



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:02 PM GMT

PDB ID : 3V27  
Title : Crystal structure of HPF bound to the 70S ribosome. This PDB entry contains coordinates for the 50S subunit of the 1st ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-11  
Resolution : 3.10 Å(reported)

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

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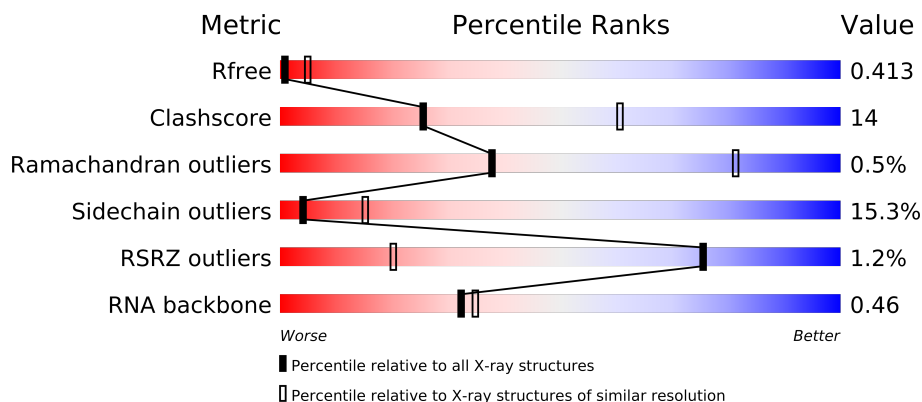
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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

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

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Mol	Chain	Length	Quality of chain
13	R	118	
14	S	112	
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92957 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2837	Total	C	N	O	P	0	0	0
			61112	27197	11440	19639	2836			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2135	1349	422	361	3			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1037	666	180	190	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	201	Total	C	N	O	S	0	0	0
			1536	980	272	282	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	1	Total	Mg	0	0
			1	1		
32	G	1	Total	Mg	0	0
			1	1		
32	Q	4	Total	Mg	0	0
			4	4		
32	D	3	Total	Mg	0	0
			3	3		
32	E	5	Total	Mg	0	0
			5	5		
32	B	23	Total	Mg	0	0
			23	23		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	V	1	Total 1	Mg 1	0	0
32	1	1	Total 1	Mg 1	0	0
32	W	2	Total 2	Mg 2	0	0
32	Z	1	Total 1	Mg 1	0	0
32	A	658	Total 658	Mg 658	0	0
32	T	2	Total 2	Mg 2	0	0
32	2	1	Total 1	Mg 1	0	0
32	5	2	Total 2	Mg 2	0	0
32	8	2	Total 2	Mg 2	0	0
32	0	1	Total 1	Mg 1	0	0
32	R	1	Total 1	Mg 1	0	0
32	9	1	Total 1	Mg 1	0	0
32	S	1	Total 1	Mg 1	0	0
32	F	2	Total 2	Mg 2	0	0

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

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

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	1678	Total 1678	O 1678	0	0
34	B	58	Total 58	O 58	0	0
34	D	18	Total 18	O 18	0	0
34	E	10	Total 10	O 10	0	0
34	F	7	Total 7	O 7	0	0
34	H	1	Total 1	O 1	0	0
34	N	2	Total 2	O 2	0	0
34	O	1	Total 1	O 1	0	0
34	P	10	Total 10	O 10	0	0
34	Q	4	Total 4	O 4	0	0
34	R	6	Total 6	O 6	0	0
34	T	1	Total 1	O 1	0	0
34	U	4	Total 4	O 4	0	0
34	V	3	Total 3	O 3	0	0
34	W	2	Total 2	O 2	0	0
34	X	2	Total 2	O 2	0	0
34	Y	3	Total 3	O 3	0	0
34	0	8	Total 8	O 8	0	0
34	1	2	Total 2	O 2	0	0
34	3	1	Total 1	O 1	0	0
34	5	5	Total 5	O 5	0	0

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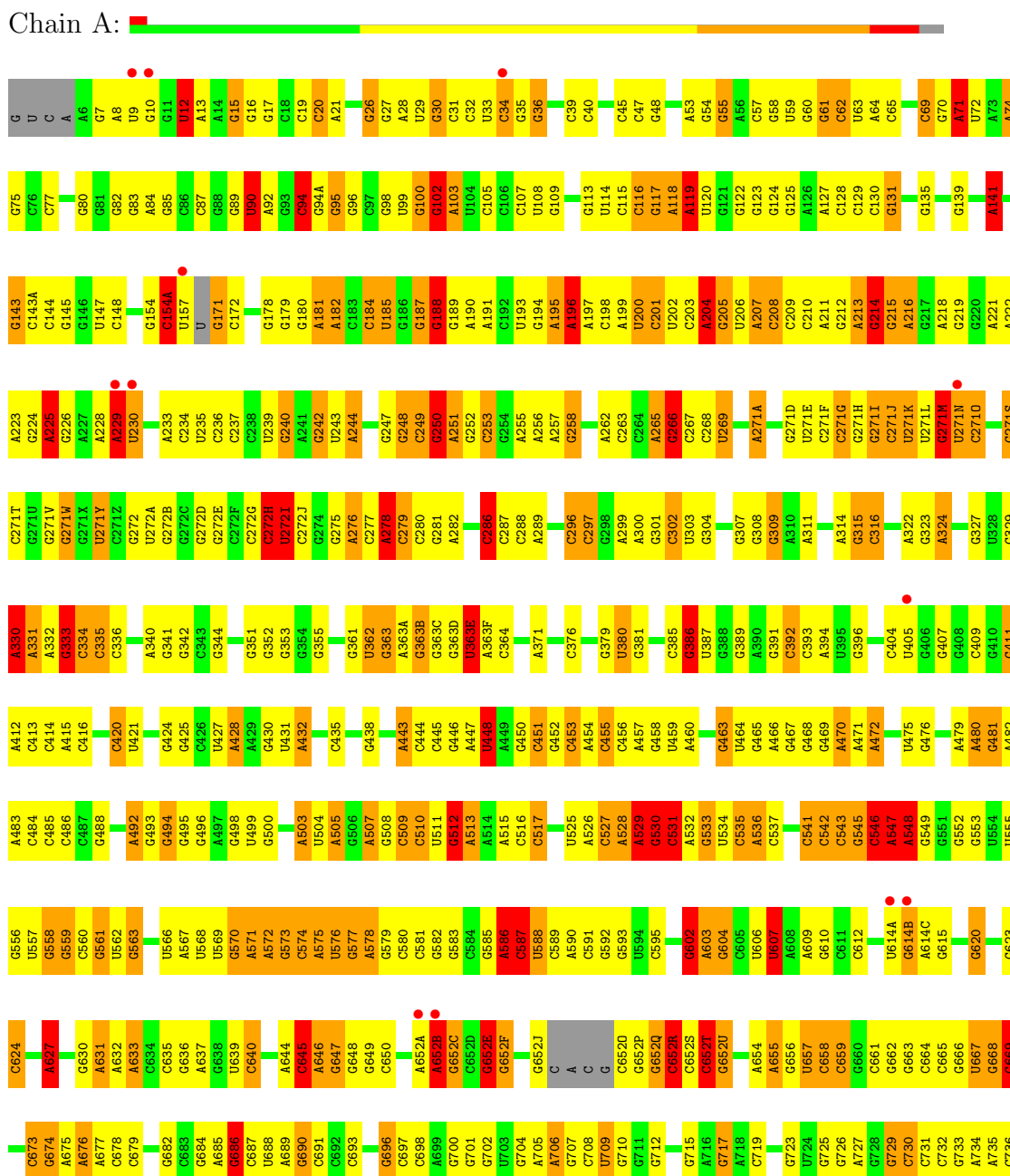
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	6	1	Total 1	O 1	0	0
34	7	3	Total 3	O 3	0	0
34	8	11	Total 11	O 11	0	0
34	9	1	Total 1	O 1	0	0

### 3 Residue-property plots

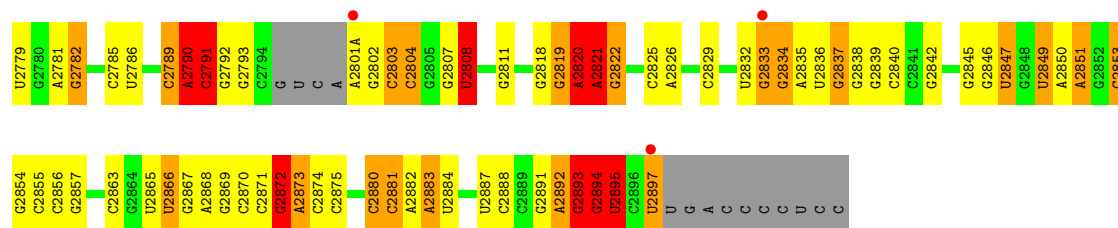
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 23S Ribosomal RNA



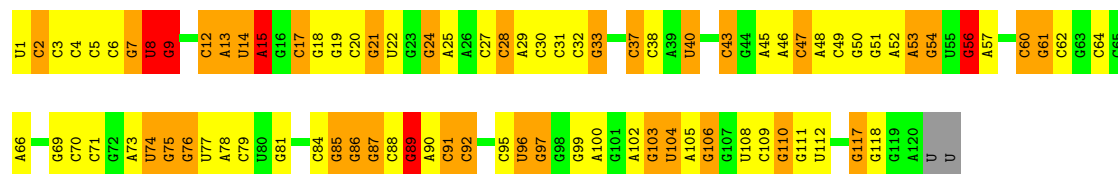
A1665	G1666	A1603	G1533	C1464	U1391	G1325	G1195	A1127	U	A1001	C936	G862	G798	C737
A1667	G1667	C1604	U1534	G1465	A1392	U1326	A1128	A1128	U	G1002	U937	A863	G799	G738
A1668	C1536	C1605	A1535	G1466	U1393	G1327	A1129	A1129	A	G1003	G938	G800	A800	G739
A1669	C1467	G1606	C1536	C1468	U1394	G1328	U1130	U1130	G	C1004	G939	G801	G939	
C1607	A1608	C1607	G1537	C1469	A1395	U1329	G1131	G1131	A	C1005	A941	U868	U802	G742
A1609	U1671	A1609	G1539	A1471	C1398	C1330	G1202	U1132	A	C1006	G942	G869	U803	G743
A1610	U1672	A1610	U1540	A1472	C1403	C1333	G1203	U1133	G	A1010	G943	A870	A804	G744
C1611	U1673	C1611	G1541	C1473	C1404	G1334	A1204	G1135	C	G1011	U944	G874	G805	G745
C1612	C1542	A1542	A1543	C1474	U1405	C1335	U1205	G1136	A	U1012	A945		C806	A746
C1613	C1675	G1613	C1543	C1475	U1406	U1336	G1206	G1137	G	U1013	G946		U807	U747
A1614	A1676	A1614	G1544	G1478	U1407	G1337	G1207	G1138	C	U1014	G947	G879	G808	G748
C1615		C1615	A1545	G1479	C1407	G1338	C1208	G1139	C	U1015	G948	G880	G809	C749
A1616		A1616	C1546		C1408	G1339	U1273	C1140	A	G1016	C949	G881	U810	A750
U1680	U1681	A1618	C1547	G1482	C1409	U1340	A1274	U1141	U	G1017	G950	G882	U811	A751
A1618	C1548	G1620	C1548	G1483	C1410	U1341	U1211	U1142	C	G1018	G951	G883	C812	A752
G1620	G1620	G1620	A1553	G1484	U1414	U1342	G1212	A1143	C	U1019	G952	G884	C815	C754
U1621	G1622	U1621	A1554	G1485	U1415	U1343	G1213	G1144	U	U1020	G953	C885	C816	C755
G1622	G1622	G1622	G1555	G1486	U1416	U1344	G1214	G1145	U	A1021	G954	C886	C817	C756
G1623	G1623	G1623	G1556	G1487	C1417	C1345	G1215		A	G1022	G955	C887	G818	C757
G1624	G1624	G1624	C1557	U1489	G1418	C1346	G1216	G1151	A	U1023	G956	C888	A819	C758
G1625	G1625	G1625	A1558	G1490	G1419	G1348	C1217	C1152	A	G1024	A957	C889	C820	G759
G1626	G1626	G1626	C1559	A1491	U1420	A1349	G1221A	C1153	G	G1025	U958	A890	A821	G760
G1627	G1627	G1627	G1560	C1494	G1421	C1350	G1222	G1154	A	U1026	A959	G892	U822	A761
G1628	G1628	G1628	G1561	A1495	G1422	C1351	G1223	A1155	G	A1027	A960	C893	G823	U762
U1629		U1629	G1562	A1496	G1423	U1352	G1224	A1156	U	A1028	C961	C894	A824	G763
A1631A		A1631A	C1564	U1497	G1424	G1356	G1225	G1157	G	A1029	G962	U895	C825	A764
A1632	A1632	A1632	C1565	A1498	U1425	U1357	G1226	C1158	C	G1030	U963	A896	U826	C766
A1633	A1633	A1633	A1566	C1499	G1426	G1358	G1227	U1159	G	G1031	G966	C897	U827	C767
A1634	A1634	A1634	C1567	A1500	A1428	A1359	G1228	G1160	U	A1032		C897	U828	U767
G1636	C1636	C1636	U1570	C1502	G1429	A1360	G1229	G1162	A	U1033	G967	A900	A829	G768
A1637	A1637	A1637	A1571	C1503	C1430	C1363	G1230	G1163	U	G1034	G968	C902	G830	G769
C1638	C1638	C1638	A1572	A1507	U1433	G1364	G1231	G1164	A	C1038	C970	C903	U831	G771
A1573	A1573	A1573	C1573	C1508	U1434	A1365	G1232	U1165	G	C1040	G972	C904	C834	U773
A1574	A1574	A1574	C1574	C1509	G1435	A1367	G1233	U1166	C	G1041	A973	U907	A835	A774
U1576	U1576	U1576	C1576	C1509	G1436	A1367	G1234	G1169	C	G1042	G974	C908	G836	G775
C1577	C1577	C1577	A1577	A1509A	C1437	G1368	G1235	G1170	A	C1043	C975	A909	C837	G776
U1578	U1578	U1578	C1578	C1509B	C1437	G1369	G1238	G1171	C	G1044	G975A	A910	C838	A777
A1579	A1579	A1579	C1579	G1510	G1441	G1370	A1241	G1173	U	A1045	G978	A911	U839	G778
A1580	A1580	A1580	C1580	C1511	G1442	U1372	A1242	A1174	G	A1046	G979	C912	C840	U779
G1581	G1581	G1581	C1581	U1512	G1443	A1373	G1243	U1175	G	G1047	A980	U913	U839	G780
C1582	C1582	C1582	U1514	C1513	G1444	G1374	G1244	G1176	G	A1048	A981	C914	A841	A781
A1583	A1583	A1583	G1517	G1517	A1445	C1375	G1245	A1177	C1109	C1049	C982	C915	C844	A782
A1584	A1584	A1584	C1376	C1376	C1446	G1377	G1246	C1178	G1110	A1050	G984	C916	G845	A783
A1585	A1585	A1585	G1377	G1377	A1447	A1378	G1247	C1179	G1112	C1052	A984	A917	U847	A784
A1586	A1586	A1586	A1378	A1378	G1448	G1379	G1248	C1180	U1113	C		G920	G848	C786
A1587	A1587	A1587	C1379	C1379	G1449	G1380	U1249	C1181	G1114	A	A988	G921	A849	U787
A1588	A1588	A1588	G1450	G1450	C1450A	G1381	G1250	C1184	G1115	G	G989	U922	A849	A788
G1593	G1593	G1593	C1451	C1451	C1452	G1382	C1251	C1185	G	A	G990	C923	C850	A789
A1594	A1594	A1594	U1526	U1526	G1453	G1383	G1252	G1186	C1116	G	C991	C924	G853	C790
C1595	C1595	C1595	G1527	G1527	C1384	C1383	A1253	G1187	G	C992	G993	G928	C856	G792
A1596	A1596	A1596	C1384	C1384	G1455	G1385	U1254	U1188	U	C994	C995	G932	C857	A793
C1597	C1597	C1597	A1528	A1528	G1456	G1386	U1255	U1189	G	C995	C996	G933	U858	G794
A1598	A1598	A1598	G1529	G1529	G1459	C1387	G1256	G1190	U	C996	C997	G934	G859	C795
C1599	C1599	C1599	C1530	C1530	A1460	C1388	C1257	G1193	G	C997	C998	U860	U860	C796
U1602	U1602	U1602	C1532	C1532	C1463	G1388	G1259	A1194	C			C935	A861	C797

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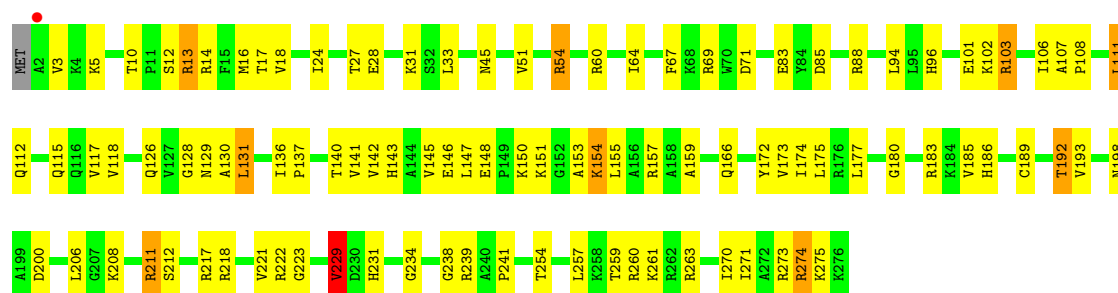
• Molecule 2: 5S Ribosomal RNA

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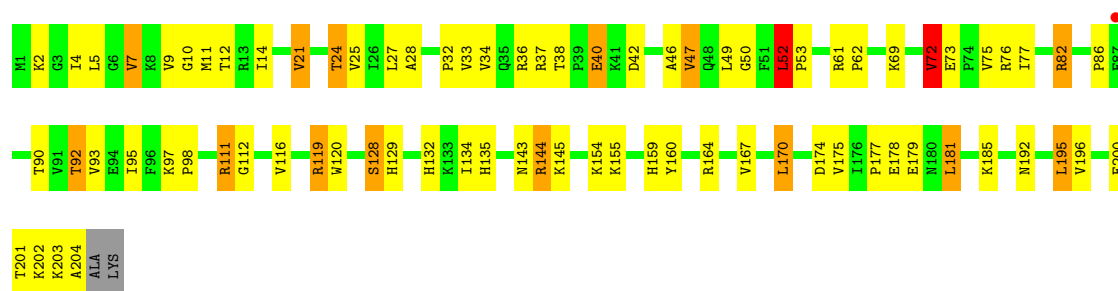
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



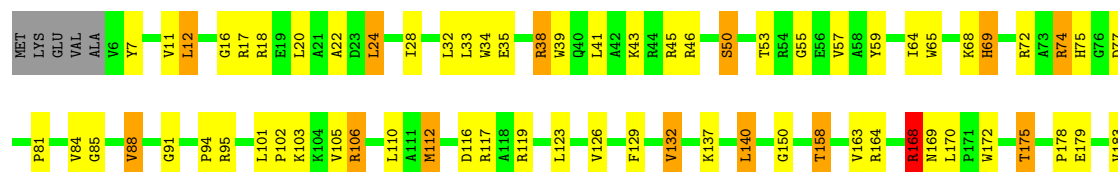
• Molecule 4: 50S Ribosomal Protein L3

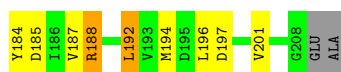
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• Molecule 5: 50S Ribosomal Protein L4

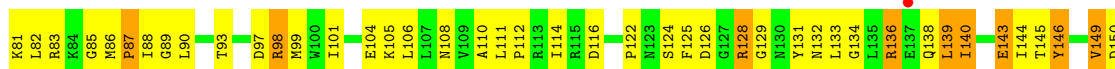
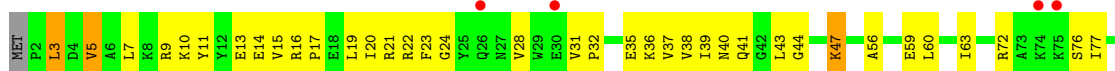
Chain F:





• Molecule 6: 50S Ribosomal Protein L5

Chain G:



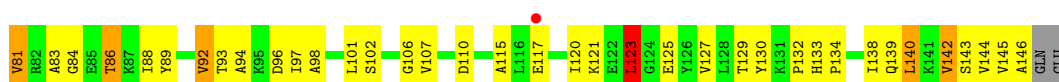
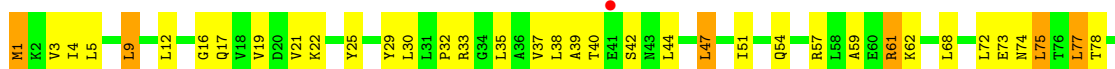
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



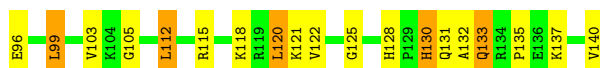
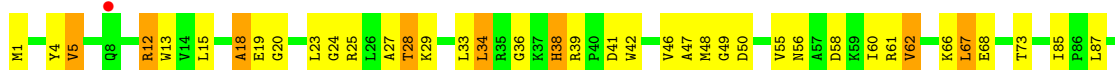
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



• Molecule 9: 50S Ribosomal Protein L13

Chain N:



• Molecule 10: 50S Ribosomal Protein L14

Chain O:

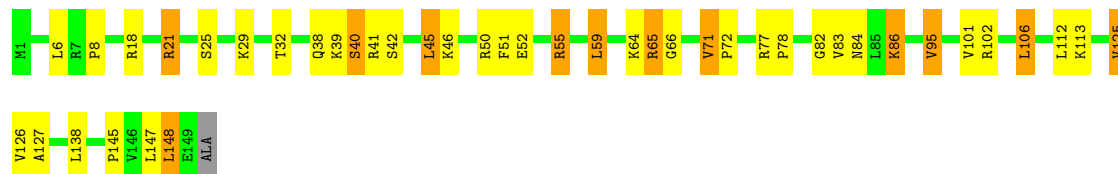






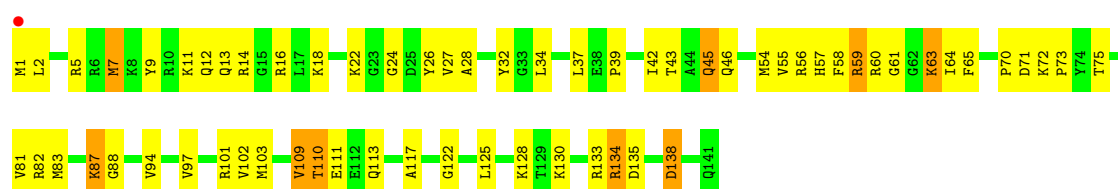
• Molecule 11: 50S Ribosomal Protein L15

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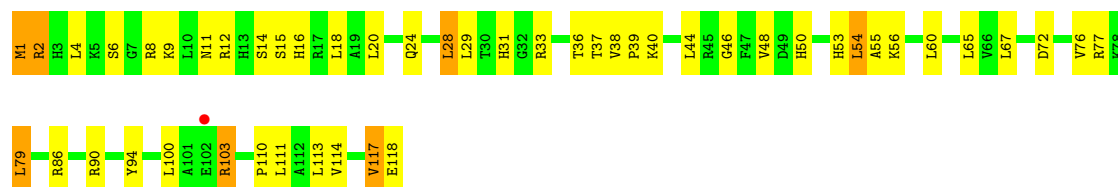
• Molecule 12: 50S Ribosomal Protein L16

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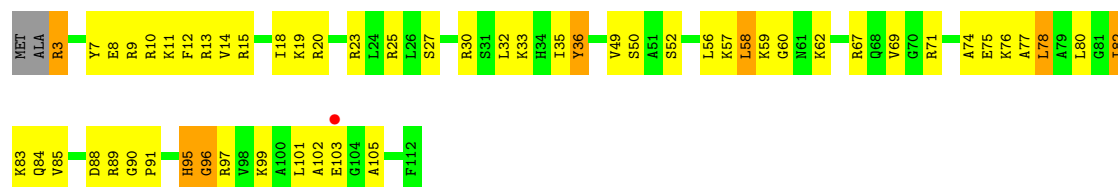
• Molecule 13: 50S Ribosomal Protein L17

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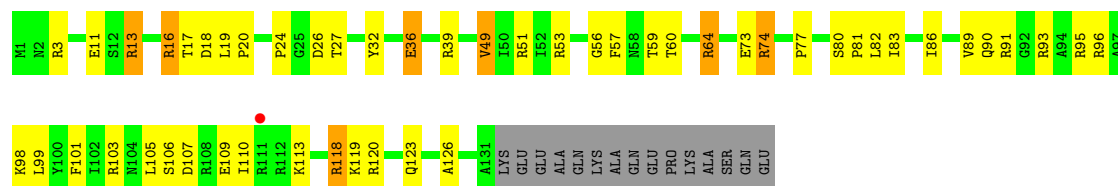
• Molecule 14: 50S Ribosomal Protein L18

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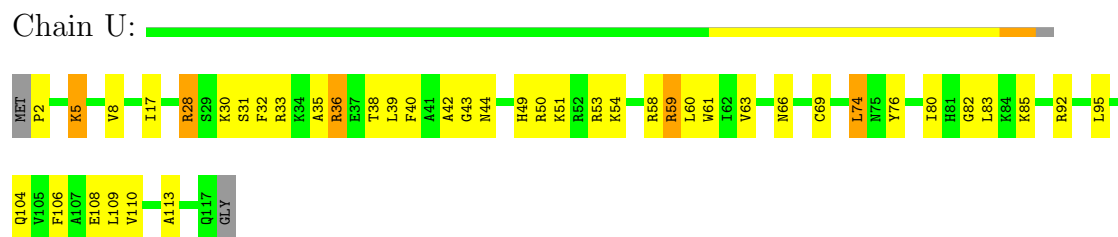


• Molecule 15: 50S Ribosomal Protein L19

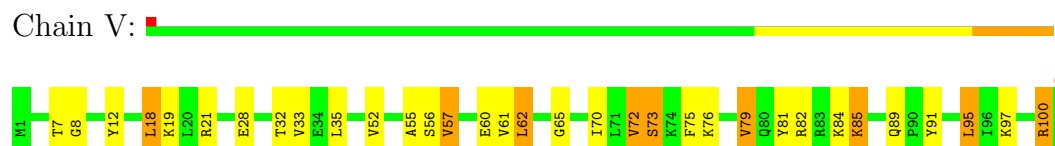
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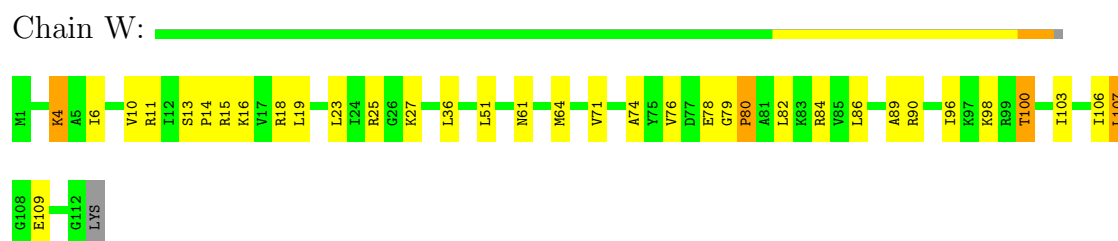
- Molecule 16: 50S Ribosomal Protein L20



