	-5.36	125.92	128.60
1	X	560	G	C1'-O4'-C4'	5.36	114.19	109.90
1	X	1009	C	N3-C2-O2	-5.36	118.15	121.90
1	X	1069	G	C3'-C2'-C1'	5.36	105.79	101.50
1	X	405	C	N1-C2-O2	5.36	122.11	118.90
1	X	1311	C	O4'-C1'-N1	5.36	112.48	108.20
1	X	2172	U	O4'-C1'-N1	5.36	112.48	108.20
1	X	2841	U	N1-C1'-C2'	5.36	120.96	114.00
1	X	601	A	P-O5'-C5'	5.35	129.46	120.90
1	X	2067	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	45	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	803	C	N1-C2-O2	5.35	122.11	118.90
1	X	1637	U	O3'-P-O5'	-5.35	93.84	104.00
1	X	2069	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	822	G	C8-N9-C4	-5.34	104.26	106.40
1	X	1652	G	N9-C4-C5	-5.34	103.26	105.40
1	X	2796	A	O4'-C1'-N9	5.34	112.48	108.20
1	X	2856	U	P-O3'-C3'	-5.34	113.29	119.70
1	X	2574	G	C8-N9-C4	-5.34	104.26	106.40
1	X	2631	C	N1-C2-O2	5.34	122.11	118.90
1	X	589	C	N1-C2-O2	5.34	122.11	118.90
1	X	701	U	O4'-C1'-N1	5.34	112.47	108.20
1	X	1231	A	P-O3'-C3'	-5.34	113.29	119.70
1	X	2060	A	N1-C6-N6	-5.34	115.39	118.60
1	X	2489	C	P-O5'-C5'	-5.34	112.36	120.90
1	X	1668	G	C6-C5-N7	-5.34	127.20	130.40
1	X	1673	C	O5'-P-OP1	5.34	117.10	110.70
1	X	233	A	O4'-C1'-N9	5.33	112.47	108.20
1	X	1392	U	N1-C1'-C2'	5.33	120.93	114.00
1	X	2776	U	P-O3'-C3'	5.33	126.10	119.70
1	X	2195	C	C6-N1-C2	-5.33	118.17	120.30
1	X	665	A	O4'-C1'-N9	5.33	112.46	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	11	G	O4'-C4'-C3'	-5.33	98.67	104.00
1	X	575	U	C3'-C2'-C1'	5.33	105.76	101.50
1	X	841	G	C5-N7-C8	-5.33	101.64	104.30
1	X	1341	G	N3-C4-C5	-5.33	125.94	128.60
1	X	598	U	O4'-C1'-N1	5.32	112.46	108.20
1	X	2188	A	O4'-C1'-N9	5.32	112.46	108.20
1	X	2856	U	N3-C2-O2	-5.32	118.47	122.20
1	X	1946	U	N3-C2-O2	-5.32	118.48	122.20
1	X	1060	C	O4'-C1'-N1	5.32	112.45	108.20
1	X	227	G	O4'-C1'-N9	5.32	112.45	108.20
1	X	621	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2417	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2621	G	C5'-C4'-C3'	5.32	124.51	116.00
1	X	613	A	N9-C1'-C2'	5.32	120.91	114.00
1	X	1428	G	O4'-C1'-N9	5.32	112.45	108.20
3	A	248	THR	CB-CA-C	5.32	125.95	111.60
1	X	2349	G	C3'-C2'-C1'	-5.31	97.25	101.50
1	X	1825	C	C5-C6-N1	5.31	123.66	121.00
1	X	998	C	N1-C2-O2	5.31	122.09	118.90
1	X	527	C	C4-C5-C6	-5.31	114.75	117.40
1	X	668	A	P-O3'-C3'	5.31	126.07	119.70
1	X	2419	C	N1-C2-O2	5.31	122.08	118.90
1	X	404	A	O4'-C1'-N9	5.30	112.44	108.20
1	X	63	A	C5'-C4'-C3'	-5.30	107.52	116.00
1	X	738	G	N3-C4-C5	-5.30	125.95	128.60
1	X	561	U	C5-C4-O4	-5.30	122.72	125.90
1	X	860	U	C1'-O4'-C4'	-5.30	105.66	109.90
1	X	1632	A	C8-N9-C4	-5.30	103.68	105.80
1	X	1730	G	C3'-C2'-C1'	-5.30	97.26	101.50
1	X	238	G	O4'-C1'-N9	5.30	112.44	108.20
2	Y	74	A	N7-C8-N9	5.30	116.45	113.80
1	X	1513	U	P-O3'-C3'	5.30	126.06	119.70
1	X	2377	U	O4'-C1'-N1	5.29	112.44	108.20
1	X	1358	C	P-O3'-C3'	5.29	126.05	119.70
1	X	469	G	N3-C4-C5	-5.29	125.95	128.60
1	X	1885	C	C4'-C3'-C2'	-5.29	97.31	102.60
1	X	2652	G	N3-C4-N9	5.29	129.18	126.00
1	X	327	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	646	C	C6-N1-C2	-5.29	118.19	120.30
1	X	1497	C	C5-C6-N1	5.29	123.64	121.00
1	X	723	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2252	A	C2-N3-C4	5.29	113.24	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	145	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	2867	G	C4-C5-N7	5.28	112.91	110.80
1	X	635	C	C6-N1-C2	-5.28	118.19	120.30
1	X	914	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1008	G	C5-C6-N1	5.28	114.14	111.50
1	X	1563	U	N1-C2-O2	5.28	126.50	122.80
1	X	230	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1398	G	P-O3'-C3'	5.28	126.03	119.70
1	X	309	G	N7-C8-N9	5.28	115.74	113.10
1	X	661	C	C6-N1-C2	-5.28	118.19	120.30
1	X	2729	A	O4'-C1'-N9	5.28	112.42	108.20
1	X	661	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1681	A	N7-C8-N9	5.28	116.44	113.80
1	X	2426	G	P-O5'-C5'	5.28	129.34	120.90
1	X	1033	G	P-O3'-C3'	5.27	126.03	119.70
1	X	2567	G	N3-C4-C5	-5.27	125.96	128.60
2	Y	38	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	1168	G	P-O5'-C5'	5.27	129.33	120.90
1	X	1742	G	P-O3'-C3'	-5.27	113.38	119.70
1	X	2004	U	O3'-P-O5'	-5.27	93.99	104.00
1	X	2026	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	2525	U	O4'-C1'-N1	5.27	112.42	108.20
1	X	1238	A	P-O5'-C5'	5.27	129.33	120.90
1	X	2607	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	418	C	P-O3'-C3'	5.27	126.02	119.70
1	X	1767	G	C5-C6-N1	5.27	114.13	111.50
1	X	2556	A	P-O3'-C3'	5.27	126.02	119.70
1	X	2598	C	N3-C2-O2	-5.27	118.21	121.90
1	X	327	C	C6-N1-C2	-5.27	118.19	120.30
1	X	664	C	C3'-C2'-C1'	5.26	105.71	101.50
1	X	1312	G	N7-C8-N9	5.26	115.73	113.10
1	X	1467	U	N1-C2-N3	-5.26	111.74	114.90
1	X	2628	C	O4'-C4'-C3'	-5.26	98.74	104.00
1	X	582	G	O3'-P-O5'	-5.26	94.00	104.00
1	X	1160	C	C6-N1-C2	-5.26	118.20	120.30
1	X	2463	G	P-O3'-C3'	-5.26	113.39	119.70
1	X	1142	G	C5-C6-O6	-5.26	125.44	128.60
1	X	2038	C	OP2-P-O3'	5.26	116.76	105.20
1	X	749	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	850	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1252	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1235	C	C6-N1-C2	-5.25	118.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1829	C	C3'-C2'-C1'	-5.25	97.30	101.50
1	X	102	C	N1-C2-O2	5.25	122.05	118.90
1	X	203	G	O4'-C1'-N9	5.25	112.40	108.20
1	X	1150	C	P-O3'-C3'	5.25	126.00	119.70
1	X	1668	G	N1-C6-O6	5.25	123.05	119.90
1	X	2698	G	O4'-C1'-N9	5.25	112.40	108.20
2	Y	111	C	P-O3'-C3'	5.25	126.00	119.70
1	X	303	C	C5-C6-N1	5.25	123.62	121.00
1	X	429	C	C6-N1-C2	-5.25	118.20	120.30
1	X	1820	G	C4'-C3'-C2'	5.25	107.85	102.60
1	X	2225	G	C3'-C2'-C1'	-5.25	97.30	101.50
1	X	2854	G	N7-C8-N9	5.25	115.72	113.10
1	X	1288	A	N9-C1'-C2'	5.25	120.82	114.00
1	X	2667	C	C5-C6-N1	5.25	123.62	121.00
1	X	2845	C	C5-C6-N1	5.25	123.62	121.00
1	X	86	U	O4'-C1'-N1	5.24	112.39	108.20
1	X	1049	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1470	G	C8-N9-C4	-5.24	104.30	106.40
1	X	1551	U	O4'-C1'-N1	5.24	112.39	108.20
1	X	1016	C	C5-C6-N1	5.24	123.62	121.00
9	G	103	TYR	C-N-CA	5.24	134.80	121.70
1	X	186	C	N1-C2-O2	5.24	122.04	118.90
1	X	488	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	846	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	1977	C	O4'-C1'-N1	5.24	112.39	108.20
2	Y	29	C	C6-N1-C2	-5.24	118.20	120.30
1	X	1083	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1683	G	N9-C1'-C2'	-5.24	106.24	112.00
1	X	1355	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	2035	G	C8-N9-C4	-5.24	104.31	106.40
1	X	2165	A	P-O3'-C3'	5.24	125.98	119.70
1	X	2321	C	N1-C2-O2	5.24	122.04	118.90
1	X	2330	G	N3-C4-C5	-5.24	125.98	128.60
1	X	2340	C	C6-N1-C2	-5.24	118.21	120.30
1	X	683	A	O4'-C1'-N9	-5.23	104.01	108.20
1	X	1312	G	C8-N9-C4	-5.23	104.31	106.40
1	X	2602	G	N3-C4-C5	-5.23	125.98	128.60
1	X	70	A	C3'-C2'-C1'	5.23	105.69	101.50
1	X	104	C	O4'-C1'-N1	5.23	112.38	108.20
1	X	572	G	C5-C6-N1	5.23	114.11	111.50
1	X	582	G	C3'-C2'-C1'	5.23	105.68	101.50
1	X	2535	C	N1-C2-O2	5.23	122.04	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	227	G	N9-C1'-C2'	5.23	120.80	114.00
1	X	1573	G	P-O3'-C3'	5.23	125.97	119.70
1	X	2246	A	C2-N3-C4	5.23	113.21	110.60
1	X	2626	U	N3-C2-O2	-5.23	118.54	122.20
1	X	148	C	O4'-C1'-N1	5.23	112.38	108.20
1	X	1563	U	N3-C2-O2	-5.23	118.54	122.20
1	X	788	G	O4'-C1'-N9	5.22	112.38	108.20
1	X	1150	C	N1-C2-O2	5.22	122.03	118.90
1	X	2326	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2432	A	C8-N9-C4	-5.22	103.71	105.80
1	X	2805	G	C8-N9-C4	-5.22	104.31	106.40
1	X	312	G	O4'-C1'-N9	5.22	112.38	108.20
1	X	1663	C	O4'-C1'-N1	5.22	112.38	108.20
1	X	2075	U	C1'-O4'-C4'	-5.22	105.72	109.90
1	X	2602	G	C5-C6-N1	5.22	114.11	111.50
1	X	689	A	C2-N3-C4	-5.22	107.99	110.60
1	X	782	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	878	C	P-O3'-C3'	5.22	125.96	119.70
1	X	1284	G	C6-C5-N7	-5.22	127.27	130.40
1	X	2632	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	2696	A	C4'-C3'-C2'	-5.22	97.38	102.60
1	X	349	G	P-O5'-C5'	5.21	129.24	120.90
1	X	1624	A	P-O3'-C3'	5.21	125.95	119.70
1	X	1663	C	O3'-P-O5'	-5.21	94.09	104.00
1	X	352	G	O4'-C1'-N9	5.21	112.37	108.20
1	X	413	G	N7-C8-N9	5.21	115.71	113.10
1	X	2550	C	P-O3'-C3'	5.21	125.95	119.70
1	X	2794	G	O5'-P-OP2	-5.21	101.01	105.70
1	X	1312	G	C6-C5-N7	-5.21	127.27	130.40
1	X	313	U	O4'-C1'-N1	5.21	112.37	108.20
1	X	2715	C	P-O5'-C5'	5.21	129.24	120.90
1	X	2843	A	C5'-C4'-C3'	-5.21	107.67	116.00
17	O	6	GLN	C-N-CA	5.21	134.72	121.70
1	X	475	U	N3-C2-O2	-5.21	118.56	122.20
1	X	967	G	O4'-C1'-N9	5.21	112.37	108.20
1	X	1064	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1271	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1549	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1824	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1284	G	C8-N9-C4	-5.21	104.32	106.40
1	X	1344	C	N1-C2-O2	5.21	122.02	118.90
1	X	2511	G	P-O5'-C5'	5.21	129.23	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2033	C	N3-C2-O2	-5.20	118.26	121.90
1	X	2326	C	P-O3'-C3'	-5.20	113.46	119.70
1	X	2671	C	P-O5'-C5'	-5.20	112.58	120.90
1	X	76	C	N1-C2-O2	5.20	122.02	118.90
1	X	1435	G	C8-N9-C4	-5.20	104.32	106.40
1	X	20	C	O4'-C1'-N1	5.20	112.36	108.20
1	X	507	A	P-O3'-C3'	-5.20	113.46	119.70
1	X	1327	C	C6-N1-C2	-5.20	118.22	120.30
1	X	1764	A	C2'-C3'-O3'	5.20	122.02	113.70
1	X	2318	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2560	G	N9-C4-C5	5.20	107.48	105.40
1	X	540	G	C4-C5-N7	-5.20	108.72	110.80
1	X	722	C	N1-C2-O2	5.20	122.02	118.90
1	X	2406	C	O4'-C1'-N1	5.19	112.36	108.20
1	X	168	A	OP1-P-O3'	5.19	116.62	105.20
1	X	1276	U	P-O3'-C3'	5.19	125.93	119.70
3	A	243	GLY	C-N-CA	5.19	134.68	121.70
1	X	682	G	C1'-O4'-C4'	-5.19	105.75	109.90
1	X	1105	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	1466	C	C2-N1-C1'	5.19	124.51	118.80
1	X	2463	G	N3-C4-C5	-5.19	126.00	128.60
1	X	831	G	C8-N9-C4	-5.19	104.33	106.40
1	X	1312	G	P-O3'-C3'	5.19	125.92	119.70
1	X	2825	A	N1-C6-N6	5.19	121.71	118.60
11	I	38	LYS	C-N-CA	5.19	134.66	121.70
1	X	2537	C	O4'-C1'-N1	5.18	112.35	108.20
1	X	34	U	P-O5'-C5'	5.18	129.19	120.90
1	X	1652	G	N1-C6-O6	5.18	123.01	119.90
1	X	430	C	C5-C6-N1	5.18	123.59	121.00
1	X	883	A	O4'-C1'-N9	5.18	112.34	108.20
2	Y	23	G	O4'-C1'-N9	5.18	112.34	108.20
1	X	1223	G	N7-C8-N9	5.18	115.69	113.10
1	X	1935	A	C2-N3-C4	5.18	113.19	110.60
1	X	7	G	C8-N9-C4	-5.18	104.33	106.40
1	X	795	A	P-O3'-C3'	5.18	125.91	119.70
1	X	2018	G	N7-C8-N9	5.18	115.69	113.10
1	X	465	C	C1'-O4'-C4'	-5.17	105.76	109.90
1	X	624	A	C2-N3-C4	5.17	113.19	110.60
1	X	951	G	C3'-C2'-C1'	-5.17	97.36	101.50
1	X	1466	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	174	A	P-O5'-C5'	5.17	129.17	120.90
1	X	597	U	C5-C4-O4	-5.17	122.80	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	765	C	N1-C2-O2	5.17	122.00	118.90
1	X	1530	U	O4'-C1'-N1	5.17	112.34	108.20
1	X	1824	C	N3-C2-O2	-5.17	118.28	121.90
1	X	2420	C	P-O5'-C5'	5.17	129.17	120.90
1	X	516	G	C4-C5-N7	5.17	112.87	110.80
1	X	652	C	C5'-C4'-C3'	-5.17	107.73	116.00
1	X	1488	G	O4'-C1'-N9	5.17	112.33	108.20
1	X	2326	C	C5-C6-N1	5.17	123.58	121.00
2	Y	92	G	C5'-C4'-O4'	5.17	115.30	109.10
1	X	7	G	C5'-C4'-C3'	-5.17	107.73	116.00
1	X	2503	G	C5-C6-O6	-5.17	125.50	128.60
1	X	956	A	O3'-P-O5'	-5.17	94.19	104.00
1	X	2854	G	C8-N9-C4	-5.17	104.33	106.40
1	X	462	G	C5-C6-N1	-5.16	108.92	111.50
1	X	540	G	N3-C4-C5	-5.16	126.02	128.60
1	X	582	G	C2-N3-C4	5.16	114.48	111.90
1	X	1000	G	O4'-C1'-C2'	-5.16	100.64	105.80
1	X	1623	C	N1-C2-O2	5.16	122.00	118.90
2	Y	14	C	C3'-C2'-C1'	5.16	105.63	101.50
1	X	545	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	1426	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2626	U	N1-C2-O2	5.16	126.41	122.80
1	X	207	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	648	A	P-O3'-C3'	5.16	125.89	119.70
1	X	1790	G	N9-C1'-C2'	5.16	120.71	114.00
1	X	2793	G	O4'-C1'-N9	5.16	112.33	108.20
1	X	780	U	O4'-C1'-N1	5.16	112.32	108.20
1	X	1010	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	811	G	P-O3'-C3'	-5.15	113.52	119.70
2	Y	45	C	N3-C2-O2	-5.15	118.29	121.90
2	Y	102	A	O4'-C1'-N9	5.15	112.32	108.20
1	X	2170	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	2825	A	P-O3'-C3'	5.15	125.88	119.70
11	I	28	LYS	C-N-CA	5.15	134.57	121.70
1	X	2776	U	O4'-C1'-N1	5.15	112.32	108.20
1	X	439	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	1138	A	P-O5'-C5'	5.15	129.13	120.90
1	X	1668	G	P-O3'-C3'	-5.15	113.53	119.70
1	X	818	G	N7-C8-N9	5.14	115.67	113.10
1	X	998	C	C5'-C4'-C3'	5.14	124.23	116.00
1	X	2264	C	P-O3'-C3'	-5.14	113.53	119.70
1	X	2478	C	C5-C6-N1	5.14	123.57	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	178	C	O4'-C1'-N1	5.14	112.31	108.20
1	X	2034	A	C5-C6-N6	-5.14	119.58	123.70
1	X	1236	G	O4'-C1'-N9	5.14	112.31	108.20
1	X	2654	A	C2-N3-C4	5.14	113.17	110.60
1	X	1714	A	O4'-C1'-N9	5.14	112.31	108.20
1	X	607	C	N3-C2-O2	-5.14	118.31	121.90
1	X	1097	A	P-O3'-C3'	5.14	125.86	119.70
1	X	2028	C	O4'-C4'-C3'	-5.14	98.86	104.00
1	X	2537	C	P-O3'-C3'	-5.14	113.54	119.70
1	X	2658	A	O4'-C1'-N9	5.14	112.31	108.20
1	X	2824	C	C2'-C3'-O3'	5.14	121.92	113.70
1	X	1930	C	N1-C2-O2	5.13	121.98	118.90
1	X	1396	C	C5-C6-N1	5.13	123.57	121.00
1	X	1219	C	O4'-C1'-N1	5.13	112.31	108.20
1	X	1268	U	P-O5'-C5'	5.13	129.11	120.90
1	X	1744	G	C6-N1-C2	-5.13	122.02	125.10