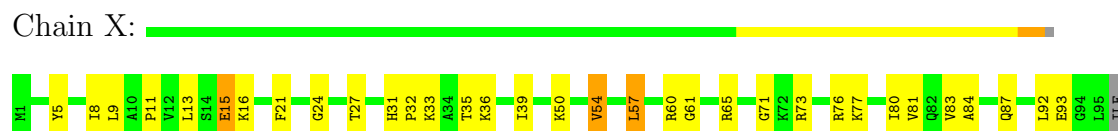
- Molecule 17: 50S Ribosomal Protein L21



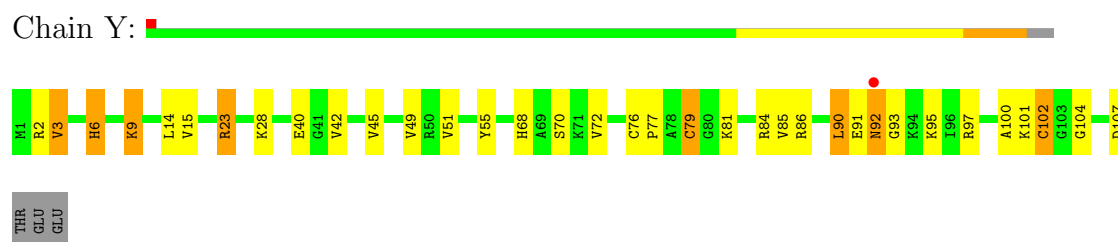
- Molecule 18: 50S Ribosomal Protein L22



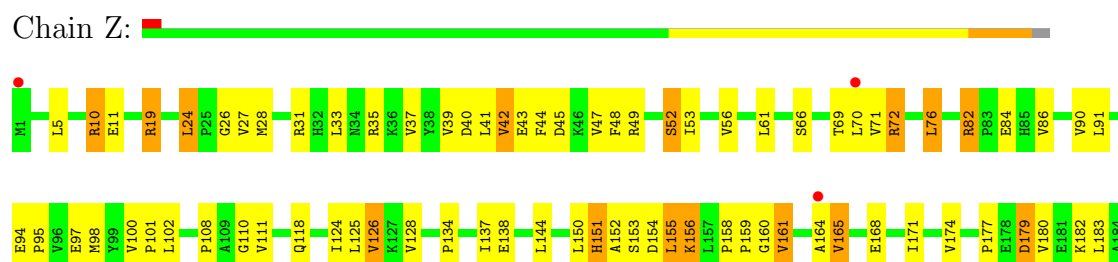
- Molecule 19: 50S Ribosomal Protein L23

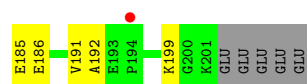


- Molecule 20: 50S Ribosomal Protein L24



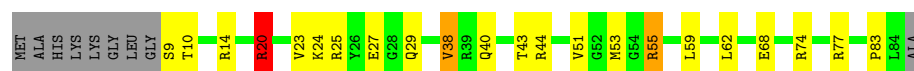
- Molecule 21: 50S Ribosomal Protein L25





• Molecule 22: 50S Ribosomal Protein L27

Chain 0:



• Molecule 23: 50S Ribosomal Protein L28

Chain 1:



• Molecule 24: 50S Ribosomal Protein L29

Chain 2:



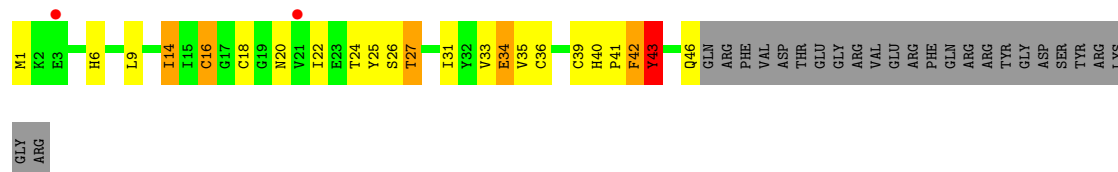
• Molecule 25: 50S Ribosomal Protein L30

Chain 3:



• Molecule 26: 50S Ribosomal Protein L31

Chain 4:



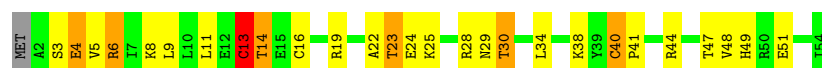
• Molecule 27: 50S Ribosomal Protein L32

Chain 5:

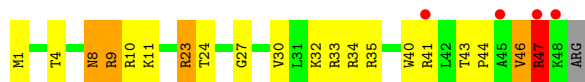


• Molecule 28: 50S Ribosomal Protein L33

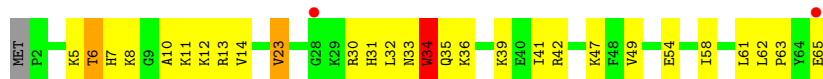
Chain 6:



## • Molecule 29: 50S Ribosomal Protein L34

Chain 7: 

## • Molecule 30: 50S Ribosomal Protein L35

Chain 8: 

## • Molecule 31: 50S Ribosomal Protein L36

Chain 9: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.10 49.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.98-3.10) 96.0 (49.98-3.10)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.216 , 0.258 0.406 , 0.413	Depositor DCC
$R_{free}$ test set	49855 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 15.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 993194 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	92957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.58	572/68445 (0.8%)	1.72	2187/106848 (2.0%)
2	B	1.13	6/2878 (0.2%)	1.53	60/4490 (1.3%)
3	D	0.90	1/2185 (0.0%)	0.91	4/2942 (0.1%)
4	E	0.90	0/1588	0.92	0/2145
5	F	0.91	0/1615	0.95	3/2188 (0.1%)
6	G	0.61	0/1393	0.79	0/1892
7	H	0.72	0/1343	0.82	1/1820 (0.1%)
8	I	0.64	0/1052	0.87	1/1441 (0.1%)
9	N	0.87	0/1139	0.87	0/1538
10	O	0.87	1/933 (0.1%)	0.88	1/1257 (0.1%)
11	P	0.84	0/1148	0.91	1/1529 (0.1%)
12	Q	0.84	0/1143	0.87	1/1527 (0.1%)
13	R	0.80	0/982	0.92	0/1312
14	S	0.67	0/875	0.88	1/1168 (0.1%)
15	T	0.83	0/1077	0.92	0/1444
16	U	1.00	1/977 (0.1%)	0.87	1/1301 (0.1%)
17	V	0.85	0/782	0.92	0/1049
18	W	1.02	0/891	0.91	0/1197
19	X	0.91	0/756	0.88	2/1016 (0.2%)
20	Y	0.80	1/798 (0.1%)	0.88	0/1073
21	Z	0.70	0/1569	0.82	1/2137 (0.0%)
22	0	0.85	0/602	0.92	1/804 (0.1%)
23	1	0.85	0/752	0.90	2/1003 (0.2%)
24	2	0.82	0/590	0.86	0/781
25	3	0.76	0/463	0.84	1/623 (0.2%)
26	4	0.68	0/358	0.84	1/487 (0.2%)
27	5	0.93	1/469 (0.2%)	1.00	0/634
28	6	0.93	2/456 (0.4%)	0.84	0/609
29	7	1.03	1/426 (0.2%)	1.12	1/561 (0.2%)
30	8	0.96	0/516	0.94	1/679 (0.1%)
31	9	0.79	0/300	0.95	0/395
All	All	1.40	586/98501 (0.6%)	1.55	2271/147890 (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	A	0	1
4	E	0	1
12	Q	0	1
14	S	0	1
19	X	0	1
21	Z	0	3
23	1	0	1
26	4	0	1
All	All	0	10

All (586) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142(A)	A	N9-C4	-12.92	1.30	1.37
1	A	945	A	N9-C4	-12.37	1.30	1.37
1	A	207	A	N9-C4	-12.29	1.30	1.37
1	A	676	A	N9-C4	-12.12	1.30	1.37
1	A	528	A	N9-C4	-12.02	1.30	1.37
1	A	1204	A	N9-C4	-9.69	1.32	1.37
1	A	2055	C	P-OP1	-9.53	1.32	1.49
1	A	1142(A)	A	N3-C4	-9.27	1.29	1.34
1	A	330	A	N9-C4	-9.14	1.32	1.37
1	A	2015	A	N7-C5	-8.94	1.33	1.39
1	A	1021	A	N9-C4	-8.86	1.32	1.37
1	A	2440	C	N1-C6	-8.80	1.31	1.37
1	A	933	A	N9-C4	-8.77	1.32	1.37
1	A	1762	A	N9-C4	8.75	1.43	1.37
1	A	2587	A	N9-C8	-8.67	1.30	1.37
1	A	1570	A	N9-C4	-8.62	1.32	1.37
1	A	1655	A	N9-C4	-8.61	1.32	1.37
1	A	1829	A	N9-C4	-8.52	1.32	1.37
1	A	732	C	N1-C6	-8.51	1.32	1.37
1	A	503	A	N3-C4	-8.48	1.29	1.34
1	A	2296	U	C4-C5	8.41	1.51	1.43
1	A	1785	A	N7-C5	-8.40	1.34	1.39
1	A	756	C	N1-C6	-8.38	1.32	1.37
1	A	933	A	N3-C4	-8.32	1.29	1.34
1	A	1210	A	N3-C4	-8.28	1.29	1.34
1	A	209	C	N1-C6	-8.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1570	A	N3-C4	-8.19	1.29	1.34
1	A	1612	C	N1-C6	-8.15	1.32	1.37
1	A	2032	G	N7-C5	-8.08	1.34	1.39
1	A	2030	A	N9-C4	-7.99	1.33	1.37
1	A	745	G	N7-C5	-7.95	1.34	1.39
1	A	209	C	N3-C4	-7.92	1.28	1.33
1	A	689	A	N9-C4	-7.89	1.33	1.37
1	A	2597	G	N7-C5	-7.88	1.34	1.39
1	A	529	A	N9-C4	-7.79	1.33	1.37
28	6	13	CYS	CB-SG	-7.75	1.69	1.82
1	A	1210	A	N7-C5	-7.60	1.34	1.39
1	A	933	A	C5-C6	-7.57	1.34	1.41
1	A	119	A	N7-C5	-7.55	1.34	1.39
1	A	1791	A	N7-C5	-7.49	1.34	1.39
1	A	472	A	N3-C4	-7.45	1.30	1.34
1	A	1755	A	N3-C4	-7.45	1.30	1.34
1	A	191	A	N7-C5	-7.43	1.34	1.39
1	A	1254	A	N3-C4	-7.43	1.30	1.34
1	A	575	A	C6-N1	-7.33	1.30	1.35
1	A	197	A	C5-C4	-7.31	1.33	1.38
1	A	2286	A	N7-C5	-7.30	1.34	1.39
1	A	567	A	N9-C4	-7.30	1.33	1.37
1	A	933	A	N7-C5	-7.29	1.34	1.39
1	A	2575	C	N1-C6	-7.29	1.32	1.37
1	A	983	A	N3-C4	-7.24	1.30	1.34
1	A	2287	A	N9-C4	-7.22	1.33	1.37
1	A	57	C	N1-C6	-7.21	1.32	1.37
1	A	2641	G	N7-C5	-7.21	1.34	1.39
1	A	2680	C	N1-C6	-7.20	1.32	1.37
1	A	1308	A	N7-C5	-7.17	1.34	1.39
1	A	804	A	C5-C4	-7.15	1.33	1.38
1	A	679	C	N1-C6	-7.14	1.32	1.37
1	A	1301	A	N7-C5	-7.11	1.34	1.39
1	A	1241	A	N9-C4	-7.11	1.33	1.37
1	A	2055	C	P-O5'	-7.10	1.52	1.59
1	A	1567	A	N9-C4	-7.09	1.33	1.37
1	A	1789	A	N7-C5	-7.08	1.35	1.39
1	A	1198	U	C2-N3	-7.07	1.32	1.37
1	A	831	G	C8-N7	-7.06	1.26	1.30
1	A	1210	A	C5-C6	-7.00	1.34	1.41
1	A	783	A	N7-C5	-6.98	1.35	1.39
1	A	2058	A	N9-C4	-6.97	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	G	P-OP1	-6.97	1.37	1.49
1	A	1674	G	N7-C5	-6.95	1.35	1.39
1	A	1901	A	C6-N1	-6.95	1.30	1.35
1	A	2335	A	C5-C4	-6.94	1.33	1.38
1	A	983	A	N9-C4	-6.90	1.33	1.37
1	A	850	C	N3-C4	-6.89	1.29	1.33
1	A	2052	G	N7-C5	-6.89	1.35	1.39
1	A	570	G	C5-C4	-6.88	1.33	1.38
1	A	804	A	N9-C4	-6.87	1.33	1.37
1	A	2248	C	N1-C6	-6.84	1.33	1.37
1	A	676	A	C5-C4	6.84	1.43	1.38
1	A	2872	G	N3-C4	-6.81	1.30	1.35
20	Y	79	CYS	CB-SG	-6.81	1.70	1.82
1	A	1225	G	N3-C4	-6.80	1.30	1.35
1	A	676	A	N3-C4	-6.77	1.30	1.34
1	A	1755	A	N9-C4	-6.77	1.33	1.37
1	A	1571	A	N9-C4	-6.76	1.33	1.37
1	A	587	C	N3-C4	-6.74	1.29	1.33
1	A	1648	C	N3-C4	-6.73	1.29	1.33
1	A	658	C	N3-C4	-6.71	1.29	1.33
1	A	1564	C	N3-C4	-6.65	1.29	1.33
1	A	1571	A	N7-C5	-6.64	1.35	1.39
1	A	1785	A	C5-C6	-6.64	1.35	1.41
1	A	676	A	N9-C8	6.63	1.43	1.37
1	A	71	A	N9-C4	-6.62	1.33	1.37
1	A	689	A	C5-C4	-6.61	1.34	1.38
1	A	1269	A	N9-C4	-6.61	1.33	1.37
1	A	204	A	N7-C5	-6.60	1.35	1.39
1	A	2015	A	N3-C4	-6.60	1.30	1.34
1	A	804	A	N3-C4	-6.59	1.30	1.34
1	A	2715	C	N1-C6	-6.59	1.33	1.37
1	A	663	G	N3-C4	-6.57	1.30	1.35
1	A	831	G	C5-C4	-6.57	1.33	1.38
1	A	371	A	N9-C4	-6.56	1.33	1.37
1	A	1142(A)	A	C5-C6	-6.56	1.35	1.41
1	A	1254	A	C6-N1	-6.56	1.30	1.35
1	A	988	A	N7-C5	-6.55	1.35	1.39
1	A	32	C	N1-C6	-6.55	1.33	1.37
1	A	1755	A	N7-C5	-6.55	1.35	1.39
1	A	472	A	N9-C4	-6.54	1.33	1.37
1	A	732	C	C4-C5	-6.53	1.37	1.43
1	A	1278	A	N9-C8	-6.53	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1653	G	N7-C5	-6.53	1.35	1.39
1	A	819	A	C6-N1	-6.52	1.30	1.35
1	A	1314	C	N1-C6	-6.52	1.33	1.37
1	A	1617	C	N1-C6	-6.52	1.33	1.37
1	A	2619	C	N1-C6	-6.51	1.33	1.37
1	A	675	A	C5-C6	-6.50	1.35	1.41
1	A	2790	A	N9-C4	6.48	1.41	1.37
1	A	32	C	N3-C4	-6.48	1.29	1.33
1	A	577	G	P-O5'	-6.46	1.53	1.59
1	A	609	A	N3-C4	-6.46	1.30	1.34
1	A	2765	A	N7-C5	-6.46	1.35	1.39
1	A	2606	C	N3-C4	-6.45	1.29	1.33
1	A	849	A	N9-C4	-6.44	1.33	1.37
1	A	1676	A	N3-C4	-6.43	1.30	1.34
1	A	1278	A	N7-C5	-6.42	1.35	1.39
1	A	1045	A	N9-C4	6.42	1.41	1.37
1	A	1322	A	N9-C4	-6.39	1.34	1.37
1	A	572	A	N3-C4	-6.39	1.31	1.34
1	A	123	G	N3-C4	-6.39	1.30	1.35
1	A	2055	C	P-OP2	-6.39	1.38	1.49
1	A	74	A	N3-C4	-6.38	1.31	1.34
1	A	561	G	C5-C4	-6.34	1.33	1.38
1	A	69	C	N1-C6	-6.33	1.33	1.37
1	A	1655	A	N3-C4	-6.33	1.31	1.34
1	A	945	A	N3-C4	-6.30	1.31	1.34
1	A	74	A	N9-C4	-6.29	1.34	1.37
1	A	1278	A	C5-C4	-6.29	1.34	1.38
1	A	2578	G	N1-C2	-6.28	1.32	1.37
1	A	793	A	N3-C4	-6.28	1.31	1.34
1	A	1046	A	N9-C4	6.28	1.41	1.37
1	A	2287	A	N3-C4	-6.27	1.31	1.34
1	A	2027	G	N1-C2	-6.27	1.32	1.37
1	A	2621	A	C6-N6	-6.27	1.28	1.33
1	A	2454	G	C5-C4	-6.26	1.33	1.38
1	A	2600	A	N7-C5	-6.25	1.35	1.39
1	A	2587	A	N7-C5	-6.25	1.35	1.39
1	A	750	A	C6-N1	-6.24	1.31	1.35
1	A	1252	G	C5-C4	-6.23	1.33	1.38
1	A	1800	C	N1-C6	-6.23	1.33	1.37
1	A	1608	A	N9-C4	-6.21	1.34	1.37
1	A	2199	A	C6-N1	-6.21	1.31	1.35
1	A	1006	C	N3-C4	-6.21	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	71	C	N1-C6	-6.21	1.33	1.37
1	A	1296	G	N1-C2	-6.20	1.32	1.37
1	A	1843	C	N1-C6	-6.18	1.33	1.37
1	A	204	A	N3-C4	-6.17	1.31	1.34
1	A	2723	C	N3-C4	-6.16	1.29	1.33
1	A	122	G	C5-C4	-6.16	1.34	1.38
1	A	463	G	N3-C4	-6.14	1.31	1.35
1	A	201	C	N1-C6	-6.13	1.33	1.37
1	A	1141	U	C2-N3	-6.12	1.33	1.37
1	A	2515	C	N1-C6	-6.12	1.33	1.37
1	A	959	A	C6-N1	-6.12	1.31	1.35
1	A	2296	U	N1-C2	6.12	1.44	1.38
1	A	2725	A	N9-C4	-6.11	1.34	1.37
1	A	189	G	N9-C4	-6.11	1.33	1.38
1	A	517	C	N1-C6	-6.11	1.33	1.37
1	A	1836	C	N3-C4	-6.10	1.29	1.33
1	A	689	A	N3-C4	-6.10	1.31	1.34
1	A	789	A	N9-C4	-6.10	1.34	1.37
1	A	2382	G	N9-C8	-6.09	1.33	1.37
1	A	2442	C	N1-C6	-6.08	1.33	1.37
1	A	1107	G	N9-C4	6.08	1.42	1.38
1	A	2058	A	N3-C4	-6.08	1.31	1.34
1	A	2505	G	N3-C4	-6.08	1.31	1.35
1	A	531	C	N1-C6	-6.07	1.33	1.37
1	A	652(B)	A	N9-C4	6.07	1.41	1.37
1	A	687	C	N3-C4	-6.07	1.29	1.33
1	A	2619	C	N3-C4	-6.07	1.29	1.33
1	A	570	G	C5-C6	-6.07	1.36	1.42
1	A	991	C	N3-C4	-6.07	1.29	1.33
1	A	567	A	N3-C4	-6.07	1.31	1.34
1	A	122	G	N7-C5	-6.06	1.35	1.39
1	A	1653	G	N9-C8	-6.05	1.33	1.37
1	A	2579	C	N3-C4	-6.04	1.29	1.33
1	A	2246	G	N1-C2	-6.02	1.32	1.37
1	A	2072	G	C8-N7	-6.02	1.27	1.30
1	A	2017	U	C2-N3	-6.01	1.33	1.37
1	A	90	U	N3-C4	6.00	1.43	1.38
1	A	745	G	C6-N1	-6.00	1.35	1.39
1	A	795	C	N1-C6	-6.00	1.33	1.37
1	A	1123	C	N1-C6	-5.99	1.33	1.37
1	A	1618	A	C6-N1	-5.99	1.31	1.35
1	A	190	A	N9-C4	-5.98	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2046	G	N7-C5	-5.98	1.35	1.39
1	A	468	G	C8-N7	-5.97	1.27	1.30
1	A	1619	G	C5-C4	-5.97	1.34	1.38
1	A	1241	A	N3-C4	-5.96	1.31	1.34
1	A	2232	U	C2-N3	-5.96	1.33	1.37
1	A	585	G	C5-C4	-5.96	1.34	1.38
2	B	76	G	N9-C4	-5.96	1.33	1.38
1	A	2541	A	N7-C5	-5.93	1.35	1.39
1	A	2607	G	C8-N7	-5.93	1.27	1.30
1	A	2768	C	N3-C4	-5.92	1.29	1.33
1	A	381	G	C5-C4	-5.92	1.34	1.38
1	A	1785	A	C6-N1	-5.91	1.31	1.35
1	A	191	A	N9-C4	-5.91	1.34	1.37
1	A	33	U	N1-C2	-5.90	1.33	1.38
1	A	940	G	N7-C5	-5.89	1.35	1.39
1	A	2082	A	N7-C5	-5.89	1.35	1.39
1	A	265	A	N7-C5	-5.89	1.35	1.39
1	A	2029	G	N9-C8	-5.89	1.33	1.37
1	A	1021	A	N3-C4	-5.88	1.31	1.34
1	A	2725	A	N3-C4	-5.88	1.31	1.34
1	A	197	A	N7-C5	-5.87	1.35	1.39
1	A	1819	A	P-O5'	-5.87	1.53	1.59
1	A	1603	A	N3-C4	-5.87	1.31	1.34
1	A	1978	A	N7-C5	-5.87	1.35	1.39
1	A	2829	C	N1-C6	-5.87	1.33	1.37
1	A	530	G	C2-N3	-5.86	1.28	1.32
1	A	21	A	N3-C4	-5.85	1.31	1.34
1	A	198	C	N1-C6	-5.85	1.33	1.37
1	A	2321	G	C2-N3	-5.85	1.28	1.32
1	A	1285	G	C5-C4	-5.84	1.34	1.38
1	A	2509	G	N7-C5	-5.84	1.35	1.39
1	A	2740	A	N3-C4	-5.84	1.31	1.34
1	A	184	C	N1-C6	-5.83	1.33	1.37
1	A	16	G	C2-N3	-5.83	1.28	1.32
1	A	2335	A	N9-C4	-5.83	1.34	1.37
1	A	194	G	C2-N3	-5.82	1.28	1.32
1	A	1938	A	N7-C5	-5.82	1.35	1.39
1	A	204	A	C6-N1	-5.82	1.31	1.35
1	A	2602	A	N9-C4	5.82	1.41	1.37
1	A	2025	C	N1-C6	-5.82	1.33	1.37
1	A	978	G	C5-C4	-5.81	1.34	1.38
1	A	330	A	N3-C4	-5.81	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1434	A	N9-C4	-5.81	1.34	1.37
1	A	2451	A	N3-C4	-5.81	1.31	1.34
1	A	1789	A	C5-C4	-5.80	1.34	1.38
1	A	2304	G	C6-N1	5.80	1.43	1.39
1	A	780	G	N9-C8	-5.79	1.33	1.37
1	A	2436	G	N1-C2	-5.78	1.33	1.37
1	A	425	G	C6-N1	-5.78	1.35	1.39
1	A	1669	A	N3-C4	-5.77	1.31	1.34
1	A	2442	C	C2-N3	-5.76	1.31	1.35
1	A	829	A	N9-C4	-5.76	1.34	1.37
1	A	71	A	C5-C4	5.76	1.42	1.38
1	A	2740	A	N7-C5	-5.75	1.35	1.39
1	A	794	G	C6-N1	-5.75	1.35	1.39
1	A	609	A	C5-C4	-5.75	1.34	1.38
1	A	2382	G	N7-C5	-5.75	1.35	1.39
1	A	389	G	C8-N7	-5.75	1.27	1.30
1	A	800	A	N3-C4	-5.74	1.31	1.34
1	A	2346	A	N7-C5	-5.74	1.35	1.39
1	A	753	C	N3-C4	-5.74	1.29	1.33
1	A	425	G	N9-C8	-5.73	1.33	1.37
1	A	989	G	N7-C5	-5.72	1.35	1.39
1	A	2000	G	C5-C4	-5.72	1.34	1.38
1	A	1890	A	N9-C4	-5.71	1.34	1.37
1	A	181	A	N3-C4	-5.71	1.31	1.34
1	A	571	A	C5-C4	-5.71	1.34	1.38
1	A	47	C	C5-C6	-5.71	1.29	1.34
1	A	344	G	C5-C4	-5.70	1.34	1.38
1	A	2267	A	N9-C4	-5.70	1.34	1.37
1	A	2507	C	C2-N3	-5.70	1.31	1.35
1	A	1367	A	C5-C4	-5.70	1.34	1.38
1	A	2676	C	N1-C6	-5.69	1.33	1.37
1	A	71	A	N9-C8	5.69	1.42	1.37
1	A	87	C	N1-C6	-5.69	1.33	1.37
1	A	1212	G	N9-C8	-5.67	1.33	1.37
1	A	1430	C	N1-C6	-5.67	1.33	1.37
1	A	119	A	N9-C8	-5.67	1.33	1.37
1	A	884	C	N1-C6	5.67	1.40	1.37
1	A	983	A	C5-C4	-5.65	1.34	1.38
1	A	492	A	N7-C5	-5.65	1.35	1.39
1	A	2322	A	C5-C6	5.65	1.46	1.41
1	A	1535	A	N9-C4	5.64	1.41	1.37
1	A	197	A	N3-C4	-5.64	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	788	A	N9-C8	-5.64	1.33	1.37
1	A	1202	C	N1-C6	-5.64	1.33	1.37
1	A	2445	G	N9-C8	-5.64	1.33	1.37
1	A	751	A	N3-C4	-5.63	1.31	1.34
1	A	1960	A	N9-C4	-5.63	1.34	1.37
1	A	55	G	N1-C2	-5.63	1.33	1.37
1	A	2452	C	N1-C6	-5.63	1.33	1.37
1	A	211	A	C5-C4	-5.63	1.34	1.38
1	A	2322	A	C6-N1	5.63	1.39	1.35
1	A	1363	C	N3-C4	-5.62	1.30	1.33
1	A	2607	G	N9-C8	-5.62	1.33	1.37
1	A	512	G	P-O5'	-5.62	1.54	1.59
1	A	98	G	N9-C4	-5.61	1.33	1.38
1	A	2515	C	C4-C5	-5.60	1.38	1.43
1	A	190	A	C5-C6	-5.59	1.36	1.41
1	A	682	G	C5-C6	-5.59	1.36	1.42
1	A	2028	U	C2-N3	-5.59	1.33	1.37
1	A	1599	C	N3-C4	-5.59	1.30	1.33
1	A	2541	A	N9-C8	-5.59	1.33	1.37
1	A	425	G	N1-C2	-5.58	1.33	1.37
1	A	815	C	N1-C6	-5.58	1.33	1.37
1	A	1989	G	N7-C5	-5.58	1.35	1.39
1	A	2695	C	N1-C6	-5.58	1.33	1.37
1	A	425	G	C5-C4	-5.58	1.34	1.38
1	A	783	A	C5-C4	-5.57	1.34	1.38
1	A	2249	U	P-O5'	-5.57	1.54	1.59
1	A	586	A	N7-C5	-5.57	1.35	1.39
1	A	960	A	C5-C6	-5.56	1.36	1.41
1	A	1570	A	C5-C6	-5.56	1.36	1.41
1	A	558	G	C5-C4	-5.56	1.34	1.38
1	A	794	G	N1-C2	-5.56	1.33	1.37
1	A	1297	C	N1-C2	-5.56	1.34	1.40
1	A	2284	C	N3-C4	-5.56	1.30	1.33
1	A	553	G	C5-C6	-5.55	1.36	1.42
1	A	1244	G	C2-N3	-5.55	1.28	1.32
1	A	1653	G	C6-N1	-5.55	1.35	1.39
1	A	90	U	C2-N3	5.54	1.41	1.37
1	A	560	C	N1-C6	-5.54	1.33	1.37
1	A	830	G	N9-C8	-5.53	1.33	1.37
1	A	2058	A	C5-C4	-5.53	1.34	1.38
1	A	1162	G	N7-C5	-5.53	1.35	1.39
1	A	451	C	N1-C6	-5.52	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1567	A	N7-C5	-5.52	1.35	1.39
1	A	1698	A	N7-C5	-5.52	1.35	1.39
1	A	2642	G	N9-C8	-5.52	1.33	1.37
1	A	2052	G	N9-C8	-5.52	1.33	1.37
1	A	1668	A	C5-C4	-5.51	1.34	1.38
1	A	2015	A	N9-C4	-5.51	1.34	1.37
1	A	113	G	N9-C4	-5.51	1.33	1.38
1	A	1250	G	N7-C5	-5.50	1.35	1.39
1	A	2431	U	N1-C2	-5.50	1.33	1.38
1	A	229	A	N9-C4	5.50	1.41	1.37
1	A	751	A	C5-C4	-5.50	1.34	1.38
1	A	1254	A	N7-C5	-5.50	1.35	1.39
1	A	480	A	N7-C5	-5.50	1.35	1.39
1	A	745	G	C5-C6	-5.49	1.36	1.42
1	A	2051	A	N3-C4	-5.49	1.31	1.34
1	A	2747	G	C6-N1	-5.49	1.35	1.39
1	A	207	A	N7-C5	-5.49	1.35	1.39
1	A	189	G	N9-C8	-5.49	1.34	1.37
1	A	975	C	N1-C6	-5.49	1.33	1.37
1	A	2011	U	N1-C2	-5.48	1.33	1.38
1	A	802	A	N7-C5	-5.48	1.35	1.39
1	A	1300	U	C3'-O3'	5.48	1.49	1.42
1	A	1490	A	N3-C4	5.48	1.38	1.34
1	A	2589	A	N9-C4	-5.48	1.34	1.37
1	A	1988	C	N1-C6	-5.48	1.33	1.37
1	A	572	A	N7-C5	-5.47	1.35	1.39
1	A	2017	U	C2-O2	-5.47	1.17	1.22
1	A	804	A	N9-C8	-5.47	1.33	1.37
1	A	1804	C	N3-C4	-5.47	1.30	1.33
10	O	21	CYS	CB-SG	-5.47	1.72	1.81
1	A	1698	A	C5-C6	-5.46	1.36	1.41
3	D	28	GLU	CG-CD	5.46	1.60	1.51
1	A	1528	A	N3-C4	-5.46	1.31	1.34
1	A	2426	A	C6-N1	-5.46	1.31	1.35
1	A	1655	A	C5-C4	-5.45	1.34	1.38
1	A	2054	A	C5-C6	-5.45	1.36	1.41
1	A	664	C	N1-C6	-5.45	1.33	1.37
1	A	1330	C	N1-C6	-5.45	1.33	1.37
1	A	1535	A	N3-C4	5.45	1.38	1.34
1	A	483	A	C6-N1	-5.45	1.31	1.35
1	A	1252	G	N3-C4	-5.45	1.31	1.35
2	B	104	U	C2-N3	-5.44	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2017	U	N1-C6	-5.44	1.33	1.38
1	A	1189	A	C5-C6	-5.44	1.36	1.41
1	A	756	C	N1-C2	-5.44	1.34	1.40
1	A	1771	C	N3-C4	-5.43	1.30	1.33
1	A	1658	C	P-OP1	-5.43	1.39	1.49
1	A	2058	A	N7-C5	-5.43	1.35	1.39
1	A	2059	A	N9-C8	-5.43	1.33	1.37
1	A	2447	G	C5-C4	-5.43	1.34	1.38
1	A	265	A	C5-C6	-5.43	1.36	1.41
1	A	778	G	N7-C5	-5.42	1.35	1.39
1	A	2053	G	C5-C4	-5.42	1.34	1.38
1	A	2686	G	C5-C4	-5.42	1.34	1.38
1	A	2572	A	C5-C4	-5.42	1.34	1.38
2	B	56	G	N7-C5	-5.42	1.35	1.39
1	A	1403	C	N3-C4	-5.42	1.30	1.33
2	B	99	G	C5-C4	-5.41	1.34	1.38
1	A	787	U	P-OP2	-5.41	1.39	1.49
1	A	1614	A	N9-C4	-5.41	1.34	1.37
1	A	1638	C	N1-C6	-5.41	1.33	1.37
1	A	1643	G	C6-N1	-5.41	1.35	1.39
1	A	1779	U	P-O5'	-5.41	1.54	1.59
1	A	1308	A	C5-C4	-5.40	1.34	1.38
1	A	204	A	C5-C6	-5.40	1.36	1.41
1	A	505	A	N9-C4	-5.40	1.34	1.37
1	A	785	G	N9-C4	-5.40	1.33	1.38
1	A	141	A	N9-C4	-5.39	1.34	1.37
1	A	734	A	N9-C4	-5.39	1.34	1.37
1	A	994	C	N1-C6	-5.39	1.33	1.37
1	A	536	A	C5-C4	-5.39	1.34	1.38
1	A	1132	A	C6-N1	-5.39	1.31	1.35
1	A	971	C	N3-C4	-5.38	1.30	1.33
1	A	466	A	P-O5'	-5.38	1.54	1.59
1	A	2323	G	C5-C4	-5.37	1.34	1.38
1	A	2251	G	N7-C5	-5.37	1.36	1.39
1	A	57	C	N3-C4	-5.37	1.30	1.33
1	A	1674	G	N9-C8	-5.37	1.34	1.37
1	A	2541	A	N3-C4	-5.36	1.31	1.34
27	5	6	VAL	CB-CG2	-5.36	1.41	1.52
1	A	2153	G	C6-N1	5.36	1.43	1.39
1	A	1674	G	C5-C4	-5.36	1.34	1.38
1	A	745	G	C5-C4	-5.35	1.34	1.38
1	A	2614	A	N9-C8	-5.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	G	C5-C4	-5.34	1.34	1.38
1	A	733	G	C5-C4	-5.34	1.34	1.38
1	A	2246	G	C2-N3	-5.34	1.28	1.32
1	A	1359	A	C6-N6	-5.33	1.29	1.33
1	A	1606	G	N9-C8	-5.33	1.34	1.37
1	A	989	G	C8-N7	-5.33	1.27	1.30
1	A	507	A	N7-C5	-5.32	1.36	1.39
1	A	1157	G	N7-C5	-5.32	1.36	1.39
1	A	981	A	N9-C4	-5.32	1.34	1.37
1	A	271(M)	G	N9-C4	5.31	1.42	1.38
1	A	1137	G	C8-N7	-5.31	1.27	1.30
1	A	1031	G	N1-C2	-5.31	1.33	1.37
1	A	690	G	N1-C2	-5.31	1.33	1.37
1	A	85	G	N7-C5	-5.30	1.36	1.39
1	A	527	C	N3-C4	-5.30	1.30	1.33
1	A	2013	A	C5-C6	-5.30	1.36	1.41
1	A	2330	G	N3-C4	-5.30	1.31	1.35
1	A	211	A	N9-C4	-5.30	1.34	1.37
1	A	2162	G	N3-C4	5.30	1.39	1.35
1	A	1268	A	C6-N1	-5.30	1.31	1.35
1	A	70	G	N1-C2	-5.29	1.33	1.37
1	A	2432	A	C5-C6	-5.29	1.36	1.41
1	A	2065	C	N1-C6	-5.28	1.33	1.37
1	A	744	G	N9-C8	-5.28	1.34	1.37
1	A	1132	A	N3-C4	-5.28	1.31	1.34
1	A	1764	G	C6-N1	-5.27	1.35	1.39
1	A	2599	G	N9-C8	-5.27	1.34	1.37
1	A	1616	A	C5-C6	-5.27	1.36	1.41
1	A	2225	A	N9-C4	-5.26	1.34	1.37
1	A	2577	A	P-OP2	-5.26	1.40	1.49
1	A	733	G	C8-N7	-5.26	1.27	1.30
1	A	978	G	C5-C6	-5.25	1.37	1.42
1	A	981	A	N7-C5	-5.25	1.36	1.39
1	A	2505	G	C2-N3	-5.25	1.28	1.32
1	A	733	G	N7-C5	-5.25	1.36	1.39
1	A	941	A	C5-C4	-5.25	1.35	1.38
1	A	1657	C	N1-C6	-5.25	1.33	1.37
1	A	13	A	C6-N1	-5.25	1.31	1.35
1	A	994	C	N3-C4	-5.25	1.30	1.33
1	A	2025	C	C4-C5	-5.25	1.38	1.43
1	A	2571	C	C2-O2	-5.25	1.19	1.24
1	A	2778	A	C6-N1	-5.25	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2087	G	C5-C6	-5.24	1.37	1.42
1	A	748	G	N9-C8	-5.24	1.34	1.37
1	A	943	U	N1-C2	-5.24	1.33	1.38
1	A	575	A	C6-N6	-5.24	1.29	1.33
1	A	788	A	N7-C5	-5.24	1.36	1.39
1	A	1225	G	C2-N3	-5.23	1.28	1.32
1	A	380	U	N1-C6	-5.22	1.33	1.38
1	A	2778	A	N7-C5	-5.22	1.36	1.39
1	A	2825	C	N1-C6	-5.22	1.34	1.37
1	A	2506	U	N1-C2	5.22	1.43	1.38
1	A	1698	A	N3-C4	-5.21	1.31	1.34
1	A	2329	G	N1-C2	-5.21	1.33	1.37
1	A	197	A	C5-C6	-5.21	1.36	1.41
1	A	952	G	C5-C4	-5.21	1.34	1.38
1	A	1195	G	C5-C4	-5.21	1.34	1.38
1	A	1262	A	C6-N6	-5.21	1.29	1.33
1	A	2602	A	O3'-P	5.21	1.67	1.61
1	A	463	G	C6-N1	-5.21	1.35	1.39
29	7	30	VAL	CA-CB	-5.21	1.43	1.54
1	A	253	C	N1-C6	-5.20	1.34	1.37
1	A	1217	C	C4-C5	-5.20	1.38	1.43
1	A	2436	G	C2-N3	-5.20	1.28	1.32
1	A	71	A	C5-C6	-5.20	1.36	1.41
1	A	1368	G	P-O5'	-5.20	1.54	1.59
1	A	278	A	C6-N1	5.20	1.39	1.35
1	A	1195	G	C2-N3	-5.20	1.28	1.32
1	A	980	A	C5-C6	-5.19	1.36	1.41
1	A	936	C	N1-C2	-5.19	1.34	1.40
1	A	1137	G	N7-C5	-5.19	1.36	1.39
1	A	2822	G	N9-C8	-5.19	1.34	1.37
1	A	2764	A	N3-C4	-5.18	1.31	1.34
1	A	2020	A	N9-C8	-5.18	1.33	1.37
1	A	2546	U	N1-C2	-5.18	1.33	1.38
1	A	2606	C	N1-C6	-5.18	1.34	1.37
1	A	15	G	N9-C8	-5.18	1.34	1.37
1	A	686	G	C5-C6	-5.18	1.37	1.42
1	A	980	A	N7-C5	-5.18	1.36	1.39
1	A	1256	G	N3-C4	-5.18	1.31	1.35
2	B	96	U	C2-N3	-5.18	1.34	1.37
1	A	2304	G	N7-C5	5.17	1.42	1.39
1	A	2376	A	N7-C5	-5.17	1.36	1.39
1	A	1204	A	C5-C6	-5.17	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1618	A	P-O5'	-5.17	1.54	1.59
1	A	733	G	C6-N1	-5.17	1.35	1.39
1	A	1184	G	C2-N3	-5.17	1.28	1.32
1	A	1889	A	N9-C4	-5.17	1.34	1.37
1	A	1933	G	C6-N1	-5.17	1.35	1.39
1	A	975	C	N3-C4	-5.16	1.30	1.33
1	A	2587	A	P-O5'	-5.16	1.54	1.59
1	A	819	A	N9-C4	-5.16	1.34	1.37
1	A	1787	A	N3-C4	-5.16	1.31	1.34
1	A	107	C	N1-C6	-5.15	1.34	1.37
1	A	753	C	C2-N3	-5.15	1.31	1.35
1	A	2422	A	N9-C4	-5.15	1.34	1.37
1	A	119	A	N9-C4	-5.15	1.34	1.37
1	A	1647	G	N9-C8	-5.15	1.34	1.37
1	A	2517	C	N1-C6	-5.15	1.34	1.37
1	A	555	U	P-O5'	-5.14	1.54	1.59
1	A	20	C	N1-C6	-5.14	1.34	1.37
1	A	1195	G	N3-C4	-5.14	1.31	1.35
1	A	1791	A	N3-C4	-5.14	1.31	1.34
1	A	2352	A	N9-C4	-5.14	1.34	1.37
1	A	2149	G	C6-N1	5.14	1.43	1.39
1	A	2542	A	N3-C4	-5.14	1.31	1.34
1	A	2288	A	N9-C4	5.14	1.41	1.37
1	A	244	A	C5-C6	-5.14	1.36	1.41
1	A	1285	G	N7-C5	-5.14	1.36	1.39
1	A	2819	G	N9-C8	-5.14	1.34	1.37
1	A	2724	C	N1-C6	-5.13	1.34	1.37
1	A	783	A	N3-C4	-5.13	1.31	1.34
16	U	69	CYS	CB-SG	-5.13	1.73	1.81
1	A	2072	G	C5-C4	-5.12	1.34	1.38
1	A	2684	U	N1-C6	-5.12	1.33	1.38
1	A	189	G	N3-C4	-5.12	1.31	1.35
1	A	2287	A	C6-N6	-5.12	1.29	1.33
1	A	204	A	C5-C4	-5.12	1.35	1.38
1	A	2245	U	C2-N3	-5.12	1.34	1.37
1	A	2699	C	N1-C6	-5.12	1.34	1.37
1	A	939	G	N3-C4	-5.11	1.31	1.35
1	A	2723	C	C2-N3	-5.11	1.31	1.35
1	A	2602	A	N7-C5	5.11	1.42	1.39
1	A	849	A	C5-C4	-5.11	1.35	1.38
1	A	1176	G	N3-C4	5.11	1.39	1.35
1	A	2711	A	N9-C4	-5.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1365	A	N9-C4	-5.10	1.34	1.37
1	A	1903	G	N7-C5	-5.10	1.36	1.39
1	A	749	C	C4-C5	-5.10	1.38	1.43
1	A	1314	C	N3-C4	-5.09	1.30	1.33
1	A	2741	A	C5-C4	-5.09	1.35	1.38
1	A	1034	G	C5-C4	-5.09	1.34	1.38
28	6	16	CYS	CB-SG	-5.09	1.73	1.81
1	A	447	A	C5-C6	-5.09	1.36	1.41
1	A	1564	C	N1-C6	-5.09	1.34	1.37
1	A	2026	C	N1-C6	-5.09	1.34	1.37
1	A	123	G	N9-C4	-5.09	1.33	1.38
1	A	1279	G	C6-N1	-5.09	1.35	1.39
1	A	1624	G	C5-C4	-5.09	1.34	1.38
1	A	2063	C	N1-C6	-5.09	1.34	1.37
1	A	1308	A	N9-C8	-5.08	1.33	1.37
1	A	745	G	N1-C2	-5.07	1.33	1.37
1	A	188	G	C8-N7	-5.07	1.27	1.30
1	A	577	G	P-OP2	-5.07	1.40	1.49
1	A	2445	G	C6-N1	-5.07	1.36	1.39
1	A	109	G	C6-N1	-5.06	1.36	1.39
1	A	1827	C	N3-C4	-5.06	1.30	1.33
1	A	533	G	C6-N1	-5.06	1.36	1.39
1	A	658	C	C2-N3	-5.06	1.31	1.35
1	A	70	G	C6-N1	-5.06	1.36	1.39
1	A	1199	U	C2-N3	-5.05	1.34	1.37
1	A	1199	U	N1-C2	-5.05	1.34	1.38
1	A	1204	A	N3-C4	-5.05	1.31	1.34
1	A	2054	A	O3'-P	-5.05	1.55	1.61
1	A	972	G	N1-C2	-5.05	1.33	1.37
1	A	934	G	N9-C8	-5.05	1.34	1.37
1	A	555	U	N1-C2	-5.04	1.34	1.38
1	A	1363	C	C4-N4	-5.04	1.29	1.33
1	A	214	G	C5-C4	-5.04	1.34	1.38
1	A	1829	A	N3-C4	-5.04	1.31	1.34
1	A	2117	A	N9-C4	5.04	1.40	1.37
1	A	1393	A	C6-N1	-5.04	1.32	1.35
1	A	1363	C	C2-O2	-5.04	1.20	1.24
1	A	1211	U	P-O5'	-5.04	1.54	1.59
1	A	763	G	P-O5'	-5.03	1.54	1.59
1	A	2575	C	N3-C4	-5.03	1.30	1.33
1	A	1611	C	N1-C6	-5.03	1.34	1.37
1	A	841	A	N3-C4	-5.03	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	940	G	N3-C4	-5.03	1.31	1.35
1	A	659	C	N1-C6	-5.03	1.34	1.37
1	A	2036	C	N1-C2	-5.03	1.35	1.40
1	A	1970	A	N9-C8	-5.02	1.33	1.37
1	A	282	A	N7-C5	-5.02	1.36	1.39
1	A	1127	A	N9-C4	-5.02	1.34	1.37
1	A	1596	A	N9-C4	-5.02	1.34	1.37
1	A	71	A	C6-N6	-5.02	1.29	1.33
1	A	562	U	C2-O2	-5.01	1.17	1.22
1	A	1251	C	N1-C6	-5.01	1.34	1.37
1	A	2778	A	N9-C4	-5.01	1.34	1.37
1	A	807	U	N1-C6	-5.01	1.33	1.38
1	A	693	C	N1-C6	-5.00	1.34	1.37
1	A	2588	G	N1-C2	-5.00	1.33	1.37