1	X	2555	G	C5-C6-N1	5.13	114.07	111.50
1	X	2828	C	O4'-C1'-N1	5.13	112.30	108.20
1	X	519	C	O4'-C1'-N1	5.13	112.30	108.20
1	X	1142	G	C5-C6-N1	5.13	114.06	111.50
1	X	1345	G	P-O3'-C3'	5.13	125.86	119.70
1	X	1876	C	N1-C2-O2	5.13	121.98	118.90
1	X	2381	A	O4'-C1'-N9	5.13	112.30	108.20
1	X	540	G	C3'-C2'-C1'	5.13	105.60	101.50
1	X	1946	U	N1-C2-O2	5.13	126.39	122.80
1	X	1681	A	C8-N9-C4	-5.12	103.75	105.80
1	X	170	U	N1-C2-O2	5.12	126.39	122.80
1	X	27	G	O4'-C1'-N9	5.12	112.30	108.20
1	X	1403	U	C3'-C2'-C1'	5.12	105.60	101.50
1	X	2229	G	C2-N3-C4	5.12	114.46	111.90
1	X	1106	A	P-O3'-C3'	5.12	125.84	119.70
1	X	2688	G	C5-C6-O6	-5.12	125.53	128.60
2	Y	67	C	P-O3'-C3'	5.12	125.84	119.70
1	X	1123	G	P-O3'-C3'	5.12	125.84	119.70
1	X	1142	G	C6-N1-C2	-5.12	122.03	125.10
1	X	2016	A	P-O3'-C3'	5.12	125.84	119.70
1	X	1407	G	C6-C5-N7	-5.12	127.33	130.40
1	X	1607	A	C3'-C2'-C1'	-5.12	97.41	101.50
1	X	1725	C	P-O5'-C5'	-5.12	112.71	120.90
1	X	2615	U	O4'-C1'-N1	5.12	112.29	108.20
2	Y	90	C	C4'-C3'-O3'	5.12	123.23	113.00
1	X	2660	C	P-O5'-C5'	5.11	129.08	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2748	C	N1-C1'-C2'	-5.11	106.37	112.00
1	X	596	C	P-O5'-C5'	-5.11	112.72	120.90
1	X	2660	C	P-O3'-C3'	5.11	125.83	119.70
1	X	499	G	C5-C6-N1	5.11	114.06	111.50
1	X	552	C	N1-C2-O2	5.11	121.97	118.90
1	X	934	G	N7-C8-N9	5.11	115.66	113.10
1	X	1666	G	C5-C6-N1	5.11	114.06	111.50
1	X	2369	U	O4'-C1'-N1	5.11	112.29	108.20
1	X	2606	G	C5'-C4'-O4'	5.11	115.23	109.10
1	X	236	C	C5-C6-N1	5.11	123.55	121.00
1	X	247	A	C5'-C4'-O4'	5.11	115.23	109.10
1	X	1337	G	P-O5'-C5'	5.11	129.07	120.90
1	X	1540	C	O4'-C1'-N1	5.11	112.28	108.20
1	X	1663	C	C2-N1-C1'	5.10	124.41	118.80
1	X	2667	C	P-O3'-C3'	5.10	125.82	119.70
1	X	1010	U	P-O5'-C5'	5.10	129.06	120.90
1	X	1097	A	O4'-C1'-N9	5.10	112.28	108.20
1	X	2032	G	C5-C6-N1	5.10	114.05	111.50
1	X	480	G	C3'-C2'-C1'	-5.10	97.42	101.50
1	X	688	A	P-O3'-C3'	5.10	125.82	119.70
1	X	333	A	O4'-C1'-N9	5.10	112.28	108.20
1	X	854	G	C3'-C2'-C1'	-5.10	97.42	101.50
1	X	2526	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	2826	C	N1-C2-O2	5.10	121.96	118.90
2	Y	19	C	N3-C2-O2	-5.10	118.33	121.90
1	X	402	A	P-O3'-C3'	-5.09	113.59	119.70
1	X	459	A	C2-N3-C4	5.09	113.15	110.60
1	X	616	U	O4'-C1'-N1	5.09	112.28	108.20
1	X	996	C	N3-C2-O2	-5.09	118.33	121.90
1	X	1254	G	N3-C4-C5	-5.09	126.05	128.60
1	X	1337	G	O5'-P-OP2	-5.09	101.11	105.70
1	X	98	U	N3-C2-O2	-5.09	118.64	122.20
1	X	542	A	N7-C8-N9	5.09	116.35	113.80
1	X	1198	C	O4'-C1'-N1	5.09	112.27	108.20
1	X	1648	C	N1-C2-O2	5.09	121.95	118.90
1	X	1870	U	O4'-C1'-N1	5.09	112.27	108.20
1	X	2774	U	P-O3'-C3'	5.09	125.81	119.70
1	X	2195	C	O4'-C1'-N1	5.08	112.27	108.20
1	X	2702	G	O4'-C1'-N9	-5.08	104.13	108.20
1	X	179	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	540	G	C2-N3-C4	5.08	114.44	111.90
1	X	757	U	OP2-P-O3'	5.08	116.39	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2015	G	C5-N7-C8	-5.08	101.76	104.30
2	Y	100	G	O4'-C1'-N9	5.08	112.27	108.20
1	X	1015	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	1321	A	C3'-C2'-C1'	-5.08	97.43	101.50
1	X	1801	C	N1-C2-O2	5.08	121.95	118.90
2	Y	53	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	1497	C	O4'-C1'-N1	5.08	112.26	108.20
1	X	516	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	625	A	P-O3'-C3'	5.08	125.79	119.70
1	X	1248	G	O4'-C1'-N9	-5.08	104.14	108.20
1	X	1266	G	P-O3'-C3'	5.07	125.79	119.70
1	X	1882	G	C8-N9-C4	-5.07	104.37	106.40
1	X	2727	G	O4'-C1'-N9	5.07	112.26	108.20
2	Y	94	G	C5'-C4'-O4'	5.07	115.19	109.10
1	X	227	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1863	U	O4'-C1'-N1	5.07	112.26	108.20
1	X	985	G	C5-C6-N1	5.07	114.03	111.50
1	X	1384	G	P-O3'-C3'	5.07	125.78	119.70
1	X	2848	A	O4'-C1'-N9	5.07	112.26	108.20
1	X	2588	U	C5'-C4'-O4'	5.07	115.18	109.10
1	X	358	C	P-O5'-C5'	5.07	129.01	120.90
1	X	807	A	O4'-C1'-N9	5.07	112.25	108.20
1	X	934	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1766	U	P-O3'-C3'	5.07	125.78	119.70
1	X	1922	U	N3-C2-O2	-5.07	118.65	122.20
1	X	2261	G	C4'-C3'-C2'	5.07	107.67	102.60
1	X	2452	U	N3-C2-O2	-5.07	118.65	122.20
1	X	16	G	N3-C4-N9	5.06	129.04	126.00
2	Y	123	U	C6-N1-C1'	-5.06	114.11	121.20
1	X	22	C	P-O3'-C3'	5.06	125.78	119.70
1	X	1037	U	C1'-O4'-C4'	-5.06	105.85	109.90
1	X	1625	A	P-O3'-C3'	5.06	125.78	119.70
1	X	1690	U	P-O5'-C5'	-5.06	112.80	120.90
1	X	2000	U	N3-C4-O4	5.06	122.94	119.40
1	X	2264	C	C3'-C2'-C1'	-5.06	97.45	101.50
1	X	2442	C	N1-C2-O2	5.06	121.94	118.90
1	X	2213	G	C8-N9-C4	-5.06	104.38	106.40
1	X	2718	A	C5'-C4'-O4'	5.06	115.17	109.10
1	X	93	A	O4'-C1'-N9	5.06	112.25	108.20
1	X	569	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	2568	A	O4'-C4'-C3'	-5.06	98.94	104.00
1	X	672	C	C3'-C2'-C1'	-5.06	97.45	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2210	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	1152	C	P-O5'-C5'	5.06	128.99	120.90
1	X	940	G	C8-N9-C4	-5.05	104.38	106.40
1	X	1608	U	P-O3'-C3'	5.05	125.77	119.70
1	X	1971	C	P-O5'-C5'	-5.05	112.81	120.90
1	X	2314	A	O4'-C1'-N9	5.05	112.24	108.20
2	Y	86	A	C5'-C4'-O4'	5.05	115.17	109.10
1	X	1965	U	C5'-C4'-C3'	-5.05	107.92	116.00
1	X	2592	U	C5'-C4'-O4'	5.05	115.16	109.10
1	X	2824	C	N1-C1'-C2'	5.05	120.57	114.00
1	X	354	C	O4'-C1'-N1	5.05	112.24	108.20
1	X	1383	C	O4'-C1'-N1	5.05	112.24	108.20
1	X	1481	U	O4'-C1'-N1	5.05	112.24	108.20
1	X	1975	G	C3'-C2'-C1'	5.05	105.54	101.50
1	X	184	A	N1-C6-N6	-5.05	115.57	118.60
1	X	998	C	C4'-C3'-C2'	-5.05	97.55	102.60
1	X	860	U	C2-N1-C1'	5.05	123.75	117.70
1	X	2468	G	C2-N3-C4	5.05	114.42	111.90
1	X	869	C	C6-N1-C2	-5.04	118.28	120.30
1	X	916	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	940	G	P-O3'-C3'	5.04	125.75	119.70
1	X	1132	C	C5-C6-N1	5.04	123.52	121.00
1	X	1619	A	P-O3'-C3'	5.04	125.75	119.70
1	X	2527	G	P-O5'-C5'	-5.04	112.83	120.90
1	X	42	G	O4'-C1'-N9	5.04	112.23	108.20
1	X	332	C	C1'-O4'-C4'	-5.04	105.87	109.90
1	X	570	G	P-O3'-C3'	5.04	125.75	119.70
1	X	598	U	O4'-C4'-C3'	-5.04	98.96	104.00
1	X	1219	C	C6-N1-C2	-5.04	118.28	120.30
1	X	1337	G	C4'-C3'-C2'	5.04	107.64	102.60
1	X	1909	U	P-O3'-C3'	5.04	125.75	119.70
1	X	1496	G	C4'-C3'-O3'	5.04	123.08	113.00
1	X	670	U	N1-C2-O2	5.04	126.33	122.80
1	X	1162	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	X	2620	G	P-O3'-C3'	5.04	125.75	119.70
1	X	1825	C	C6-N1-C2	-5.04	118.28	120.30
1	X	1881	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	1973	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1470	G	C5-C6-O6	-5.04	125.58	128.60
1	X	1689	U	N3-C2-O2	-5.04	118.68	122.20
1	X	2311	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	2702	G	C5-N7-C8	-5.04	101.78	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2831	A	C2-N3-C4	5.04	113.12	110.60
3	A	203	ASN	CB-CA-C	5.04	120.47	110.40
1	X	615	C	O4'-C1'-N1	5.03	112.23	108.20
1	X	689	A	C4-C5-N7	5.03	113.22	110.70
1	X	2527	G	N3-C4-C5	-5.03	126.08	128.60
2	Y	119	G	O4'-C1'-N9	5.03	112.23	108.20
1	X	684	C	C4-C5-C6	5.03	119.92	117.40
1	X	2340	C	O4'-C1'-N1	5.03	112.23	108.20
1	X	303	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	636	G	C5'-C4'-C3'	-5.03	107.95	116.00
1	X	2038	C	P-O3'-C3'	5.03	125.74	119.70
1	X	2340	C	C5-C6-N1	5.03	123.52	121.00
1	X	1663	C	C3'-C2'-C1'	5.03	105.52	101.50
1	X	11	G	N7-C8-N9	5.03	115.61	113.10
1	X	311	A	O4'-C1'-N9	5.03	112.22	108.20
1	X	1010	U	N3-C2-O2	-5.03	118.68	122.20
1	X	1122	A	O4'-C1'-N9	5.03	112.22	108.20
1	X	1570	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	2015	G	C5-C6-N1	5.03	114.01	111.50
1	X	2635	U	N3-C2-O2	-5.03	118.68	122.20
1	X	2780	A	P-O5'-C5'	5.03	128.94	120.90
1	X	518	A	P-O5'-C5'	5.02	128.94	120.90
1	X	1731	C	C3'-C2'-C1'	-5.02	97.48	101.50
1	X	2062	U	O4'-C1'-N1	5.02	112.22	108.20
2	Y	77	G	P-O5'-C5'	5.02	128.94	120.90
1	X	2254	C	N1-C2-O2	5.02	121.91	118.90
1	X	2740	C	N1-C2-O2	5.02	121.91	118.90
1	X	677	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	2582	G	C6-C5-N7	-5.02	127.39	130.40
1	X	622	U	O4'-C1'-N1	5.02	112.22	108.20
1	X	661	C	N3-C2-O2	-5.02	118.39	121.90
1	X	978	U	O4'-C1'-N1	5.02	112.22	108.20
1	X	834	A	P-O3'-C3'	-5.02	113.68	119.70
1	X	1128	G	P-O5'-C5'	5.02	128.93	120.90
1	X	1679	U	N3-C2-O2	-5.02	118.69	122.20
1	X	2619	G	N1-C6-O6	5.02	122.91	119.90
1	X	416	U	C1'-O4'-C4'	-5.02	105.89	109.90
1	X	863	C	C6-N1-C2	-5.02	118.29	120.30
1	X	1785	A	P-O5'-C5'	-5.02	112.87	120.90
1	X	1429	A	O4'-C1'-N9	5.01	112.21	108.20
1	X	1603	A	P-O3'-C3'	5.01	125.72	119.70
1	X	534	U	P-O5'-C5'	5.01	128.92	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	941	U	C4'-C3'-C2'	-5.01	97.59	102.60
1	X	1661	C	N1-C2-O2	5.01	121.91	118.90
1	X	1932	G	O4'-C1'-N9	5.01	112.21	108.20
1	X	216	U	N3-C2-O2	-5.01	118.69	122.20
1	X	1533	G	N7-C8-N9	5.01	115.60	113.10
1	X	1886	G	C8-N9-C4	-5.01	104.40	106.40
2	Y	12	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	19	C	P-O3'-C3'	-5.01	113.69	119.70
1	X	581	A	O3'-P-O5'	-5.01	94.49	104.00
1	X	1652	G	N3-C4-N9	5.01	129.00	126.00
1	X	349	G	O4'-C1'-N9	5.00	112.20	108.20
1	X	631	G	C1'-O4'-C4'	-5.00	105.90	109.90
1	X	2487	G	C8-N9-C4	-5.00	104.40	106.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1251	G	Sidechain
1	X	699	G	Sidechain
1	X	967	G	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	535	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	83	0
4	B	1539	0	1600	57	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	17	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	997	0	1046	30	0
11	I	1067	0	1103	39	0
12	J	1090	0	1125	31	0
13	K	878	0	930	24	0
14	L	779	0	820	19	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	23	0
19	Q	726	0	753	11	0
20	R	825	0	881	26	0
21	S	1345	0	1372	30	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	15	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1080	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (1080) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.38	1.03
1:X:558:G:H4'	1:X:559:C:H5'	1.40	1.02
1:X:1448:A:H61	1:X:1574:A:H61	1.09	1.00
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.46	0.96
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.49	0.95
1:X:1542:G:H22	1:X:1562:G:H1	1.13	0.94
1:X:1007:A:H4'	16:N:93:LYS:HB3	1.46	0.94
1:X:1919:A:H2	1:X:1926:U:H3	1.09	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.31	0.93
11:I:62:LYS:HE2	11:I:64:GLY:HA3	1.53	0.91
32:X:2929:1F4:H59	32:X:2929:1F4:H60	1.51	0.90
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.07	0.89
1:X:77:C:H42	1:X:106:G:H1	1.21	0.88
15:M:79:ARG:HH11	15:M:79:ARG:HG3	1.36	0.88
1:X:1770:U:H5	1:X:1775:A:N7	1.70	0.88
14:L:38:ILE:HG13	14:L:39:TYR:H	1.39	0.88
4:B:116:VAL:HG22	4:B:136:ARG:NE	1.88	0.87
21:S:71:MET:HA	21:S:78:PRO:HA	1.58	0.85
4:B:131:SER:HB3	4:B:134:TRP:CD1	2.11	0.85
3:A:252:LYS:HD2	3:A:253:PRO:HD3	1.59	0.84
1:X:1817:U:H4'	3:A:252:LYS:HE2	1.59	0.83
1:X:1266:G:N7	11:I:32:ARG:NH1	2.25	0.83
13:K:10:LEU:HD21	13:K:17:ARG:HB2	1.61	0.82
3:A:248:THR:HB	3:A:249:PRO:HD3	1.60	0.82
1:X:2371:A:H2	1:X:2403:C:H42	1.28	0.82
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.62	0.82
1:X:38:G:H1	1:X:453:U:H3	1.25	0.81
1:X:1278:A:H2	1:X:1997:A:H62	1.26	0.80
9:G:33:ILE:HB	9:G:34:PRO:CD	2.11	0.80
1:X:2387:U:H2'	1:X:2388:G:H8	1.45	0.80
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.47	0.79
1:X:1342:U:H5''	1:X:1343:C:H5	1.48	0.78
1:X:559:C:H2'	1:X:560:G:O4'	1.84	0.78
3:A:43:ARG:HD2	3:A:43:ARG:N	1.99	0.78
32:X:2929:1F4:H3	32:X:2929:1F4:C39	2.13	0.78
1:X:823:U:OP1	11:I:32:ARG:NH1	2.17	0.78
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.66	0.78
16:N:66:ASN:HB3	16:N:76:TYR:H	1.50	0.77
1:X:640:C:H4'	1:X:660:G:H21	1.49	0.77
15:M:59:GLY:HA3	15:M:64:LYS:HA	1.65	0.77
3:A:172:TYR:HA	3:A:186:HIS:HA	1.66	0.76
1:X:224:G:OP2	1:X:226:C:N4	2.17	0.76
5:C:29:GLU:HB2	11:I:18:ARG:HH12	1.50	0.76
1:X:673:G:H5'	5:C:93:TYR:CE1	2.20	0.76
14:L:33:ARG:HD2	14:L:38:ILE:HD13	1.66	0.76
1:X:689:A:H8	1:X:2052:G:H21	1.33	0.76
26:Z:35:GLN:O	26:Z:37:HIS:N	2.19	0.76
21:S:6:LYS:H	21:S:7:PRO:HD3	1.48	0.75
1:X:1007:A:H1'	17:O:6:GLN:HG2	1.67	0.75
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:K:10:LEU:CD2	13:K:17:ARG:HB2	2.15	0.75
4:B:134:TRP:H	4:B:134:TRP:HD1	1.32	0.75
15:M:79:ARG:HH11	15:M:79:ARG:CG	2.00	0.75
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.52	0.75
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.70	0.73
25:W:12:ARG:HH11	25:W:12:ARG:HG2	1.52	0.73
1:X:1919:A:H2	1:X:1926:U:N3	1.84	0.73
1:X:1329:U:H2'	1:X:1330:G:H8	1.52	0.73
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.70	0.73
1:X:652:C:H42	1:X:657:A:H61	1.35	0.73
15:M:79:ARG:HG3	15:M:79:ARG:NH1	2.02	0.73
9:G:100:TYR:HB2	9:G:116:ARG:HH12	1.51	0.72
17:O:57:GLN:H	17:O:97:GLY:HA3	1.53	0.72
1:X:2387:U:H2'	1:X:2388:G:C8	2.23	0.72
11:I:62:LYS:CE	11:I:64:GLY:HA3	2.19	0.72
1:X:1329:U:H2'	1:X:1330:G:C8	2.25	0.72
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.20	0.71
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.70	0.71
11:I:62:LYS:HE2	11:I:64:GLY:CA	2.20	0.71
1:X:2241:U:H5	22:T:17:ASN:OD1	1.72	0.71
1:X:617:U:H5	1:X:632:A:H2	1.38	0.70
3:A:231:HIS:HD2	3:A:233:HIS:H	1.38	0.70
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.73	0.70
1:X:617:U:C5	1:X:632:A:C2	2.80	0.70
1:X:1673:C:H2'	1:X:1674:C:H6	1.55	0.70
3:A:243:GLY:C	3:A:244:ARG:HD3	2.11	0.70