All (2271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	U	N3-C4-O4	-24.18	102.47	119.40
1	A	2296	U	C2-N3-C4	-20.65	114.61	127.00
1	A	2296	U	C5-C6-N1	-20.40	112.50	122.70
1	A	2296	U	C2-N1-C1'	-18.50	95.50	117.70
1	A	676	A	C2-N3-C4	-18.16	101.52	110.60
1	A	2296	U	C5-C4-O4	18.02	136.71	125.90
1	A	945	A	C5-N7-C8	-17.19	95.31	103.90
1	A	330	A	C2-N3-C4	-16.40	102.40	110.60
1	A	2322	A	N9-C4-C5	15.93	112.17	105.80
1	A	528	A	C2-N3-C4	-14.74	103.23	110.60
1	A	587	C	C6-N1-C2	-14.72	114.41	120.30
1	A	1142(A)	A	C2-N3-C4	-14.71	103.25	110.60
1	A	2296	U	N1-C2-N3	13.85	123.21	114.90
1	A	1049	C	C6-N1-C2	-13.36	114.95	120.30
1	A	528	A	N3-C4-N9	-13.17	116.86	127.40
1	A	2322	A	C6-N1-C2	-13.05	110.77	118.60
1	A	945	A	N7-C8-N9	13.03	120.31	113.80
1	A	71	A	C2-N3-C4	-12.91	104.15	110.60
1	A	141	A	C5-N7-C8	-12.77	97.52	103.90
1	A	2296	U	C6-N1-C1'	12.76	139.06	121.20
1	A	2286	A	N1-C6-N6	12.72	126.23	118.60
1	A	856	C	C6-N1-C2	-12.70	115.22	120.30
1	A	528	A	N3-C4-C5	12.66	135.66	126.80
1	A	676	A	N3-C4-C5	12.62	135.64	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	A	C5-N7-C8	-12.39	97.70	103.90
1	A	975	C	C6-N1-C2	-12.23	115.41	120.30
1	A	2296	U	N3-C2-O2	-12.18	113.67	122.20
1	A	945	A	C2-N3-C4	-12.12	104.54	110.60
1	A	1049	C	C5-C6-N1	12.09	127.04	121.00
1	A	1021	A	C2-N3-C4	-12.08	104.56	110.60
1	A	676	A	C5-C6-N1	-11.91	111.74	117.70
1	A	2322	A	C8-N9-C4	-11.83	101.07	105.80
1	A	945	A	C4-C5-N7	11.57	116.48	110.70
1	A	2286	A	C6-C5-N7	-11.49	124.25	132.30
1	A	1762	A	C8-N9-C4	-11.37	101.25	105.80
1	A	2335	A	C5-C6-N1	11.28	123.34	117.70
1	A	141	A	N7-C8-N9	11.23	119.42	113.80
1	A	265	A	C5-N7-C8	-11.15	98.33	103.90
1	A	857	C	C6-N1-C2	-11.02	115.89	120.30
1	A	1698	A	C2-N3-C4	-10.94	105.13	110.60
1	A	1359	A	N1-C6-N6	-10.90	112.06	118.60
1	A	928	G	N1-C6-O6	10.88	126.43	119.90
1	A	933	A	C5-N7-C8	-10.83	98.48	103.90
1	A	71	A	C5-N7-C8	-10.79	98.51	103.90
1	A	141	A	N1-C6-N6	10.66	125.00	118.60
1	A	2723	C	N3-C4-C5	10.46	126.08	121.90
1	A	1204	A	C2-N3-C4	-10.41	105.40	110.60
1	A	2322	A	C4-C5-N7	-10.37	105.52	110.70
1	A	2296	U	N3-C4-C5	10.29	120.78	114.60
1	A	2322	A	N1-C6-N6	-10.28	112.43	118.60
2	B	30	C	C6-N1-C2	-10.24	116.20	120.30
1	A	330	A	N1-C2-N3	10.24	134.42	129.30
1	A	2371	G	N1-C6-O6	10.23	126.04	119.90
1	A	1108	U	N3-C2-O2	-10.22	115.05	122.20
1	A	915	C	C6-N1-C2	-10.12	116.25	120.30
1	A	90	U	C5-C6-N1	10.07	127.73	122.70
1	A	2319	G	C8-N9-C4	-10.02	102.39	106.40
1	A	1243	G	N1-C6-O6	9.92	125.85	119.90
1	A	1227	G	N1-C6-O6	9.91	125.85	119.90
1	A	2040	C	C6-N1-C2	9.90	124.26	120.30
1	A	884	C	C5-C6-N1	9.89	125.94	121.00
1	A	141	A	C4-C5-N7	9.83	115.62	110.70
1	A	1107	G	C4-N9-C1'	9.82	139.26	126.50
1	A	1210	A	C6-C5-N7	-9.80	125.44	132.30
1	A	676	A	N3-C4-N9	-9.79	119.56	127.40
1	A	265	A	N7-C8-N9	9.79	118.69	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2287	A	C2-N3-C4	-9.78	105.71	110.60
1	A	2719	G	C8-N9-C4	9.76	110.31	106.40
1	A	1107	G	C8-N9-C1'	-9.73	114.35	127.00
1	A	209	C	C5-C6-N1	-9.57	116.22	121.00
1	A	570	G	C8-N9-C4	9.54	110.22	106.40
1	A	409	C	C6-N1-C2	9.54	124.11	120.30
1	A	154(A)	C	N1-C2-O2	9.47	124.58	118.90
1	A	754	C	C5-C4-N4	-9.46	113.58	120.20
1	A	1248	G	C5-C6-O6	-9.46	122.92	128.60
1	A	1626	G	C5-C6-O6	9.46	134.27	128.60
2	B	104	U	C5-C6-N1	-9.45	117.97	122.70
1	A	2107	C	C2-N3-C4	9.44	124.62	119.90
1	A	2581	G	C5-C6-O6	9.44	134.26	128.60
1	A	265	A	C6-C5-N7	-9.41	125.71	132.30
1	A	2017	U	N1-C2-N3	9.41	120.55	114.90
1	A	47	C	C6-N1-C2	9.40	124.06	120.30
1	A	2251	G	C8-N9-C4	-9.38	102.65	106.40
1	A	463	G	C5-C6-O6	9.34	134.21	128.60
1	A	835	A	C2-N3-C4	9.34	115.27	110.60
1	A	202	U	N3-C4-O4	-9.33	112.87	119.40
1	A	194	G	N3-C2-N2	-9.33	113.37	119.90
1	A	265	A	N1-C6-N6	9.30	124.18	118.60
1	A	265	A	C4-C5-N7	9.30	115.35	110.70
1	A	2375	G	C8-N9-C4	9.29	110.11	106.40
1	A	1142(A)	A	N3-C4-C5	9.27	133.29	126.80
1	A	1437	C	C6-N1-C2	-9.26	116.59	120.30
1	A	1612	C	C6-N1-C2	9.26	124.01	120.30
1	A	391	G	N1-C6-O6	9.24	125.45	119.90
1	A	508	G	N1-C6-O6	9.20	125.42	119.90
1	A	2015	A	C8-N9-C4	-9.19	102.12	105.80
1	A	933	A	C4-C5-N7	9.19	115.30	110.70
1	A	465	G	C8-N9-C4	-9.19	102.72	106.40
1	A	2572	A	C8-N9-C4	9.16	109.47	105.80
1	A	1142(A)	A	N1-C6-N6	9.15	124.09	118.60
1	A	945	A	C8-N9-C4	-9.13	102.15	105.80
1	A	1490	A	C8-N9-C4	9.13	109.45	105.80
1	A	928	G	C6-C5-N7	-9.10	124.94	130.40
1	A	1210	A	C5-N7-C8	-9.08	99.36	103.90
1	A	1142(A)	A	C5-N7-C8	-9.06	99.37	103.90
1	A	2036	C	C6-N1-C2	-9.05	116.68	120.30
1	A	570	G	N9-C4-C5	-9.05	101.78	105.40
1	A	2502	G	C5-C6-N1	9.04	116.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1618	A	N1-C6-N6	-9.04	113.18	118.60
1	A	94	C	C6-N1-C2	-9.03	116.69	120.30
1	A	759	G	N1-C6-O6	9.02	125.31	119.90
1	A	1391	U	N1-C2-O2	9.02	129.11	122.80
1	A	2581	G	N1-C6-O6	-9.01	114.49	119.90
1	A	2322	A	N1-C2-N3	9.00	133.80	129.30
1	A	1210	A	N7-C8-N9	8.99	118.30	113.80
1	A	179	G	N1-C6-O6	8.99	125.29	119.90
1	A	2572	A	N7-C8-N9	-8.99	109.31	113.80
1	A	2273	A	C8-N9-C4	-8.98	102.21	105.80
1	A	982	C	N3-C2-O2	-8.97	115.62	121.90
1	A	1210	A	N1-C6-N6	8.97	123.98	118.60
1	A	71	A	N7-C8-N9	8.96	118.28	113.80
1	A	391	G	C4-C5-N7	8.96	114.39	110.80
1	A	1142(A)	A	C5-C6-N1	-8.96	113.22	117.70
1	A	1243	G	C2-N3-C4	-8.96	107.42	111.90
1	A	452	G	C5-C6-O6	8.96	133.97	128.60
1	A	572	A	C8-N9-C4	-8.95	102.22	105.80
1	A	2729	G	N1-C6-O6	8.95	125.27	119.90
1	A	141	A	C6-C5-N7	-8.93	126.05	132.30
1	A	574	C	C6-N1-C2	-8.91	116.74	120.30
1	A	1992	G	C4-C5-N7	-8.91	107.24	110.80
1	A	945	A	N3-C4-C5	8.89	133.03	126.80
1	A	2250	G	C8-N9-C4	-8.86	102.86	106.40
1	A	2371	G	C5-C6-O6	-8.85	123.29	128.60
1	A	689	A	C8-N9-C4	8.82	109.33	105.80
1	A	676	A	N7-C8-N9	8.82	118.21	113.80
1	A	794	G	N1-C6-O6	-8.82	114.61	119.90
1	A	1779	U	C6-N1-C2	8.81	126.28	121.00
1	A	2538	C	C6-N1-C2	8.80	123.82	120.30
1	A	2522	U	N3-C4-O4	8.79	125.55	119.40
1	A	675	A	N1-C6-N6	8.77	123.86	118.60
1	A	759	G	C5-C6-O6	-8.76	123.34	128.60
1	A	2791	C	C6-N1-C2	-8.76	116.80	120.30
1	A	777	A	C5-N7-C8	8.75	108.28	103.90
1	A	2041	U	N3-C2-O2	-8.75	116.08	122.20
1	A	2646	C	C6-N1-C2	8.74	123.80	120.30
1	A	391	G	N9-C4-C5	-8.73	101.91	105.40
1	A	1845	G	N1-C6-O6	-8.71	114.67	119.90
1	A	389	G	N9-C4-C5	-8.71	101.92	105.40
1	A	2440	C	C4-C5-C6	8.69	121.75	117.40
1	A	1022	G	C4-C5-N7	-8.69	107.32	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2286	A	C4-C5-C6	8.69	121.34	117.00
1	A	124	G	C4-C5-N7	8.68	114.27	110.80
1	A	1107	G	N3-C4-N9	8.68	131.21	126.00
1	A	698	C	N1-C2-O2	-8.67	113.70	118.90
1	A	1779	U	C6-N1-C1'	-8.67	109.06	121.20
1	A	2607	G	N1-C2-N2	-8.67	108.40	116.20
1	A	885	C	N1-C2-O2	8.64	124.08	118.90
1	A	528	A	C5-C6-N1	-8.62	113.39	117.70
1	A	154(A)	C	N3-C4-N4	-8.61	111.97	118.00
1	A	735	A	C8-N9-C4	8.61	109.24	105.80
1	A	884	C	C2-N3-C4	8.61	124.20	119.90
1	A	1001	A	C8-N9-C4	8.56	109.22	105.80
1	A	1698	A	C6-C5-N7	-8.56	126.31	132.30
1	A	2429	G	C8-N9-C4	-8.56	102.98	106.40
1	A	2440	C	N3-C4-C5	-8.56	118.48	121.90
1	A	386	G	C8-N9-C4	-8.54	102.98	106.40
1	A	1021	A	C5-N7-C8	-8.54	99.63	103.90
1	A	1222	C	N3-C4-C5	8.54	125.31	121.90
1	A	205	G	N9-C4-C5	-8.51	102.00	105.40
1	A	1565	C	C6-N1-C2	8.51	123.70	120.30
1	A	330	A	N3-C4-C5	8.51	132.75	126.80
1	A	1313	U	C6-N1-C2	-8.50	115.90	121.00
1	A	1645	G	C8-N9-C4	-8.48	103.01	106.40
1	A	510	C	N3-C4-C5	-8.46	118.51	121.90
1	A	1604	C	N1-C2-O2	-8.46	113.82	118.90
1	A	1248	G	N1-C6-O6	8.46	124.97	119.90
1	A	2286	A	C2-N3-C4	-8.45	106.37	110.60
1	A	1695	G	C4-C5-N7	8.44	114.17	110.80
1	A	455	C	N1-C2-O2	8.42	123.95	118.90
1	A	2725	A	C2-N3-C4	-8.42	106.39	110.60
1	A	676	A	C4-C5-N7	8.42	114.91	110.70
29	7	47	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	154(A)	C	N3-C2-O2	-8.40	116.02	121.90
1	A	684	G	N3-C2-N2	-8.38	114.04	119.90
1	A	1216	G	C6-C5-N7	-8.37	125.38	130.40
1	A	1315	C	N3-C2-O2	-8.37	116.04	121.90
1	A	975	C	N3-C2-O2	-8.36	116.05	121.90
1	A	1049	C	C2-N1-C1'	8.35	127.98	118.80
1	A	2723	C	N3-C4-N4	-8.35	112.16	118.00
2	B	4	C	C6-N1-C2	8.34	123.64	120.30
1	A	2318	G	C8-N9-C4	-8.34	103.06	106.40
1	A	2375	G	N7-C8-N9	-8.33	108.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	910	A	C8-N9-C4	8.32	109.13	105.80
1	A	1762	A	N7-C8-N9	8.32	117.96	113.80
1	A	804	A	C8-N9-C4	8.31	109.12	105.80
1	A	988	A	N1-C6-N6	8.30	123.58	118.60
1	A	2286	A	N7-C8-N9	8.30	117.95	113.80
1	A	508	G	C5-C6-O6	-8.28	123.63	128.60
1	A	2321	G	N3-C2-N2	-8.28	114.10	119.90
1	A	145	G	C8-N9-C4	8.28	109.71	106.40
1	A	2619	C	C5-C6-N1	-8.27	116.86	121.00
1	A	959	A	C5-C6-N6	8.27	130.32	123.70
1	A	1695	G	N1-C6-O6	8.27	124.86	119.90
2	B	76	G	C8-N9-C4	8.26	109.70	106.40
1	A	188	G	C2-N3-C4	-8.26	107.77	111.90
1	A	1210	A	C8-N9-C4	-8.26	102.50	105.80
1	A	645	C	N1-C2-O2	8.25	123.85	118.90
1	A	959	A	N1-C6-N6	-8.25	113.65	118.60
1	A	2206	G	C4-N9-C1'	-8.25	115.78	126.50
1	A	2100	G	N3-C4-N9	8.24	130.95	126.00
1	A	971	C	C6-N1-C2	-8.24	117.00	120.30
1	A	678	C	C6-N1-C2	8.24	123.60	120.30
1	A	844	C	C6-N1-C2	8.23	123.59	120.30
1	A	1022	G	N9-C4-C5	8.23	108.69	105.40
1	A	849	A	C8-N9-C4	8.23	109.09	105.80
1	A	1655	A	C8-N9-C4	8.22	109.09	105.80
5	F	74	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	1021	A	C5-C6-N1	-8.20	113.60	117.70
1	A	2206	G	N3-C4-C5	8.19	132.69	128.60
16	U	28	ARG	NE-CZ-NH1	-8.19	116.21	120.30
1	A	782	A	C6-N1-C2	-8.18	113.69	118.60
1	A	130	C	C6-N1-C2	8.18	123.57	120.30
1	A	2700	C	C6-N1-C2	8.17	123.57	120.30
1	A	745	G	N3-C4-C5	-8.16	124.52	128.60
1	A	1328	G	C8-N9-C4	8.16	109.66	106.40
1	A	2689	U	C5-C4-O4	8.15	130.79	125.90
1	A	2105	C	C6-N1-C2	-8.13	117.05	120.30
1	A	1977	A	C8-N9-C4	8.13	109.05	105.80
1	A	2349	G	C8-N9-C4	-8.11	103.16	106.40
1	A	272(D)	G	C8-N9-C4	8.09	109.64	106.40
1	A	2261	C	C4-C5-C6	8.09	121.44	117.40
1	A	1452	A	C8-N9-C4	8.08	109.03	105.80
1	A	1695	G	C5-N7-C8	-8.08	100.26	104.30
1	A	552	G	C8-N9-C4	8.08	109.63	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2084	C	C5-C6-N1	-8.08	116.96	121.00
1	A	1314	C	C2-N1-C1'	8.07	127.68	118.80
1	A	207	A	C2-N3-C4	-8.07	106.56	110.60
1	A	612	C	C6-N1-C2	8.07	123.53	120.30
1	A	527	C	N3-C2-O2	-8.06	116.25	121.90
1	A	2596	U	N1-C2-O2	-8.05	117.16	122.80
2	B	85	G	C5-C6-O6	-8.05	123.77	128.60
1	A	1695	G	C6-C5-N7	-8.05	125.57	130.40
1	A	205	G	N3-C2-N2	8.04	125.53	119.90
1	A	2242	G	N3-C2-N2	-8.04	114.27	119.90
1	A	1617	C	N3-C4-C5	-8.04	118.68	121.90
1	A	2306	C	C2-N1-C1'	8.03	127.63	118.80
1	A	745	G	N3-C4-N9	8.03	130.82	126.00
1	A	2497	A	C6-N1-C2	-8.03	113.78	118.60
1	A	2044	C	N1-C2-O2	-8.02	114.09	118.90
1	A	2010	G	N1-C6-O6	8.02	124.71	119.90
1	A	13	A	N1-C6-N6	-8.01	113.79	118.60
1	A	587	C	N3-C4-C5	-8.01	118.70	121.90
1	A	928	G	C5-C6-O6	-8.00	123.80	128.60
1	A	1647	G	N1-C6-O6	8.00	124.70	119.90
1	A	1217	C	C6-N1-C2	7.99	123.50	120.30
1	A	271(J)	C	C6-N1-C2	7.99	123.49	120.30
1	A	185	U	C5-C6-N1	-7.98	118.71	122.70
1	A	71	A	C8-N9-C4	-7.97	102.61	105.80
1	A	2087	G	N1-C6-O6	7.95	124.67	119.90
1	A	2286	A	C5-N7-C8	-7.95	99.93	103.90
1	A	2080	G	C8-N9-C4	7.94	109.58	106.40
1	A	2689	U	N3-C4-O4	-7.94	113.84	119.40
2	B	61	G	N3-C2-N2	-7.94	114.34	119.90
1	A	2307	G	N7-C8-N9	7.94	117.07	113.10
1	A	2404	C	C6-N1-C2	7.93	123.47	120.30
1	A	844	C	C5-C6-N1	-7.92	117.04	121.00
1	A	1372	U	N3-C2-O2	-7.92	116.66	122.20
1	A	1992	G	N9-C4-C5	7.91	108.56	105.40
1	A	546	C	C5-C6-N1	7.88	124.94	121.00
1	A	475	U	C6-N1-C2	-7.88	116.28	121.00
1	A	1570	A	C2-N3-C4	-7.87	106.67	110.60
1	A	1283	G	C5-C6-O6	7.85	133.31	128.60
1	A	1047	G	N3-C4-N9	7.85	130.71	126.00
1	A	2623	G	N3-C4-C5	-7.85	124.68	128.60
1	A	1128	A	C6-N1-C2	-7.84	113.90	118.60
1	A	1698	A	C5-N7-C8	-7.84	99.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	G	N9-C4-C5	-7.83	102.27	105.40
1	A	982	C	N1-C2-O2	7.83	123.60	118.90
1	A	2496	C	N1-C2-O2	-7.82	114.21	118.90
1	A	972	G	C5-C6-O6	7.81	133.29	128.60
1	A	572	A	N9-C4-C5	7.81	108.92	105.80
1	A	737	C	C6-N1-C2	7.81	123.42	120.30
1	A	2488	A	C8-N9-C4	7.80	108.92	105.80
1	A	202	U	N3-C4-C5	7.79	119.27	114.60
1	A	2505	G	C5-C6-N1	-7.78	107.61	111.50
1	A	2306	C	N1-C2-O2	7.77	123.56	118.90
1	A	729	G	C5-N7-C8	-7.75	100.42	104.30
1	A	2538	C	C5-C6-N1	-7.75	117.12	121.00
1	A	2863	C	C6-N1-C2	7.75	123.40	120.30
1	A	2791	C	N1-C2-O2	7.74	123.55	118.90
1	A	1657	C	N1-C2-O2	-7.74	114.26	118.90
1	A	689	A	N7-C8-N9	-7.73	109.94	113.80
1	A	287	C	C6-N1-C2	7.72	123.39	120.30
1	A	676	A	N1-C6-N6	7.72	123.23	118.60
1	A	455	C	N3-C2-O2	-7.72	116.50	121.90
1	A	2200	C	N3-C2-O2	-7.72	116.50	121.90
1	A	1343	G	N7-C8-N9	7.71	116.96	113.10
1	A	2296	U	O4'-C1'-N1	7.71	114.37	108.20
1	A	729	G	C4-C5-N7	7.71	113.89	110.80
1	A	102	G	C8-N9-C4	-7.70	103.32	106.40
1	A	2182	G	C6-N1-C2	7.70	129.72	125.10
1	A	655	A	C8-N9-C4	-7.69	102.72	105.80
1	A	2364	C	C6-N1-C2	7.68	123.37	120.30
1	A	2579	C	C5-C6-N1	-7.68	117.16	121.00
1	A	528	A	C5-N7-C8	-7.68	100.06	103.90
2	B	117	G	C8-N9-C4	7.67	109.47	106.40
1	A	745	G	C5-C6-N1	7.67	115.33	111.50
1	A	1602	U	N3-C4-C5	-7.67	110.00	114.60
1	A	2144	U	C5-C6-N1	7.67	126.53	122.70
1	A	2694	G	N3-C4-C5	-7.64	124.78	128.60
1	A	1490	A	N9-C4-C5	-7.64	102.75	105.80
1	A	655	A	N7-C8-N9	7.63	117.62	113.80
1	A	2041	U	N1-C2-N3	7.63	119.48	114.90
1	A	2286	A	C5-C6-N1	-7.63	113.89	117.70
1	A	1254	A	C8-N9-C4	-7.62	102.75	105.80
2	B	76	G	N3-C4-C5	7.62	132.41	128.60
1	A	465	G	N3-C4-C5	-7.62	124.79	128.60
2	B	7	G	N1-C6-O6	7.62	124.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	945	A	N3-C4-N9	-7.61	121.31	127.40
1	A	756	C	N3-C4-C5	-7.61	118.86	121.90
1	A	2619	C	C6-N1-C2	7.60	123.34	120.30
1	A	1314	C	C6-N1-C1'	-7.59	111.69	120.80
1	A	655	A	C5-N7-C8	-7.59	100.11	103.90
1	A	2200	C	N1-C2-O2	7.59	123.45	118.90
1	A	530	G	N3-C4-C5	7.58	132.39	128.60
1	A	530	G	C4-C5-N7	7.58	113.83	110.80
1	A	1779	U	N1-C2-N3	-7.58	110.35	114.90
1	A	2641	G	C6-C5-N7	-7.58	125.85	130.40
1	A	789	A	C8-N9-C4	7.57	108.83	105.80
1	A	2028	U	N3-C4-C5	7.56	119.14	114.60
1	A	2791	C	C5-C6-N1	7.55	124.77	121.00
1	A	2768	C	C5-C6-N1	-7.54	117.23	121.00
1	A	1464	C	C6-N1-C2	-7.54	117.28	120.30
1	A	556	G	C8-N9-C4	7.54	109.42	106.40
1	A	693	C	C6-N1-C2	-7.54	117.28	120.30
1	A	735	A	N7-C8-N9	-7.54	110.03	113.80
1	A	2597	G	C8-N9-C4	-7.53	103.39	106.40
1	A	202	U	C5-C6-N1	-7.53	118.94	122.70
1	A	468	G	C8-N9-C4	7.53	109.41	106.40
14	S	96	GLY	N-CA-C	-7.53	94.28	113.10
1	A	793	A	N1-C6-N6	7.52	123.11	118.60
1	A	2567	G	C8-N9-C4	7.52	109.41	106.40
1	A	297	C	N3-C4-C5	-7.52	118.89	121.90
1	A	2764	A	N1-C6-N6	-7.51	114.09	118.60
1	A	936	C	C6-N1-C2	7.51	123.31	120.30
1	A	265	A	C8-N9-C4	-7.51	102.80	105.80
1	A	188	G	N9-C4-C5	-7.51	102.40	105.40
1	A	452	G	N1-C6-O6	-7.51	115.40	119.90
1	A	1108	U	N1-C2-O2	7.50	128.05	122.80
1	A	1616	A	C5-C6-N6	-7.50	117.70	123.70
1	A	533	G	N3-C2-N2	-7.50	114.65	119.90
1	A	664	C	C6-N1-C2	7.50	123.30	120.30
1	A	577	G	C2-N3-C4	-7.50	108.15	111.90
1	A	1047	G	N3-C2-N2	7.50	125.15	119.90
1	A	62	C	C6-N1-C2	7.49	123.30	120.30
1	A	1616	A	N1-C6-N6	7.49	123.10	118.60
1	A	893	C	N1-C2-O2	7.49	123.39	118.90
1	A	1162	G	C8-N9-C4	-7.47	103.41	106.40
2	B	37	C	C6-N1-C2	-7.47	117.31	120.30
1	A	675	A	C4-C5-N7	7.47	114.43	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2449	U	N3-C4-O4	7.46	124.62	119.40
1	A	141	A	C8-N9-C4	-7.45	102.82	105.80
1	A	386	G	C4-C5-N7	7.45	113.78	110.80
1	A	562	U	N1-C2-N3	7.45	119.37	114.90
1	A	2711	A	C8-N9-C4	7.45	108.78	105.80
1	A	652(T)	C	C2-N3-C4	7.44	123.62	119.90
1	A	1582	C	N3-C2-O2	-7.43	116.70	121.90
1	A	574	C	C5-C6-N1	7.43	124.72	121.00
1	A	2893	G	C2-N3-C4	7.43	115.61	111.90
1	A	1901	A	N1-C6-N6	-7.43	114.14	118.60
1	A	810	U	N1-C2-O2	-7.42	117.60	122.80
1	A	933	A	C8-N9-C4	-7.42	102.83	105.80
1	A	2464	C	C6-N1-C1'	-7.42	111.90	120.80
1	A	209	C	C6-N1-C2	7.41	123.26	120.30
1	A	1994	C	N3-C4-N4	-7.40	112.82	118.00
1	A	2286	A	C4-C5-N7	7.40	114.40	110.70
1	A	463	G	N9-C4-C5	7.39	108.36	105.40
1	A	1653	G	N3-C4-C5	-7.39	124.91	128.60
1	A	760	G	N1-C6-O6	7.39	124.33	119.90
1	A	1258	C	N3-C4-C5	7.38	124.85	121.90
1	A	2335	A	C8-N9-C4	7.38	108.75	105.80
1	A	2018	G	C8-N9-C4	-7.37	103.45	106.40
1	A	2785	C	C6-N1-C2	-7.36	117.36	120.30
1	A	1301	A	C8-N9-C4	-7.36	102.86	105.80
1	A	1558	A	C8-N9-C4	7.36	108.74	105.80
1	A	2312	U	N3-C2-O2	-7.35	117.06	122.20
1	A	1990	C	N1-C2-O2	-7.35	114.49	118.90
1	A	1937	A	N1-C2-N3	7.34	132.97	129.30
1	A	362	U	C5-C4-O4	-7.34	121.50	125.90
1	A	2041	U	C4-C5-C6	7.34	124.10	119.70
1	A	2689	U	C5-C6-N1	-7.33	119.04	122.70