4:B:110:GLY:O	13:K:3:HIS:CD2	2.45	0.70
1:X:2039:G:N2	26:Z:4:HIS:O	2.22	0.69
4:B:14:ILE:HG22	4:B:21:ILE:HB	1.74	0.69
1:X:1561:A:H3'	1:X:1562:G:C8	2.27	0.69
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.73	0.69
23:U:48:LYS:CG	23:U:49:LYS:H	2.04	0.69
1:X:1832:G:H1	1:X:1885:C:H42	1.37	0.69
1:X:2063:A:H4'	23:U:39:LYS:HG2	1.73	0.69
3:A:231:HIS:CD2	3:A:233:HIS:H	2.11	0.69
14:L:33:ARG:NH1	14:L:38:ILE:HB	2.08	0.68
1:X:1466:C:H2'	1:X:1467:U:O4'	1.93	0.68
1:X:1278:A:N6	1:X:1996:A:H5''	2.08	0.68
1:X:501:G:H2'	1:X:502:A:C8	2.28	0.68
1:X:577:U:H2'	1:X:579:G:OP2	1.94	0.68
1:X:2770:A:H4'	1:X:2771:C:H5'	1.74	0.67
9:G:61:ARG:NH1	9:G:66:HIS:H	1.90	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1882:G:N2	1:X:1885:C:H41	1.92	0.67
1:X:1278:A:H61	1:X:1996:A:H5''	1.60	0.67
25:W:12:ARG:CG	25:W:12:ARG:HH11	2.06	0.67
1:X:2767:C:H1'	4:B:62:PRO:HG3	1.77	0.67
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.30	0.67
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.76	0.67
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.27	0.67
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.76	0.67
9:G:104:THR:OG1	9:G:110:LEU:HB3	1.95	0.67
3:A:43:ARG:HE	3:A:55:GLY:HA2	1.60	0.67
20:R:7:GLY:HA3	20:R:42:ARG:O	1.94	0.67
1:X:1885:C:C4'	3:A:244:ARG:HD2	2.24	0.66
1:X:168:A:H2'	1:X:169:C:C6	2.30	0.66
1:X:341:A:HO2'	1:X:342:G:H8	1.41	0.66
32:X:2929:1F4:H3	32:X:2929:1F4:H51	1.76	0.66
1:X:1342:U:H5''	1:X:1343:C:C5	2.31	0.66
32:X:2929:1F4:C50	32:X:2929:1F4:H60	2.23	0.66
1:X:617:U:H5	1:X:632:A:C2	2.14	0.66
12:J:15:ARG:HD2	12:J:74:PRO:HD2	1.77	0.66
25:W:4:LYS:HG2	25:W:52:GLU:HB3	1.78	0.65
1:X:1673:C:C5'	4:B:136:ARG:HD3	2.26	0.65
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.10	0.65
4:B:194:GLY:HA2	15:M:2:GLN:HB3	1.77	0.65
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.78	0.65
1:X:2266:A:H62	1:X:2323:U:H3	1.43	0.65
1:X:2551:A:N7	4:B:145:LYS:HB2	2.10	0.65
1:X:320:A:N3	1:X:340:G:O2'	2.29	0.65
1:X:1811:A:H5''	3:A:161:THR:HG21	1.78	0.65
1:X:1673:C:H2'	1:X:1674:C:C6	2.31	0.64
1:X:797:A:C5	3:A:229:VAL:HG21	2.31	0.64
11:I:17:LYS:O	11:I:18:ARG:HB2	1.97	0.64
20:R:25:LEU:H	20:R:80:LYS:HA	1.62	0.64
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.78	0.64
12:J:48:ILE:HD12	12:J:71:PRO:HG3	1.80	0.64
5:C:48:ARG:C	5:C:50:GLN:H	2.00	0.64
1:X:1744:G:OP1	15:M:100:ARG:HD2	1.97	0.64
16:N:66:ASN:HB2	16:N:70:ARG:NH1	2.13	0.64
1:X:1609:G:H2'	1:X:1610:A:C8	2.32	0.64
12:J:28:VAL:HG23	12:J:137:VAL:HB	1.80	0.64
1:X:482:A:H2'	1:X:483:A:O4'	1.96	0.64
1:X:742:G:C6	3:A:208:LYS:HB3	2.33	0.64
12:J:28:VAL:HG12	12:J:29:ALA:H	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.31	0.63
1:X:1745:C:P	15:M:101:ARG:HH22	2.20	0.63
1:X:841:G:H2'	1:X:842:A:C8	2.33	0.63
1:X:764:A:H5'	18:P:111:ARG:HA	1.79	0.63
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.32	0.63
1:X:800:U:H5''	1:X:801:A:H5'	1.81	0.63
1:X:1674:C:H2'	1:X:1675:C:C6	2.34	0.63
1:X:451:A:H2'	1:X:452:G:C8	2.34	0.62
15:M:60:SER:HB3	15:M:63:ARG:HH22	1.64	0.62
3:A:67:PHE:HB3	3:A:153:ALA:H	1.64	0.62
18:P:32:ARG:HA	18:P:121:THR:HG22	1.81	0.62
4:B:152:LYS:H	9:G:106:TYR:HB3	1.64	0.62
11:I:108:LEU:HD23	11:I:129:ALA:HB1	1.82	0.62
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.81	0.62
4:B:152:LYS:HB2	9:G:106:TYR:CB	2.27	0.62
23:U:32:ARG:HG2	23:U:33:LYS:N	2.13	0.62
21:S:3:LEU:HD11	21:S:56:VAL:HG13	1.80	0.62
1:X:797:A:N7	3:A:229:VAL:HG21	2.15	0.62
6:D:143:TYR:HA	6:D:146:VAL:HG22	1.82	0.62
24:V:28:LEU:HD12	24:V:43:VAL:HG22	1.81	0.62
1:X:1753:A:O5'	1:X:1753:A:H8	1.82	0.61
13:K:3:HIS:HB3	13:K:5:LYS:HD2	1.81	0.61
11:I:28:LYS:NZ	11:I:36:GLY:HA2	2.16	0.61
10:H:124:MET:O	10:H:127:VAL:HG12	2.00	0.61
2:Y:28:A:H8	2:Y:29:C:C5	2.17	0.61
1:X:670:U:H2'	1:X:671:A:C8	2.35	0.61
23:U:51:ILE:HA	23:U:59:THR:O	2.01	0.61
1:X:2083:G:H1	1:X:2172:U:H3	1.48	0.61
1:X:746:G:N7	1:X:774:A:C6	2.69	0.61
25:W:7:ARG:HB2	25:W:50:LEU:HA	1.82	0.61
1:X:341:A:O2'	1:X:342:G:H8	1.83	0.61
1:X:564:U:H2'	1:X:565:A:C8	2.36	0.61
1:X:1574:A:O2'	1:X:1575:C:H3'	2.00	0.61
1:X:226:C:OP2	1:X:2373:C:O2'	2.19	0.60
1:X:450:C:H2'	1:X:451:A:C8	2.35	0.60
23:U:52:ARG:NE	23:U:79:GLU:HA	2.16	0.60
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.33	0.60
15:M:17:GLU:O	15:M:21:THR:OG1	2.17	0.60
1:X:1437:A:H2'	1:X:1438:G:H8	1.64	0.60
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.83	0.60
3:A:223:GLY:HA2	3:A:226:MET:SD	2.40	0.60
1:X:512:A:H4'	18:P:15:LYS:HB3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:47:THR:HA	5:C:82:VAL:HB	1.83	0.60
12:J:62:GLY:HA3	12:J:64:LYS:HE3	1.84	0.60
1:X:2543:A:H5'	1:X:2627:G:H4'	1.82	0.60
1:X:960:U:H2'	1:X:961:G:C8	2.37	0.60
5:C:176:ASN:HD22	5:C:179:ASP:H	1.48	0.60
1:X:504:G:H4'	18:P:27:VAL:HG12	1.84	0.60
1:X:412:U:H5''	23:U:68:ARG:HH22	1.67	0.60
1:X:168:A:H2'	1:X:169:C:H6	1.67	0.59
1:X:2484:G:H22	32:X:2929:1F4:H56	1.67	0.59
5:C:34:GLN:HB3	5:C:38:ARG:HH11	1.66	0.59
5:C:54:THR:HG21	5:C:72:ARG:HB3	1.84	0.59
1:X:954:U:OP2	11:I:38:LYS:HG2	2.01	0.59
1:X:2528:G:H2'	1:X:2529:G:H8	1.66	0.59
1:X:38:G:H21	5:C:42:THR:HG21	1.66	0.59
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.85	0.59
1:X:530:G:H2'	1:X:531:G:C8	2.37	0.59
1:X:1782:A:N6	1:X:1820:G:O2'	2.35	0.59
16:N:66:ASN:HB2	16:N:70:ARG:HH11	1.67	0.59
18:P:27:VAL:HG23	18:P:125:THR:HG22	1.85	0.59
20:R:45:LYS:HA	20:R:76:LEU:O	2.02	0.59
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.84	0.59
21:S:93:GLU:HB3	21:S:121:GLN:HG3	1.83	0.59
1:X:187:U:H2'	1:X:188:G:C8	2.37	0.59
10:H:78:SER:HA	10:H:91:PHE:O	2.03	0.59
1:X:1885:C:H4'	3:A:244:ARG:HD2	1.83	0.58
22:T:45:PHE:HD2	22:T:77:ARG:HB3	1.67	0.58
17:O:36:LYS:HE2	17:O:56:VAL:HG22	1.85	0.58
3:A:252:LYS:CD	3:A:253:PRO:HD3	2.32	0.58
16:N:66:ASN:CB	16:N:76:TYR:H	2.17	0.58
1:X:689:A:H2	1:X:815:A:H61	1.51	0.58
1:X:165:G:H2'	1:X:166:G:O4'	2.04	0.58
1:X:501:G:H2'	1:X:502:A:H8	1.65	0.58
5:C:38:ARG:HH12	5:C:176:ASN:HD21	1.51	0.58
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.86	0.58
1:X:2504:G:H21	30:4:1:MET:HE2	1.67	0.58
4:B:4:ILE:HG22	4:B:96:PHE:HE1	1.67	0.58
15:M:82:PRO:HG2	15:M:85:SER:HB2	1.85	0.58
1:X:1030:U:HO2'	1:X:1032:A:H2	1.50	0.58
1:X:1999:U:O2'	26:Z:7:PRO:O	2.21	0.58
1:X:553:C:H42	1:X:559:C:H42	1.49	0.58
1:X:1656:U:H4'	1:X:2678:C:H4'	1.84	0.58
1:X:742:G:H2'	1:X:1766:U:H1'	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1584:G:N3	3:A:58:HIS:CE1	2.72	0.58
1:X:405:C:H2'	1:X:406:G:H8	1.69	0.58
4:B:26:VAL:HG11	4:B:198:LEU:HD11	1.85	0.58
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.83	0.58
1:X:1505:U:HO2'	1:X:1506:C:H6	1.51	0.58
1:X:1468:A:H5'	1:X:1472:C:N4	2.19	0.57
1:X:114:C:O2'	1:X:124:A:N3	2.37	0.57
23:U:48:LYS:HG2	23:U:49:LYS:H	1.68	0.57
20:R:48:VAL:HG12	20:R:50:GLY:H	1.69	0.57
1:X:1071:U:H4'	1:X:1072:U:H3'	1.85	0.57
5:C:58:MET:HB2	5:C:70:GLY:O	2.04	0.57
5:C:119:ALA:H	5:C:189:ASP:HA	1.69	0.57
1:X:482:A:O5'	1:X:482:A:H8	1.88	0.57
1:X:1040:A:H5''	12:J:129:GLN:HE22	1.69	0.57
23:U:56:GLN:HE21	23:U:57:VAL:HG23	1.70	0.57
25:W:12:ARG:HG3	25:W:50:LEU:HD21	1.85	0.57
23:U:48:LYS:CG	23:U:49:LYS:N	2.68	0.57
1:X:1437:A:H2'	1:X:1438:G:C8	2.40	0.57
12:J:25:GLY:HA3	12:J:102:ARG:HA	1.87	0.57
7:E:127:GLU:HG3	7:E:130:ARG:HB2	1.87	0.57
1:X:712:A:H2'	1:X:713:G:O4'	2.05	0.57
5:C:43:ALA:CB	5:C:86:PRO:HB2	2.29	0.57
10:H:13:ASN:HD21	10:H:109:ARG:HG2	1.70	0.57
1:X:2081:U:H3	1:X:2174:G:H1	1.53	0.57
1:X:1845:A:H2'	1:X:1846:A:C8	2.40	0.56
19:Q:68:PHE:O	19:Q:70:GLY:N	2.38	0.56
1:X:1699:A:H61	1:X:1723:U:H3	1.51	0.56
1:X:1787:U:H2'	1:X:1788:C:C6	2.41	0.56
1:X:829:C:H2'	1:X:830:C:C6	2.40	0.56
3:A:36:ALA:HB1	3:A:62:TYR:O	2.04	0.56
1:X:1982:C:H5''	1:X:2703:C:O2'	2.05	0.56
1:X:1033:G:H22	1:X:1153:A:H2	1.53	0.56
1:X:559:C:H2'	1:X:560:G:C1'	2.35	0.56
14:L:27:LEU:HD23	14:L:44:ASP:HA	1.87	0.56
23:U:14:VAL:O	23:U:15:VAL:HG22	2.06	0.56
1:X:1173:G:H4'	17:O:22:VAL:HG23	1.86	0.56
1:X:530:G:H2'	1:X:531:G:H8	1.69	0.56
5:C:149:LEU:HD11	5:C:170:LEU:HD13	1.87	0.56
1:X:1268:U:C2	5:C:66:ASN:HA	2.41	0.56
1:X:215:G:H21	1:X:632:A:H8	1.52	0.56
13:K:3:HIS:CE1	13:K:5:LYS:HZ2	2.23	0.56
20:R:22:VAL:HG11	20:R:80:LYS:HD2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2653:A:H2'	10:H:41:ASN:ND2	2.21	0.56
1:X:2266:A:N6	1:X:2323:U:H3	2.04	0.56
1:X:1348:C:H2'	1:X:1349:A:C8	2.40	0.56
32:X:2929:1F4:O18	32:X:2929:1F4:H9	2.06	0.55
11:I:97:ARG:O	11:I:98:LEU:HB2	2.06	0.55
1:X:2516:U:H2'	1:X:2517:C:C6	2.40	0.55
16:N:66:ASN:HB3	16:N:76:TYR:CB	2.35	0.55
1:X:187:U:H2'	1:X:188:G:H8	1.70	0.55
1:X:1468:A:H5'	1:X:1472:C:H41	1.71	0.55
1:X:1454:U:H2'	1:X:1455:C:C6	2.41	0.55
3:A:38:PRO:HA	3:A:61:LEU:HD23	1.88	0.55
1:X:1770:U:C5	1:X:1775:A:N7	2.62	0.55
1:X:1882:G:H21	1:X:1885:C:H41	1.53	0.55
1:X:1348:C:H2'	1:X:1349:A:H8	1.71	0.55
1:X:1948:C:H5''	1:X:1949:A:H2'	1.89	0.55
20:R:52:ASN:HD21	20:R:71:GLN:HE21	1.55	0.55
1:X:2212:U:H2'	1:X:2213:G:C8	2.41	0.55
1:X:1595:A:H2'	1:X:1596:A:O4'	2.07	0.55
16:N:84:LYS:HG3	16:N:92:ARG:HH22	1.70	0.55
22:T:41:ARG:HA	22:T:41:ARG:HE	1.72	0.55
6:D:104:ILE:HA	6:D:108:LEU:HD12	1.88	0.55
1:X:559:C:C2'	1:X:560:G:O4'	2.54	0.54
9:G:106:TYR:O	9:G:110:LEU:HG	2.06	0.54
1:X:774:A:H8	1:X:774:A:O5'	1.90	0.54
5:C:136:TRP:O	5:C:140:ASN:ND2	2.40	0.54
18:P:97:VAL:HG22	18:P:124:ILE:HG23	1.87	0.54
1:X:2484:G:N2	32:X:2929:1F4:H56	2.22	0.54
1:X:1032:A:H3'	1:X:1032:A:C8	2.42	0.54
16:N:37:GLN:HA	16:N:40:LEU:HD12	1.90	0.54
1:X:75:C:H5''	24:V:48:ARG:HG3	1.89	0.54
1:X:1135:C:H2'	1:X:1136:G:O4'	2.06	0.54
1:X:333:A:H2'	5:C:162:ARG:HH12	1.72	0.54
1:X:1264:C:OP1	16:N:10:ARG:HG3	2.08	0.54
1:X:2659:C:H5'	4:B:189:PRO:HA	1.90	0.54
32:X:2929:1F4:C54	32:X:2929:1F4:H18	2.38	0.54
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.90	0.54
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.90	0.54
3:A:60:ARG:HD3	3:A:86:PRO:O	2.06	0.54
1:X:219:G:N2	1:X:231:G:H2'	2.22	0.54
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.90	0.54
1:X:2196:U:H5'	1:X:2197:U:OP2	2.08	0.54
9:G:67:ARG:CG	9:G:70:PHE:HA	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:356:A:H2'	1:X:357:A:C8	2.43	0.54
1:X:29:U:H5''	16:N:7:GLY:HA2	1.90	0.54
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.90	0.54
1:X:2627:G:H2'	1:X:2628:C:O4'	2.08	0.54
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.91	0.53
32:X:2929:1F4:C39	32:X:2929:1F4:H9	2.38	0.53
1:X:760:U:O2	1:X:1997:A:H1'	2.08	0.53
10:H:77:THR:HA	10:H:94:ASN:HB3	1.89	0.53
21:S:123:VAL:HG23	21:S:161:ALA:HB2	1.90	0.53
16:N:6:THR:O	16:N:9:VAL:HG23	2.08	0.53
1:X:171:G:H2'	1:X:172:A:O4'	2.08	0.53
1:X:2482:A:H4'	1:X:2483:U:OP1	2.08	0.53
1:X:1134:C:H2'	1:X:1135:C:H6	1.74	0.53
15:M:29:PRO:HB2	15:M:99:VAL:HG21	1.90	0.53
3:A:182:LEU:HD12	3:A:269:PHE:HB2	1.90	0.53
13:K:87:TYR:CE1	13:K:94:TYR:HD2	2.27	0.53
1:X:2459:C:H2'	1:X:2459:C:O2	2.08	0.53
21:S:95:SER:HB3	21:S:119:ASN:HD22	1.74	0.53
1:X:1673:C:H5'	4:B:136:ARG:HD3	1.91	0.53
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.44	0.53
1:X:1223:G:H5'	1:X:1225:G:O4'	2.08	0.53
14:L:38:ILE:HG13	14:L:39:TYR:N	2.17	0.53
21:S:6:LYS:N	21:S:7:PRO:HD3	2.20	0.53
5:C:48:ARG:C	5:C:50:GLN:N	2.61	0.53
10:H:83:ARG:CZ	10:H:89:ILE:HD11	2.38	0.53
1:X:1076:U:H3	1:X:1080:A:H2'	1.74	0.53
20:R:26:SER:H	20:R:30:LYS:HG3	1.73	0.53
1:X:732:G:H2'	1:X:733:G:C8	2.43	0.53
2:Y:9:G:H1	2:Y:116:C:H42	1.56	0.53
4:B:5:LEU:HG	4:B:195:LEU:HD11	1.91	0.53
18:P:62:ARG:HE	26:Z:25:LEU:HD11	1.74	0.53
1:X:761:G:OP2	18:P:109:ARG:HG3	2.08	0.53
1:X:555:U:H5'	1:X:556:A:C8	2.43	0.53
11:I:102:LYS:O	11:I:104:ARG:N	2.35	0.53
1:X:2041:A:H61	32:X:2929:1F4:H46	1.73	0.53
23:U:32:ARG:HG2	23:U:33:LYS:H	1.72	0.53
1:X:633:G:H2'	1:X:634:G:H8	1.73	0.53
9:G:105:GLY:O	9:G:106:TYR:C	2.46	0.52
1:X:577:U:H5''	1:X:956:A:N6	2.23	0.52
1:X:1468:A:O5'	1:X:1468:A:C8	2.62	0.52
25:W:3:ILE:HG23	25:W:51:LEU:HD22	1.92	0.52
1:X:2270:U:H2'	1:X:2271:C:C6	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2225:G:H2'	1:X:2226:A:C8	2.43	0.52
1:X:1287:A:H2'	1:X:1288:A:H5''	1.91	0.52
3:A:45:ASN:CG	3:A:46:ARG:H	2.12	0.52
1:X:796:A:H8	1:X:797:A:H4'	1.74	0.52
10:H:70:VAL:CG2	10:H:98:ILE:HG23	2.38	0.52
4:B:131:SER:O	4:B:132:LYS:HG2	2.10	0.52
1:X:1998:A:O5'	1:X:1998:A:H8	1.92	0.52
1:X:1378:A:H1'	23:U:16:ASN:HD21	1.74	0.52
3:A:79:VAL:HG21	3:A:111:LEU:HD22	1.91	0.52
3:A:245:VAL:HG12	3:A:250:TRP:O	2.09	0.52
1:X:1039:A:N6	1:X:1136:G:H2'	2.24	0.52
1:X:2505:G:H1	1:X:2516:U:H3	1.58	0.52
1:X:760:U:C5	26:Z:3:LYS:HG3	2.44	0.52
1:X:1609:G:H2'	1:X:1610:A:H8	1.73	0.52
4:B:31:CYS:HB3	4:B:49:ILE:HG23	1.90	0.52
12:J:37:ALA:O	12:J:100:PRO:HA	2.09	0.52
1:X:110:U:H3'	1:X:111:G:C8	2.44	0.52
1:X:768:U:H2'	1:X:769:C:O4'	2.09	0.52
1:X:2860:C:H2'	1:X:2861:A:O4'	2.09	0.52
13:K:17:ARG:HH11	13:K:20:LEU:CD2	2.23	0.52
2:Y:46:G:H5'	6:D:92:ARG:HH12	1.73	0.52
23:U:51:ILE:HG23	23:U:59:THR:HA	1.92	0.52
23:U:51:ILE:HG12	23:U:59:THR:HB	1.92	0.52
1:X:2372:A:H5''	11:I:61:PRO:HB3	1.92	0.52
1:X:568:G:H2'	1:X:569:C:O4'	2.09	0.52
14:L:8:ARG:HG3	14:L:9:ARG:H	1.74	0.52
8:F:117:ALA:HB1	8:F:122:ALA:HB1	1.92	0.52
1:X:1859:A:H2'	1:X:1860:A:C8	2.45	0.52
1:X:83:A:H2	1:X:97:U:O2	1.92	0.52
4:B:152:LYS:H	9:G:106:TYR:CB	2.22	0.52
1:X:465:C:O2'	1:X:483:A:N6	2.42	0.52
1:X:1856:U:OP1	1:X:2389:G:O2'	2.26	0.52
13:K:28:LEU:HD12	13:K:48:VAL:HG21	1.92	0.52
1:X:1465:G:N2	1:X:1477:C:O2	2.41	0.52
10:H:27:SER:HA	10:H:50:ILE:HD12	1.90	0.52
17:O:40:VAL:HG12	17:O:43:GLU:HA	1.91	0.52
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.91	0.52