1	A	1815	A	N1-C6-N6	-7.33	114.20	118.60
1	A	265	A	C2-N3-C4	-7.32	106.94	110.60
1	A	1123	C	C6-N1-C2	7.32	123.23	120.30
1	A	736	C	C5-C4-N4	-7.32	115.08	120.20
1	A	211	A	C8-N9-C4	7.31	108.72	105.80
1	A	673	C	C6-N1-C2	7.31	123.22	120.30
1	A	124	G	C2-N3-C4	-7.31	108.25	111.90
1	A	674	G	N1-C6-O6	7.30	124.28	119.90
1	A	271(M)	G	N3-C4-C5	-7.30	124.95	128.60
1	A	777	A	C2-N3-C4	7.30	114.25	110.60
1	A	1819	A	N1-C6-N6	-7.29	114.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	G	N1-C2-N2	-7.29	109.64	116.20
1	A	2321	G	N9-C4-C5	7.28	108.31	105.40
1	A	975	C	N3-C4-C5	-7.27	118.99	121.90
1	A	1471	A	C8-N9-C4	-7.27	102.89	105.80
1	A	1963	U	C2-N1-C1'	7.27	126.43	117.70
1	A	47	C	N3-C4-C5	7.26	124.81	121.90
1	A	933	A	N7-C8-N9	7.26	117.43	113.80
1	A	2840	C	N3-C4-C5	7.26	124.80	121.90
1	A	135	G	C8-N9-C4	7.26	109.30	106.40
1	A	1204	A	C5-N7-C8	-7.26	100.27	103.90
1	A	2296	U	C4-C5-C6	7.26	124.05	119.70
1	A	102	G	C4-N9-C1'	7.25	135.92	126.50
1	A	745	G	C6-N1-C2	-7.25	120.75	125.10
1	A	1367	A	C8-N9-C4	7.24	108.70	105.80
1	A	1359	A	N9-C4-C5	7.24	108.69	105.80
2	B	104	U	C2-N3-C4	-7.24	122.66	127.00
1	A	765	G	N1-C6-O6	7.24	124.24	119.90
1	A	1334	G	C8-N9-C4	-7.24	103.51	106.40
1	A	2206	G	C8-N9-C1'	7.23	136.40	127.00
1	A	570	G	C4-C5-N7	7.23	113.69	110.80
1	A	1555	G	N1-C6-O6	7.22	124.23	119.90
1	A	2361	A	N1-C6-N6	7.22	122.93	118.60
1	A	2015	A	N9-C4-C5	7.21	108.69	105.80
1	A	446	G	N1-C6-O6	7.21	124.22	119.90
1	A	1189	A	N1-C6-N6	7.20	122.92	118.60
1	A	207	A	N3-C4-C5	7.20	131.84	126.80
1	A	733	G	C5-N7-C8	7.20	107.90	104.30
1	A	747	U	C5-C4-O4	-7.20	121.58	125.90
1	A	2017	U	N3-C2-O2	-7.19	117.17	122.20
1	A	1992	G	N1-C6-O6	-7.18	115.59	119.90
1	A	777	A	C4-C5-N7	-7.18	107.11	110.70
1	A	2028	U	C6-N1-C2	7.18	125.31	121.00
1	A	2251	G	N3-C4-C5	-7.17	125.02	128.60
1	A	2312	U	N1-C2-O2	7.16	127.81	122.80
1	A	2316	C	C6-N1-C2	-7.16	117.44	120.30
1	A	2041	U	C5-C6-N1	-7.15	119.12	122.70
22	0	20	ARG	NE-CZ-NH1	-7.15	116.72	120.30
1	A	330	A	C5-N7-C8	-7.15	100.33	103.90
1	A	570	G	C5-C6-O6	-7.15	124.31	128.60
1	A	2182	G	N3-C4-N9	-7.15	121.71	126.00
1	A	652(E)	G	C6-N1-C2	7.14	129.39	125.10
1	A	575	A	N1-C2-N3	7.14	132.87	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	G	C4-C5-N7	-7.14	107.94	110.80
1	A	2335	A	C6-N1-C2	-7.14	114.32	118.60
1	A	675	A	N9-C4-C5	-7.13	102.95	105.80
1	A	1189	A	C5-N7-C8	-7.13	100.33	103.90
1	A	2020	A	C8-N9-C4	7.13	108.65	105.80
1	A	1610	A	N1-C6-N6	7.12	122.87	118.60
1	A	676	A	C6-N1-C2	7.12	122.87	118.60
1	A	386	G	N7-C8-N9	7.12	116.66	113.10
1	A	1107	G	N3-C4-C5	-7.12	125.04	128.60
1	A	910	A	N9-C4-C5	-7.11	102.95	105.80
1	A	1992	G	N3-C4-C5	-7.11	125.05	128.60
1	A	1790	C	N1-C2-O2	-7.11	114.64	118.90
1	A	2761	G	C8-N9-C4	-7.10	103.56	106.40
1	A	691	C	N3-C4-C5	7.10	124.74	121.90
1	A	1604	C	N3-C2-O2	7.10	126.87	121.90
1	A	1180	C	C6-N1-C2	7.10	123.14	120.30
1	A	702	G	C2-N3-C4	-7.10	108.35	111.90
1	A	1045	A	C2-N3-C4	7.09	114.15	110.60
1	A	2755	C	C5-C6-N1	7.09	124.55	121.00
1	A	536	A	C8-N9-C4	7.09	108.64	105.80
1	A	1951	U	N3-C4-C5	-7.08	110.35	114.60
1	A	595	C	N3-C4-N4	7.08	122.96	118.00
1	A	2251	G	N9-C4-C5	7.08	108.23	105.40
1	A	1681	G	C4-C5-N7	7.07	113.63	110.80
2	B	89	G	C5-C6-O6	-7.07	124.36	128.60
1	A	2319	G	N7-C8-N9	7.06	116.63	113.10
1	A	1698	A	N1-C2-N3	7.06	132.83	129.30
1	A	90	U	N3-C4-O4	7.06	124.34	119.40
1	A	2503	A	N1-C2-N3	-7.05	125.78	129.30
1	A	1745	C	N1-C2-O2	-7.04	114.67	118.90
1	A	1989	G	N1-C6-O6	7.04	124.12	119.90
1	A	821	A	C8-N9-C4	-7.03	102.99	105.80
1	A	1243	G	C4-C5-N7	7.03	113.61	110.80
1	A	2609	U	N1-C2-O2	-7.03	117.88	122.80
1	A	148	C	C2-N3-C4	-7.03	116.39	119.90
1	A	1229	G	N1-C6-O6	7.03	124.12	119.90
1	A	1776	G	C8-N9-C4	7.03	109.21	106.40
1	A	884	C	C6-N1-C2	-7.02	117.49	120.30
1	A	1940	U	N3-C4-O4	7.02	124.32	119.40
1	A	1835	G	C8-N9-C4	-7.02	103.59	106.40
1	A	1249	U	N1-C2-O2	-7.02	117.89	122.80
1	A	141	A	C2-N3-C4	-7.02	107.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271(A)	A	C8-N9-C4	7.02	108.61	105.80
1	A	1358	G	N1-C6-O6	-7.02	115.69	119.90
1	A	1784	A	C8-N9-C4	7.02	108.61	105.80
1	A	2073	C	C5-C6-N1	-7.01	117.49	121.00
1	A	673	C	N3-C4-C5	7.01	124.70	121.90
1	A	2351	G	C8-N9-C1'	-7.01	117.89	127.00
1	A	2100	G	N3-C4-C5	-7.01	125.10	128.60
1	A	2307	G	C8-N9-C4	-7.01	103.60	106.40
1	A	729	G	C8-N9-C4	-7.00	103.60	106.40
1	A	1343	G	C5-N7-C8	-7.00	100.80	104.30
1	A	102	G	N7-C8-N9	7.00	116.60	113.10
1	A	729	G	N7-C8-N9	7.00	116.60	113.10
1	A	362	U	C2-N3-C4	-6.99	122.81	127.00
1	A	1558	A	C2-N3-C4	-6.99	107.11	110.60
1	A	1250	G	N1-C6-O6	6.99	124.09	119.90
1	A	804	A	N7-C8-N9	-6.99	110.31	113.80
1	A	391	G	C6-C5-N7	-6.99	126.21	130.40
1	A	425	G	N3-C4-C5	-6.98	125.11	128.60
1	A	1776	G	N9-C4-C5	-6.98	102.61	105.40
1	A	1698	A	N7-C8-N9	6.98	117.29	113.80
1	A	1628	G	C8-N9-C4	-6.98	103.61	106.40
1	A	1625	C	N3-C4-C5	6.98	124.69	121.90
1	A	1315	C	C6-N1-C2	-6.98	117.51	120.30
1	A	1643	G	N1-C6-O6	-6.97	115.72	119.90
1	A	767	U	N3-C2-O2	-6.97	117.32	122.20
1	A	2191	G	C5-C6-O6	-6.96	124.42	128.60
1	A	2579	C	C4-C5-C6	6.96	120.88	117.40
1	A	1184	G	N3-C2-N2	-6.96	115.03	119.90
1	A	1145	C	C6-N1-C2	-6.96	117.52	120.30
1	A	940	G	N1-C6-O6	6.96	124.07	119.90
1	A	71	A	N3-C4-N9	-6.95	121.84	127.40
1	A	33	U	C2-N1-C1'	-6.95	109.36	117.70
1	A	690	G	C5-C6-N1	6.95	114.97	111.50
1	A	1757	U	C5-C4-O4	-6.95	121.73	125.90
1	A	793	A	C5-N7-C8	-6.95	100.43	103.90
1	A	975	C	C5-C4-N4	6.95	125.06	120.20
1	A	1313	U	C2-N1-C1'	6.94	126.03	117.70
1	A	2346	A	C6-N1-C2	-6.94	114.43	118.60
1	A	1340	U	C5-C6-N1	-6.94	119.23	122.70
1	A	2837	G	C5-C6-O6	-6.94	124.44	128.60
1	A	1006	C	C5-C4-N4	6.93	125.05	120.20
1	A	575	A	C2-N3-C4	-6.93	107.13	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	A	N1-C6-N6	-6.92	114.45	118.60
1	A	751	A	C8-N9-C4	6.92	108.57	105.80
1	A	1210	A	C4-C5-C6	6.92	120.46	117.00
1	A	2803	C	C6-N1-C2	-6.92	117.53	120.30
1	A	1939	U	N3-C4-C5	6.92	118.75	114.60
1	A	2689	U	N1-C2-N3	6.91	119.05	114.90
1	A	2728	U	C5-C6-N1	-6.91	119.25	122.70
1	A	934	G	C8-N9-C4	6.91	109.16	106.40
1	A	2182	G	C5-C6-O6	6.91	132.74	128.60
1	A	188	G	C6-C5-N7	-6.90	126.26	130.40
1	A	645	C	C2-N1-C1'	6.90	126.39	118.80
1	A	2036	C	C5-C6-N1	6.89	124.44	121.00
1	A	803	U	C5-C6-N1	-6.88	119.26	122.70
1	A	530	G	N3-C2-N2	-6.87	115.09	119.90
1	A	2471	C	N1-C2-O2	6.87	123.02	118.90
1	A	2723	C	C2-N3-C4	-6.87	116.46	119.90
1	A	196	A	C4-C5-N7	6.87	114.13	110.70
1	A	475	U	N3-C4-C5	-6.87	110.48	114.60
1	A	1269	A	N9-C4-C5	-6.87	103.05	105.80
1	A	807	U	C5-C4-O4	-6.87	121.78	125.90
1	A	1207	C	C6-N1-C2	6.87	123.05	120.30
1	A	2011	U	N3-C2-O2	6.87	127.00	122.20
1	A	910	A	N1-C6-N6	6.86	122.72	118.60
1	A	2371	G	C4-C5-N7	6.86	113.54	110.80
1	A	1710	C	C6-N1-C2	6.85	123.04	120.30
1	A	988	A	N9-C4-C5	-6.84	103.06	105.80
1	A	1041	C	C6-N1-C2	-6.84	117.56	120.30
1	A	1210	A	C2-N3-C4	-6.84	107.18	110.60
2	B	37	C	N3-C4-C5	-6.83	119.17	121.90
1	A	547	A	C2-N3-C4	6.83	114.02	110.60
1	A	2059	A	N7-C8-N9	-6.83	110.38	113.80
1	A	207	A	C5-N7-C8	-6.83	100.49	103.90
1	A	1243	G	C6-C5-N7	-6.83	126.30	130.40
1	A	512	G	N1-C6-O6	-6.82	115.81	119.90
1	A	2705	A	C8-N9-C4	6.81	108.53	105.80
1	A	2442	C	C2-N3-C4	-6.81	116.49	119.90
1	A	2397	G	C8-N9-C4	-6.81	103.67	106.40
1	A	1021	A	N3-C4-C5	6.81	131.56	126.80
1	A	2582	G	N1-C6-O6	-6.81	115.81	119.90
2	B	27	C	C6-N1-C2	-6.81	117.58	120.30
1	A	213	A	N1-C6-N6	6.80	122.68	118.60
1	A	678	C	N3-C4-C5	6.80	124.62	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1758	G	N1-C6-O6	6.80	123.98	119.90
1	A	578	A	N9-C4-C5	6.80	108.52	105.80
1	A	1210	A	C4-C5-N7	6.80	114.10	110.70
1	A	1605	C	N3-C2-O2	-6.80	117.14	121.90
1	A	2363	C	C6-N1-C2	6.80	123.02	120.30
1	A	446	G	N3-C4-N9	6.79	130.07	126.00
1	A	2571	C	N1-C2-O2	-6.79	114.83	118.90
1	A	744	G	C5-C6-N1	-6.79	108.11	111.50
1	A	1405	U	N3-C4-O4	-6.79	114.65	119.40
1	A	2821	A	N1-C6-N6	6.79	122.67	118.60
1	A	786	C	C5-C6-N1	-6.78	117.61	121.00
1	A	2897	U	C2-N1-C1'	6.78	125.84	117.70
1	A	1047	G	N3-C4-C5	-6.78	125.21	128.60
1	A	885	C	C2-N1-C1'	6.78	126.25	118.80
1	A	458	G	N9-C4-C5	6.77	108.11	105.40
1	A	2351	G	C4-N9-C1'	6.77	135.30	126.50
1	A	1204	A	N3-C4-C5	6.76	131.53	126.80
1	A	1021	A	N1-C6-N6	6.76	122.66	118.60
1	A	530	G	N3-C4-N9	-6.76	121.94	126.00
1	A	188	G	C5-C6-N1	-6.76	108.12	111.50
1	A	2321	G	C8-N9-C4	-6.75	103.70	106.40
1	A	2041	U	C2-N3-C4	-6.75	122.95	127.00
1	A	2571	C	N1-C2-N3	6.75	123.92	119.20
1	A	1674	G	C5-C6-O6	-6.74	124.55	128.60
1	A	1698	A	C4-C5-N7	6.74	114.07	110.70
1	A	785	G	N3-C2-N2	-6.74	115.18	119.90
1	A	1790	C	C2-N3-C4	-6.73	116.53	119.90
1	A	1983	C	N1-C2-O2	-6.73	114.86	118.90
1	A	1283	G	N1-C6-O6	-6.73	115.86	119.90
1	A	258	G	N1-C2-N2	-6.72	110.15	116.20
1	A	2321	G	N1-C2-N2	6.72	122.25	116.20
1	A	525	U	C6-N1-C2	-6.72	116.97	121.00
1	A	2020	A	N7-C8-N9	-6.72	110.44	113.80
1	A	945	A	C6-C5-N7	-6.71	127.61	132.30
1	A	94	C	C5-C6-N1	6.70	124.35	121.00
1	A	1026	U	N1-C2-O2	6.70	127.49	122.80
1	A	204	A	C8-N9-C4	-6.70	103.12	105.80
1	A	1142(A)	A	N3-C4-N9	-6.70	122.04	127.40
1	A	940	G	C6-C5-N7	-6.70	126.38	130.40
1	A	2575	C	N3-C4-C5	-6.70	119.22	121.90
1	A	465	G	C4-C5-C6	6.70	122.82	118.80
1	A	2593	U	N3-C4-O4	-6.70	114.71	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2609	U	C2-N3-C4	-6.70	122.98	127.00
1	A	682	G	C4-C5-N7	6.69	113.48	110.80
1	A	839	U	C5-C4-O4	6.69	129.92	125.90
1	A	972	G	N1-C6-O6	-6.69	115.88	119.90
1	A	1038	C	N3-C2-O2	-6.69	117.22	121.90
1	A	1254	A	N1-C2-N3	6.68	132.64	129.30
1	A	754	C	N3-C4-C5	6.68	124.57	121.90
1	A	1653	G	C4-N9-C1'	6.68	135.19	126.50
1	A	2107	C	N3-C4-C5	-6.68	119.23	121.90
1	A	1758	G	N3-C2-N2	-6.67	115.23	119.90
2	B	81	G	N1-C6-O6	6.67	123.90	119.90
1	A	2519	U	N1-C2-O2	-6.67	118.13	122.80
1	A	1934	C	C6-N1-C2	6.66	122.97	120.30
1	A	1327	C	C6-N1-C2	-6.66	117.64	120.30
1	A	17	G	N1-C6-O6	-6.66	115.90	119.90
1	A	60	G	N1-C6-O6	6.66	123.89	119.90
1	A	1999	C	C2-N3-C4	-6.66	116.57	119.90
1	A	12	U	N3-C2-O2	-6.65	117.54	122.20
1	A	1217	C	N3-C2-O2	6.65	126.55	121.90
1	A	2100	G	C4-N9-C1'	6.64	135.14	126.50
1	A	675	A	C5-C6-N6	-6.64	118.39	123.70
1	A	2676	C	C6-N1-C2	6.64	122.96	120.30
1	A	1022	G	C6-C5-N7	6.64	134.38	130.40
1	A	213	A	C8-N9-C4	6.64	108.45	105.80
1	A	330	A	N3-C4-N9	-6.63	122.09	127.40
1	A	698	C	N3-C2-O2	6.63	126.54	121.90
1	A	577	G	N1-C6-O6	6.63	123.88	119.90
1	A	2371	G	N9-C4-C5	-6.63	102.75	105.40
1	A	669	G	C8-N9-C4	6.62	109.05	106.40
1	A	1345	C	C6-N1-C2	-6.62	117.65	120.30
1	A	2020	A	C5-N7-C8	6.62	107.21	103.90
1	A	592	G	C8-N9-C4	-6.62	103.75	106.40
1	A	2609	U	C5-C6-N1	-6.62	119.39	122.70
1	A	2464	C	C5-C4-N4	-6.62	115.57	120.20
1	A	885	C	C6-N1-C1'	-6.61	112.86	120.80
1	A	1132	A	C2-N3-C4	-6.61	107.29	110.60
1	A	47	C	C5-C4-N4	-6.61	115.57	120.20
1	A	2582	G	N7-C8-N9	6.61	116.41	113.10
1	A	793	A	N7-C8-N9	6.61	117.10	113.80
1	A	1613	G	N3-C2-N2	6.61	124.53	119.90
1	A	2832	U	C2-N1-C1'	6.61	125.63	117.70
1	A	1359	A	C5-C6-N1	6.60	121.00	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1217	C	C5-C4-N4	-6.60	115.58	120.20
1	A	2250	G	N9-C4-C5	6.60	108.04	105.40
1	A	458	G	C8-N9-C4	-6.60	103.76	106.40
1	A	750	A	C8-N9-C4	-6.60	103.16	105.80
1	A	1013	C	N1-C2-O2	-6.60	114.94	118.90
1	A	2182	G	C6-C5-N7	6.60	134.36	130.40
1	A	2000	G	N7-C8-N9	-6.59	109.80	113.10
1	A	2725	A	N1-C2-N3	6.59	132.60	129.30
1	A	71	A	N3-C4-C5	6.58	131.41	126.80
1	A	148	C	N3-C4-C5	6.58	124.53	121.90
1	A	1275	A	N1-C6-N6	6.58	122.55	118.60
1	A	1778	U	C5-C6-N1	-6.58	119.41	122.70
1	A	90	U	C2-N3-C4	6.58	130.95	127.00
1	A	1142(A)	A	C4-C5-N7	6.57	113.99	110.70
1	A	552	G	N7-C8-N9	-6.57	109.81	113.10
1	A	2572	A	C5-N7-C8	6.57	107.19	103.90
1	A	2304	G	C6-C5-N7	6.56	134.34	130.40
1	A	124	G	C5-C6-O6	-6.56	124.66	128.60
1	A	391	G	C5-C6-O6	-6.56	124.66	128.60
1	A	1536	C	C6-N1-C2	-6.56	117.68	120.30
1	A	13	A	C8-N9-C4	-6.56	103.18	105.80
1	A	1342	A	C5-C6-N1	6.56	120.98	117.70
1	A	2306	C	C5-C6-N1	6.56	124.28	121.00
1	A	1229	G	C5-C6-O6	-6.55	124.67	128.60
1	A	796	C	N3-C4-C5	6.55	124.52	121.90
2	B	7	G	C4-C5-N7	6.55	113.42	110.80
1	A	1391	U	N3-C2-O2	-6.55	117.62	122.20
1	A	769	G	C8-N9-C4	6.55	109.02	106.40
1	A	527	C	N3-C4-N4	-6.55	113.42	118.00
1	A	530	G	C5-N7-C8	-6.55	101.03	104.30
1	A	2607	G	N1-C2-N3	6.54	127.82	123.90
1	A	1207	C	C5-C6-N1	-6.54	117.73	121.00
1	A	1698	A	N1-C6-N6	6.54	122.52	118.60
1	A	2623	G	C5-C6-O6	6.54	132.52	128.60
1	A	1125	G	C8-N9-C1'	-6.53	118.51	127.00
1	A	1328	G	N9-C4-C5	-6.53	102.79	105.40
2	B	89	G	N1-C6-O6	6.53	123.82	119.90
1	A	2107	C	C5-C4-N4	6.53	124.77	120.20
1	A	2087	G	C4-C5-N7	6.53	113.41	110.80
1	A	2206	G	N3-C4-N9	-6.53	122.08	126.00
1	A	1334	G	N9-C4-C5	6.52	108.01	105.40
1	A	1822	G	C8-N9-C4	6.52	109.01	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	G	N7-C8-N9	-6.51	109.84	113.10
1	A	2224	G	N1-C6-O6	6.51	123.81	119.90
1	A	210	C	C6-N1-C2	6.51	122.90	120.30
1	A	2767	C	C6-N1-C2	6.51	122.90	120.30
1	A	1222	C	C5-C4-N4	-6.51	115.64	120.20
1	A	1189	A	C6-C5-N7	-6.50	127.75	132.30
1	A	2391	G	C4-C5-N7	-6.50	108.20	110.80
1	A	324	A	C8-N9-C4	6.50	108.40	105.80
1	A	1279	G	N1-C6-O6	-6.50	116.00	119.90
1	A	271(O)	C	C5-C6-N1	-6.50	117.75	121.00
1	A	1625	C	C6-N1-C2	6.50	122.90	120.30
1	A	2334	G	C8-N9-C4	6.50	109.00	106.40
2	B	30	C	C5-C6-N1	6.50	124.25	121.00
1	A	2037	G	N1-C6-O6	-6.50	116.00	119.90
1	A	2039	C	C5-C6-N1	6.50	124.25	121.00
1	A	2068	U	N3-C4-C5	6.50	118.50	114.60
1	A	674	G	C5-C6-O6	-6.49	124.70	128.60
1	A	1325	G	N3-C4-N9	6.49	129.90	126.00
1	A	2306	C	C2-N3-C4	6.49	123.15	119.90
1	A	2498	C	C6-N1-C2	6.49	122.89	120.30
1	A	1141	U	N1-C2-N3	6.49	118.79	114.90
1	A	1674	G	N1-C6-O6	6.49	123.79	119.90
1	A	205	G	N1-C2-N2	-6.49	110.36	116.20
1	A	1141	U	N3-C2-O2	-6.49	117.66	122.20
1	A	1343	G	C8-N9-C4	-6.49	103.81	106.40
2	B	87	G	C8-N9-C4	6.49	108.99	106.40
1	A	2849	U	C5-C6-N1	-6.48	119.46	122.70
1	A	71	A	N1-C2-N3	6.48	132.54	129.30
1	A	205	G	C8-N9-C4	6.48	108.99	106.40
1	A	624	C	C6-N1-C2	6.48	122.89	120.30
1	A	830	G	C4-C5-N7	-6.48	108.21	110.80
1	A	1137	G	C5-C6-N1	-6.48	108.26	111.50
1	A	2107	C	C6-N1-C2	-6.48	117.71	120.30
1	A	2659	G	C8-N9-C4	-6.47	103.81	106.40
1	A	33	U	C5-C4-O4	6.47	129.78	125.90
1	A	1001	A	N7-C8-N9	-6.47	110.56	113.80
1	A	968	G	C8-N9-C4	6.47	108.99	106.40
1	A	2129	C	C6-N1-C2	-6.47	117.71	120.30
1	A	2336	A	C2-N3-C4	6.47	113.83	110.60
1	A	2501	C	C6-N1-C2	6.47	122.89	120.30
1	A	62	C	C5-C6-N1	-6.46	117.77	121.00
1	A	2318	G	N7-C8-N9	6.46	116.33	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	G	N9-C4-C5	6.46	107.98	105.40
1	A	1304	C	C6-N1-C2	6.46	122.89	120.30
1	A	2198	A	C8-N9-C4	6.46	108.38	105.80
1	A	966	G	N1-C2-N2	-6.46	110.39	116.20
1	A	195	A	N1-C6-N6	6.45	122.47	118.60
1	A	389	G	N3-C2-N2	6.45	124.42	119.90
1	A	1970	A	C8-N9-C4	6.45	108.38	105.80
1	A	2503	A	C2-N3-C4	6.45	113.83	110.60
1	A	2259	G	N1-C6-O6	6.45	123.77	119.90
1	A	1610	A	N9-C4-C5	-6.45	103.22	105.80
1	A	333	G	C4-N9-C1'	6.45	134.88	126.50
1	A	2840	C	N3-C4-N4	-6.45	113.49	118.00
1	A	2385	C	C2-N3-C4	-6.44	116.68	119.90
1	A	2441	C	N3-C2-O2	-6.44	117.39	121.90
1	A	213	A	N9-C4-C5	-6.43	103.23	105.80
1	A	560	C	N1-C2-O2	-6.43	115.04	118.90
1	A	196	A	N1-C6-N6	6.43	122.46	118.60
1	A	974	G	N3-C4-C5	-6.43	125.39	128.60
1	A	2312	U	C2-N1-C1'	6.43	125.41	117.70
1	A	781	A	C8-N9-C4	6.43	108.37	105.80
1	A	984	A	N9-C4-C5	-6.43	103.23	105.80
1	A	1041	C	C5-C6-N1	6.43	124.21	121.00
1	A	1342	A	C6-N1-C2	-6.43	114.74	118.60
1	A	1464	C	N3-C4-C5	-6.42	119.33	121.90
1	A	1576	U	N3-C2-O2	-6.42	117.70	122.20
1	A	2065	C	N3-C2-O2	-6.42	117.40	121.90
1	A	1802	A	C2-N3-C4	-6.42	107.39	110.60
1	A	2587	A	N1-C6-N6	6.42	122.45	118.60
1	A	776	G	C6-N1-C2	-6.42	121.25	125.10
1	A	1616	A	C4-C5-N7	6.42	113.91	110.70
1	A	2819	G	C8-N9-C4	6.42	108.97	106.40
1	A	251	A	N1-C6-N6	-6.42	114.75	118.60
1	A	229	A	C8-N9-C4	-6.41	103.23	105.80
1	A	553	G	C4-C5-N7	6.41	113.37	110.80
1	A	1648	C	N3-C2-O2	-6.41	117.41	121.90
1	A	1273	U	N1-C2-N3	6.41	118.75	114.90
1	A	1658	C	C5-C4-N4	-6.41	115.71	120.20
1	A	2277	G	C5-C6-O6	6.41	132.44	128.60
1	A	2067	G	N3-C4-C5	-6.41	125.40	128.60
1	A	2751	G	C5-C6-O6	6.41	132.44	128.60
1	A	696	G	N9-C4-C5	-6.40	102.84	105.40
1	A	870	A	N7-C8-N9	-6.40	110.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1231	G	C2-N3-C4	-6.40	108.70	111.90
1	A	2539	C	C6-N1-C2	6.40	122.86	120.30
1	A	47	C	C2-N3-C4	-6.40	116.70	119.90
1	A	1216	G	C4-C5-N7	6.40	113.36	110.80
1	A	1813	G	N1-C6-O6	6.40	123.74	119.90
1	A	2897	U	C5-C6-N1	6.39	125.90	122.70