1:X:504:G:H21	18:P:78:ASN:HD21	1.57	0.52
1:X:2528:G:H5''	1:X:2528:G:C8	2.45	0.52
1:X:2594:U:C2	26:Z:7:PRO:HA	2.45	0.52
14:L:36:LYS:HB3	14:L:64:LYS:HB2	1.92	0.52
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:450:C:H2'	1:X:451:A:H8	1.73	0.52
1:X:1623:C:H4'	1:X:1624:A:O5'	2.10	0.52
1:X:216:U:H2'	1:X:217:U:O4'	2.10	0.52
4:B:116:VAL:CG2	4:B:136:ARG:HE	2.15	0.51
3:A:43:ARG:HB3	3:A:54:ILE:HG12	1.91	0.51
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.42	0.51
2:Y:43:G:H5'	2:Y:44:C:H5''	1.91	0.51
1:X:400:U:H5	23:U:21:ARG:HH12	1.57	0.51
1:X:1804:U:H2'	1:X:1805:G:H8	1.73	0.51
1:X:627:A:H2'	1:X:628:A:C8	2.46	0.51
1:X:611:C:H5''	1:X:611:C:H6	1.75	0.51
1:X:413:G:H8	1:X:413:G:O5'	1.93	0.51
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.93	0.51
9:G:93:LYS:HB3	9:G:96:ASP:HB3	1.92	0.51
21:S:117:VAL:HG22	21:S:168:VAL:HA	1.91	0.51
20:R:59:LYS:HG2	20:R:62:MET:HB3	1.93	0.51
15:M:69:ARG:HG3	15:M:78:GLU:HG3	1.93	0.51
32:X:2929:1F4:C23	32:X:2929:1F4:C41	2.88	0.51
1:X:451:A:H2'	1:X:452:G:H8	1.74	0.51
1:X:388:G:H2'	1:X:389:G:H8	1.75	0.51
1:X:1016:C:O2'	9:G:56:THR:HG21	2.11	0.51
5:C:24:SER:HA	5:C:27:LEU:HD12	1.93	0.51
1:X:2042:A:OP1	5:C:66:ASN:ND2	2.44	0.51
6:D:4:LEU:HG	6:D:5:LYS:H	1.74	0.51
6:D:114:PHE:HZ	6:D:176:PRO:HG2	1.74	0.51
1:X:2545:A:H61	10:H:40:GLY:HA3	1.74	0.51
7:E:6:LYS:HB3	7:E:69:ARG:HD3	1.93	0.51
1:X:699:G:C8	1:X:699:G:H5'	2.46	0.51
1:X:840:U:O2	1:X:2225:G:H4'	2.11	0.51
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.11	0.51
17:O:8:GLY:H	17:O:20:ILE:HD13	1.75	0.51
1:X:2289:A:H3'	1:X:2290:A:H8	1.75	0.51
1:X:1542:G:N2	1:X:1562:G:H1	1.94	0.51
1:X:334:G:OP1	1:X:349:G:N2	2.44	0.51
15:M:44:ARG:HE	15:M:46:ARG:HH21	1.58	0.51
3:A:58:HIS:O	3:A:58:HIS:ND1	2.44	0.50
1:X:1736:C:H2'	1:X:1737:G:C8	2.46	0.50
20:R:105:ARG:HH22	20:R:112:LYS:HA	1.76	0.50
1:X:1584:G:H4'	3:A:59:LYS:HG2	1.94	0.50
1:X:935:C:H2'	1:X:936:A:C8	2.45	0.50
5:C:22:VAL:HG22	5:C:106:MET:HG3	1.92	0.50
21:S:3:LEU:HD13	21:S:32:PHE:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1454:U:H2'	1:X:1455:C:H6	1.76	0.50
17:O:15:SER:HA	17:O:95:ILE:O	2.11	0.50
32:X:2929:1F4:C50	32:X:2929:1F4:C52	2.90	0.50
1:X:1834:G:H1	1:X:1881:U:H3	1.59	0.50
4:B:61:LYS:HB3	4:B:62:PRO:HD3	1.93	0.50
23:U:52:ARG:HD3	23:U:70:LEU:HD22	1.92	0.50
4:B:4:ILE:HG12	4:B:28:ALA:HB1	1.94	0.50
1:X:2271:C:P	14:L:18:ARG:HH21	2.35	0.50
12:J:26:ASP:HB3	12:J:68:ARG:HH22	1.76	0.50
13:K:17:ARG:HH11	13:K:20:LEU:HD22	1.76	0.50
1:X:1656:U:H2'	1:X:1657:A:H5''	1.94	0.50
1:X:620:G:N2	1:X:630:G:H1'	2.26	0.50
1:X:2002:A:N7	26:Z:9:LYS:HD2	2.26	0.50
16:N:24:PHE:O	16:N:29:SER:HB3	2.11	0.50
4:B:35:GLN:HB2	4:B:48:GLN:HB3	1.93	0.50
1:X:1142:G:C1'	9:G:103:TYR:HD2	2.25	0.50
3:A:246:PRO:HD2	3:A:249:PRO:O	2.12	0.50
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.47	0.50
5:C:148:VAL:HB	5:C:167:VAL:HG12	1.93	0.50
3:A:182:LEU:HB2	3:A:268:ARG:O	2.11	0.50
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.93	0.50
1:X:969:U:H5''	12:J:17:ARG:HH11	1.77	0.50
15:M:33:VAL:HG22	15:M:51:GLU:HB2	1.93	0.50
21:S:51:LEU:HB3	21:S:65:LEU:HD12	1.94	0.50
20:R:92:THR:HB	20:R:95:ARG:HH22	1.75	0.50
1:X:884:C:H2'	1:X:885:A:H8	1.77	0.50
1:X:2056:C:H4'	3:A:228:PRO:HB2	1.93	0.49
26:Z:30:LEU:HD22	26:Z:39:LYS:HB3	1.94	0.49
5:C:164:VAL:C	5:C:166:TRP:H	2.15	0.49
23:U:48:LYS:HG2	23:U:49:LYS:N	2.27	0.49
1:X:2861:A:O2'	26:Z:31:THR:HG23	2.12	0.49
1:X:504:G:H4'	18:P:27:VAL:CG1	2.42	0.49
21:S:127:PRO:C	21:S:129:ARG:H	2.16	0.49
1:X:1448:A:H61	1:X:1574:A:N6	1.93	0.49
14:L:15:ARG:HD2	14:L:91:ARG:HD2	1.95	0.49
1:X:2597:G:H21	4:B:150:VAL:HG11	1.77	0.49
5:C:4:ILE:HG22	5:C:13:ARG:HH21	1.77	0.49
8:F:112:MET:HA	8:F:115:LEU:HD12	1.94	0.49
26:Z:45:ILE:HG21	26:Z:57:VAL:HG23	1.94	0.49
1:X:1326:U:H2'	1:X:1626:A:C2	2.48	0.49
1:X:1979:C:H4'	1:X:1980:A:OP1	2.13	0.49
1:X:1632:A:H5'	1:X:1632:A:H8	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:K:11:ASN:HD21	13:K:17:ARG:NH1	2.09	0.49
1:X:2653:A:C2'	10:H:41:ASN:ND2	2.75	0.49
1:X:1089:C:H5'	8:F:132:ARG:HH12	1.77	0.49
10:H:113:PRO:HB3	10:H:134:LEU:HD12	1.94	0.49
1:X:2546:G:H2'	1:X:2547:C:C6	2.48	0.49
3:A:66:ASP:HB3	3:A:105:ILE:HD12	1.93	0.49
21:S:5:ALA:HB1	21:S:7:PRO:HD3	1.94	0.49
1:X:2039:G:H2'	1:X:2039:G:N3	2.28	0.49
21:S:56:VAL:HG12	21:S:57:GLU:H	1.78	0.49
9:G:90:LEU:HD23	9:G:94:LYS:HA	1.94	0.49
1:X:1750:A:H1'	1:X:2690:A:C2	2.47	0.49
2:Y:50:U:OP1	14:L:94:TYR:HA	2.13	0.49
1:X:347:C:H4'	20:R:15:HIS:CD2	2.48	0.49
3:A:58:HIS:O	3:A:59:LYS:HB3	2.11	0.49
2:Y:92:G:H8	2:Y:92:G:OP2	1.95	0.49
16:N:74:MET:HG2	16:N:78:THR:HG22	1.94	0.49
16:N:66:ASN:HD22	16:N:70:ARG:HH12	1.60	0.49
1:X:1030:U:H3	1:X:1153:A:H62	1.61	0.49
1:X:2035:G:H4'	4:B:143:GLN:O	2.13	0.49
3:A:164:GLN:HB3	3:A:176:ARG:HB3	1.94	0.49
1:X:1478:U:H2'	1:X:1479:G:H8	1.78	0.49
10:H:112:GLY:O	10:H:131:PRO:HD2	2.13	0.49
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.59	0.49
16:N:75:ASN:ND2	16:N:78:THR:H	2.10	0.49
1:X:229:G:OP1	11:I:49:PHE:HE1	1.96	0.49
1:X:1509:A:H8	1:X:1510:A:C8	2.30	0.49
17:O:71:ILE:HD11	17:O:86:HIS:HB2	1.94	0.48
1:X:1469:U:P	1:X:1471:G:OP2	2.71	0.48
1:X:2779:C:H2'	1:X:2780:A:C8	2.48	0.48
4:B:27:LEU:HD23	4:B:51:TYR:OH	2.12	0.48
32:X:2929:1F4:H3	32:X:2929:1F4:O18	2.12	0.48
1:X:1333:G:N2	1:X:1344:C:N4	2.61	0.48
1:X:793:G:H21	1:X:796:A:H62	1.61	0.48
1:X:643:A:H4'	11:I:67:ASN:HB3	1.95	0.48
6:D:60:ILE:HD12	6:D:61:THR:HG23	1.95	0.48
1:X:463:C:H42	1:X:467:U:H5	1.60	0.48
18:P:102:THR:HG21	18:P:118:LYS:HB3	1.95	0.48
3:A:37:LEU:HD13	3:A:38:PRO:HD2	1.95	0.48
1:X:611:C:H4'	5:C:98:GLN:HE22	1.79	0.48
1:X:1608:U:H2'	1:X:1609:G:C8	2.48	0.48
1:X:2857:C:H5'	13:K:96:ARG:HG3	1.94	0.48
11:I:30:ALA:HB3	11:I:34:HIS:HE1	1.70	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:4:LYS:CG	25:W:52:GLU:HB3	2.43	0.48
1:X:1478:U:H2'	1:X:1479:G:C8	2.48	0.48
1:X:1515:U:H2'	1:X:1516:A:H8	1.79	0.48
3:A:165:VAL:HA	3:A:175:VAL:HG12	1.94	0.48
16:N:50:ARG:O	16:N:53:LYS:HG2	2.13	0.48
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.29	0.48
1:X:794:A:H5'	3:A:218:LYS:NZ	2.29	0.48
23:U:48:LYS:HG3	23:U:49:LYS:H	1.79	0.48
1:X:654:A:H2	1:X:655:A:H3'	1.78	0.48
1:X:1202:U:H2'	1:X:1203:A:H8	1.78	0.48
1:X:958:G:H2'	1:X:959:C:C6	2.49	0.48
1:X:2821:G:H2'	1:X:2822:U:C6	2.49	0.48
1:X:503:G:H2'	1:X:504:G:O4'	2.14	0.48
1:X:1093:U:H5'	8:F:117:ALA:HA	1.96	0.48
20:R:38:LEU:HB3	20:R:47:VAL:HB	1.95	0.48
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.96	0.48
1:X:82:G:N1	1:X:100:G:H2'	2.29	0.48
14:L:31:VAL:HG21	14:L:100:VAL:HG23	1.96	0.48
20:R:23:ILE:HG22	20:R:33:THR:HB	1.95	0.48
1:X:527:C:OP1	26:Z:16:ARG:NH2	2.46	0.48
1:X:1167:A:H61	16:N:48:ARG:HG2	1.79	0.48
3:A:118:ASN:HD22	3:A:119:ALA:N	2.12	0.48
1:X:621:U:H2'	1:X:622:U:C6	2.49	0.48
1:X:1918:G:H1'	1:X:1947:G:N2	2.28	0.48
11:I:130:ILE:HG22	11:I:140:VAL:HG21	1.96	0.48
10:H:26:ASN:CB	10:H:38:GLY:H	2.26	0.48
1:X:2045:A:O5'	1:X:2045:A:H8	1.96	0.48
23:U:65:ASN:HA	23:U:68:ARG:HD3	1.96	0.48
1:X:1687:C:OP2	1:X:2529:G:OP1	2.32	0.47
1:X:1736:C:H2'	1:X:1737:G:H8	1.79	0.47
6:D:8:TYR:O	6:D:12:VAL:HB	2.14	0.47
1:X:881:U:H2'	1:X:882:C:C6	2.49	0.47
1:X:1497:C:C6	1:X:1497:C:H5''	2.50	0.47
23:U:52:ARG:HE	23:U:79:GLU:HA	1.77	0.47
1:X:1515:U:H2'	1:X:1516:A:C8	2.49	0.47
2:Y:21:C:H2'	2:Y:22:U:O4'	2.13	0.47
24:V:42:ARG:NH1	24:V:45:GLN:OE1	2.47	0.47
1:X:1674:C:H2'	1:X:1675:C:H6	1.76	0.47
32:X:2929:1F4:H11	32:X:2929:1F4:C41	2.44	0.47
10:H:116:ARG:HH11	15:M:38:LYS:HD3	1.79	0.47
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.96	0.47
1:X:1406:A:N6	19:Q:15:LYS:HG2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:I:62:LYS:NZ	11:I:64:GLY:HA3	2.28	0.47
9:G:67:ARG:HE	9:G:70:PHE:HA	1.78	0.47
20:R:22:VAL:HG13	20:R:81:VAL:O	2.14	0.47
3:A:118:ASN:HD22	3:A:119:ALA:H	1.61	0.47
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.96	0.47
7:E:67:LEU:O	7:E:71:LEU:HG	2.15	0.47
1:X:1673:C:H5'	4:B:136:ARG:HH11	1.78	0.47
4:B:133:LYS:HG2	4:B:137:ARG:HB3	1.96	0.47
1:X:2362:G:H2'	1:X:2363:G:C8	2.49	0.47
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.80	0.47
3:A:186:HIS:HB2	3:A:188:GLU:CG	2.44	0.47
10:H:90:ARG:HG2	15:M:78:GLU:HB2	1.96	0.47
1:X:2394:G:H4'	11:I:65:PHE:HB3	1.96	0.47
1:X:588:G:H2'	1:X:589:C:H6	1.78	0.47
1:X:1507:A:H2'	1:X:1508:G:H8	1.79	0.47
1:X:1168:G:O2'	25:W:28:ILE:HG12	2.15	0.47
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.28	0.47
4:B:149:ARG:NH1	9:G:106:TYR:HB2	2.29	0.47
11:I:58:ALA:O	11:I:59:ARG:CB	2.62	0.47
9:G:61:ARG:HH11	9:G:66:HIS:H	1.61	0.47
3:A:208:LYS:C	3:A:209:ALA:O	2.53	0.47
3:A:208:LYS:O	3:A:209:ALA:O	2.32	0.47
1:X:388:G:H2'	1:X:389:G:C8	2.50	0.47
1:X:2014:A:C6	1:X:2477:C:H1'	2.49	0.47
21:S:131:PRO:HG3	21:S:155:PRO:HG2	1.97	0.47
21:S:23:ALA:HA	21:S:83:PHE:O	2.14	0.47
1:X:2048:C:H1'	1:X:2428:U:O2	2.14	0.47
4:B:5:LEU:HD12	4:B:197:VAL:HG22	1.97	0.47
1:X:588:G:H2'	1:X:589:C:C6	2.49	0.47
1:X:2493:U:H2'	1:X:2494:C:C6	2.50	0.47
1:X:7:G:H2'	1:X:8:A:C8	2.50	0.47
1:X:203:G:H21	1:X:205:A:H62	1.63	0.47
13:K:97:ILE:HA	13:K:112:LEU:O	2.14	0.47
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.96	0.47
1:X:1584:G:N3	3:A:58:HIS:HE1	2.10	0.47
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.79	0.47
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.96	0.47
1:X:1255:A:H2'	1:X:1256:C:C6	2.50	0.47
1:X:745:C:H2'	1:X:746:G:O4'	2.14	0.47
6:D:63:GLN:HG3	6:D:95:ARG:HH21	1.79	0.47
16:N:49:ASP:HA	16:N:52:ASN:HB2	1.97	0.47
1:X:609:U:H4'	11:I:18:ARG:HE	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2653:A:H4'	10:H:42:LYS:HB2	1.97	0.46
19:Q:12:ILE:H	19:Q:12:ILE:HD13	1.80	0.46
9:G:61:ARG:HG2	9:G:65:LYS:HE3	1.96	0.46
12:J:28:VAL:HG13	12:J:135:ARG:HG2	1.98	0.46
2:Y:94:G:H5'	21:S:74:ARG:HH12	1.79	0.46
16:N:88:ILE:CG1	17:O:49:GLU:HB2	2.45	0.46
9:G:116:ARG:HA	9:G:119:LEU:HD12	1.98	0.46
1:X:2604:G:H2'	1:X:2605:C:O4'	2.15	0.46
1:X:1329:U:H5'	1:X:1405:A:H1'	1.97	0.46
3:A:244:ARG:N	3:A:244:ARG:HD3	2.30	0.46
22:T:45:PHE:CD2	22:T:77:ARG:HB3	2.47	0.46
1:X:2286:G:C2	1:X:2287:G:H1'	2.50	0.46
25:W:47:VAL:HB	25:W:50:LEU:HD12	1.98	0.46
9:G:66:HIS:HA	16:N:67:ALA:HB1	1.98	0.46
20:R:35:LYS:HE3	20:R:37:LEU:HB3	1.98	0.46
1:X:118:U:H4'	1:X:119:G:H5''	1.97	0.46
22:T:48:GLY:HA3	22:T:79:ILE:O	2.15	0.46
1:X:876:A:H2'	1:X:877:G:C8	2.50	0.46
21:S:19:ILE:HD12	21:S:79:ILE:HA	1.97	0.46
1:X:1148:G:H2'	1:X:1149:G:O4'	2.14	0.46
15:M:13:LEU:HA	15:M:13:LEU:HD12	1.70	0.46
4:B:117:MET:HG3	4:B:136:ARG:HG3	1.98	0.46
11:I:32:ARG:HB3	17:O:79:GLN:NE2	2.31	0.46
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.97	0.46
1:X:2574:G:N2	1:X:2577:A:C8	2.82	0.46
16:N:72:HIS:HB2	16:N:110:VAL:HG11	1.96	0.46
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.69	0.46
1:X:1333:G:N2	1:X:1344:C:H41	2.14	0.46
1:X:649:G:H22	1:X:661:C:H1'	1.80	0.46
1:X:1978:U:H1'	10:H:3:MET:HE1	1.97	0.46
1:X:1169:C:H4'	25:W:28:ILE:O	2.16	0.46
1:X:547:U:H2'	1:X:548:G:C8	2.50	0.46
14:L:63:ASN:HB3	14:L:66:ASP:HB2	1.96	0.46
19:Q:20:MET:HG2	19:Q:92:ALA:O	2.16	0.46
1:X:2522:G:H2'	1:X:2523:G:C8	2.50	0.46
1:X:1505:U:O2'	1:X:1506:C:H6	1.98	0.46
11:I:77:LEU:HD13	11:I:110:ALA:HA	1.98	0.46
1:X:2784:A:C6	1:X:2866:A:C8	3.04	0.46
11:I:121:HIS:HA	11:I:141:VAL:HB	1.98	0.46
1:X:2691:C:O2'	1:X:2693:U:H5'	2.16	0.46
26:Z:33:CYS:HB2	26:Z:46:CYS:SG	2.56	0.46
1:X:609:U:H5'	11:I:18:ARG:HD3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:333:A:H2'	5:C:162:ARG:NH1	2.30	0.46
1:X:540:G:H1'	1:X:2004:U:O2'	2.16	0.46
19:Q:66:GLY:O	19:Q:68:PHE:N	2.34	0.46
1:X:636:G:H5''	1:X:636:G:C8	2.51	0.46
22:T:71:ASN:HD21	22:T:74:LYS:HG2	1.81	0.46
1:X:2062:U:H2'	1:X:2063:A:C8	2.52	0.45
1:X:1032:A:H3'	1:X:1032:A:H8	1.78	0.45
17:O:25:LEU:HB2	17:O:32:LYS:HE2	1.98	0.45
1:X:784:U:H2'	1:X:785:U:C6	2.51	0.45
1:X:2352:A:H2'	1:X:2353:G:H8	1.81	0.45
1:X:172:A:H61	1:X:175:C:H3'	1.81	0.45
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.98	0.45
1:X:240:U:H2'	1:X:241:C:O4'	2.16	0.45
4:B:32:PRO:HA	4:B:89:ASP:HB3	1.98	0.45
12:J:21:ASP:HA	12:J:99:LYS:HE2	1.97	0.45
14:L:66:ASP:C	14:L:68:ALA:H	2.19	0.45
12:J:42:TRP:CD1	12:J:97:VAL:HG12	2.51	0.45
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.98	0.45
1:X:2371:A:H1'	11:I:59:ARG:HG3	1.97	0.45
1:X:673:G:H5'	5:C:93:TYR:CD1	2.52	0.45
1:X:1805:G:N3	3:A:50:THR:CG2	2.80	0.45
25:W:19:THR:HG21	25:W:46:THR:HG22	1.98	0.45
5:C:5:ASN:HB3	5:C:10:ASN:HA	1.99	0.45
1:X:313:U:H2'	1:X:314:G:H8	1.81	0.45
1:X:2210:C:OP1	23:U:45:ASN:HA	2.17	0.45
1:X:2843:A:H5''	1:X:2843:A:C8	2.51	0.45
1:X:523:A:O2'	16:N:11:ARG:HD2	2.16	0.45
1:X:1673:C:H5'	4:B:136:ARG:NH1	2.31	0.45
1:X:631:G:H1	5:C:97:ARG:NH1	2.14	0.45
1:X:322:A:N6	1:X:339:U:H2'	2.31	0.45
1:X:1845:A:N1	1:X:2070:G:H1'	2.31	0.45
1:X:428:A:H2'	1:X:429:C:O4'	2.17	0.45
1:X:674:U:H2'	1:X:675:C:O4'	2.17	0.45
2:Y:28:A:C8	2:Y:29:C:C5	3.02	0.45
1:X:635:C:O2'	1:X:670:U:H5''	2.17	0.45
1:X:1805:G:N3	3:A:50:THR:HG22	2.31	0.45
1:X:710:C:H2'	1:X:711:C:C6	2.52	0.45
17:O:48:GLY:C	17:O:50:ASP:H	2.20	0.45
1:X:1234:C:H2'	1:X:1235:C:H6	1.82	0.45
1:X:1997:A:H2'	1:X:1998:A:C8	2.51	0.45
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.82	0.45
1:X:1832:G:H1	1:X:1885:C:N4	2.09	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1981:A:H2'	1:X:1982:C:O4'	2.16	0.45
20:R:105:ARG:NH2	20:R:112:LYS:HA	2.32	0.45
3:A:83:GLU:N	3:A:92:ILE:O	2.46	0.45
7:E:11:VAL:HG11	7:E:50:LEU:HD13	1.98	0.45
18:P:105:ARG:HB3	18:P:105:ARG:HE	1.64	0.45
23:U:19:ILE:HA	23:U:42:GLN:HA	1.98	0.45
12:J:31:GLY:HA2	12:J:108:ALA:HB2	1.99	0.45
1:X:1573:G:H3'	1:X:1574:A:O4'	2.17	0.45
12:J:42:TRP:CG	12:J:95:VAL:HG11	2.52	0.45
9:G:154:GLU:C	9:G:157:PRO:HD2	2.36	0.45
5:C:74:VAL:HG23	5:C:76:THR:H	1.81	0.45
10:H:11:ALA:O	10:H:110:VAL:HA	2.17	0.45
3:A:134:ARG:HG3	3:A:135:PHE:HD2	1.81	0.45
9:G:34:PRO:HA	9:G:69:ASP:CG	2.37	0.45
1:X:1164:C:H5'	16:N:76:TYR:CE2	2.52	0.45
1:X:2579:A:H2'	1:X:2580:C:C6	2.52	0.45
1:X:2222:U:H2'	1:X:2223:U:C6	2.52	0.45
1:X:2661:G:O6	1:X:2708:U:H1'	2.17	0.45
15:M:79:ARG:CG	15:M:79:ARG:NH1	2.68	0.45
1:X:640:C:C4'	1:X:660:G:H21	2.23	0.45
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.98	0.45
1:X:593:C:N4	1:X:594:G:C6	2.85	0.45
9:G:70:PHE:HB2	16:N:64:ARG:HE	1.83	0.44
1:X:636:G:O2'	1:X:669:G:H4'	2.17	0.44
1:X:1367:A:H2'	1:X:1368:G:O4'	2.17	0.44
20:R:97:GLN:HB2	20:R:101:GLY:HA2	1.99	0.44
1:X:1045:G:N2	1:X:1133:G:H1'	2.31	0.44
4:B:119:ARG:HG2	4:B:120:TRP:CE2	2.52	0.44
1:X:1494:G:H2'	1:X:1495:G:O4'	2.17	0.44
1:X:1769:U:H2'	1:X:1775:A:N6	2.31	0.44
3:A:79:VAL:HG21	3:A:111:LEU:CD2	2.47	0.44
1:X:2252:A:H2'	1:X:2253:A:C8	2.52	0.44
20:R:25:LEU:N	20:R:80:LYS:HA	2.30	0.44
3:A:208:LYS:HE3	3:A:208:LYS:HA	2.00	0.44
1:X:1202:U:H5'	17:O:78:VAL:HG22	1.98	0.44
1:X:2195:C:H5"	1:X:2195:C:H6	1.82	0.44
1:X:1373:G:N2	1:X:2192:U:H3	2.15	0.44
3:A:147:LEU:HD22	3:A:183:ARG:HH22	1.82	0.44
12:J:73:LYS:H	12:J:94:TRP:HD1	1.65	0.44
1:X:1117:G:H2'	1:X:1118:G:H8	1.80	0.44
2:Y:72:C:H2'	2:Y:73:C:H6	1.82	0.44
1:X:224:G:H4'	1:X:399:G:C5	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1834:G:H1'	3:A:244:ARG:HH22	1.82	0.44
1:X:956:A:C4	1:X:2427:A:C2	3.06	0.44
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.98	0.44
1:X:339:U:O4	1:X:343:A:C8	2.70	0.44
1:X:796:A:H4'	1:X:2567:G:H4'	1.99	0.44
10:H:70:VAL:HG21	10:H:98:ILE:HG23	1.98	0.44
18:P:41:VAL:HG22	18:P:60:ILE:HG21	1.99	0.44
3:A:231:HIS:ND1	3:A:247:VAL:HA	2.31	0.44
3:A:42:GLY:H	3:A:43:ARG:NH1	2.15	0.44
5:C:46:ARG:HD2	5:C:51:VAL:HB	1.99	0.44
1:X:1833:U:H2'	1:X:1834:G:C8	2.53	0.44
2:Y:89:G:N2	2:Y:92:G:C8	2.86	0.44
12:J:98:VAL:HG11	12:J:104:MET:HG2	2.00	0.44
1:X:358:C:H6	1:X:358:C:O5'	2.01	0.44
1:X:2056:C:H5'	3:A:229:VAL:HG22	2.00	0.44
4:B:5:LEU:HD22	4:B:49:ILE:HG22	1.99	0.44
4:B:54:LYS:HD3	4:B:59:VAL:HG22	1.99	0.44
1:X:1819:U:OP2	3:A:222:ARG:NH2	2.50	0.44
1:X:819:C:OP2	11:I:41:SER:HA	2.17	0.44
12:J:77:LYS:O	12:J:88:LYS:HD2	2.18	0.44
1:X:2609:G:H2'	1:X:2610:G:C8	2.52	0.44
22:T:40:GLN:HE21	22:T:57:HIS:HB3	1.83	0.44
1:X:1524:C:H3'	1:X:1525:A:H8	1.82	0.44
13:K:76:VAL:HA	13:K:79:VAL:HG12	2.00	0.44
3:A:67:PHE:HB3	3:A:153:ALA:N	2.31	0.44
1:X:1223:G:H5''	1:X:1224:A:H3'	2.00	0.44
1:X:2002:A:N1	1:X:2018:G:O6	2.51	0.44
12:J:44:LYS:HB3	12:J:46:ASN:ND2	2.33	0.44
1:X:1725:C:H42	1:X:1741:G:H1	1.64	0.44
1:X:490:A:N3	1:X:492:G:H5''	2.33	0.44
7:E:164:PHE:O	7:E:166:GLY:N	2.51	0.44
3:A:43:ARG:HG3	3:A:54:ILE:O	2.18	0.44
3:A:209:ALA:C	3:A:211:ARG:H	2.21	0.44
18:P:72:LEU:HD12	18:P:126:ILE:HD13	2.00	0.44
12:J:78:LYS:HE2	12:J:81:GLU:HA	2.00	0.44
10:H:24:VAL:HG13	10:H:45:ALA:HB2	1.99	0.44
21:S:3:LEU:HB3	21:S:34:LEU:HB3	1.99	0.44
14:L:8:ARG:CG	14:L:9:ARG:H	2.31	0.44
19:Q:51:ILE:HD11	19:Q:81:ARG:HD3	2.00	0.44
11:I:8:PRO:HB2	11:I:14:LYS:NZ	2.32	0.44
19:Q:39:LYS:HG2	19:Q:43:GLN:HE21	1.83	0.43
1:X:2506:C:H5'	30:4:33:LYS:HD2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2506:C:H5''	30:4:30:VAL:HB	2.00	0.43
1:X:1101:U:H2'	1:X:1102:G:C8	2.53	0.43
5:C:107:ALA:HB1	5:C:180:ILE:HD11	2.00	0.43
3:A:247:VAL:CG2	3:A:248:THR:N	2.81	0.43
1:X:760:U:C6	26:Z:3:LYS:HG3	2.53	0.43
1:X:1333:G:N7	1:X:1342:U:H5'	2.32	0.43
5:C:95:LEU:CD2	5:C:96:PRO:HD2	2.48	0.43
21:S:117:VAL:HG23	21:S:168:VAL:HG13	2.00	0.43
13:K:34:ILE:HG13	13:K:113:ILE:HG23	2.01	0.43
5:C:150:LEU:HA	5:C:187:VAL:HB	2.00	0.43
1:X:2324:G:H5''	1:X:2326:C:O4'	2.18	0.43
9:G:43:VAL:HB	9:G:167:LYS:HG2	1.99	0.43
1:X:1230:C:H2'	1:X:1231:A:H8	1.83	0.43
4:B:134:TRP:CD1	4:B:134:TRP:N	2.76	0.43
11:I:54:SER:HA	11:I:58:ALA:HB3	2.00	0.43
1:X:2551:A:O5'	1:X:2553:G:H4'	2.18	0.43
1:X:114:C:H2'	1:X:115:G:C8	2.53	0.43
3:A:145:LEU:HB3	3:A:155:LEU:HD12	2.00	0.43
6:D:117:ILE:HD13	6:D:130:LEU:HD11	2.00	0.43
3:A:202:LYS:C	3:A:204:ILE:H	2.22	0.43
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.45	0.43
1:X:342:G:O3'	1:X:343:A:C8	2.71	0.43
1:X:695:G:N2	1:X:808:C:O2	2.44	0.43
5:C:127:ASP:HB2	5:C:128:ALA:H	1.64	0.43
32:X:2929:1F4:C41	32:X:2929:1F4:C16	2.97	0.43
1:X:1996:A:H5'	18:P:118:LYS:NZ	2.33	0.43
12:J:62:GLY:H	21:S:175:ARG:N	2.16	0.43
1:X:2594:U:H2'	1:X:2595:C:H6	1.83	0.43
5:C:30:VAL:HG11	5:C:177:VAL:HG21	2.00	0.43
2:Y:91:A:H2'	2:Y:92:G:C8	2.54	0.43
1:X:84:G:N3	1:X:101:A:C2	2.86	0.43
1:X:314:G:H2'	1:X:315:G:C8	2.53	0.43
1:X:538:A:H5''	9:G:139:ARG:HE	1.83	0.43
1:X:1577:G:H2'	1:X:1578:U:O4'	2.19	0.43
5:C:133:PHE:HB2	5:C:160:ALA:HB1	2.00	0.43
3:A:245:VAL:N	3:A:252:LYS:HE3	2.34	0.43
1:X:339:U:H4'	20:R:77:HIS:ND1	2.34	0.43
1:X:1782:A:O3'	3:A:206:LEU:HB2	2.18	0.43
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.95	0.43
17:O:69:ILE:HG22	17:O:86:HIS:HB3	2.00	0.43
5:C:74:VAL:O	5:C:77:PHE:HB2	2.18	0.43
1:X:1539:U:H2'	1:X:1540:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:4:19:ARG:HD2	30:4:24:LEU:HD22	2.01	0.43
1:X:2006:G:H4'	1:X:2596:C:O3'	2.19	0.43
1:X:2277:A:H2'	1:X:2278:A:O4'	2.18	0.43
10:H:22:ILE:HD11	10:H:54:SER:HB2	1.99	0.43
1:X:2066:G:N2	1:X:2216:G:H1'	2.34	0.43
1:X:2170:C:H2'	1:X:2171:U:H4'	2.01	0.43
1:X:1919:A:C2	1:X:1926:U:N3	2.74	0.43
12:J:61:ARG:HD3	21:S:174:PRO:HB2	1.99	0.43
3:A:63:ARG:O	3:A:65:ILE:HD12	2.18	0.43
1:X:2825:A:H2'	1:X:2826:C:C6	2.54	0.43
18:P:25:PHE:C	18:P:25:PHE:CD2	2.90	0.43
1:X:742:G:N1	3:A:208:LYS:HD3	2.33	0.43
3:A:45:ASN:CG	3:A:46:ARG:N	2.72	0.43
10:H:27:SER:OG	10:H:49:ASP:HA	2.19	0.43
1:X:1283:C:H5''	1:X:1284:G:O5'	2.19	0.43
1:X:1148:G:O2'	9:G:134:MET:HG3	2.18	0.43
15:M:22:ARG:HD2	15:M:83:PHE:O	2.19	0.43
10:H:19:ILE:HG22	10:H:55:VAL:HA	2.01	0.43
32:X:2929:1F4:H53	32:X:2929:1F4:H9	2.00	0.43
16:N:66:ASN:HB3	16:N:76:TYR:N	2.27	0.43
1:X:1643:A:H61	1:X:1656:U:H3	1.67	0.43
5:C:148:VAL:O	5:C:167:VAL:HA	2.19	0.43
10:H:10:VAL:HG11	10:H:98:ILE:HD12	2.00	0.43
1:X:1469:U:OP1	1:X:1471:G:OP2	2.36	0.43
1:X:205:A:C8	1:X:205:A:H3'	2.54	0.43
13:K:33:ARG:HD3	13:K:112:LEU:HD22	2.01	0.43
1:X:551:A:H2'	1:X:552:C:O4'	2.19	0.43
20:R:24:VAL:HB	20:R:29:HIS:O	2.19	0.43
1:X:2320:G:H2'	1:X:2321:C:O4'	2.19	0.43
4:B:11:MET:HA	4:B:23:VAL:O	2.19	0.43
1:X:504:G:N2	18:P:78:ASN:HD21	2.17	0.43
1:X:1268:U:H5	5:C:68:ARG:HB2	1.84	0.43
1:X:882:C:H2'	1:X:883:A:O4'	2.19	0.43
1:X:1497:C:H5''	1:X:1497:C:H6	1.84	0.43
25:W:27:LYS:O	25:W:30:ASP:HB2	2.19	0.43
2:Y:32:C:H1'	2:Y:59:A:H61	1.84	0.43
2:Y:107:C:H2'	2:Y:108:G:O4'	2.19	0.43
20:R:18:LYS:HD3	20:R:18:LYS:H	1.84	0.43
1:X:487:G:H4'	1:X:512:A:N1	2.34	0.42
1:X:1978:U:H3'	1:X:1979:C:H2'	2.01	0.42
1:X:1373:G:H22	1:X:2192:U:H3	1.67	0.42
3:A:201:HIS:CD2	3:A:204:ILE:HD12	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:130:THR:HG23	5:C:160:ALA:HA	2.00	0.42
21:S:149:ALA:HB3	21:S:164:PRO:HA	1.99	0.42
7:E:33:LEU:HD13	7:E:136:ILE:HG22	2.01	0.42
9:G:45:ASP:HA	9:G:83:ILE:HG13	2.01	0.42
13:K:90:ARG:HA	13:K:91:PRO:HD3	1.89	0.42
1:X:2235:G:N2	1:X:2254:C:C4	2.87	0.42
25:W:12:ARG:CG	25:W:12:ARG:NH1	2.76	0.42
1:X:322:A:H3'	1:X:323:G:H8	1.83	0.42
26:Z:6:VAL:HG22	26:Z:7:PRO:HD2	2.00	0.42
7:E:6:LYS:H	7:E:65:HIS:HE1	1.66	0.42
1:X:636:G:H8	1:X:636:G:H5''	1.84	0.42
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.52	0.42
1:X:719:A:H2'	1:X:720:A:O4'	2.19	0.42
7:E:126:PRO:HG2	7:E:130:ARG:HH22	1.85	0.42
20:R:93:ARG:HG2	20:R:108:VAL:HA	2.01	0.42
1:X:2011:U:H2'	1:X:2012:A:O4'	2.19	0.42
1:X:812:G:H3'	1:X:813:A:H2'	2.01	0.42
1:X:2024:U:H2'	1:X:2025:A:O4'	2.20	0.42
1:X:2489:C:C4	1:X:2490:U:C5	3.08	0.42
1:X:5:A:H2'	1:X:6:A:C8	2.54	0.42
1:X:2220:A:H2'	1:X:2221:G:C8	2.54	0.42
1:X:1371:G:H8	1:X:1371:G:O5'	2.02	0.42
18:P:46:ARG:HG3	18:P:95:ALA:HB3	2.01	0.42
1:X:2427:A:HO2'	1:X:2428:U:H5	1.64	0.42
1:X:346:C:O2	1:X:347:C:C5	2.72	0.42
2:Y:108:G:H4'	21:S:26:LYS:HB3	2.02	0.42
1:X:441:A:H3'	1:X:442:A:H8	1.84	0.42
1:X:638:A:C8	11:I:74:VAL:HG11	2.55	0.42
10:H:64:VAL:HG22	10:H:106:ARG:NH1	2.35	0.42
15:M:34:ARG:HH22	15:M:90:GLN:N	2.17	0.42
1:X:1656:U:C2'	1:X:1657:A:H5''	2.50	0.42
14:L:44:ASP:HB2	14:L:51:LEU:HD13	2.01	0.42
2:Y:91:A:H8	2:Y:91:A:OP2	2.03	0.42
1:X:958:G:H2'	1:X:959:C:H6	1.84	0.42
1:X:877:G:H2'	1:X:878:C:C6	2.55	0.42
5:C:117:LEU:HD23	5:C:187:VAL:HG22	2.01	0.42
5:C:122:GLY:C	5:C:124:ASP:H	2.22	0.42
1:X:2200:G:H2'	1:X:2201:G:C8	2.55	0.42
1:X:1332:G:C6	1:X:1333:G:N1	2.88	0.42
3:A:43:ARG:H	3:A:43:ARG:HD2	1.78	0.42
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.49	0.42
11:I:119:THR:HG23	11:I:139:ARG:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2683:C:H2'	1:X:2684:A:O4'	2.19	0.42
1:X:50:G:H4'	1:X:51:A:H5'	2.02	0.42
1:X:700:C:H2'	1:X:701:U:O4'	2.20	0.42
4:B:131:SER:HB3	4:B:134:TRP:HD1	1.79	0.42
4:B:152:LYS:N	9:G:106:TYR:HB3	2.33	0.42
17:O:12:TYR:HB2	17:O:40:VAL:H	1.84	0.42
1:X:2545:A:H61	10:H:40:GLY:CA	2.32	0.42
1:X:1737:G:H2'	1:X:1738:U:C6	2.55	0.42
2:Y:89:G:H5''	2:Y:90:C:OP2	2.19	0.42
1:X:205:A:H8	1:X:205:A:H3'	1.84	0.42
1:X:810:U:H2'	1:X:811:G:O4'	2.20	0.42
16:N:13:ARG:HA	16:N:16:LYS:HE2	2.02	0.42
1:X:2658:A:H4'	4:B:165:VAL:HG11	2.02	0.42
2:Y:102:A:H2'	2:Y:103:A:C8	2.54	0.42
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.85	0.42
1:X:2241:U:C5	22:T:17:ASN:OD1	2.63	0.42
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.49	0.42
1:X:2528:G:H2'	1:X:2529:G:C8	2.49	0.42
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.19	0.42
14:L:68:ALA:HB1	14:L:102:ALA:HB3	2.01	0.42
1:X:2352:A:H2'	1:X:2353:G:C8	2.54	0.42
1:X:1381:G:H8	1:X:1381:G:O5'	2.03	0.42
11:I:82:ASP:H	11:I:114:ILE:HG21	1.84	0.42
1:X:2687:G:H2'	1:X:2688:G:H8	1.85	0.42
3:A:173:VAL:HG23	3:A:187:SER:HB3	2.02	0.42
1:X:590:C:H2'	1:X:591:G:C8	2.55	0.42
1:X:1279:G:O2'	1:X:1995:G:O6	2.26	0.42
1:X:631:G:H4'	1:X:632:A:H5'	2.02	0.42
4:B:193:GLY:O	15:M:2:GLN:N	2.53	0.42
23:U:31:GLY:HA2	23:U:32:ARG:HH11	1.85	0.42
5:C:33:TRP:CE3	5:C:95:LEU:HD12	2.54	0.42
1:X:1804:U:H2'	1:X:1805:G:C8	2.54	0.42
9:G:157:PRO:C	9:G:159:SER:H	2.23	0.42
5:C:194:GLU:O	5:C:195:ILE:HG12	2.20	0.42
1:X:1314:A:H2	1:X:1642:G:N3	2.17	0.42
1:X:1100:G:H21	1:X:1113:C:H42	1.67	0.42
1:X:666:U:O2'	1:X:667:U:H5''	2.20	0.42
1:X:1035:G:C8	1:X:1036:G:H2'	2.55	0.42
1:X:1774:A:C6	1:X:2566:A:C2	3.08	0.42
1:X:688:A:N3	1:X:2422:C:O2'	2.46	0.42
1:X:1765:C:O5'	1:X:1765:C:H6	2.03	0.42
1:X:708:G:OP1	1:X:1393:G:O2'	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1447:U:HO2'	1:X:1448:A:H8	1.65	0.42
15:M:38:LYS:HB3	15:M:46:ARG:HB3	2.01	0.42
5:C:180:ILE:HG13	5:C:181:LEU:N	2.35	0.42
1:X:1929:U:H2'	1:X:1930:C:C6	2.54	0.42
9:G:170:PRO:HB2	9:G:171:LEU:H	1.75	0.42
13:K:76:VAL:O	13:K:80:MET:HB2	2.20	0.41
9:G:132:PHE:HZ	9:G:142:ARG:HA	1.85	0.41
11:I:28:LYS:HZ1	11:I:36:GLY:HA2	1.83	0.41
1:X:554:U:H4'	1:X:555:U:OP2	2.20	0.41
10:H:132:GLU:HG2	10:H:134:LEU:HG	2.02	0.41
1:X:1167:A:C5	16:N:51:ARG:HD3	2.55	0.41
20:R:29:HIS:CD2	20:R:51:VAL:HG22	2.55	0.41
5:C:94:THR:HG22	5:C:100:ARG:HH12	1.84	0.41
13:K:8:ARG:O	13:K:9:LYS:HB3	2.20	0.41
1:X:1302:C:H2'	1:X:1303:U:H6	1.85	0.41
1:X:149:A:H2'	1:X:150:A:H8	1.84	0.41
32:X:2929:1F4:H18	32:X:2929:1F4:C53	2.50	0.41
1:X:224:G:H4'	1:X:399:G:C4	2.55	0.41
1:X:2796:A:H2'	1:X:2797:G:C8	2.55	0.41
1:X:54:G:C2	1:X:114:C:C2	3.08	0.41
1:X:1975:G:N2	1:X:1979:C:O2'	2.52	0.41
1:X:622:U:H2'	1:X:623:G:O4'	2.21	0.41
24:V:32:ALA:HB2	24:V:37:LEU:HG	2.02	0.41
1:X:2053:G:H2'	1:X:2054:A:C8	2.54	0.41
23:U:47:HIS:HB2	23:U:48:LYS:H	1.71	0.41
12:J:6:LYS:O	12:J:71:PRO:HD2	2.20	0.41
1:X:1032:A:C3'	1:X:1032:A:C8	3.03	0.41
1:X:1287:A:H2	1:X:1661:C:O2	2.03	0.41
1:X:1385:C:H2'	1:X:1386:A:O4'	2.20	0.41
1:X:2859:U:N3	26:Z:52:TYR:CE1	2.88	0.41
1:X:692:C:H2'	1:X:693:A:C8	2.55	0.41
1:X:1973:C:H2'	1:X:1974:U:O4'	2.21	0.41
1:X:1249:G:O2'	1:X:1250:A:H8	2.03	0.41
1:X:1266:G:C8	11:I:32:ARG:NH1	2.85	0.41
1:X:649:G:H2'	1:X:650:U:C6	2.55	0.41
1:X:237:G:H1'	1:X:632:A:H1'	2.02	0.41
25:W:4:LYS:HE3	25:W:52:GLU:O	2.20	0.41
1:X:1811:A:H3'	3:A:178:PRO:HB2	2.02	0.41
12:J:64:LYS:HG2	21:S:112:LEU:HD22	2.02	0.41
1:X:960:U:H2'	1:X:961:G:H8	1.82	0.41
1:X:934:G:H1'	22:T:26:PHE:CD1	2.55	0.41
1:X:2209:G:H4'	23:U:46:LEU:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:I:60:LEU:HA	11:I:60:LEU:HD12	1.89	0.41
12:J:6:LYS:HE3	12:J:7:ARG:HE	1.86	0.41
1:X:1687:C:H6	1:X:1687:C:O5'	2.02	0.41
1:X:1224:A:H4'	1:X:1225:G:OP2	2.20	0.41
1:X:1381:G:H2'	1:X:1799:A:H61	1.86	0.41
6:D:75:SER:HB2	6:D:79:LEU:HB2	2.03	0.41
12:J:36:ILE:HG13	12:J:103:VAL:HA	2.03	0.41
1:X:2590:U:O4'	32:X:2929:1F4:H32	2.21	0.41
11:I:28:LYS:HZ3	11:I:36:GLY:HA2	1.86	0.41
23:U:65:ASN:N	23:U:65:ASN:OD1	2.54	0.41
1:X:2556:A:H5''	1:X:2557:G:H5'	2.02	0.41
1:X:2225:G:H2'	1:X:2226:A:H8	1.85	0.41
13:K:96:ARG:O	13:K:113:ILE:HA	2.20	0.41
4:B:104:ALA:HB3	4:B:170:LEU:HD12	2.02	0.41
1:X:1792:C:N4	1:X:2185:U:H5'	2.36	0.41
3:A:213:ARG:HD2	3:A:213:ARG:HA	1.97	0.41
5:C:171:PRO:O	5:C:173:ALA:N	2.54	0.41
1:X:1117:G:H2'	1:X:1118:G:C8	2.55	0.41
15:M:34:ARG:NH1	15:M:91:VAL:HB	2.36	0.41
1:X:2519:C:O2'	1:X:2720:A:N3	2.44	0.41
1:X:2633:A:N1	1:X:2644:A:H5''	2.35	0.41
1:X:946:U:H2'	1:X:947:C:C6	2.56	0.41
9:G:62:ILE:HG23	9:G:135:LEU:HD21	2.02	0.41
1:X:1:G:H2'	1:X:1:G:N3	2.36	0.41