1	A	760	G	C5-C6-O6	-6.39	124.77	128.60
1	A	1639	U	N3-C2-O2	-6.39	117.73	122.20
1	A	296	C	N3-C4-C5	6.38	124.45	121.90
1	A	2429	G	N9-C4-C5	6.38	107.95	105.40
1	A	1695	G	N7-C8-N9	6.38	116.29	113.10
1	A	179	G	C8-N9-C4	6.38	108.95	106.40
1	A	2043	C	N1-C2-O2	-6.38	115.07	118.90
1	A	2633	G	N1-C6-O6	-6.38	116.07	119.90
1	A	1261	C	N3-C2-O2	6.38	126.36	121.90
1	A	464	U	C5-C4-O4	6.37	129.72	125.90
1	A	1204	A	C5-C6-N1	-6.37	114.51	117.70
1	A	1325	G	C5-C6-O6	-6.37	124.78	128.60
1	A	2182	G	C4-N9-C1'	-6.37	118.22	126.50
1	A	1790	C	C5-C4-N4	-6.37	115.74	120.20
1	A	2607	G	C4-C5-C6	6.37	122.62	118.80
1	A	453	C	C6-N1-C2	6.37	122.85	120.30
1	A	731	C	C6-N1-C2	6.37	122.85	120.30
1	A	886	C	C5-C6-N1	6.37	124.19	121.00
1	A	302	C	C6-N1-C2	-6.37	117.75	120.30
1	A	1269	A	C4-C5-N7	6.37	113.88	110.70
1	A	2837	G	N1-C6-O6	6.37	123.72	119.90
1	A	206	U	N1-C2-O2	-6.36	118.34	122.80
1	A	2080	G	N9-C4-C5	-6.36	102.86	105.40
1	A	2571	C	C2-N3-C4	-6.36	116.72	119.90
1	A	278	A	C6-N1-C2	-6.36	114.78	118.60
1	A	893	C	C2-N1-C1'	6.36	125.80	118.80
1	A	1982	C	C5-C6-N1	6.36	124.18	121.00
1	A	2430	A	C6-N1-C2	-6.36	114.78	118.60
1	A	1555	G	C6-C5-N7	-6.36	126.58	130.40
1	A	2761	G	N7-C8-N9	6.36	116.28	113.10
2	B	85	G	C4-C5-N7	6.36	113.34	110.80
1	A	272(D)	G	N7-C8-N9	-6.36	109.92	113.10
1	A	576	U	N3-C2-O2	-6.36	117.75	122.20
1	A	679	C	C6-N1-C2	6.35	122.84	120.30
1	A	2369	A	C5-C6-N1	6.35	120.88	117.70
1	A	760	G	C4-C5-N7	6.35	113.34	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2791	C	C2-N1-C1'	6.35	125.78	118.80
1	A	48	G	C5-C6-N1	-6.35	108.33	111.50
1	A	1791	A	C6-C5-N7	-6.35	127.86	132.30
1	A	840	C	C6-N1-C2	6.34	122.84	120.30
1	A	1125	G	C4-N9-C1'	6.34	134.75	126.50
1	A	2259	G	C2-N3-C4	-6.34	108.73	111.90
1	A	61	G	C8-N9-C4	6.34	108.94	106.40
1	A	2803	C	C5-C6-N1	6.34	124.17	121.00
1	A	512	G	C5-C6-O6	6.34	132.40	128.60
2	B	7	G	C5-C6-O6	-6.34	124.80	128.60
1	A	2628	C	C6-N1-C2	6.34	122.83	120.30
1	A	2719	G	N7-C8-N9	-6.34	109.93	113.10
1	A	1243	G	C5-C6-N1	-6.34	108.33	111.50
1	A	1938	A	C4-C5-C6	6.34	120.17	117.00
1	A	2778	A	C2-N3-C4	-6.34	107.43	110.60
1	A	570	G	N7-C8-N9	-6.33	109.93	113.10
1	A	1478	G	N3-C4-N9	6.33	129.80	126.00
1	A	200	U	C2-N3-C4	-6.33	123.20	127.00
1	A	2181	G	N3-C4-N9	-6.33	122.20	126.00
1	A	1437	C	N3-C4-C5	-6.33	119.37	121.90
1	A	829	A	C8-N9-C4	6.33	108.33	105.80
1	A	558	G	C8-N9-C4	6.33	108.93	106.40
1	A	745	G	C6-C5-N7	-6.33	126.61	130.40
1	A	2306	C	C6-N1-C1'	-6.33	113.21	120.80
1	A	2721	A	C6-N1-C2	-6.32	114.81	118.60
1	A	778	G	N1-C6-O6	-6.32	116.11	119.90
1	A	1404	C	N3-C2-O2	-6.32	117.48	121.90
1	A	2296	U	C1'-O4'-C4'	-6.32	104.84	109.90
1	A	794	G	C5-C6-O6	6.32	132.39	128.60
1	A	1696	G	C8-N9-C4	6.32	108.93	106.40
1	A	1782	C	C5-C4-N4	-6.32	115.78	120.20
1	A	2680	C	N3-C4-N4	6.32	122.42	118.00
1	A	777	A	N1-C6-N6	-6.32	114.81	118.60
1	A	2612	C	C6-N1-C2	6.32	122.83	120.30
1	A	2617	C	C6-N1-C2	6.32	122.83	120.30
1	A	2719	G	N9-C4-C5	-6.32	102.87	105.40
1	A	756	C	C4-C5-C6	6.31	120.56	117.40
1	A	1202	C	N1-C2-O2	-6.31	115.11	118.90
1	A	2182	G	C8-N9-C1'	6.31	135.21	127.00
1	A	2577	A	N1-C2-N3	-6.31	126.14	129.30
1	A	1189	A	N7-C8-N9	6.31	116.95	113.80
1	A	1189	A	C8-N9-C4	-6.31	103.28	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614(B)	G	C6-C5-N7	6.31	134.19	130.40
1	A	147	U	C5-C6-N1	-6.31	119.55	122.70
1	A	189	G	C8-N9-C4	6.31	108.92	106.40
1	A	2789	C	C6-N1-C2	6.31	122.82	120.30
1	A	657	U	C5-C6-N1	-6.30	119.55	122.70
1	A	2087	G	C5-C6-O6	-6.30	124.82	128.60
1	A	60	G	C5-C6-O6	-6.30	124.82	128.60
1	A	1044	G	N3-C4-C5	-6.30	125.45	128.60
1	A	129	C	C2-N3-C4	-6.30	116.75	119.90
1	A	753	C	N3-C2-O2	-6.30	117.49	121.90
1	A	1593	G	C5-C6-N1	6.30	114.65	111.50
1	A	1881	C	C6-N1-C2	-6.30	117.78	120.30
1	A	202	U	C6-N1-C2	6.29	124.78	121.00
1	A	723	G	C8-N9-C4	6.29	108.92	106.40
1	A	1896	G	N1-C6-O6	6.29	123.68	119.90
1	A	389	G	C4-C5-N7	6.29	113.32	110.80
1	A	659	C	C5-C6-N1	-6.29	117.85	121.00
1	A	1785	A	C2-N3-C4	-6.29	107.45	110.60
1	A	528	A	C8-N9-C1'	6.29	139.01	127.70
1	A	262	A	C6-N1-C2	-6.28	114.83	118.60
1	A	1791	A	N1-C6-N6	6.28	122.37	118.60
1	A	2487	G	N1-C6-O6	6.28	123.67	119.90
1	A	386	G	C5-N7-C8	-6.28	101.16	104.30
1	A	2335	A	O4'-C1'-N9	6.28	113.22	108.20
1	A	2371	G	C6-C5-N7	-6.28	126.63	130.40
1	A	148	C	C6-N1-C2	6.27	122.81	120.30
1	A	1616	A	N9-C4-C5	-6.27	103.29	105.80
1	A	271(J)	C	N3-C4-C5	6.27	124.41	121.90
1	A	1227	G	C5-C6-O6	-6.27	124.84	128.60
1	A	1661	G	N1-C2-N3	6.27	127.66	123.90
1	A	1021	A	N7-C8-N9	6.26	116.93	113.80
1	A	2623	G	C4-C5-N7	-6.26	108.29	110.80
2	B	8	U	C6-N1-C2	-6.26	117.24	121.00
1	A	661	C	C6-N1-C2	-6.26	117.80	120.30
1	A	71	A	C4-C5-N7	6.26	113.83	110.70
1	A	988	A	C6-C5-N7	-6.26	127.92	132.30
1	A	1005	C	N3-C4-C5	6.25	124.40	121.90
1	A	1256	G	N1-C2-N3	6.25	127.65	123.90
1	A	2036	C	C6-N1-C1'	6.25	128.31	120.80
1	A	2510	C	N3-C2-O2	-6.25	117.53	121.90
1	A	859	G	N1-C6-O6	6.25	123.65	119.90
1	A	109	G	N1-C6-O6	-6.25	116.15	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	A	N7-C8-N9	-6.25	110.68	113.80
1	A	2059	A	C5-N7-C8	6.25	107.02	103.90
1	A	2700	C	N3-C4-C5	6.25	124.40	121.90
1	A	526	A	C8-N9-C4	-6.24	103.30	105.80
1	A	1431	U	C5-C6-N1	6.24	125.82	122.70
1	A	2179	C	N1-C2-O2	6.24	122.65	118.90
1	A	2683	C	C6-N1-C2	-6.24	117.80	120.30
1	A	2712(A)	A	C2-N3-C4	-6.24	107.48	110.60
1	A	982	C	N3-C4-N4	-6.24	113.63	118.00
1	A	194	G	N3-C4-C5	6.24	131.72	128.60
1	A	640	C	N3-C4-C5	-6.24	119.40	121.90
1	A	793	A	C8-N9-C4	-6.24	103.30	105.80
1	A	988	A	C5-C6-N6	-6.24	118.71	123.70
1	A	2338	G	N1-C6-O6	6.24	123.64	119.90
1	A	2729	G	C5-C6-N1	-6.24	108.38	111.50
1	A	416	C	N3-C4-C5	6.24	124.39	121.90
1	A	2439	A	C2-N3-C4	-6.24	107.48	110.60
1	A	2621	A	C5-C6-N1	6.24	120.82	117.70
1	A	446	G	N9-C4-C5	-6.24	102.91	105.40
1	A	2502	G	C6-N1-C2	-6.24	121.36	125.10
1	A	2015	A	C2-N3-C4	-6.23	107.48	110.60
1	A	2011	U	N1-C2-O2	-6.23	118.44	122.80
1	A	2587	A	C8-N9-C4	6.22	108.29	105.80
1	A	652(F)	G	N1-C6-O6	6.22	123.63	119.90
1	A	2164	C	N3-C4-C5	-6.22	119.41	121.90
1	A	2100	G	C6-C5-N7	-6.22	126.67	130.40
1	A	745	G	C5-C6-O6	-6.22	124.87	128.60
1	A	799	G	C6-N1-C2	-6.22	121.37	125.10
1	A	196	A	C5-N7-C8	-6.21	100.79	103.90
1	A	1698	A	C8-N9-C4	-6.21	103.31	105.80
1	A	2292	C	N3-C4-C5	6.21	124.39	121.90
1	A	960	A	N1-C6-N6	6.21	122.33	118.60
1	A	2692	C	N3-C4-C5	6.21	124.39	121.90
1	A	2769	C	N3-C4-C5	6.21	124.38	121.90
1	A	586	A	C8-N9-C4	-6.21	103.32	105.80
1	A	763	G	C6-N1-C2	-6.21	121.38	125.10
1	A	1243	G	N3-C4-C5	6.21	131.70	128.60
1	A	2353	G	N9-C4-C5	-6.21	102.92	105.40
1	A	1803	A	C2-N3-C4	6.21	113.70	110.60
1	A	2555	U	N1-C2-O2	-6.21	118.46	122.80
1	A	529	A	C5-N7-C8	-6.20	100.80	103.90
1	A	1864	U	N3-C2-O2	6.20	126.54	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	G	C8-N9-C4	6.20	108.88	106.40
1	A	1602	U	C4-C5-C6	6.20	123.42	119.70
1	A	2353	G	C8-N9-C4	6.20	108.88	106.40
1	A	2425	A	C8-N9-C4	-6.20	103.32	105.80
1	A	2768	C	C2-N3-C4	-6.20	116.80	119.90
2	B	118	G	C8-N9-C4	6.20	108.88	106.40
1	A	1304	C	N3-C4-C5	6.19	124.38	121.90
1	A	2296	U	C6-N1-C2	6.19	124.71	121.00
1	A	2059	A	C8-N9-C4	6.19	108.28	105.80
1	A	2454	G	N7-C8-N9	-6.19	110.01	113.10
1	A	989	G	N9-C4-C5	-6.19	102.92	105.40
1	A	1021	A	N1-C2-N3	6.19	132.39	129.30
1	A	1992	G	C5-C6-O6	6.19	132.31	128.60
1	A	1979	C	C5-C6-N1	6.18	124.09	121.00
1	A	729	G	N1-C6-O6	6.18	123.61	119.90
1	A	984	A	C8-N9-C4	6.18	108.27	105.80
1	A	1128	A	C8-N9-C4	-6.18	103.33	105.80
1	A	1578	U	C5-C4-O4	6.18	129.61	125.90
1	A	2018	G	N7-C8-N9	6.18	116.19	113.10
1	A	558	G	N7-C8-N9	-6.17	110.01	113.10
1	A	2487	G	C5-C6-O6	-6.17	124.89	128.60
1	A	2808	U	N3-C4-O4	6.17	123.72	119.40
1	A	272(H)	C	C5-C6-N1	6.17	124.09	121.00
1	A	1262	A	C8-N9-C4	-6.17	103.33	105.80
1	A	2782	G	N1-C6-O6	6.17	123.60	119.90
1	A	2768	C	N3-C2-O2	-6.17	117.58	121.90
1	A	623	G	C8-N9-C4	6.17	108.87	106.40
1	A	1655	A	N7-C8-N9	-6.17	110.72	113.80
1	A	1858	G	C8-N9-C4	-6.17	103.93	106.40
1	A	1200	C	C5-C6-N1	-6.16	117.92	121.00
1	A	1304	C	C2-N3-C4	-6.16	116.82	119.90
1	A	1350	C	C6-N1-C2	6.16	122.77	120.30
1	A	1667	G	C5-C6-O6	-6.16	124.90	128.60
1	A	688	U	N1-C2-O2	-6.16	118.49	122.80
1	A	12	U	N1-C2-O2	6.16	127.11	122.80
1	A	1755	A	N9-C4-C5	6.16	108.26	105.80
1	A	2764	A	N9-C4-C5	6.16	108.26	105.80
1	A	1950	G	C5-C6-O6	6.15	132.29	128.60
1	A	678	C	C2-N3-C4	-6.15	116.83	119.90
1	A	764	A	C8-N9-C4	-6.15	103.34	105.80
1	A	2621	A	C4-C5-C6	-6.15	113.92	117.00
1	A	278	A	C5-C6-N6	-6.15	118.78	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	U	N1-C2-N3	6.15	118.59	114.90
1	A	2286	A	C8-N9-C4	-6.15	103.34	105.80
1	A	1178	C	C5-C6-N1	6.14	124.07	121.00
1	A	1448	G	N1-C6-O6	6.14	123.59	119.90
1	A	2582	G	C5-C6-O6	6.14	132.28	128.60
1	A	1819	A	C4-C5-N7	-6.14	107.63	110.70
1	A	2220	G	C8-N9-C4	-6.14	103.94	106.40
1	A	2592	G	C8-N9-C4	-6.13	103.95	106.40
1	A	272(H)	C	C5-C4-N4	-6.13	115.91	120.20
1	A	452	G	N3-C4-C5	-6.13	125.53	128.60
1	A	380	U	C5-C6-N1	-6.13	119.64	122.70
1	A	2300	G	N3-C4-N9	6.13	129.68	126.00
1	A	2596	U	N1-C2-N3	6.13	118.58	114.90
1	A	2446	G	C5-C6-O6	-6.12	124.93	128.60
1	A	475	U	N3-C2-O2	-6.12	117.92	122.20
1	A	2257	U	N3-C2-O2	6.12	126.48	122.20
1	A	363(B)	G	N3-C4-N9	6.12	129.67	126.00
1	A	1200	C	C2-N3-C4	-6.12	116.84	119.90
1	A	1531	C	C6-N1-C2	-6.12	117.85	120.30
1	A	667	U	N1-C2-O2	-6.12	118.52	122.80
1	A	2445	G	C5-C6-O6	6.12	132.27	128.60
1	A	201	C	C6-N1-C2	6.11	122.74	120.30
1	A	1936	A	C8-N9-C4	-6.11	103.36	105.80
1	A	1536	C	C2-N1-C1'	6.11	125.52	118.80
1	A	2100	G	C8-N9-C1'	-6.11	119.06	127.00
1	A	2103	C	C2-N3-C4	6.10	122.95	119.90
1	A	196	A	N9-C4-C5	-6.10	103.36	105.80
1	A	592	G	N9-C4-C5	6.10	107.84	105.40
1	A	1681	G	C6-C5-N7	-6.10	126.74	130.40
1	A	1268	A	C2-N3-C4	-6.10	107.55	110.60
1	A	2013	A	C5-N7-C8	-6.09	100.85	103.90
1	A	682	G	C6-C5-N7	-6.09	126.75	130.40
1	A	2049	G	C2-N3-C4	-6.09	108.86	111.90
1	A	2286	A	N1-C2-N3	6.09	132.34	129.30
1	A	2875	C	C6-N1-C2	6.09	122.74	120.30
2	B	92	C	C5-C6-N1	6.09	124.04	121.00
1	A	1137	G	N1-C6-O6	6.09	123.55	119.90
1	A	1816	G	N9-C4-C5	-6.09	102.97	105.40
3	D	131	LEU	CB-CG-CD2	-6.09	100.65	111.00
1	A	742	G	C8-N9-C4	6.08	108.83	106.40
1	A	1391	U	C2-N1-C1'	6.08	125.00	117.70
1	A	143	G	C4-N9-C1'	-6.08	118.59	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	759	G	C8-N9-C4	6.08	108.83	106.40
1	A	2273	A	C5-N7-C8	-6.08	100.86	103.90
1	A	2856	C	C6-N1-C2	-6.08	117.87	120.30
1	A	546	C	C6-N1-C2	-6.08	117.87	120.30
1	A	2225	A	C4-C5-C6	-6.08	113.96	117.00
1	A	2397	G	N7-C8-N9	6.08	116.14	113.10
1	A	122	G	N1-C6-O6	6.08	123.55	119.90
1	A	468	G	N9-C4-C5	-6.08	102.97	105.40
1	A	679	C	C2-N3-C4	-6.08	116.86	119.90
1	A	2015	A	C4-C5-C6	6.08	120.04	117.00
1	A	533	G	N1-C2-N3	6.07	127.54	123.90
1	A	1315	C	N1-C2-N3	6.07	123.45	119.20
1	A	2003	G	C5-C6-N1	6.07	114.54	111.50
1	A	886	C	N1-C2-O2	6.07	122.54	118.90
1	A	2287	A	C5-N7-C8	-6.07	100.86	103.90
1	A	2464	C	C2-N1-C1'	6.07	125.48	118.80
1	A	2672	G	N1-C6-O6	6.07	123.54	119.90
1	A	239	U	C5-C6-N1	-6.07	119.67	122.70
1	A	763	G	C4-C5-N7	-6.07	108.37	110.80
1	A	527	C	C5-C4-N4	6.07	124.45	120.20
1	A	2004	G	C5-N7-C8	-6.07	101.27	104.30
1	A	2707	G	C4-C5-N7	6.07	113.23	110.80
1	A	1478	G	N3-C2-N2	6.06	124.14	119.90
1	A	2279	G	N1-C2-N2	-6.06	110.74	116.20
1	A	2587	A	N1-C2-N3	6.06	132.33	129.30
1	A	1530	C	C6-N1-C1'	-6.06	113.53	120.80
1	A	1142(A)	A	N1-C2-N3	6.06	132.33	129.30
1	A	1471	A	N7-C8-N9	6.06	116.83	113.80
1	A	1900	A	C2-N3-C4	6.06	113.63	110.60
1	A	2065	C	N3-C4-C5	-6.06	119.48	121.90
1	A	2607	G	C8-N9-C1'	-6.06	119.12	127.00
1	A	1358	G	N3-C4-C5	-6.05	125.57	128.60
1	A	2312	U	C5-C6-N1	6.05	125.73	122.70
1	A	535	C	C2-N1-C1'	-6.05	112.14	118.80
1	A	1276	A	C2-N3-C4	-6.05	107.57	110.60
1	A	1368	G	N9-C4-C5	6.05	107.82	105.40
1	A	1970	A	C8-N9-C1'	-6.05	116.81	127.70
1	A	2072	G	C6-C5-N7	-6.05	126.77	130.40
1	A	2279	G	N3-C2-N2	6.05	124.13	119.90
1	A	2575	C	C4-C5-C6	6.05	120.42	117.40
1	A	1698	A	C5-C6-N1	-6.05	114.68	117.70
1	A	2026	C	N3-C4-C5	-6.04	119.48	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	U	C2-N1-C1'	6.04	124.95	117.70
1	A	20	C	C2-N3-C4	-6.04	116.88	119.90
1	A	94	C	C2-N1-C1'	6.04	125.45	118.80
1	A	1245	G	N1-C6-O6	-6.04	116.27	119.90
1	A	1130	U	C4-C5-C6	6.04	123.32	119.70
1	A	1864	U	N1-C2-O2	-6.04	118.57	122.80
1	A	1608	A	C2-N3-C4	-6.04	107.58	110.60
1	A	1242	A	C8-N9-C4	6.04	108.22	105.80
1	A	2304	G	C4-N9-C1'	-6.03	118.66	126.50
2	B	61	G	N1-C2-N2	6.03	121.63	116.20
1	A	2200	C	C2-N1-C1'	6.03	125.43	118.80
1	A	2238	G	C2-N3-C4	6.03	114.91	111.90
1	A	2578	G	N1-C2-N3	6.03	127.52	123.90
1	A	751	A	C6-N1-C2	-6.03	114.98	118.60
1	A	131	G	C4-C5-N7	6.02	113.21	110.80
1	A	752	A	N1-C2-N3	6.02	132.31	129.30
1	A	2319	G	N3-C4-N9	-6.02	122.39	126.00
1	A	975	C	C4-C5-C6	6.02	120.41	117.40
1	A	1632	A	N1-C6-N6	6.02	122.21	118.60
1	A	385	C	N3-C4-C5	-6.01	119.50	121.90
1	A	624	C	N3-C4-C5	6.01	124.30	121.90
1	A	941	A	C2-N3-C4	6.01	113.61	110.60
1	A	940	G	C8-N9-C4	-6.01	104.00	106.40
1	A	595	C	C5-C4-N4	-6.00	116.00	120.20
1	A	737	C	N3-C2-O2	6.00	126.10	121.90
1	A	1159	U	N1-C2-N3	6.00	118.50	114.90
1	A	2361	A	C5-C6-N6	-6.00	118.90	123.70
1	A	392	C	N3-C4-C5	6.00	124.30	121.90
1	A	723	G	N9-C4-C5	-6.00	103.00	105.40
1	A	2319	G	N9-C4-C5	6.00	107.80	105.40
1	A	1243	G	N9-C4-C5	-6.00	103.00	105.40
1	A	706	A	C8-N9-C4	6.00	108.20	105.80
1	A	920	G	N1-C2-N2	-5.99	110.81	116.20
1	A	2727	G	N1-C6-O6	5.99	123.50	119.90
1	A	684	G	N1-C2-N2	5.99	121.59	116.20
1	A	893	C	C6-N1-C1'	-5.99	113.61	120.80
1	A	1273	U	N3-C4-O4	-5.99	115.21	119.40
1	A	1721	G	C4-C5-N7	5.99	113.20	110.80
1	A	1819	A	N9-C4-C5	5.99	108.20	105.80
1	A	782	A	C5-C6-N6	-5.99	118.91	123.70
1	A	1531	C	C5-C6-N1	5.99	123.99	121.00
1	A	1952	A	C8-N9-C4	-5.99	103.40	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	912	C	C6-N1-C2	-5.99	117.91	120.30
1	A	2497	A	C5-C6-N1	5.98	120.69	117.70
1	A	1643	G	C5-C6-O6	5.98	132.19	128.60
8	I	123	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	1779	U	N1-C2-O2	5.98	126.99	122.80
1	A	448	U	C6-N1-C2	-5.98	117.41	121.00
1	A	180	G	C5-C6-O6	-5.98	125.01	128.60
1	A	794	G	N1-C2-N2	-5.97	110.82	116.20
1	A	500	G	C5-C6-O6	5.97	132.18	128.60
1	A	2028	U	N3-C4-O4	-5.97	115.22	119.40
1	A	1811	G	N3-C2-N2	-5.97	115.72	119.90
1	A	2791	C	N3-C2-O2	-5.97	117.72	121.90
1	A	1760	A	N1-C6-N6	-5.97	115.02	118.60
1	A	652(T)	C	N1-C2-O2	5.97	122.48	118.90
1	A	990	A	C2-N3-C4	-5.97	107.62	110.60
1	A	2621	A	N1-C6-N6	-5.97	115.02	118.60
2	B	117	G	N7-C8-N9	-5.96	110.12	113.10
1	A	1546	C	C2-N1-C1'	5.96	125.36	118.80
1	A	2522	U	N3-C4-C5	-5.96	111.02	114.60
1	A	1773	A	C2-N3-C4	5.96	113.58	110.60
1	A	194	G	C5-C6-N1	-5.96	108.52	111.50
1	A	2292	C	C2-N3-C4	-5.96	116.92	119.90
1	A	892	G	C6-N1-C2	5.96	128.67	125.10
1	A	215	G	N1-C2-N3	5.96	127.47	123.90
1	A	945	A	C1'-O4'-C4'	-5.96	105.14	109.90
1	A	746	A	N1-C6-N6	5.95	122.17	118.60
1	A	988	A	C4-C5-N7	5.95	113.68	110.70
1	A	114	U	C2-N1-C1'	5.94	124.83	117.70
1	A	508	G	N9-C4-C5	-5.94	103.02	105.40
1	A	516	C	N1-C2-O2	-5.94	115.33	118.90
1	A	2680	C	C6-N1-C2	5.94	122.68	120.30
1	A	2894	G	C4-C5-N7	5.94	113.17	110.80
1	A	268	C	N3-C4-N4	5.93	122.15	118.00
1	A	2518	A	C8-N9-C4	-5.93	103.43	105.80
1	A	2335	A	C5-C6-N6	-5.93	118.95	123.70
1	A	1298	C	N3-C4-C5	5.93	124.27	121.90
2	B	97	G	N7-C8-N9	-5.93	110.14	113.10
1	A	386	G	C6-C5-N7	-5.93	126.84	130.40
1	A	951	C	C6-N1-C2	5.93	122.67	120.30
1	A	1208	C	C5-C4-N4	-5.93	116.05	120.20
1	A	1300	U	P-O3'-C3'	5.93	126.81	119.70
1	A	2641	G	C4-N9-C1'	5.93	134.21	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	A	C5-C6-N6	-5.92	118.96	123.70
1	A	1565	C	N3-C4-C5	5.92	124.27	121.90
1	A	777	A	N3-C4-C5	-5.92	122.65	126.80
1	A	989	G	C4-C5-N7	5.92	113.17	110.80
1	A	1681	G	N1-C6-O6	5.92	123.45	119.90
1	A	1132	A	N1-C2-N3	5.91	132.26	129.30
1	A	1208	C	N1-C2-O2	-5.91	115.35	118.90
1	A	1858	G	N7-C8-N9	5.91	116.06	113.10
1	A	271(M)	G	N3-C4-N9	5.91	129.55	126.00
1	A	2609	U	C4-C5-C6	5.91	123.25	119.70
1	A	886	C	C2-N1-C1'	5.91	125.30	118.80
1	A	271(G)	C	C6-N1-C2	-5.91	117.94	120.30
1	A	578	A	C8-N9-C4	-5.91	103.44	105.80
1	A	2391	G	N9-C4-C5	5.91	107.76	105.40
1	A	2581	G	N3-C2-N2	5.90	124.03	119.90
1	A	431	U	C5-C6-N1	5.90	125.65	122.70
1	A	826	U	N3-C4-C5	-5.90	111.06	114.60
1	A	2277	G	N1-C6-O6	-5.90	116.36	119.90
1	A	1290	C	C6-N1-C2	-5.90	117.94	120.30
1	A	792	G	C8-N9-C1'	-5.90	119.33	127.00
1	A	179	G	C5-C6-O6	-5.89	125.06	128.60