21:S:141:MET:SD	21:S:147:ILE:HG12	2.61	0.41
1:X:654:A:C2	1:X:655:A:H3'	2.56	0.41
9:G:53:ARG:HH22	9:G:171:LEU:HD12	1.85	0.41
1:X:2395:C:H2'	1:X:2396:C:H5''	2.02	0.41
12:J:14:PHE:CE1	12:J:90:ALA:HB2	2.56	0.41
1:X:1132:C:H6	1:X:1132:C:O5'	2.03	0.41
14:L:31:VAL:HG23	14:L:38:ILE:HD11	2.01	0.41
1:X:322:A:H3'	1:X:323:G:C8	2.55	0.41
20:R:22:VAL:HG22	20:R:83:LEU:H	1.85	0.41
12:J:27:TYR:HB2	12:J:137:VAL:HG21	2.02	0.41
21:S:107:GLU:HG3	21:S:112:LEU:HA	2.02	0.41
23:U:14:VAL:HB	23:U:15:VAL:H	1.75	0.41
1:X:762:A:H4'	1:X:1284:G:N3	2.36	0.41
16:N:68:GLY:HA2	16:N:71:LEU:HD23	2.02	0.41
4:B:105:THR:HB	4:B:166:THR:HG23	2.03	0.41
7:E:24:PHE:HB2	7:E:37:TYR:HD1	1.85	0.41
1:X:1009:C:H2'	1:X:1010:U:O4'	2.21	0.41
1:X:494:A:C8	20:R:56:LYS:HD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:1106:A:H2'	1:X:1107:A:H8	1.86	0.41
4:B:55:ALA:HB3	4:B:58:LYS:HD2	2.01	0.41
1:X:95:G:H4'	24:V:41:HIS:ND1	2.35	0.41
1:X:1494:G:HO2'	1:X:1574:A:H2	1.66	0.41
1:X:657:A:H3'	1:X:657:A:C8	2.56	0.41
1:X:1467:U:H3'	1:X:1467:U:H6	1.85	0.41
5:C:176:ASN:ND2	5:C:179:ASP:H	2.16	0.41
1:X:188:G:H2'	1:X:189:A:C8	2.56	0.41
1:X:1469:U:H5'	1:X:1470:G:N7	2.36	0.41
1:X:98:U:H1'	1:X:100:G:C4	2.56	0.41
1:X:1533:G:H2'	1:X:1534:A:H8	1.86	0.41
17:O:19:VAL:HG13	17:O:90:PHE:CD1	2.56	0.41
14:L:76:ALA:HB2	14:L:107:ALA:HA	2.02	0.41
1:X:874:A:H2'	1:X:875:G:O4'	2.21	0.41
1:X:2357:A:H1'	14:L:88:VAL:HG11	2.02	0.41
22:T:38:VAL:CG1	22:T:59:LEU:HD12	2.50	0.41
1:X:1615:C:OP2	19:Q:35:LYS:HD2	2.20	0.41
1:X:956:A:C5	1:X:2427:A:C2	3.09	0.40
5:C:30:VAL:HA	5:C:95:LEU:HD11	2.02	0.40
1:X:99:U:H5''	1:X:100:G:C8	2.57	0.40
16:N:88:ILE:HG13	17:O:49:GLU:HB2	2.03	0.40
24:V:2:LYS:H	24:V:3:PRO:CD	2.33	0.40
1:X:1835:C:H2'	1:X:1836:C:C6	2.56	0.40
1:X:2526:U:H2'	1:X:2527:G:C8	2.57	0.40
28:2:14:LYS:CA	28:2:15:THR:CA	2.98	0.40
18:P:19:LYS:HB3	18:P:19:LYS:HE2	1.76	0.40
1:X:2796:A:OP2	13:K:5:LYS:NZ	2.55	0.40
22:T:41:ARG:HA	22:T:41:ARG:NE	2.34	0.40
1:X:957:G:H2'	1:X:958:G:H8	1.86	0.40
3:A:147:LEU:HD22	3:A:183:ARG:NH2	2.35	0.40
1:X:1835:C:O2'	3:A:254:THR:HB	2.21	0.40
19:Q:56:MET:SD	19:Q:57:ASN:N	2.91	0.40
21:S:53:ASP:HA	21:S:63:PRO:HA	2.03	0.40
23:U:43:ARG:HH21	23:U:43:ARG:HB2	1.85	0.40
1:X:1248:G:O5'	1:X:1248:G:H8	2.04	0.40
32:X:2929:1F4:O46	32:X:2929:1F4:H7	2.22	0.40
1:X:649:G:N2	1:X:660:G:N2	2.69	0.40
1:X:651:C:H2'	1:X:652:C:H6	1.86	0.40
12:J:70:PHE:HA	12:J:71:PRO:HD3	1.95	0.40
2:Y:22:U:H3	2:Y:65:A:H61	1.68	0.40
3:A:202:LYS:C	3:A:204:ILE:N	2.75	0.40
23:U:20:ARG:HB2	23:U:43:ARG:HD2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:166:GLN:HB2	3:A:174:ILE:HG22	2.03	0.40
26:Z:36:CYS:HB3	26:Z:49:CYS:HB3	1.94	0.40
1:X:2419:C:N3	1:X:2420:C:H1'	2.37	0.40
1:X:2064:U:H2'	1:X:2065:A:C8	2.56	0.40
26:Z:42:SER:O	26:Z:44:HIS:HD2	2.03	0.40
16:N:42:ALA:O	16:N:46:GLU:N	2.51	0.40
1:X:1796:A:N3	3:A:50:THR:HG23	2.36	0.40
1:X:877:G:H2'	1:X:878:C:H6	1.86	0.40
1:X:1519:G:H2'	1:X:1520:G:H8	1.86	0.40
21:S:36:ARG:O	21:S:40:ASP:HB2	2.22	0.40
1:X:506:G:H4'	18:P:21:ARG:HH21	1.85	0.40
1:X:1467:U:H5''	1:X:1467:U:C6	2.57	0.40
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.21	0.40
9:G:103:TYR:HB3	9:G:107:GLN:HE21	1.85	0.40
17:O:10:LYS:HE3	17:O:11:GLN:HG2	2.03	0.40
1:X:1255:A:H2'	1:X:1256:C:H6	1.86	0.40
1:X:2422:C:H2'	1:X:2423:G:C8	2.56	0.40
16:N:95:LEU:HA	16:N:98:ILE:HD12	2.04	0.40
4:B:181:LEU:HD21	15:M:12:LEU:CD2	2.51	0.40
7:E:140:LEU:O	7:E:144:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	2	26
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	9	61
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	8
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	5	48
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	3	38
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	4	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	1	15
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	10	63
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	9
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	1	21
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	3	38
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	1	13
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	3	36
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	2	34
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	9
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	6	55
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	10
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	6
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	2	33
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	2	34
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	3
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	7	57
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	12	67
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	1	21
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	7	58
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	25

All (235) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	209	ALA
3	A	217	ARG
3	A	248	THR
3	A	249	PRO
3	A	250	TRP
3	A	271	VAL
5	C	4	ILE
5	C	20	PRO
5	C	60	GLY
5	C	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	129	LYS
5	C	164	VAL
5	C	165	SER
5	C	172	VAL
5	C	195	ILE
6	D	10	ASP
6	D	81	GLN
6	D	122	PHE
7	E	165	VAL
9	G	33	ILE
9	G	67	ARG
9	G	92	GLY
9	G	97	ASP
9	G	104	THR
9	G	170	PRO
10	H	27	SER
11	I	18	ARG
11	I	47	ALA
11	I	49	PHE
11	I	64	GLY
11	I	98	LEU
11	I	99	VAL
11	I	103	ASN
12	J	80	ALA
12	J	82	THR
12	J	88	LYS
13	K	6	ALA
13	K	92	GLY
14	L	21	THR
14	L	61	SER
14	L	68	ALA
14	L	95	LYS
15	M	29	PRO
16	N	8	ILE
16	N	95	LEU
17	O	7	THR
17	O	10	LYS
17	O	22	VAL
17	O	48	GLY
19	Q	6	ILE
19	Q	61	LYS
19	Q	63	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Q	67	ARG
19	Q	69	ILE
20	R	11	ASN
20	R	15	HIS
20	R	60	PRO
20	R	82	ALA
20	R	107	ALA
21	S	6	LYS
21	S	26	LYS
21	S	56	VAL
21	S	91	PRO
21	S	156	GLU
22	T	19	LYS
23	U	15	VAL
23	U	19	ILE
23	U	32	ARG
23	U	34	THR
23	U	56	GLN
23	U	60	VAL
26	Z	4	HIS
26	Z	36	CYS
26	Z	53	ASP
3	A	35	GLU
3	A	58	HIS
3	A	220	HIS
4	B	132	LYS
5	C	22	VAL
5	C	83	ALA
5	C	121	ASP
5	C	190	ALA
5	C	196	VAL
6	D	124	GLY
7	E	59	GLN
7	E	173	ALA
9	G	37	ASP
9	G	105	GLY
9	G	107	GLN
9	G	158	HIS
10	H	5	GLN
10	H	29	ILE
11	I	36	GLY
11	I	54	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	I	62	LYS
11	I	68	VAL
12	J	11	ARG
12	J	83	ARG
12	J	87	GLY
12	J	91	VAL
13	K	4	GLY
13	K	9	LYS
14	L	31	VAL
14	L	40	ALA
14	L	94	TYR
15	M	26	ASP
15	M	31	ASP
15	M	39	VAL
15	M	57	ILE
16	N	7	GLY
16	N	87	ASN
17	O	8	GLY
17	O	9	GLY
17	O	14	VAL
18	P	9	ARG
18	P	85	MET
19	Q	12	ILE
19	Q	84	GLU
20	R	85	ASP
20	R	98	ILE
22	T	11	LYS
23	U	29	GLY
23	U	41	VAL
23	U	76	LYS
24	V	2	LYS
24	V	36	GLN
30	4	3	VAL
3	A	254	THR
3	A	269	PHE
4	B	129	HIS
4	B	146	THR
5	C	9	GLN
5	C	10	ASN
5	C	15	ILE
5	C	67	ALA
5	C	113	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	114	GLY
5	C	163	ASN
5	C	189	ASP
6	D	71	LYS
6	D	119	PRO
9	G	34	PRO
11	I	91	ASP
12	J	81	GLU
14	L	33	ARG
14	L	52	ALA
15	M	74	GLY
16	N	92	ARG
16	N	94	VAL
17	O	11	GLN
17	O	49	GLU
18	P	132	GLY
19	Q	62	ARG
19	Q	74	ASP
19	Q	89	GLU
20	R	14	LEU
20	R	83	LEU
20	R	87	GLU
20	R	96	LYS
21	S	88	TYR
21	S	128	ARG
22	T	74	LYS
23	U	27	ASP
26	Z	24	ALA
26	Z	37	HIS
3	A	54	ILE
3	A	55	GLY
5	C	13	ARG
5	C	18	PRO
5	C	194	GLU
6	D	40	LEU
7	E	19	ALA
7	E	65	HIS
8	F	118	GLY
9	G	159	SER
11	I	59	ARG
11	I	65	PHE
11	I	90	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	J	17	ARG
12	J	29	ALA
13	K	95	THR
14	L	60	LYS
17	O	31	ASP
17	O	36	LYS
17	O	78	VAL
19	Q	87	SER
20	R	63	THR
21	S	33	ALA
21	S	74	ARG
22	T	13	GLY
22	T	27	GLY
3	A	247	VAL
3	A	255	LYS
4	B	90	SER
5	C	55	GLY
5	C	68	ARG
7	E	7	GLN
7	E	55	PRO
7	E	92	VAL
11	I	37	GLN
11	I	115	SER
12	J	21	ASP
14	L	53	ALA
17	O	30	GLY
20	R	6	ALA
20	R	108	VAL
23	U	26	ALA
23	U	47	HIS
25	W	14	GLY
3	A	187	SER
4	B	137	ARG
5	C	126	ALA
9	G	165	VAL
11	I	86	THR
13	K	93	GLY
14	L	39	TYR
16	N	65	ILE
18	P	20	LEU
20	R	50	GLY
21	S	125	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	U	12	ASN
9	G	68	PRO
12	J	28	VAL
20	R	51	VAL
7	E	126	PRO
8	F	96	VAL
11	I	9	THR
21	S	174	PRO
8	F	120	VAL
20	R	111	GLY
3	A	270	ILE
9	G	138	GLY
19	Q	66	GLY
23	U	14	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	145 (78%)	40 (22%)	1	10
4	B	155/157 (99%)	119 (77%)	36 (23%)	1	8
5	C	157/163 (96%)	112 (71%)	45 (29%)	0	4
6	D	153/156 (98%)	130 (85%)	23 (15%)	4	27
7	E	136/144 (94%)	115 (85%)	21 (15%)	4	25
8	F	51/107 (48%)	49 (96%)	2 (4%)	43	85
9	G	118/146 (81%)	94 (80%)	24 (20%)	2	11
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	9
11	I	108/121 (89%)	79 (73%)	29 (27%)	1	5
12	J	110/115 (96%)	89 (81%)	21 (19%)	2	14
13	K	90/93 (97%)	76 (84%)	14 (16%)	4	25
14	L	74/82 (90%)	51 (69%)	23 (31%)	0	4
15	M	94/134 (70%)	71 (76%)	23 (24%)	1	7
16	N	96/97 (99%)	76 (79%)	20 (21%)	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	O	75/79 (95%)	56 (75%)	19 (25%)	1	7
18	P	109/115 (95%)	91 (84%)	18 (16%)	3	22
19	Q	75/76 (99%)	60 (80%)	15 (20%)	2	12
20	R	91/96 (95%)	75 (82%)	16 (18%)	3	18
21	S	149/192 (78%)	117 (78%)	32 (22%)	1	10
22	T	62/67 (92%)	53 (86%)	9 (14%)	5	28
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	1
24	V	54/55 (98%)	43 (80%)	11 (20%)	2	11
25	W	48/48 (100%)	37 (77%)	11 (23%)	1	8
26	Z	51/53 (96%)	41 (80%)	10 (20%)	2	13
30	4	35/35 (100%)	29 (83%)	6 (17%)	3	20
All	All	2436/2715 (90%)	1921 (79%)	515 (21%)	1	10

All (515) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	37	LEU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	46	ARG
3	A	48	ARG
3	A	49	ILE
3	A	52	ARG
3	A	63	ARG
3	A	68	LYS
3	A	69	ARG
3	A	88	ARG
3	A	96	HIS
3	A	105	ILE
3	A	111	LEU
3	A	118	ASN
3	A	131	LEU
3	A	145	LEU
3	A	157	ARG
3	A	162	SER
3	A	169	GLU
3	A	183	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	186	HIS
3	A	196	VAL
3	A	203	ASN
3	A	208	LYS
3	A	212	SER
3	A	218	LYS
3	A	222	ARG
3	A	226	MET
3	A	240	THR
3	A	244	ARG
3	A	245	VAL
3	A	247	VAL
3	A	248	THR
3	A	250	TRP
3	A	252	LYS
3	A	254	THR
3	A	259	THR
3	A	270	ILE
4	B	2	LYS
4	B	4	ILE
4	B	5	LEU
4	B	14	ILE
4	B	27	LEU
4	B	34	VAL
4	B	35	GLN
4	B	37	LYS
4	B	41	THR
4	B	49	ILE
4	B	69	LYS
4	B	72	VAL
4	B	75	THR
4	B	103	ASP
4	B	107	THR
4	B	113	THR
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	136	ARG
4	B	137	ARG
4	B	140	SER
4	B	141	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	145	LYS
4	B	149	ARG
4	B	150	VAL
4	B	152	LYS
4	B	154	LYS
4	B	162	MET
4	B	163	GLU
4	B	165	VAL
4	B	192	ASN
4	B	198	LEU
4	B	200	SER
4	B	203	LYS
5	C	3	GLN
5	C	7	ILE
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	45	THR
5	C	48	ARG
5	C	51	VAL
5	C	52	SER
5	C	53	LYS
5	C	59	TYR
5	C	64	THR
5	C	66	ASN
5	C	71	ASP
5	C	72	ARG
5	C	76	THR
5	C	89	ARG
5	C	91	TYR
5	C	94	THR
5	C	95	LEU
5	C	97	ARG
5	C	118	VAL
5	C	121	ASP
5	C	123	PHE
5	C	124	ASP
5	C	127	ASP
5	C	130	THR
5	C	134	ILE
5	C	136	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	138	LYS
5	C	140	ASN
5	C	143	ASP
5	C	148	VAL
5	C	151	VAL
5	C	153	ASP
5	C	154	ASP
5	C	162	ARG
5	C	164	VAL
5	C	166	TRP
5	C	175	VAL
5	C	180	ILE
5	C	181	LEU
5	C	188	ILE
5	C	194	GLU
6	D	11	GLN
6	D	33	LYS
6	D	40	LEU
6	D	45	GLU
6	D	57	LEU
6	D	60	ILE
6	D	63	GLN
6	D	67	ILE
6	D	71	LYS
6	D	80	ARG
6	D	89	VAL
6	D	95	ARG
6	D	112	ARG
6	D	115	ARG
6	D	125	ARG
6	D	130	LEU
6	D	134	GLU
6	D	136	LEU
6	D	148	LYS
6	D	150	ARG
6	D	153	ASP
6	D	171	GLN
6	D	175	LEU
7	E	15	VAL
7	E	21	ASP
7	E	35	VAL
7	E	40	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	44	ARG
7	E	50	LEU
7	E	59	GLN
7	E	67	LEU
7	E	69	ARG
7	E	72	VAL
7	E	81	ASP
7	E	86	ASN
7	E	97	LYS
7	E	98	LEU
7	E	121	VAL
7	E	130	ARG
7	E	133	VAL
7	E	139	GLN
7	E	140	LEU
7	E	141	VAL
7	E	155	ASP
8	F	78	ILE
8	F	101	TRP
9	G	31	THR
9	G	38	GLU
9	G	41	TRP
9	G	56	THR
9	G	61	ARG
9	G	62	ILE
9	G	63	ARG
9	G	70	PHE
9	G	75	ILE
9	G	91	THR
9	G	95	LEU
9	G	101	THR
9	G	102	ARG
9	G	104	THR
9	G	112	THR
9	G	113	GLU
9	G	116	ARG
9	G	122	HIS
9	G	132	PHE
9	G	137	LYS
9	G	145	HIS
9	G	154	GLU
9	G	165	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	G	168	THR
10	H	1	MET
10	H	7	ARG
10	H	9	ASP
10	H	10	VAL
10	H	23	ARG
10	H	29	ILE
10	H	41	ASN
10	H	57	ASP
10	H	83	ARG
10	H	85	ASP
10	H	88	THR
10	H	89	ILE
10	H	90	ARG
10	H	94	ASN
10	H	102	GLN
10	H	106	ARG
10	H	109	ARG
10	H	116	ARG
10	H	117	GLU
10	H	119	ARG
10	H	124	MET
10	H	126	ILE
10	H	127	VAL
11	I	4	HIS
11	I	6	LEU
11	I	13	ARG
11	I	18	ARG
11	I	21	ARG
11	I	26	THR
11	I	29	THR
11	I	32	ARG
11	I	39	SER
11	I	40	ARG
11	I	45	LYS
11	I	50	GLU
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	60	LEU
11	I	62	LYS
11	I	65	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	I	77	LEU
11	I	78	SER
11	I	83	LEU
11	I	85	ASP
11	I	86	THR
11	I	93	LEU
11	I	98	LEU
11	I	99	VAL
11	I	101	ARG
11	I	108	LEU
11	I	142	LEU
12	J	7	ARG
12	J	8	THR
12	J	11	ARG
12	J	17	ARG
12	J	32	ASP
12	J	43	ILE
12	J	44	LYS
12	J	52	ARG
12	J	54	VAL
12	J	64	LYS
12	J	73	LYS
12	J	81	GLU
12	J	93	TYR
12	J	94	TRP
12	J	95	VAL
12	J	120	ARG
12	J	126	LEU
12	J	129	GLN
12	J	131	LYS
12	J	134	LYS
12	J	140	GLU
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	51	LEU
13	K	60	LEU
13	K	73	LYS
13	K	83	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	K	94	TYR
13	K	99	ARG
13	K	109	THR
13	K	115	LEU
14	L	8	ARG
14	L	11	LEU
14	L	12	ARG
14	L	13	THR
14	L	15	ARG
14	L	18	ARG
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS
14	L	37	HIS
14	L	43	ILE
14	L	64	LYS
14	L	66	ASP
14	L	67	THR
14	L	87	VAL
14	L	88	VAL
14	L	89	PHE
14	L	90	ASP
14	L	91	ARG
14	L	93	SER
14	L	94	TYR
14	L	99	ARG
14	L	108	ARG
15	M	5	ILE
15	M	6	LYS
15	M	7	ILE
15	M	12	LEU
15	M	13	LEU
15	M	14	ARG
15	M	31	ASP
15	M	34	ARG
15	M	35	VAL
15	M	40	ARG
15	M	54	VAL
15	M	57	ILE
15	M	63	ARG
15	M	68	VAL
15	M	69	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	M	78	GLU
15	M	79	ARG
15	M	89	ASN
15	M	93	ILE
15	M	95	GLU
15	M	98	LYS
15	M	99	VAL
15	M	100	ARG
16	N	3	ARG
16	N	5	LYS
16	N	8	ILE
16	N	9	VAL
16	N	13	ARG
16	N	18	LEU
16	N	22	LYS
16	N	25	TRP
16	N	40	LEU
16	N	51	ARG
16	N	58	ARG
16	N	60	LEU
16	N	71	LEU
16	N	88	ILE
16	N	90	LEU
16	N	92	ARG
16	N	93	LYS
16	N	95	LEU
16	N	102	GLU
16	N	111	ASP
17	O	13	ARG
17	O	18	ASP
17	O	20	ILE
17	O	21	ARG
17	O	22	VAL
17	O	25	LEU
17	O	26	GLN
17	O	28	GLU
17	O	39	PHE
17	O	40	VAL
17	O	46	VAL
17	O	47	PHE
17	O	50	ASP
17	O	56	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	O	62	GLU
17	O	69	ILE
17	O	76	SER
17	O	78	VAL
17	O	88	GLN
18	P	9	ARG
18	P	11	LYS
18	P	32	ARG
18	P	60	ILE
18	P	62	ARG
18	P	71	VAL
18	P	72	LEU
18	P	84	GLU
18	P	86	LEU
18	P	87	GLU
18	P	91	PHE
18	P	109	ARG
18	P	111	ARG
18	P	113	SER
18	P	118	LYS
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
19	Q	7	LEU
19	Q	12	ILE
19	Q	14	GLU
19	Q	26	SER
19	Q	38	ILE
19	Q	40	ASP
19	Q	42	ILE
19	Q	56	MET
19	Q	58	VAL
19	Q	63	LYS
19	Q	65	VAL
19	Q	67	ARG
19	Q	81	ARG
19	Q	82	LEU
19	Q	84	GLU
20	R	13	LYS
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R	26	SER
20	R	80	LYS
20	R	81	VAL
20	R	87	GLU
20	R	88	THR
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
20	R	112	LYS
20	R	113	THR
21	S	2	GLU
21	S	13	LYS
21	S	14	LEU
21	S	15	ASP
21	S	22	VAL
21	S	24	TYR
21	S	26	LYS
21	S	41	ARG
21	S	46	GLN
21	S	48	THR
21	S	51	LEU
21	S	53	ASP
21	S	54	ILE
21	S	65	LEU
21	S	66	VAL
21	S	67	LYS
21	S	71	MET
21	S	76	ARG
21	S	79	ILE
21	S	94	VAL
21	S	95	SER
21	S	113	VAL
21	S	120	LEU
21	S	128	ARG
21	S	132	GLN
21	S	133	GLU
21	S	139	THR
21	S	152	ILE
21	S	155	PRO
21	S	160	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	S	163	ASP
21	S	166	LEU
22	T	5	LYS
22	T	16	SER
22	T	17	ASN
22	T	41	ARG
22	T	46	LYS
22	T	49	GLN
22	T	62	LEU
22	T	64	ASP
22	T	85	GLN
23	U	8	THR
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	23	LYS
23	U	32	ARG
23	U	37	ILE
23	U	40	ARG
23	U	42	GLN
23	U	43	ARG
23	U	45	ASN
23	U	47	HIS
23	U	52	ARG
23	U	57	VAL
23	U	62	LEU
23	U	63	SER
23	U	65	ASN
23	U	70	LEU
23	U	75	TYR
23	U	78	ILE
23	U	79	GLU
24	V	6	MET
24	V	7	ARG
24	V	13	ASP
24	V	14	PHE
24	V	21	ARG
24	V	25	LEU
24	V	28	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	V	41	HIS
24	V	53	LEU
24	V	60	LEU
24	V	65	GLU
25	W	4	LYS
25	W	6	VAL
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	26	ARG
25	W	32	ARG
25	W	34	VAL
25	W	36	ASP
25	W	37	THR
25	W	46	THR
26	Z	3	LYS
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	14	SER
26	Z	18	MET
26	Z	25	LEU
26	Z	35	GLN
26	Z	40	LYS
26	Z	57	VAL
30	4	2	LYS
30	4	9	LYS
30	4	14	CYS
30	4	17	VAL
30	4	25	VAL
30	4	30	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	ASN
3	A	118	ASN
3	A	201	HIS
3	A	231	HIS
4	B	129	HIS
4	B	180	ASN
5	C	61	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	66	ASN
5	C	98	GLN
5	C	140	ASN
5	C	176	ASN
6	D	63	GLN
6	D	129	ASN
7	E	18	ASN
7	E	59	GLN
7	E	65	HIS
7	E	86	ASN
9	G	73	ASN
9	G	76	GLN
10	H	41	ASN
11	I	34	HIS
11	I	37	GLN
12	J	46	ASN
12	J	129	GLN
13	K	13	ASN
14	L	41	GLN
14	L	49	GLN
15	M	58	ASN
15	M	90	GLN
16	N	31	GLN
16	N	66	ASN
16	N	75	ASN
17	O	6	GLN
17	O	11	GLN
17	O	79	GLN
17	O	88	GLN
18	P	78	ASN
18	P	81	HIS
18	P	115	ASN
19	Q	43	GLN
19	Q	44	GLN
19	Q	57	ASN
20	R	10	HIS
20	R	15	HIS
20	R	29	HIS
20	R	44	GLN
20	R	64	ASN
20	R	71	GLN
21	S	80	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	S	119	ASN
22	T	3	HIS
22	T	17	ASN
22	T	35	ASN
22	T	49	GLN
22	T	71	ASN
23	U	56	GLN
25	W	54	GLN
26	Z	23	HIS
26	Z	43	HIS
26	Z	44	HIS
26	Z	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	701 (26%)	250 (9%)
2	Y	121/123 (98%)	41 (33%)	12 (9%)
All	All	2804/3003 (93%)	742 (26%)	262 (9%)

All (742) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	13	A
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	54	G
1	X	62	U
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	73	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	84	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	97	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	107	G
1	X	108	G
1	X	111	G
1	X	112	U
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A
1	X	127	C
1	X	129	A
1	X	136	A
1	X	137	A
1	X	138	G
1	X	143	A
1	X	147	G
1	X	154	U
1	X	157	G
1	X	158	A
1	X	173	A
1	X	174	A
1	X	176	A
1	X	177	U
1	X	181	A
1	X	182	G
1	X	191	G
1	X	192	G
1	X	193	A
1	X	199	A
1	X	203	G
1	X	205	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	206	U
1	X	207	U
1	X	209	G
1	X	219	G
1	X	225	G
1	X	227	G
1	X	228	A
1	X	229	G
1	X	238	G
1	X	239	A
1	X	241	C
1	X	242	A
1	X	243	G
1	X	245	C
1	X	246	C
1	X	248	A
1	X	310	A
1	X	312	G
1	X	319	G
1	X	321	A
1	X	322	A
1	X	323	G
1	X	332	C
1	X	333	A
1	X	334	G
1	X	335	A
1	X	338	G
1	X	340	G
1	X	342	G
1	X	343	A
1	X	349	G
1	X	358	C
1	X	360	A
1	X	361	G
1	X	388	G
1	X	396	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	409	G
1	X	411	C
1	X	414	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	416	U
1	X	417	C
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	433	G
1	X	441	A
1	X	455	A
1	X	456	C
1	X	458	G
1	X	459	A
1	X	461	A
1	X	463	C
1	X	467	U
1	X	468	A
1	X	469	G
1	X	470	U
1	X	484	G
1	X	490	A
1	X	492	G
1	X	495	C
1	X	504	G
1	X	506	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	522	G
1	X	523	A
1	X	534	U
1	X	539	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	557	U
1	X	558	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	559	C
1	X	560	G
1	X	572	G
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	596	C
1	X	597	U
1	X	601	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	623	G
1	X	625	A
1	X	627	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	636	G
1	X	645	G
1	X	648	A
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A
1	X	657	A
1	X	658	G
1	X	664	C
1	X	665	A
1	X	667	U
1	X	668	A
1	X	677	G
1	X	681	A
1	X	683	A
1	X	684	C
1	X	690	A
1	X	695	G
1	X	697	G
1	X	699	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	700	C
1	X	703	A
1	X	717	G
1	X	723	C
1	X	725	C
1	X	727	U
1	X	728	G
1	X	729	A
1	X	730	C
1	X	731	A
1	X	732	G
1	X	739	G
1	X	742	G
1	X	743	A
1	X	751	G
1	X	753	U
1	X	754	G
1	X	760	U
1	X	777	A
1	X	778	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	801	A
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	814	G
1	X	815	A
1	X	816	U
1	X	818	G
1	X	824	U
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	842	A
1	X	843	G
1	X	859	U
1	X	860	U
1	X	872	G
1	X	879	A
1	X	883	A
1	X	886	A
1	X	891	A
1	X	919	U
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	941	U
1	X	943	U
1	X	944	A
1	X	952	A
1	X	956	A
1	X	957	G
1	X	967	G
1	X	968	C
1	X	969	U
1	X	970	A
1	X	972	C
1	X	979	A
1	X	984	A
1	X	985	G
1	X	994	A
1	X	995	A
1	X	996	C
1	X	998	C
1	X	1001	A
1	X	1002	C
1	X	1006	C
1	X	1007	A
1	X	1010	U
1	X	1014	G
1	X	1016	C
1	X	1019	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1020	A
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1028	G
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1053	G
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1068	A
1	X	1069	G
1	X	1072	U
1	X	1073	G
1	X	1077	U
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	1101	U
1	X	1108	U
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1125	G
1	X	1127	C
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1141	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1161	U
1	X	1168	G
1	X	1182	U
1	X	1184	G
1	X	1185	C
1	X	1186	G
1	X	1187	A
1	X	1189	G
1	X	1192	A
1	X	1194	U
1	X	1209	G
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1250	A
1	X	1251	G
1	X	1261	G
1	X	1262	U
1	X	1263	G
1	X	1264	C
1	X	1266	G
1	X	1269	G
1	X	1282	A
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1302	C
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1319	C
1	X	1326	U
1	X	1334	A
1	X	1342	U
1	X	1345	G
1	X	1346	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1353	A
1	X	1354	A
1	X	1357	U
1	X	1358	C
1	X	1359	G
1	X	1365	U
1	X	1372	A
1	X	1378	A
1	X	1379	A
1	X	1381	G
1	X	1392	U
1	X	1399	C
1	X	1404	C
1	X	1409	U
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	1439	G
1	X	1440	G
1	X	1441	A
1	X	1442	C
1	X	1443	G
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	1474	A
1	X	1475	U
1	X	1476	G
1	X	1489	C
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1506	C
1	X	1508	G
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	1529	C
1	X	1531	C
1	X	1533	G
1	X	1545	G
1	X	1548	U
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	1582	A
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	1609	G
1	X	1613	G
1	X	1614	C
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	1635	G
1	X	1648	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1651	U
1	X	1656	U
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1685	A
1	X	1686	A
1	X	1691	G
1	X	1695	U
1	X	1699	A
1	X	1710	U
1	X	1711	C
1	X	1713	G
1	X	1714	A
1	X	1717	A
1	X	1732	U
1	X	1733	U
1	X	1734	C
1	X	1746	A
1	X	1749	G
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1773	C
1	X	1776	A
1	X	1777	A
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1800	A
1	X	1801	C
1	X	1807	A
1	X	1808	C
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1813	A
1	X	1821	A
1	X	1825	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1830	C
1	X	1831	G
1	X	1839	A
1	X	1840	A
1	X	1852	G
1	X	1861	G
1	X	1867	A
1	X	1874	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	1921	A
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1937	G
1	X	1938	U
1	X	1939	U
1	X	1943	A
1	X	1946	U
1	X	1947	G
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1964	A
1	X	1965	U
1	X	1976	U
1	X	1980	A
1	X	2003	A
1	X	2006	G
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2033	C
1	X	2035	G
1	X	2038	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2063	A
1	X	2076	G
1	X	2078	G
1	X	2079	A
1	X	2089	C
1	X	2166	G
1	X	2171	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2193	C
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2214	G
1	X	2217	G
1	X	2218	G
1	X	2228	U
1	X	2229	G
1	X	2246	A
1	X	2247	A
1	X	2257	A
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2268	G
1	X	2283	G
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2289	A
1	X	2291	U
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2305	C
1	X	2306	A
1	X	2313	G
1	X	2315	A
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2330	G
1	X	2333	A
1	X	2340	C
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2374	C
1	X	2381	A
1	X	2385	U
1	X	2389	G
1	X	2396	C
1	X	2397	A
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2406	C
1	X	2407	G
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2415	G
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2438	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2447	G
1	X	2448	A
1	X	2453	C
1	X	2455	A
1	X	2457	A
1	X	2459	C
1	X	2461	G
1	X	2463	G
1	X	2466	G
1	X	2470	U
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2498	U
1	X	2499	C
1	X	2508	G
1	X	2514	G
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2552	C
1	X	2557	G
1	X	2561	G
1	X	2564	U
1	X	2565	C
1	X	2580	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2590	U
1	X	2591	C
1	X	2593	A
1	X	2594	U
1	X	2608	A
1	X	2609	G
1	X	2611	A
1	X	2613	A
1	X	2615	U
1	X	2616	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2618	A
1	X	2621	G
1	X	2633	A
1	X	2634	G
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	2706	U
1	X	2713	A
1	X	2718	A
1	X	2719	U
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2735	C
1	X	2737	A
1	X	2745	A
1	X	2758	A
1	X	2759	U
1	X	2760	G
1	X	2769	C
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2776	U
1	X	2778	U
1	X	2779	C
1	X	2780	A
1	X	2793	G
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2800	C
1	X	2808	U
1	X	2824	C
1	X	2825	A
1	X	2841	U
1	X	2843	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2861	A
1	X	2864	C
1	X	2866	A
1	X	2868	G
1	X	2877	A
2	Y	11	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	38	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	49	C
2	Y	52	G
2	Y	53	G
2	Y	54	U
2	Y	58	G
2	Y	59	A
2	Y	69	G
2	Y	75	A
2	Y	76	U
2	Y	77	G
2	Y	86	A
2	Y	88	C
2	Y	89	G
2	Y	90	C
2	Y	91	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	92	G
2	Y	99	G
2	Y	102	A
2	Y	106	U
2	Y	110	U
2	Y	111	C
2	Y	112	A
2	Y	115	G
2	Y	116	C
2	Y	123	U

All (262) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	33	C
1	X	34	U
1	X	48	A
1	X	61	U
1	X	62	U
1	X	70	A
1	X	71	A
1	X	73	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	173	A
1	X	176	A
1	X	181	A
1	X	190	A
1	X	198	A
1	X	204	A
1	X	242	A
1	X	247	A
1	X	312	G
1	X	321	A
1	X	322	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	332	C
1	X	333	A
1	X	334	G
1	X	339	U
1	X	341	A
1	X	342	G
1	X	343	A
1	X	387	A
1	X	396	U
1	X	399	G
1	X	400	U
1	X	408	U
1	X	416	U
1	X	417	C
1	X	425	A
1	X	447	U
1	X	454	G
1	X	458	G
1	X	466	A
1	X	467	U
1	X	469	G
1	X	513	A
1	X	522	G
1	X	539	A
1	X	540	G
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	582	G
1	X	583	C
1	X	596	C
1	X	631	G
1	X	648	A
1	X	657	A
1	X	664	C