1	A	424	G	C5-C6-O6	-5.89	125.06	128.60
1	A	844	C	N3-C4-C5	5.89	124.26	121.90
1	A	297	C	N3-C4-N4	5.89	122.12	118.00
1	A	1422	G	C2-N3-C4	5.89	114.84	111.90
1	A	2381	C	N1-C2-N3	5.89	123.32	119.20
1	A	2226	C	C6-N1-C2	5.89	122.66	120.30
3	D	229	VAL	CB-CA-C	-5.89	100.22	111.40
1	A	2319	G	C5-N7-C8	-5.88	101.36	104.30
1	A	2335	A	N9-C4-C5	-5.88	103.45	105.80
1	A	1721	G	C8-N9-C4	-5.88	104.05	106.40
1	A	240	G	C5-C6-N1	5.88	114.44	111.50
1	A	271(S)	G	N1-C6-O6	5.88	123.43	119.90
1	A	667	U	N3-C4-O4	5.88	123.51	119.40
1	A	256	A	C8-N9-C4	5.88	108.15	105.80
1	A	819	A	N1-C6-N6	-5.88	115.08	118.60
1	A	1428	C	C4-C5-C6	5.88	120.34	117.40
1	A	1479	G	N1-C6-O6	5.88	123.43	119.90
1	A	2297	C	C5-C4-N4	5.88	124.31	120.20
1	A	2729	G	C6-C5-N7	-5.88	126.88	130.40
1	A	209	C	C4-C5-C6	5.87	120.34	117.40
1	A	752	A	P-O3'-C3'	5.87	126.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2129	C	N1-C2-O2	5.87	122.42	118.90
1	A	736	C	N1-C2-O2	-5.87	115.38	118.90
1	A	1230	C	C6-N1-C2	5.87	122.65	120.30
1	A	610	G	C8-N9-C4	5.86	108.75	106.40
1	A	1128	A	C5-C6-N1	5.86	120.63	117.70
1	A	1926	U	N3-C2-O2	-5.86	118.09	122.20
1	A	756	C	N1-C2-O2	-5.86	115.38	118.90
1	A	1128	A	N9-C4-C5	5.86	108.14	105.80
1	A	330	A	C5-C6-N1	-5.86	114.77	117.70
1	A	1951	U	N3-C4-O4	5.86	123.50	119.40
1	A	1405	U	C5-C6-N1	-5.86	119.77	122.70
1	A	845	G	N3-C4-N9	5.86	129.51	126.00
1	A	846	C	C2-N3-C4	-5.86	116.97	119.90
1	A	1989	G	C6-C5-N7	-5.86	126.89	130.40
1	A	2260	C	N1-C2-N3	5.85	123.30	119.20
1	A	751	A	N7-C8-N9	-5.85	110.87	113.80
1	A	822	U	N3-C2-O2	-5.85	118.10	122.20
1	A	1304	C	C5-C6-N1	-5.85	118.07	121.00
1	A	2441	C	C2-N3-C4	-5.85	116.97	119.90
1	A	2751	G	C8-N9-C4	-5.85	104.06	106.40
1	A	2857	G	N1-C6-O6	5.85	123.41	119.90
1	A	679	C	N1-C2-O2	-5.85	115.39	118.90
1	A	2201	C	C2-N3-C4	-5.85	116.97	119.90
1	A	1677	A	C2-N3-C4	-5.85	107.68	110.60
1	A	2004	G	N7-C8-N9	5.85	116.02	113.10
1	A	1645	G	N9-C4-C5	5.84	107.74	105.40
1	A	508	G	C6-C5-N7	-5.84	126.89	130.40
1	A	1004	C	C6-N1-C2	-5.84	117.96	120.30
1	A	1351	C	N1-C2-O2	-5.84	115.39	118.90
1	A	1367	A	N7-C8-N9	-5.84	110.88	113.80
1	A	2087	G	C2-N3-C4	-5.84	108.98	111.90
1	A	2453	A	N1-C6-N6	-5.84	115.09	118.60
1	A	1290	C	N3-C2-O2	-5.84	117.81	121.90
1	A	1382	G	C8-N9-C4	5.84	108.74	106.40
1	A	1653	G	N3-C4-N9	5.84	129.50	126.00
1	A	2740	A	N1-C2-N3	5.84	132.22	129.30
1	A	1297	C	N1-C2-O2	-5.84	115.40	118.90
1	A	1519	G	C8-N9-C4	-5.84	104.07	106.40
1	A	1779	U	C5-C4-O4	-5.84	122.40	125.90
1	A	2546	U	N3-C4-C5	-5.84	111.10	114.60
1	A	793	A	C5-C6-N6	-5.83	119.03	123.70
1	A	1211	U	N3-C2-O2	5.83	126.28	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	807	U	N3-C4-O4	5.83	123.48	119.40
1	A	2044	C	N3-C2-O2	5.83	125.98	121.90
1	A	2455	G	C5-C6-O6	-5.83	125.10	128.60
12	Q	87	LYS	CD-CE-NZ	5.83	125.11	111.70
1	A	1271	G	C5-C6-N1	-5.83	108.58	111.50
1	A	848	G	C4-N9-C1'	5.83	134.08	126.50
1	A	640	C	C6-N1-C2	-5.83	117.97	120.30
1	A	2017	U	C6-N1-C2	-5.82	117.51	121.00
1	A	1021	A	C4-C5-N7	5.82	113.61	110.70
1	A	2348	U	N3-C4-C5	5.82	118.09	114.60
1	A	2617	C	C5-C6-N1	-5.82	118.09	121.00
1	A	1680	U	C6-N1-C2	-5.82	117.51	121.00
1	A	2146	C	N1-C2-O2	5.82	122.39	118.90
1	A	968	G	N7-C8-N9	-5.82	110.19	113.10
1	A	2746	U	C5-C4-O4	5.82	129.39	125.90
1	A	141	A	C5-C6-N6	-5.82	119.05	123.70
1	A	1432	C	N3-C4-N4	5.82	122.07	118.00
1	A	2049	G	N3-C4-C5	5.82	131.51	128.60
1	A	1333	C	N1-C2-O2	-5.81	115.41	118.90
1	A	1359	A	C4-C5-C6	-5.81	114.09	117.00
1	A	746	A	C5-N7-C8	-5.81	101.00	103.90
1	A	1207	C	C4-C5-C6	5.81	120.31	117.40
1	A	2849	U	N1-C2-O2	-5.81	118.73	122.80
1	A	1387	C	C6-N1-C2	-5.81	117.98	120.30
1	A	2304	G	C5-C6-N1	5.81	114.40	111.50
1	A	1578	U	N3-C2-O2	-5.80	118.14	122.20
1	A	2073	C	C4-C5-C6	5.80	120.30	117.40
1	A	446	G	C5-C6-O6	-5.80	125.12	128.60
1	A	510	C	C5-C4-N4	5.80	124.26	120.20
1	A	115	C	N1-C2-O2	-5.80	115.42	118.90
1	A	2230	G	N1-C2-N2	5.80	121.42	116.20
1	A	1963	U	C5-C6-N1	5.79	125.60	122.70
1	A	2592	G	N3-C4-C5	-5.79	125.70	128.60
1	A	723	G	C5-C6-O6	-5.79	125.12	128.60
1	A	1938	A	C8-N9-C4	-5.79	103.48	105.80
1	A	1142(A)	A	C6-C5-N7	-5.79	128.25	132.30
1	A	1769	G	C5-C6-O6	-5.79	125.12	128.60
1	A	571	A	C5-C6-N6	-5.79	119.07	123.70
1	A	1937	A	C6-N1-C2	-5.79	115.13	118.60
1	A	475	U	N1-C2-N3	5.79	118.37	114.90
1	A	2273	A	N7-C8-N9	5.79	116.69	113.80
1	A	188	G	C8-N9-C4	5.79	108.71	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	G	C4-C5-N7	-5.79	108.49	110.80
1	A	496	G	N9-C4-C5	-5.78	103.09	105.40
1	A	794	G	N1-C2-N3	5.78	127.37	123.90
1	A	674	G	C4-C5-N7	5.78	113.11	110.80
1	A	1273	U	C2-N3-C4	-5.78	123.53	127.00
2	B	15	A	N1-C6-N6	5.78	122.07	118.60
1	A	2054	A	C5-C6-N6	-5.78	119.08	123.70
1	A	2712(A)	A	N1-C6-N6	5.77	122.06	118.60
1	A	1117	G	C5-C6-O6	-5.77	125.14	128.60
1	A	2304	G	C8-N9-C1'	5.77	134.50	127.00
1	A	2745	C	C2-N1-C1'	5.77	125.15	118.80
1	A	991	C	N1-C2-O2	-5.77	115.44	118.90
1	A	2370	G	N1-C6-O6	-5.77	116.44	119.90
1	A	1266	G	C4-C5-N7	5.76	113.11	110.80
1	A	2609	U	N1-C2-N3	5.76	118.36	114.90
1	A	951	C	C5-C6-N1	-5.76	118.12	121.00
1	A	2454	G	C8-N9-C4	5.76	108.70	106.40
1	A	2790	A	C8-N9-C4	-5.76	103.50	105.80
1	A	1180	C	C5-C6-N1	-5.76	118.12	121.00
1	A	2298	A	N1-C6-N6	-5.76	115.14	118.60
1	A	1022	G	N3-C2-N2	-5.76	115.87	119.90
1	A	2430	A	N1-C2-N3	5.76	132.18	129.30
1	A	1269	A	C5-N7-C8	-5.76	101.02	103.90
1	A	2004	G	C8-N9-C4	-5.76	104.10	106.40
1	A	1998	G	C5-C6-N1	-5.75	108.62	111.50
1	A	633	A	N1-C6-N6	5.75	122.05	118.60
1	A	803	U	C4-C5-C6	5.75	123.15	119.70
1	A	1478	G	N1-C2-N2	-5.75	111.02	116.20
1	A	1658	C	N3-C4-N4	5.75	122.03	118.00
1	A	2300	G	N3-C4-C5	-5.75	125.72	128.60
1	A	13	A	N9-C4-C5	5.75	108.10	105.80
1	A	1398	C	N1-C2-O2	-5.75	115.45	118.90
1	A	2322	A	N3-C4-C5	-5.75	122.77	126.80
1	A	1254	A	N9-C4-C5	5.75	108.10	105.80
1	A	2840	C	C2-N3-C4	-5.75	117.03	119.90
1	A	677	A	C2-N3-C4	-5.74	107.73	110.60
1	A	193	U	N1-C2-N3	5.74	118.34	114.90
1	A	848	G	C8-N9-C1'	-5.74	119.54	127.00
1	A	1791	A	C2-N3-C4	-5.74	107.73	110.60
1	A	2626	C	N3-C4-C5	5.74	124.20	121.90
1	A	810	U	N3-C2-O2	5.74	126.22	122.20
1	A	1805	U	N3-C4-O4	5.74	123.42	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2589	A	C8-N9-C4	5.74	108.10	105.80
1	A	1938	A	C6-N1-C2	-5.74	115.16	118.60
1	A	510	C	C4-C5-C6	5.74	120.27	117.40
1	A	712	G	C8-N9-C4	5.74	108.69	106.40
2	B	97	G	C5-N7-C8	5.73	107.17	104.30
1	A	2014	A	N1-C6-N6	5.73	122.04	118.60
1	A	2590	A	C5-N7-C8	-5.73	101.03	103.90
1	A	2732	G	C5-C6-O6	-5.73	125.16	128.60
1	A	2785	C	N3-C2-O2	-5.73	117.89	121.90
1	A	2442	C	C5-C6-N1	-5.73	118.14	121.00
2	B	5	C	C6-N1-C2	5.73	122.59	120.30
1	A	1801	G	C5-C6-O6	-5.72	125.17	128.60
1	A	2260	C	C2-N3-C4	-5.72	117.04	119.90
1	A	463	G	N1-C6-O6	-5.72	116.47	119.90
1	A	664	C	C5-C6-N1	-5.72	118.14	121.00
1	A	2682	U	C5-C4-O4	-5.72	122.47	125.90
1	A	1543	C	N1-C2-O2	5.72	122.33	118.90
1	A	2676	C	C5-C6-N1	-5.72	118.14	121.00
1	A	607	U	C6-N1-C2	5.71	124.43	121.00
1	A	2066	C	C5-C6-N1	5.71	123.86	121.00
1	A	324	A	N7-C8-N9	-5.71	110.94	113.80
1	A	1225	G	N3-C4-N9	-5.71	122.57	126.00
1	A	1858	G	N3-C4-C5	-5.71	125.75	128.60
1	A	2694	G	N3-C4-N9	5.71	129.43	126.00
19	X	57	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	1261	C	N1-C2-O2	-5.71	115.47	118.90
1	A	2261	C	N3-C4-C5	-5.71	119.62	121.90
2	B	61	G	N1-C6-O6	5.71	123.32	119.90
1	A	431	U	C2-N1-C1'	5.71	124.55	117.70
2	B	14	U	C5-C6-N1	-5.71	119.85	122.70
1	A	841	A	N1-C2-N3	5.70	132.15	129.30
1	A	1341	U	N3-C2-O2	-5.70	118.21	122.20
1	A	2764	A	C5-C6-N6	5.70	128.26	123.70
1	A	2883	A	C8-N9-C4	5.70	108.08	105.80
1	A	1125	G	N3-C4-N9	5.70	129.42	126.00
2	B	74	U	N1-C2-N3	5.70	118.32	114.90
1	A	2577	A	C4-C5-C6	-5.70	114.15	117.00
1	A	48	G	C5-C6-O6	5.70	132.02	128.60
1	A	1828	G	C8-N9-C4	5.70	108.68	106.40
1	A	2189	U	N1-C2-O2	5.70	126.79	122.80
1	A	2491	U	C6-N1-C2	5.70	124.42	121.00
1	A	1586	A	N7-C8-N9	5.69	116.65	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	734	A	N1-C6-N6	5.69	122.02	118.60
1	A	2893	G	C8-N9-C1'	5.69	134.40	127.00
1	A	806	C	N3-C4-C5	5.69	124.18	121.90
1	A	1139	G	N1-C6-O6	-5.69	116.49	119.90
1	A	1858	G	C4-N9-C1'	5.69	133.90	126.50
1	A	2445	G	N1-C6-O6	-5.69	116.49	119.90
1	A	2623	G	N1-C6-O6	-5.69	116.49	119.90
23	1	46	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	2086	U	C5-C4-O4	5.69	129.31	125.90
1	A	194	G	C2-N3-C4	-5.69	109.06	111.90
1	A	2832	U	C6-N1-C1'	-5.69	113.24	121.20
1	A	2186	G	C5-C6-N1	-5.69	108.66	111.50
1	A	26	G	C8-N9-C4	-5.68	104.13	106.40
1	A	508	G	C4-C5-N7	5.68	113.07	110.80
1	A	1368	G	C8-N9-C4	-5.68	104.13	106.40
1	A	2597	G	C6-C5-N7	-5.68	126.99	130.40
1	A	1244	G	N3-C2-N2	-5.68	115.92	119.90
1	A	870	A	C8-N9-C4	5.68	108.07	105.80
1	A	1443	G	N1-C6-O6	5.68	123.31	119.90
1	A	1998	G	C2-N3-C4	-5.68	109.06	111.90
1	A	2338	G	C5-C6-O6	-5.68	125.19	128.60
1	A	2499	C	C6-N1-C2	-5.68	118.03	120.30
1	A	476	G	C5-C6-N1	-5.67	108.66	111.50
1	A	528	A	C6-N1-C2	5.67	122.00	118.60
1	A	512	G	C4-C5-N7	-5.67	108.53	110.80
1	A	874	G	N3-C4-C5	5.67	131.44	128.60
1	A	938	G	C8-N9-C4	5.67	108.67	106.40
1	A	1586	A	C4-C5-C6	5.67	119.84	117.00
1	A	431	U	N3-C4-O4	5.67	123.37	119.40
1	A	363(E)	U	C6-N1-C2	-5.67	117.60	121.00
1	A	734	A	C5-N7-C8	-5.67	101.07	103.90
1	A	2699	C	C5-C4-N4	-5.67	116.23	120.20
1	A	2821	A	N9-C4-C5	-5.66	103.53	105.80
1	A	2182	G	C4-C5-N7	-5.66	108.53	110.80
1	A	577	G	C6-C5-N7	-5.66	127.00	130.40
1	A	1374	G	N1-C6-O6	5.66	123.30	119.90
1	A	2826	A	C2-N3-C4	-5.66	107.77	110.60
1	A	1845	G	C5-C6-O6	5.66	132.00	128.60
1	A	1459	G	C8-N9-C4	-5.66	104.14	106.40
1	A	1799	G	P-O3'-C3'	5.65	126.48	119.70
1	A	1345	C	N1-C2-O2	-5.65	115.51	118.90
1	A	954	G	N3-C4-C5	-5.65	125.78	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1797	C	C6-N1-C2	5.65	122.56	120.30
1	A	577	G	C5-C6-N1	-5.65	108.68	111.50
1	A	932	G	N9-C4-C5	5.65	107.66	105.40
1	A	1409	C	C6-N1-C2	5.64	122.56	120.30
1	A	1982	C	C6-N1-C2	-5.64	118.04	120.30
1	A	99	U	C6-N1-C2	5.64	124.39	121.00
1	A	250	G	C5-C6-O6	-5.64	125.22	128.60
1	A	1407	C	N1-C2-O2	-5.64	115.52	118.90
1	A	2866	U	C5-C4-O4	5.64	129.29	125.90
1	A	1316	U	N1-C2-O2	5.64	126.75	122.80
1	A	1779	U	C2-N1-C1'	5.64	124.47	117.70
1	A	1992	G	P-O3'-C3'	5.64	126.47	119.70
1	A	1758	G	C5-C6-O6	-5.63	125.22	128.60
1	A	308	G	C4-N9-C1'	5.63	133.82	126.50
1	A	1002	G	C8-N9-C4	-5.63	104.15	106.40
1	A	2471	C	N3-C2-O2	-5.63	117.96	121.90
1	A	1900	A	C8-N9-C4	-5.63	103.55	105.80
1	A	185	U	N1-C2-N3	5.62	118.27	114.90
1	A	512	G	O4'-C1'-N9	5.62	112.70	108.20
1	A	1001	A	C4-C5-C6	-5.62	114.19	117.00
1	A	2055	C	C2-N1-C1'	-5.62	112.61	118.80
1	A	907	U	N1-C2-O2	5.62	126.74	122.80
1	A	201	C	C2-N3-C4	-5.62	117.09	119.90
1	A	706	A	N9-C4-C5	-5.62	103.55	105.80
1	A	1322	A	N1-C2-N3	-5.62	126.49	129.30
1	A	116	C	C4-C5-C6	5.62	120.21	117.40
1	A	1256	G	C4-N9-C1'	5.62	133.81	126.50
1	A	1278	A	C4-C5-C6	5.62	119.81	117.00
1	A	2857	G	C8-N9-C4	-5.62	104.15	106.40
1	A	1187	G	N1-C6-O6	-5.62	116.53	119.90
1	A	1797	C	C5-C4-N4	-5.62	116.27	120.20
1	A	2055	C	C6-N1-C1'	5.62	127.54	120.80
1	A	58	G	N1-C2-N3	5.61	127.27	123.90
1	A	1824	G	C5-N7-C8	5.61	107.11	104.30
1	A	1916	A	C8-N9-C4	5.61	108.05	105.80
1	A	799	G	N1-C2-N3	5.61	127.27	123.90
1	A	1022	G	N3-C4-N9	-5.61	122.63	126.00
1	A	1049	C	N1-C2-O2	5.61	122.27	118.90
1	A	1187	G	C8-N9-C4	-5.61	104.16	106.40
1	A	1637	A	C8-N9-C4	-5.61	103.56	105.80
1	A	1785	A	C6-C5-N7	-5.61	128.37	132.30
1	A	271(W)	G	N1-C6-O6	-5.61	116.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1298	C	N3-C4-N4	-5.61	114.08	118.00
1	A	739	G	C5-C6-O6	-5.60	125.24	128.60
1	A	932	G	N3-C4-N9	-5.60	122.64	126.00
1	A	1242	A	N1-C6-N6	5.60	121.96	118.60
1	A	1989	G	C5-C6-O6	-5.60	125.24	128.60
1	A	2554	U	N1-C2-O2	-5.60	118.88	122.80
1	A	2676	C	C2-N3-C4	-5.60	117.10	119.90
1	A	1170	G	C6-C5-N7	-5.60	127.04	130.40
1	A	1333	C	N3-C4-C5	5.60	124.14	121.90
1	A	1374	G	N3-C2-N2	-5.60	115.98	119.90
1	A	1829	A	C2-N3-C4	-5.60	107.80	110.60
2	B	86	G	C5-C6-O6	-5.60	125.24	128.60
1	A	1358	G	C4-C5-N7	-5.60	108.56	110.80
1	A	496	G	C8-N9-C4	5.59	108.64	106.40
1	A	729	G	C5-C6-O6	-5.59	125.24	128.60
1	A	2550	G	N3-C2-N2	-5.59	115.98	119.90
1	A	2610	C	N3-C4-C5	5.59	124.14	121.90
1	A	509	C	C4-C5-C6	5.59	120.19	117.40
1	A	837	C	C6-N1-C2	-5.59	118.06	120.30
7	H	71	LEU	N-CA-C	-5.59	95.90	111.00
1	A	959	A	C4-C5-N7	-5.59	107.91	110.70
1	A	1022	G	C8-N9-C1'	5.59	134.27	127.00
1	A	425	G	C5-N7-C8	5.59	107.09	104.30
1	A	1021	A	C6-C5-N7	-5.59	128.39	132.30
1	A	2441	C	C5-C6-N1	-5.59	118.21	121.00
1	A	1261	C	N3-C4-C5	-5.58	119.67	121.90
1	A	2416	C	N1-C2-O2	-5.58	115.55	118.90
2	B	97	G	C8-N9-C4	5.58	108.63	106.40
1	A	2087	G	C6-C5-N7	-5.58	127.05	130.40
1	A	560	C	C2-N3-C4	-5.58	117.11	119.90
1	A	2179	C	C2-N1-C1'	5.58	124.94	118.80
1	A	2733	A	N1-C6-N6	5.58	121.95	118.60
1	A	614(B)	G	C4-C5-N7	-5.58	108.57	110.80
1	A	746	A	C4-C5-N7	5.58	113.49	110.70
1	A	13	A	C5-C6-N6	5.58	128.16	123.70
1	A	1349	A	N1-C6-N6	5.58	121.94	118.60
1	A	1779	U	N3-C4-C5	5.57	117.94	114.60
1	A	2593	U	C5-C4-O4	5.57	129.24	125.90
1	A	2661	G	N3-C4-C5	-5.57	125.81	128.60
1	A	1488	G	N1-C6-O6	5.57	123.24	119.90
1	A	1653	G	C4-C5-C6	5.57	122.14	118.80
30	8	34	TRP	N-CA-C	-5.57	95.96	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	C	C4-C5-C6	5.57	120.19	117.40
1	A	1597	A	N7-C8-N9	-5.57	111.02	113.80
1	A	1999	C	N1-C2-O2	-5.57	115.56	118.90
1	A	1193	G	C8-N9-C4	5.57	108.63	106.40
1	A	2351	G	N3-C4-N9	5.57	129.34	126.00
1	A	2696	U	N3-C4-O4	-5.57	115.50	119.40
1	A	2538	C	C2-N3-C4	-5.56	117.12	119.90
1	A	2545	G	N3-C2-N2	-5.56	116.00	119.90
2	B	64	C	C2-N1-C1'	-5.56	112.68	118.80
1	A	1803	A	C8-N9-C4	-5.56	103.58	105.80
1	A	2587	A	N9-C4-C5	-5.56	103.58	105.80
1	A	2342	C	C5-C6-N1	5.56	123.78	121.00
1	A	496	G	N1-C6-O6	5.55	123.23	119.90
1	A	1204	A	C4-C5-N7	5.55	113.48	110.70
1	A	2297	C	C6-N1-C1'	5.55	127.47	120.80
1	A	2641	G	N7-C8-N9	5.55	115.88	113.10
1	A	1021	A	N3-C4-N9	-5.55	122.96	127.40
1	A	1939	U	C4-C5-C6	-5.55	116.37	119.70
1	A	263	C	N1-C2-O2	5.55	122.23	118.90
1	A	1250	G	C5-C6-O6	-5.55	125.27	128.60
1	A	2611	U	C5-C4-O4	-5.55	122.57	125.90
1	A	1900	A	C5-C6-N1	5.55	120.47	117.70
1	A	1403	C	C2-N1-C1'	-5.55	112.70	118.80
1	A	1822	G	N7-C8-N9	-5.55	110.33	113.10
1	A	90	U	N1-C2-N3	-5.54	111.57	114.90
1	A	1322	A	N1-C6-N6	5.54	121.92	118.60
1	A	2567	G	N7-C8-N9	-5.54	110.33	113.10
1	A	2607	G	N3-C2-N2	5.54	123.78	119.90
1	A	425	G	N3-C4-N9	5.54	129.32	126.00
1	A	966	G	N3-C2-N2	5.54	123.78	119.90
1	A	1816	G	C4-C5-N7	5.54	113.02	110.80
1	A	2271	G	N3-C4-N9	5.54	129.32	126.00
1	A	1805	U	C4-C5-C6	5.54	123.02	119.70
1	A	154(A)	C	C5-C4-N4	5.54	124.07	120.20
1	A	1581	G	C4-N9-C1'	5.54	133.69	126.50
1	A	179	G	N9-C4-C5	-5.53	103.19	105.40
1	A	1800	C	N3-C4-C5	-5.53	119.69	121.90
1	A	768	G	N3-C4-N9	5.53	129.32	126.00
26	4	42	PHE	C-N-CA	5.53	135.53	121.70
1	A	2354	G	C5-N7-C8	-5.53	101.54	104.30
1	A	830	G	C5-N7-C8	5.53	107.06	104.30
1	A	1489	U	N1-C2-O2	-5.53	118.93	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2430	A	C8-N9-C4	-5.53	103.59	105.80
1	A	2605	U	N1-C2-N3	5.53	118.22	114.90
1	A	648	G	N3-C2-N2	-5.52	116.03	119.90
1	A	1391	U	C6-N1-C1'	-5.52	113.47	121.20
1	A	1530	C	C5-C4-N4	-5.52	116.33	120.20
1	A	2314	C	C2-N1-C1'	-5.52	112.72	118.80
1	A	1271	G	N1-C6-O6	5.52	123.21	119.90
1	A	1628	G	N7-C8-N9	5.52	115.86	113.10
1	A	1641	A	N1-C2-N3	5.52	132.06	129.30
1	A	2043	C	C6-N1-C2	-5.52	118.09	120.30
1	A	2590	A	N3-C4-C5	5.52	130.67	126.80
1	A	2716	U	N1-C2-O2	5.52	126.67	122.80
1	A	2252	G	C8-N9-C4	5.52	108.61	106.40
2	B	104	U	C6-N1-C2	5.52	124.31	121.00
2	B	104	U	N3-C4-C5	5.52	117.91	114.60
1	A	1405	U	N3-C4-C5	5.52	117.91	114.60
1	A	2225	A	C5-C6-N1	5.52	120.46	117.70
1	A	688	U	C2-N3-C4	-5.51	123.69	127.00
1	A	990	A	N9-C4-C5	-5.51	103.59	105.80
1	A	2895	U	C5-C6-N1	5.51	125.46	122.70
1	A	122	G	C6-C5-N7	-5.51	127.10	130.40
1	A	1561	G	C5-C6-O6	-5.50	125.30	128.60
1	A	1752	C	N3-C2-O2	5.50	125.75	121.90
1	A	1962	C	C5-C6-N1	5.50	123.75	121.00
1	A	675	A	C5-N7-C8	-5.50	101.15	103.90
1	A	33	U	C5-C6-N1	-5.50	119.95	122.70
1	A	1912	A	C8-N9-C4	-5.50	103.60	105.80
1	A	2623	G	C8-N9-C4	-5.50	104.20	106.40
1	A	652(F)	G	C5-C6-O6	-5.50	125.30	128.60
1	A	754	C	N3-C4-N4	5.50	121.85	118.00
1	A	1022	G	C4-N9-C1'	-5.50	119.35	126.50
1	A	2162	G	N3-C4-N9	5.50	129.30	126.00
1	A	2370	G	C6-N1-C2	-5.50	121.80	125.10
1	A	2881	C	N3-C2-O2	5.50	125.75	121.90
1	A	446	G	C8-N9-C1'	-5.49	119.86	127.00