1	X	672	C
1	X	682	G
1	X	683	A
1	X	687	G
1	X	698	A
1	X	717	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	731	A
1	X	765	C
1	X	775	U
1	X	777	A
1	X	788	G
1	X	802	A
1	X	803	C
1	X	806	A
1	X	813	A
1	X	824	U
1	X	840	U
1	X	841	G
1	X	842	A
1	X	858	G
1	X	859	U
1	X	878	C
1	X	883	A
1	X	886	A
1	X	925	U
1	X	938	G
1	X	939	C
1	X	943	U
1	X	956	A
1	X	969	U
1	X	970	A
1	X	972	C
1	X	995	A
1	X	1000	G
1	X	1019	U
1	X	1036	G
1	X	1037	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1072	U
1	X	1080	A
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A
1	X	1122	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1129	A
1	X	1139	A
1	X	1142	G
1	X	1143	A
1	X	1152	C
1	X	1185	C
1	X	1186	G
1	X	1191	G
1	X	1223	G
1	X	1249	G
1	X	1250	A
1	X	1266	G
1	X	1278	A
1	X	1288	A
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1333	G
1	X	1337	G
1	X	1345	G
1	X	1353	A
1	X	1357	U
1	X	1404	C
1	X	1409	U
1	X	1412	C
1	X	1433	A
1	X	1434	U
1	X	1439	G
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1467	U
1	X	1473	U
1	X	1474	A
1	X	1475	U
1	X	1489	C
1	X	1496	G
1	X	1508	G
1	X	1513	U
1	X	1562	G
1	X	1570	C
1	X	1574	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	1575	C
1	X	1583	A
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1607	A
1	X	1613	G
1	X	1618	U
1	X	1624	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1685	A
1	X	1686	A
1	X	1710	U
1	X	1711	C
1	X	1732	U
1	X	1749	G
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1791	C
1	X	1795	C
1	X	1799	A
1	X	1800	A
1	X	1810	U
1	X	1811	A
1	X	1820	G
1	X	1830	C
1	X	1839	A
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1937	G
1	X	1938	U
1	X	1953	A
1	X	1975	G
1	X	2018	G
1	X	2032	G
1	X	2075	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2165	A
1	X	2189	A
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	2295	C
1	X	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A
1	X	2314	A
1	X	2323	U
1	X	2343	C
1	X	2363	G
1	X	2370	G
1	X	2381	A
1	X	2396	C
1	X	2401	A
1	X	2409	A
1	X	2447	G
1	X	2482	A
1	X	2497	A
1	X	2508	G
1	X	2528	G
1	X	2545	A
1	X	2560	G
1	X	2561	G
1	X	2564	U
1	X	2580	C
1	X	2593	A
1	X	2608	A
1	X	2615	U
1	X	2660	C
1	X	2669	C
1	X	2691	C
1	X	2693	U
1	X	2731	G
1	X	2736	U
1	X	2758	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	2759	U
1	X	2770	A
1	X	2778	U
1	X	2795	A
1	X	2807	U
1	X	2808	U
1	X	2824	C
1	X	2832	G
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
2	Y	14	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	58	G
2	Y	86	A
2	Y	90	C
2	Y	92	G
2	Y	94	G
2	Y	111	C
2	Y	116	C
2	Y	117	G

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 [i](#)

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	1F4	X	2929	-	62,62,62	1.22	4 (6%)	95,95,95	3.39	47 (49%)

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	1F4	X	2929	-	-	0/74/119/119	0/3/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	C41-N40	4.34	1.39	1.33
32	X	2929	1F4	C52-C51	3.20	1.44	1.39
32	X	2929	1F4	C22-C9	2.46	1.58	1.52
32	X	2929	1F4	O46-C44	2.06	1.24	1.21

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C5-O17-C41	-13.94	99.90	108.91
32	X	2929	1F4	C51-C47-N45	-11.68	98.37	112.97
32	X	2929	1F4	C6-C5-C4	-6.73	102.72	110.30
32	X	2929	1F4	C4-N40-C41	-6.52	106.10	112.50
32	X	2929	1F4	C6-O10-C11	6.42	129.97	118.17
32	X	2929	1F4	C58-C49-C50	-6.27	104.57	110.73
32	X	2929	1F4	O43-C44-N45	5.96	117.96	111.02
32	X	2929	1F4	C22-C9-C7	-5.39	103.00	111.22
32	X	2929	1F4	C57-C49-C58	5.05	115.94	109.44
32	X	2929	1F4	C21-C14-C13	4.65	120.37	111.46
32	X	2929	1F4	C49-C50-N45	-4.63	99.00	104.37
32	X	2929	1F4	O17-C41-N40	4.51	112.94	109.39
32	X	2929	1F4	O43-C13-C14	4.43	119.16	107.48
32	X	2929	1F4	C48-C47-N45	4.42	107.03	102.95
32	X	2929	1F4	C9-C7-C2	-4.24	108.70	115.89
32	X	2929	1F4	C9-C8-C14	4.21	120.20	113.60
32	X	2929	1F4	O18-C9-C8	4.12	115.63	108.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	O42-C41-N40	-4.12	124.25	129.22
32	X	2929	1F4	C57-C49-C48	-4.04	105.87	111.23
32	X	2929	1F4	C22-C9-C8	-3.94	104.32	110.00
32	X	2929	1F4	C5-C4-N40	-3.61	95.86	99.92
32	X	2929	1F4	C54-N55-C56	3.61	123.32	116.85
32	X	2929	1F4	C21-C14-C8	3.58	120.06	112.86
32	X	2929	1F4	C51-C56-N55	-3.51	118.45	124.22
32	X	2929	1F4	O46-C44-N45	-3.44	120.22	124.31
32	X	2929	1F4	C2-C3-C1	3.32	125.24	118.99
32	X	2929	1F4	O20-C28-O29	-3.31	102.43	110.69
32	X	2929	1F4	C19-C2-C7	-3.25	104.01	109.97
32	X	2929	1F4	C7-C9-C8	2.97	113.41	110.03
32	X	2929	1F4	C28-O20-C8	-2.91	111.22	116.28
32	X	2929	1F4	C24-C5-C4	2.88	119.29	117.03
32	X	2929	1F4	O10-C6-C23	2.87	113.37	107.52
32	X	2929	1F4	C49-C48-C47	-2.87	101.42	105.36
32	X	2929	1F4	C16-C1-C4	-2.72	110.11	114.39
32	X	2929	1F4	C13-O43-C44	2.62	120.33	116.74
32	X	2929	1F4	C1-C4-N40	-2.61	108.63	113.13
32	X	2929	1F4	C28-O29-C30	-2.56	108.70	112.87
32	X	2929	1F4	C58-C49-C48	2.54	114.61	111.23
32	X	2929	1F4	C5-C4-C1	2.53	122.97	117.61
32	X	2929	1F4	C48-C47-C51	-2.51	108.23	113.43
32	X	2929	1F4	C24-C5-C6	2.50	116.81	112.22
32	X	2929	1F4	C31-C32-C33	2.44	113.61	110.12
32	X	2929	1F4	C23-C6-C5	-2.36	112.26	115.53
32	X	2929	1F4	O15-C3-C2	-2.24	116.59	121.15
32	X	2929	1F4	O17-C5-C6	2.22	109.37	105.02
32	X	2929	1F4	C50-N45-C47	-2.18	108.31	111.60
32	X	2929	1F4	C16-C1-C3	2.16	112.41	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	X	2686/2880 (93%)	-0.24	53 (1%) 62 36	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.22	3 (2%) 54 31	83, 135, 170, 191	0
3	A	240/274 (87%)	0.04	3 (1%) 74 47	68, 115, 146, 172	0
4	B	205/211 (97%)	-0.09	1 (0%) 88 71	45, 73, 105, 154	0
5	C	197/205 (96%)	0.08	5 (2%) 54 31	57, 114, 154, 187	0
6	D	177/180 (98%)	0.07	3 (1%) 67 40	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.19	0 100 100	92, 143, 192, 206	0
8	F	71/144 (49%)	1.26	13 (18%) 2 2	211, 236, 252, 257	0
9	G	142/174 (81%)	-0.07	0 100 100	72, 97, 144, 161	0
10	H	134/134 (100%)	-0.13	0 100 100	50, 70, 97, 121	0
11	I	141/156 (90%)	0.42	11 (7%) 13 8	67, 129, 174, 204	0
12	J	136/141 (96%)	0.45	6 (4%) 33 18	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.11	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	0.06	0 100 100	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.23	0 100 100	50, 73, 111, 145	0
16	N	117/118 (99%)	-0.14	0 100 100	59, 90, 128, 159	0
17	O	94/100 (94%)	-0.09	0 100 100	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.20	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	0.02	2 (2%) 59 34	73, 106, 162, 195	0
20	R	110/115 (95%)	0.08	4 (3%) 41 23	88, 117, 170, 178	0
21	S	175/237 (73%)	0.48	14 (8%) 12 8	121, 155, 175, 190	0
22	T	84/91 (92%)	0.46	10 (11%) 5 5	79, 107, 186, 200	0
23	U	72/81 (88%)	0.26	5 (6%) 17 9	92, 128, 153, 161	0
24	V	66/67 (98%)	0.25	5 (7%) 14 8	100, 132, 211, 216	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.14	1 (1%) 65 39	80, 98, 126, 152	0
26	Z	58/60 (96%)	0.03	2 (3%) 43 24	49, 70, 105, 114	0
27	1	53/55 (96%)	2.01	15 (28%) 1 1	8, 32, 62, 93	0
28	2	46/47 (97%)	4.61	40 (86%) 0 1	3, 15, 38, 59	0
29	3	63/66 (95%)	2.74	35 (55%) 0 1	3, 25, 40, 61	0
30	4	37/37 (100%)	3.53	26 (70%) 0 1	228, 254, 266, 269	0
All	All	5997/6561 (91%)	0.04	257 (4%) 32 19	3, 100, 196, 276	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	19.9
30	4	25	VAL	10.6
28	2	37	LYS	10.0
28	2	27	GLY	9.8
24	V	1	MET	9.8
1	X	731	A	9.6
30	4	24	LEU	9.2
28	2	33	ARG	9.0
28	2	4	THR	8.8
29	3	42	ARG	8.7
28	2	22	MET	8.0
28	2	32	ALA	7.9
28	2	25	LYS	7.8
29	3	32	GLN	7.7
29	3	35	GLY	7.7
30	4	17	VAL	7.5
1	X	1089	C	7.4
28	2	8	ASN	7.3
28	2	24	THR	7.2
28	2	23	LYS	7.1
29	3	8	LYS	6.9
29	3	31	HIS	6.8
27	1	44	ALA	6.8
27	1	26	LYS	6.7
27	1	25	THR	6.5
2	Y	123	U	6.5
28	2	11	LYS	6.5
1	X	1091	C	6.4
27	1	43	VAL	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	X	1067	G	6.3
29	3	22	VAL	6.3
28	2	36	ALA	6.2
30	4	32	HIS	6.2
28	2	7	PRO	6.2
28	2	38	GLY	6.0
22	T	9	SER	5.9
30	4	34	GLN	5.8
11	I	9	THR	5.6
28	2	9	ASN	5.6
27	1	24	THR	5.6
12	J	84	MET	5.6
28	2	6	GLN	5.4
1	X	1106	A	5.4
1	X	1079	G	5.4
28	2	28	ARG	5.4
29	3	2	PRO	5.4
30	4	29	ASN	5.4
28	2	13	ALA	5.3
30	4	35	ARG	5.3
1	X	1090	C	5.3
30	4	22	ARG	5.1
28	2	5	TYR	5.1
27	1	23	THR	5.0
28	2	29	ASN	5.0
29	3	10	ALA	5.0
8	F	98	LYS	5.0
28	2	2	LYS	5.0
28	2	26	SER	4.9
29	3	6	THR	4.9
1	X	1086	C	4.9
1	X	248	A	4.9
30	4	19	ARG	4.9
26	Z	2	ALA	4.8
30	4	16	VAL	4.7
11	I	8	PRO	4.7
1	X	2776	U	4.7
11	I	4	HIS	4.6
28	2	16	HIS	4.5
1	X	1068	A	4.5
30	4	27	CYS	4.4
29	3	40	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	F	137	THR	4.3
29	3	51	ALA	4.2
28	2	20	ALA	4.1
1	X	1107	A	4.1
30	4	23	VAL	4.1
29	3	63	PRO	4.1
11	I	52	GLY	4.0
29	3	9	MET	4.0
19	Q	64	ARG	4.0
29	3	7	HIS	4.0
1	X	1109	A	3.9
28	2	15	THR	3.9
3	A	203	ASN	3.8
29	3	36	LYS	3.8
1	X	1078	A	3.8
30	4	20	HIS	3.8
29	3	60	LEU	3.7
28	2	41	GLN	3.7
30	4	28	SER	3.7
30	4	36	GLN	3.7
28	2	40	HIS	3.6
29	3	33	ASN	3.6
30	4	21	GLY	3.6
1	X	1077	U	3.6
1	X	1099	A	3.6
30	4	10	MET	3.6
1	X	2289	A	3.6
29	3	3	LYS	3.6
22	T	10	SER	3.5
8	F	125	ASN	3.5
29	3	59	LYS	3.5
6	D	145	MET	3.5
3	A	250	TRP	3.5
29	3	34	THR	3.4
29	3	64	ARG	3.4
11	I	29	THR	3.4
24	V	2	LYS	3.4
4	B	205	SER	3.4
11	I	10	PRO	3.3
30	4	6	SER	3.3
24	V	3	PRO	3.3
22	T	8	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	S	23	ALA	3.2
28	2	19	ARG	3.2
11	I	5	ASP	3.2
11	I	6	LEU	3.2
12	J	85	GLY	3.2
1	X	730	C	3.2
30	4	18	ARG	3.2
27	1	11	LYS	3.2
8	F	84	ILE	3.2
1	X	1084	A	3.2
27	1	47	HIS	3.2
1	X	2169	A	3.1
23	U	27	ASP	3.1
5	C	47	THR	3.1
1	X	1104	G	3.1
1	X	1186	G	3.1
8	F	121	GLU	3.1
21	S	24	TYR	3.1
30	4	14	CYS	3.0
1	X	891	A	3.0
1	X	1073	G	3.0
1	X	1094	C	3.0
21	S	165	GLU	3.0
30	4	11	CYS	3.0
1	X	2777	A	3.0
28	2	3	ARG	3.0
8	F	114	ASP	2.9
28	2	10	ARG	2.9
5	C	123	PHE	2.9
28	2	34	ARG	2.9
27	1	41	ASP	2.9
1	X	1085	G	2.9
12	J	82	THR	2.9
30	4	26	ILE	2.9
1	X	1080	A	2.9
20	R	99	VAL	2.9
5	C	197	GLU	2.9
20	R	100	ASP	2.9
29	3	18	GLY	2.8
1	X	2778	U	2.8
21	S	29	ASN	2.8
1	X	1088	A	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	1	46	LYS	2.7
28	2	12	ARG	2.7
28	2	43	THR	2.7
1	X	665	A	2.7
1	X	358	C	2.6
1	X	1093	U	2.6
30	4	7	VAL	2.6
1	X	1524	C	2.6
12	J	86	LYS	2.6
8	F	111	LYS	2.6
29	3	57	ARG	2.6
1	X	435	A	2.6
23	U	47	HIS	2.6
22	T	6	GLY	2.6
22	T	15	ASP	2.6
29	3	5	LYS	2.6
1	X	2174	G	2.5
23	U	25	ARG	2.5
28	2	30	ILE	2.5
29	3	27	SER	2.5
21	S	12	GLN	2.5
29	3	11	LYS	2.5
22	T	4	LYS	2.5
1	X	361	G	2.5
27	1	9	ILE	2.5
20	R	102	LYS	2.5
1	X	74	G	2.5
1	X	1098	G	2.5
6	D	146	VAL	2.5
27	1	31	THR	2.5
21	S	85	MET	2.5
12	J	81	GLU	2.5
3	A	261	ARG	2.5
1	X	728	G	2.5
1	X	225	G	2.5
1	X	1081	A	2.5
11	I	63	ARG	2.5
8	F	107	ILE	2.4
1	X	2329	C	2.4
27	1	22	TYR	2.4
28	2	31	LEU	2.4
22	T	11	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	2	21	ARG	2.4
8	F	108	ALA	2.4
29	3	39	ASP	2.4
26	Z	3	LYS	2.4
1	X	1951	G	2.4
22	T	20	TYR	2.4
29	3	4	MET	2.4
29	3	47	GLY	2.3
8	F	97	GLY	2.3
29	3	19	THR	2.3
11	I	96	TYR	2.3
21	S	27	GLU	2.3
8	F	99	LEU	2.3
21	S	28	ASN	2.3
11	I	33	GLY	2.2
29	3	55	TRP	2.2
1	X	1913	G	2.2
29	3	53	ALA	2.2
1	X	1114	A	2.2
30	4	33	LYS	2.2
22	T	5	LYS	2.2
28	2	42	LEU	2.2
1	X	727	U	2.2
30	4	12	ASP	2.2
1	X	1108	U	2.2
27	1	20	PHE	2.2
28	2	39	ARG	2.2
22	T	17	ASN	2.2
29	3	61	MET	2.2
1	X	169	C	2.1
23	U	28	GLY	2.1
28	2	1	MET	2.1
1	X	170	U	2.1
1	X	1087	C	2.1
20	R	98	ILE	2.1
2	Y	2	C	2.1
21	S	14	LEU	2.1
24	V	6	MET	2.1
1	X	1072	U	2.1
2	Y	68	A	2.1
21	S	11	LYS	2.1
29	3	26	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	U	39	LYS	2.1
21	S	164	PRO	2.1
12	J	90	ALA	2.1
21	S	15	ASP	2.1
5	C	48	ARG	2.1
21	S	143	ILE	2.1
8	F	112	MET	2.1
1	X	356	A	2.0
30	4	15	LYS	2.0
28	2	17	GLY	2.0
5	C	20	PRO	2.0
21	S	163	ASP	2.0
25	W	6	VAL	2.0
8	F	126	THR	2.0
19	Q	94	GLN	2.0
24	V	4	SER	2.0
6	D	43	SER	2.0
29	3	25	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	Y	203	1/1	1.04	134.09	59,59,59,59	0
31	MG	X	2912	1/1	0.65	109.67	71,71,71,71	0
31	MG	X	2921	1/1	0.68	76.20	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	2908	1/1	2.36	61.45	37,37,37,37	0
31	MG	X	2926	1/1	1.75	56.01	45,45,45,45	0
31	MG	X	2928	1/1	0.76	53.57	61,61,61,61	0
31	MG	X	2909	1/1	0.66	51.87	97,97,97,97	0
31	MG	X	2919	1/1	0.86	41.55	30,30,30,30	0
31	MG	X	2913	1/1	0.98	40.79	60,60,60,60	0
31	MG	X	2917	1/1	1.09	36.99	55,55,55,55	0
31	MG	M	201	1/1	1.34	32.55	23,23,23,23	0
31	MG	X	2920	1/1	0.65	30.81	113,113,113,113	0
31	MG	X	2924	1/1	1.21	27.74	70,70,70,70	0
31	MG	X	2918	1/1	1.28	26.91	42,42,42,42	0
31	MG	X	2916	1/1	1.15	25.06	37,37,37,37	0
31	MG	X	2905	1/1	0.50	24.26	65,65,65,65	0
31	MG	Y	204	1/1	1.00	22.71	86,86,86,86	0
31	MG	X	2903	1/1	0.62	22.17	89,89,89,89	0
31	MG	X	2907	1/1	0.83	21.72	51,51,51,51	0
31	MG	X	2927	1/1	0.59	21.40	64,64,64,64	0
31	MG	X	2915	1/1	0.72	17.75	57,57,57,57	0
31	MG	Y	202	1/1	1.50	17.40	88,88,88,88	0
31	MG	Y	206	1/1	0.32	15.69	78,78,78,78	0
31	MG	X	2901	1/1	0.61	14.84	50,50,50,50	0
31	MG	X	2910	1/1	0.68	14.76	41,41,41,41	0
31	MG	X	2906	1/1	0.98	14.02	58,58,58,58	0
31	MG	X	2922	1/1	0.81	10.50	44,44,44,44	0
31	MG	X	2911	1/1	0.29	6.53	68,68,68,68	0
31	MG	X	2923	1/1	0.36	5.84	34,34,34,34	0
31	MG	Y	205	1/1	0.42	5.30	82,82,82,82	0
31	MG	Y	201	1/1	0.40	3.88	98,98,98,98	0
31	MG	X	2904	1/1	0.29	3.65	110,110,110,110	0
31	MG	X	2914	1/1	0.59	3.59	27,27,27,27	0
31	MG	X	2902	1/1	0.37	2.93	94,94,94,94	0
32	1F4	X	2929	58/58	0.22	-0.18	20,20,20,20	0
31	MG	X	2925	1/1	0.13	-0.24	122,122,122,122	0

6.5 Other polymers ⓘ

There are no such residues in this entry.