1	A	826	U	C4-C5-C6	5.49	122.99	119.70
1	A	2238	G	N3-C4-C5	-5.49	125.86	128.60
2	B	47	C	N3-C4-N4	5.49	121.84	118.00
1	A	2157	G	N9-C4-C5	5.49	107.59	105.40
1	A	928	G	C4-C5-N7	5.49	112.99	110.80
1	A	945	A	N1-C6-N6	5.49	121.89	118.60
1	A	2496	C	N3-C2-O2	5.49	125.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	A	N9-C4-C5	5.48	107.99	105.80
1	A	1313	U	N3-C2-O2	-5.48	118.36	122.20
1	A	1626	G	N1-C6-O6	-5.48	116.61	119.90
1	A	1269	A	C8-N9-C4	5.48	107.99	105.80
1	A	1948	G	N1-C6-O6	-5.48	116.61	119.90
1	A	2590	A	C4-C5-N7	5.48	113.44	110.70
1	A	945	A	N1-C2-N3	5.48	132.04	129.30
1	A	1306	C	N3-C4-C5	5.48	124.09	121.90
1	A	1992	G	C8-N9-C4	-5.48	104.21	106.40
1	A	230	U	C2-N1-C1'	5.47	124.27	117.70
1	A	1942	C	C6-N1-C1'	5.47	127.37	120.80
1	A	736	C	N3-C4-N4	5.47	121.83	118.00
1	A	1621	U	N3-C4-O4	5.47	123.23	119.40
1	A	2506	U	N3-C2-O2	-5.47	118.37	122.20
1	A	631	A	N1-C6-N6	5.47	121.88	118.60
1	A	488	G	C5-N7-C8	5.47	107.03	104.30
1	A	1275	A	N1-C2-N3	5.47	132.03	129.30
1	A	1330	C	N3-C4-N4	5.47	121.83	118.00
1	A	768	G	N3-C4-C5	-5.47	125.87	128.60
1	A	1295	C	C6-N1-C2	-5.47	118.11	120.30
1	A	1320	C	N1-C2-O2	-5.47	115.62	118.90
1	A	1588	C	C6-N1-C2	-5.47	118.11	120.30
1	A	2032	G	C4-C5-C6	5.47	122.08	118.80
1	A	1553	A	N9-C4-C5	5.46	107.99	105.80
1	A	1624	G	C5-C6-N1	5.46	114.23	111.50
1	A	2804	C	C5-C6-N1	5.46	123.73	121.00
1	A	1930	G	C4-N9-C1'	-5.46	119.40	126.50
1	A	2084	C	C4-C5-C6	5.46	120.13	117.40
1	A	2032	G	N1-C6-O6	5.46	123.18	119.90
1	A	948	G	C8-N9-C4	-5.46	104.22	106.40
1	A	1257	C	N3-C2-O2	-5.46	118.08	121.90
1	A	139	G	C8-N9-C4	-5.46	104.22	106.40
1	A	443	A	C8-N9-C4	-5.46	103.62	105.80
1	A	1343	G	C4-N9-C1'	5.46	133.59	126.50
1	A	835	A	N1-C2-N3	-5.46	126.57	129.30
1	A	856	C	C5-C6-N1	5.46	123.73	121.00
1	A	1653	G	C8-N9-C1'	-5.46	119.91	127.00
1	A	885	C	C5-C4-N4	-5.45	116.38	120.20
1	A	2373	G	C8-N9-C4	5.45	108.58	106.40
1	A	847	U	C2-N3-C4	-5.45	123.73	127.00
1	A	928	G	N7-C8-N9	5.45	115.82	113.10
1	A	1140	C	N1-C2-O2	5.45	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1048	A	N1-C6-N6	-5.45	115.33	118.60
1	A	1216	G	N1-C2-N2	-5.45	111.30	116.20
1	A	1257	C	N1-C2-N3	5.45	123.01	119.20
1	A	1316	U	N3-C2-O2	-5.44	118.39	122.20
1	A	1829	A	C8-N9-C4	5.44	107.98	105.80
1	A	2307	G	C5-N7-C8	-5.44	101.58	104.30
1	A	454	A	N1-C6-N6	5.44	121.86	118.60
1	A	2035	G	C8-N9-C4	-5.44	104.22	106.40
1	A	528	A	C4-C5-C6	-5.44	114.28	117.00
1	A	1204	A	N3-C4-N9	-5.44	123.05	127.40
1	A	1348	G	N1-C6-O6	5.44	123.16	119.90
1	A	2358	G	N1-C6-O6	-5.44	116.64	119.90
1	A	928	G	C4-C5-C6	5.44	122.06	118.80
1	A	2286	A	C4-N9-C1'	5.44	136.09	126.30
2	B	6	C	N1-C2-O2	5.44	122.16	118.90
1	A	1049	C	C4-C5-C6	-5.44	114.68	117.40
1	A	1845	G	C4-C5-N7	-5.43	108.63	110.80
1	A	309	G	N1-C6-O6	-5.43	116.64	119.90
1	A	645	C	C6-N1-C2	-5.43	118.13	120.30
1	A	1547	C	C5-C6-N1	-5.43	118.28	121.00
1	A	2251	G	N1-C6-O6	-5.43	116.64	119.90
21	Z	151	HIS	N-CA-C	5.43	125.67	111.00
1	A	2000	G	C8-N9-C4	5.43	108.57	106.40
1	A	2264	C	C5-C6-N1	-5.43	118.28	121.00
1	A	2769	C	N3-C2-O2	-5.43	118.10	121.90
1	A	2084	C	C6-N1-C2	5.43	122.47	120.30
11	P	148	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	2000	G	C5-N7-C8	5.43	107.01	104.30
1	A	663	G	C8-N9-C4	-5.42	104.23	106.40
1	A	2271	G	N3-C4-C5	-5.42	125.89	128.60
1	A	2866	U	C4-C5-C6	5.42	122.95	119.70
1	A	742	G	N9-C4-C5	-5.42	103.23	105.40
1	A	147	U	N1-C2-N3	5.42	118.15	114.90
1	A	525	U	N1-C2-N3	5.42	118.15	114.90
1	A	2680	C	C5-C4-N4	-5.42	116.41	120.20
1	A	1233	C	C5-C6-N1	5.42	123.71	121.00
1	A	1785	A	C4-C5-C6	5.42	119.71	117.00
1	A	1319	G	N1-C2-N3	5.42	127.15	123.90
1	A	1845	G	N3-C4-C5	-5.42	125.89	128.60
1	A	351	G	C8-N9-C4	5.42	108.57	106.40
1	A	1022	G	N1-C6-O6	-5.42	116.65	119.90
1	A	1471	A	N1-C2-N3	5.42	132.01	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	A	N9-C4-C5	-5.42	103.63	105.80
1	A	645	C	C5-C6-N1	5.42	123.71	121.00
1	A	1034	G	C4-C5-N7	-5.42	108.63	110.80
1	A	2287	A	N1-C2-N3	5.42	132.01	129.30
1	A	2351	G	N3-C4-C5	-5.42	125.89	128.60
1	A	2441	C	N3-C4-C5	5.41	124.06	121.90
1	A	171	G	C6-N1-C2	5.41	128.34	125.10
1	A	178	G	N1-C2-N3	5.41	127.15	123.90
1	A	333	G	C8-N9-C1'	-5.41	119.97	127.00
1	A	2240	C	N1-C2-O2	5.41	122.14	118.90
1	A	2894	G	C5-N7-C8	-5.41	101.59	104.30
1	A	33	U	C6-N1-C2	5.41	124.24	121.00
1	A	1206	G	N1-C2-N3	5.41	127.14	123.90
1	A	915	C	N3-C2-O2	-5.41	118.12	121.90
1	A	2489	G	N3-C4-C5	-5.40	125.90	128.60
1	A	800	A	C6-N1-C2	-5.40	115.36	118.60
1	A	2628	C	N3-C4-C5	5.40	124.06	121.90
1	A	717	G	N3-C4-C5	5.40	131.30	128.60
1	A	1436	G	C6-C5-N7	-5.40	127.16	130.40
1	A	654	A	C8-N9-C4	5.40	107.96	105.80
1	A	801	G	N9-C4-C5	5.40	107.56	105.40
1	A	2727	G	C5-C6-O6	-5.40	125.36	128.60
1	A	432	A	C8-N9-C4	-5.39	103.64	105.80
1	A	1133	U	N3-C4-C5	5.39	117.84	114.60
1	A	393	C	N1-C2-O2	-5.39	115.67	118.90
1	A	1536	C	N3-C4-C5	-5.39	119.74	121.90
1	A	676	A	C1'-O4'-C4'	-5.39	105.59	109.90
1	A	763	G	C5-N7-C8	5.39	106.99	104.30
1	A	1231	G	N1-C2-N3	5.39	127.13	123.90
1	A	2276	G	N3-C2-N2	-5.39	116.13	119.90
1	A	2894	G	C5-C6-N1	5.39	114.19	111.50
1	A	776	G	N1-C2-N3	5.38	127.13	123.90
1	A	1324	G	N1-C6-O6	5.38	123.13	119.90
1	A	1448	G	C8-N9-C4	5.38	108.55	106.40
1	A	941	A	N1-C2-N3	-5.38	126.61	129.30
1	A	1448	G	C5-C6-O6	-5.38	125.37	128.60
1	A	1490	A	N7-C8-N9	-5.38	111.11	113.80
1	A	1681	G	C5-N7-C8	-5.38	101.61	104.30
1	A	2031	A	C5-C6-N6	-5.38	119.39	123.70
1	A	2129	C	N3-C2-O2	-5.38	118.13	121.90
1	A	2515	C	N3-C4-N4	5.38	121.77	118.00
1	A	2762	G	C5-C6-O6	-5.38	125.37	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1189	A	C4-C5-N7	5.38	113.39	110.70
1	A	2790	A	C2-N3-C4	5.38	113.29	110.60
1	A	1231	G	C5-C6-N1	-5.38	108.81	111.50
1	A	2443	C	C6-N1-C2	-5.38	118.15	120.30
1	A	2767	C	C5-C6-N1	-5.38	118.31	121.00
1	A	2224	G	C5-C6-O6	-5.38	125.38	128.60
1	A	2536	G	N1-C2-N3	5.38	127.13	123.90
1	A	2346	A	C5-C6-N6	-5.38	119.40	123.70
1	A	2590	A	C2-N3-C4	-5.38	107.91	110.60
1	A	1428	C	N1-C2-O2	-5.37	115.68	118.90
1	A	2319	G	N3-C2-N2	-5.37	116.14	119.90
1	A	1276	A	N1-C6-N6	5.37	121.82	118.60
1	A	1905	C	C6-N1-C2	-5.37	118.15	120.30
1	A	2740	A	C4-C5-C6	5.37	119.69	117.00
1	A	2517	C	C2-N3-C4	-5.37	117.22	119.90
1	A	2105	C	C5-C6-N1	5.37	123.68	121.00
1	A	2430	A	N7-C8-N9	5.37	116.48	113.80
1	A	2453	A	C5-C6-N1	5.37	120.39	117.70
10	O	8	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	69	C	C5-C6-N1	-5.36	118.32	121.00
1	A	874	G	N1-C6-O6	5.36	123.12	119.90
1	A	782	A	C5-C6-N1	5.36	120.38	117.70
1	A	874	G	C5-C6-O6	-5.36	125.38	128.60
1	A	994	C	C5-C6-N1	-5.36	118.32	121.00
1	A	1365	A	C5-N7-C8	-5.36	101.22	103.90
1	A	2373	G	C2-N3-C4	-5.36	109.22	111.90
1	A	730	C	C6-N1-C2	-5.36	118.16	120.30
1	A	476	G	N1-C6-O6	5.36	123.11	119.90
1	A	2335	A	C4-C5-C6	-5.36	114.32	117.00
1	A	804	A	N1-C6-N6	5.36	121.81	118.60
1	A	2016	U	N3-C2-O2	5.36	125.95	122.20
2	B	8	U	C5-C6-N1	5.36	125.38	122.70
1	A	702	G	N1-C6-O6	5.35	123.11	119.90
1	A	2694	G	C4-N9-C1'	5.35	133.46	126.50
1	A	2820	A	N1-C6-N6	5.35	121.81	118.60
3	D	263	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	762	U	N1-C2-O2	5.35	126.55	122.80
1	A	1558	A	P-O3'-C3'	5.35	126.12	119.70
1	A	380	U	C6-N1-C2	5.35	124.21	121.00
1	A	697	C	N3-C4-N4	5.35	121.74	118.00
1	A	1407	C	N3-C4-C5	-5.35	119.76	121.90
1	A	1673	U	C5-C6-N1	-5.35	120.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1687	G	C8-N9-C4	-5.35	104.26	106.40
2	B	95	C	C6-N1-C2	-5.35	118.16	120.30
1	A	1010	A	C8-N9-C4	5.35	107.94	105.80
1	A	614(B)	G	C4-N9-C1'	-5.35	119.55	126.50
1	A	1858	G	C6-C5-N7	-5.34	127.19	130.40
1	A	553	G	C2-N3-C4	-5.34	109.23	111.90
1	A	2074	U	N1-C2-O2	5.34	126.54	122.80
1	A	53	A	C5-N7-C8	-5.34	101.23	103.90
1	A	185	U	C2-N3-C4	-5.34	123.80	127.00
1	A	960	A	N9-C4-C5	-5.34	103.66	105.80
1	A	77	C	N3-C2-O2	-5.34	118.16	121.90
1	A	700	G	N1-C2-N3	5.34	127.10	123.90
1	A	733	G	N7-C8-N9	-5.34	110.43	113.10
1	A	1573	G	N3-C2-N2	5.34	123.64	119.90
1	A	1653	G	P-O3'-C3'	5.34	126.11	119.70
1	A	956	G	C5-C6-N1	-5.34	108.83	111.50
1	A	568	U	C5-C4-O4	-5.33	122.70	125.90
1	A	1721	G	N7-C8-N9	5.33	115.77	113.10
1	A	1613	G	N1-C2-N2	-5.33	111.40	116.20
1	A	2607	G	C5-C6-N1	-5.33	108.83	111.50
1	A	69	C	C4-C5-C6	5.33	120.06	117.40
1	A	130	C	C5-C6-N1	-5.33	118.33	121.00
1	A	1225	G	N9-C4-C5	5.33	107.53	105.40
1	A	1609	A	C6-N1-C2	-5.33	115.40	118.60
1	A	2429	G	N7-C8-N9	5.33	115.77	113.10
1	A	2602	A	C6-N1-C2	-5.33	115.40	118.60
2	B	60	C	N3-C4-C5	-5.33	119.77	121.90
1	A	750	A	N7-C8-N9	5.33	116.46	113.80
1	A	1460	A	C2-N3-C4	5.33	113.26	110.60
1	A	2420	C	C6-N1-C2	5.33	122.43	120.30
1	A	102	G	C8-N9-C1'	-5.33	120.08	127.00
1	A	1231	G	N1-C6-O6	5.33	123.10	119.90
1	A	1238	G	C5-C6-O6	-5.33	125.41	128.60
1	A	1406	U	C5-C6-N1	5.33	125.36	122.70
1	A	1693	U	C5-C6-N1	-5.33	120.04	122.70
1	A	1983	C	C5-C4-N4	-5.32	116.47	120.20
1	A	465	G	C4-N9-C1'	5.32	133.42	126.50
1	A	1942	C	C2-N1-C1'	-5.32	112.95	118.80
1	A	1661	G	C6-N1-C2	-5.32	121.91	125.10
1	A	2331	G	C5-C6-O6	-5.32	125.41	128.60
1	A	1336	A	C5-C6-N1	5.32	120.36	117.70
5	F	168	ARG	NE-CZ-NH1	5.32	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	U	N1-C2-N3	5.31	118.09	114.90
1	A	1130	U	N3-C4-C5	-5.31	111.41	114.60
1	A	1632	A	C5-C6-N6	-5.31	119.45	123.70
1	A	2312	U	C6-N1-C2	-5.31	117.81	121.00
1	A	2356	C	C6-N1-C2	5.31	122.42	120.30
1	A	2587	A	C2-N3-C4	-5.31	107.94	110.60
1	A	775	G	N3-C2-N2	5.31	123.62	119.90
1	A	1404	C	N1-C2-O2	5.31	122.09	118.90
1	A	2242	G	N3-C4-N9	-5.31	122.82	126.00
1	A	982	C	C6-N1-C2	-5.31	118.18	120.30
1	A	1414	G	C8-N9-C4	-5.31	104.28	106.40
1	A	1631(A)	A	C8-N9-C4	-5.30	103.68	105.80
1	A	2067	G	N3-C4-N9	5.30	129.18	126.00
1	A	2287	A	C4-C5-N7	5.30	113.35	110.70
1	A	1187	G	N9-C4-C5	5.30	107.52	105.40
1	A	452	G	N1-C2-N3	5.30	127.08	123.90
1	A	102	G	N3-C4-C5	-5.30	125.95	128.60
1	A	757	U	N3-C2-O2	-5.30	118.49	122.20
1	A	888	C	C5-C6-N1	5.30	123.65	121.00
1	A	1762	A	N3-C4-C5	-5.30	123.09	126.80
1	A	2033	A	N1-C6-N6	-5.30	115.42	118.60
1	A	1618	A	C5-C6-N6	5.30	127.94	123.70
1	A	1845	G	N1-C2-N2	-5.30	111.43	116.20
1	A	207	A	N3-C4-N9	-5.30	123.16	127.40
1	A	856	C	N3-C4-C5	-5.30	119.78	121.90
1	A	949	C	C6-N1-C2	5.30	122.42	120.30
1	A	2080	G	N7-C8-N9	-5.30	110.45	113.10
1	A	889	C	N1-C2-O2	5.29	122.08	118.90
1	A	2348	U	C6-N1-C2	5.29	124.18	121.00
1	A	796	C	C6-N1-C2	5.29	122.42	120.30
1	A	1657	C	N3-C2-O2	5.29	125.61	121.90
25	3	56	VAL	CB-CA-C	-5.29	101.34	111.40
1	A	266	G	C8-N9-C4	5.29	108.52	106.40
1	A	2613	U	N3-C2-O2	-5.29	118.50	122.20
1	A	696	G	C8-N9-C4	5.29	108.52	106.40
1	A	59	U	N1-C2-N3	5.29	118.07	114.90
1	A	645	C	N3-C2-O2	-5.29	118.20	121.90
1	A	1204	A	C3'-C2'-C1'	-5.29	97.27	101.50
1	A	1318	C	N1-C2-O2	-5.29	115.73	118.90
1	A	2079	U	C4-C5-C6	5.29	122.87	119.70
1	A	394	A	C2-N3-C4	-5.29	107.96	110.60
1	A	652(T)	C	C5-C4-N4	5.29	123.90	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1222	C	C6-N1-C2	5.29	122.41	120.30
1	A	389	G	C8-N9-C1'	-5.28	120.13	127.00
1	A	587	C	N1-C2-N3	5.28	122.90	119.20
1	A	966	G	N1-C6-O6	-5.28	116.73	119.90
1	A	1608	A	N3-C4-N9	-5.28	123.17	127.40
1	A	884	C	N3-C4-C5	-5.28	119.79	121.90
1	A	2764	A	C8-N9-C4	-5.28	103.69	105.80
1	A	108	U	N1-C2-O2	5.28	126.50	122.80
1	A	765	G	N3-C2-N2	-5.28	116.20	119.90
1	A	839	U	C6-N1-C2	-5.28	117.83	121.00
1	A	861	A	N1-C2-N3	-5.28	126.66	129.30
1	A	2088	G	N3-C2-N2	-5.28	116.20	119.90
1	A	936	C	C5-C6-N1	-5.28	118.36	121.00
1	A	1654	A	C5-C6-N6	5.28	127.92	123.70
1	A	2488	A	N7-C8-N9	-5.28	111.16	113.80
1	A	512	G	N9-C4-C5	5.28	107.51	105.40
1	A	607	U	C5-C6-N1	-5.28	120.06	122.70
1	A	886	C	C6-N1-C2	-5.28	118.19	120.30
1	A	2297	C	C6-N1-C2	-5.28	118.19	120.30
2	B	70	C	C6-N1-C2	-5.28	118.19	120.30
2	B	91	C	C6-N1-C2	5.28	122.41	120.30
1	A	2013	A	C4-C5-N7	5.27	113.34	110.70
1	A	2607	G	N3-C4-N9	5.27	129.16	126.00
1	A	351	G	N1-C6-O6	5.27	123.06	119.90
1	A	2398	U	N3-C4-C5	-5.27	111.44	114.60
1	A	446	G	C6-C5-N7	-5.27	127.24	130.40
1	A	2510	C	N1-C2-N3	5.27	122.89	119.20
1	A	32	C	N3-C2-O2	-5.26	118.22	121.90
1	A	849	A	N7-C8-N9	-5.26	111.17	113.80
1	A	1531	C	C2-N1-C1'	5.26	124.59	118.80
1	A	2254	C	C6-N1-C2	5.26	122.41	120.30
1	A	2114	A	N7-C8-N9	5.26	116.43	113.80
1	A	60	G	C6-C5-N7	-5.26	127.24	130.40
1	A	171	G	N3-C2-N2	5.26	123.58	119.90
1	A	363(B)	G	N9-C4-C5	-5.26	103.30	105.40
1	A	1487	G	C8-N9-C4	-5.26	104.30	106.40
1	A	1965	C	N1-C2-O2	5.26	122.06	118.90
1	A	2487	G	N9-C4-C5	-5.26	103.30	105.40
1	A	548	A	N9-C4-C5	-5.26	103.70	105.80
1	A	690	G	C8-N9-C4	5.26	108.50	106.40
1	A	1187	G	C2-N3-C4	5.26	114.53	111.90
1	A	1241	A	C2-N3-C4	-5.26	107.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1994	C	N3-C4-C5	5.26	124.00	121.90
1	A	2048	G	C5-C6-N1	-5.26	108.87	111.50
1	A	2157	G	C8-N9-C1'	5.26	133.83	127.00
1	A	2350	C	N3-C4-N4	5.25	121.68	118.00
1	A	392	C	C6-N1-C2	5.25	122.40	120.30
1	A	1341	U	N1-C2-O2	5.25	126.48	122.80
1	A	2348	U	N1-C2-O2	5.25	126.48	122.80
1	A	686	G	C6-C5-N7	-5.25	127.25	130.40
1	A	1688	U	N1-C2-N3	5.25	118.05	114.90
1	A	2303	G	C8-N9-C4	-5.25	104.30	106.40
1	A	2623	G	N9-C4-C5	5.25	107.50	105.40
1	A	790	C	N3-C2-O2	5.25	125.58	121.90
1	A	2037	G	C5-C6-O6	5.25	131.75	128.60
1	A	2425	A	C5-N7-C8	-5.25	101.28	103.90
1	A	760	G	C5-N7-C8	-5.25	101.68	104.30
1	A	1050	A	C8-N9-C4	-5.25	103.70	105.80
1	A	2157	G	N3-C4-N9	-5.25	122.85	126.00
1	A	1582	C	N1-C2-O2	5.25	122.05	118.90
1	A	1981	A	N9-C4-C5	5.25	107.90	105.80
1	A	1415	U	N3-C4-O4	-5.25	115.73	119.40
19	X	54	VAL	CB-CA-C	-5.24	101.44	111.40
23	1	21	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	2261	C	N3-C2-O2	-5.24	118.23	121.90
1	A	525	U	N3-C4-C5	-5.24	111.46	114.60
1	A	1324	G	C5-C6-O6	-5.24	125.46	128.60
1	A	2322	A	C5-C6-N1	5.24	120.32	117.70
1	A	2626	C	C2-N3-C4	-5.24	117.28	119.90
1	A	2081	C	C4-C5-C6	5.24	120.02	117.40
1	A	676	A	O4'-C1'-N9	5.24	112.39	108.20
1	A	2602	A	C5-C6-N1	5.24	120.32	117.70
1	A	124	G	N3-C4-C5	5.23	131.22	128.60
1	A	915	C	C2-N1-C1'	5.23	124.56	118.80
1	A	2763	G	C6-C5-N7	-5.23	127.26	130.40
1	A	1308	A	C4-C5-C6	5.23	119.62	117.00
1	A	1490	A	N1-C6-N6	5.23	121.74	118.60
1	A	1586	A	C8-N9-C4	-5.23	103.71	105.80
1	A	747	U	C2-N3-C4	-5.23	123.86	127.00
1	A	1012	U	N3-C2-O2	-5.23	118.54	122.20
1	A	1112	G	C5-C6-N1	-5.22	108.89	111.50
1	A	1283	G	N1-C2-N2	-5.22	111.50	116.20
1	A	2065	C	C4-C5-C6	5.22	120.01	117.40
1	A	2782	G	C6-C5-N7	-5.22	127.27	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	87	G	N7-C8-N9	-5.22	110.49	113.10
1	A	182	A	C8-N9-C4	-5.22	103.71	105.80
1	A	2273	A	N1-C2-N3	-5.22	126.69	129.30
1	A	2558	C	N3-C4-C5	5.22	123.99	121.90
2	B	17	C	C6-N1-C2	5.22	122.39	120.30
1	A	2152	G	C4-N9-C1'	-5.22	119.72	126.50
1	A	2335	A	N7-C8-N9	-5.22	111.19	113.80
1	A	391	G	C8-N9-C1'	-5.22	120.22	127.00
1	A	1974	C	N3-C4-C5	5.22	123.99	121.90
1	A	2582	G	C8-N9-C4	-5.21	104.31	106.40
1	A	1670	C	C2-N3-C4	-5.21	117.29	119.90
1	A	2403	C	C6-N1-C2	-5.21	118.22	120.30
1	A	571	A	C8-N9-C4	5.21	107.88	105.80
1	A	592	G	C5-C6-O6	5.21	131.73	128.60
1	A	702	G	N1-C2-N3	5.21	127.03	123.90
1	A	1698	A	C4-C5-C6	5.21	119.61	117.00
1	A	2331	G	N1-C6-O6	5.21	123.03	119.90
1	A	2412	A	N1-C6-N6	-5.21	115.47	118.60
1	A	775	G	N1-C2-N2	-5.21	111.51	116.20
1	A	1129	A	C8-N9-C4	-5.21	103.72	105.80
1	A	469	G	C5-C6-O6	-5.21	125.48	128.60
1	A	857	C	N1-C2-N3	5.21	122.84	119.20
1	A	190	A	N1-C2-N3	-5.21	126.70	129.30
1	A	958	U	C6-N1-C2	-5.21	117.88	121.00
1	A	1342	A	C8-N9-C4	-5.21	103.72	105.80
2	B	60	C	C6-N1-C2	-5.21	118.22	120.30
1	A	1006	C	N3-C4-N4	-5.20	114.36	118.00
1	A	1822	G	N1-C2-N3	5.20	127.02	123.90
1	A	2602	A	P-O3'-C3'	5.20	125.94	119.70
1	A	1131	G	C4-C5-N7	5.20	112.88	110.80
1	A	2328	A	C8-N9-C4	5.20	107.88	105.80
1	A	996	A	N1-C6-N6	-5.20	115.48	118.60
1	A	1254	A	C4-C5-C6	5.20	119.60	117.00
1	A	2421	G	C6-C5-N7	-5.20	127.28	130.40
1	A	2487	G	C6-C5-N7	-5.20	127.28	130.40
1	A	2681	C	N3-C2-O2	-5.20	118.26	121.90
1	A	577	G	C4-C5-N7	5.19	112.88	110.80
1	A	1279	G	C5-C6-N1	5.19	114.10	111.50
1	A	327	G	N9-C4-C5	-5.19	103.32	105.40
1	A	2581	G	C4-N9-C1'	5.19	133.25	126.50
1	A	974	G	C8-N9-C4	-5.19	104.33	106.40
1	A	988	A	C5-N7-C8	-5.19	101.31	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2689	U	C2-N1-C1'	-5.19	111.48	117.70
1	A	147	U	C2-N3-C4	-5.19	123.89	127.00
1	A	181	A	N1-C6-N6	-5.19	115.49	118.60
1	A	528	A	C4-N9-C1'	-5.18	116.97	126.30
1	A	1265	A	C6-N1-C2	-5.18	115.49	118.60
1	A	2144	U	C6-N1-C2	-5.18	117.89	121.00
1	A	2641	G	C8-N9-C4	-5.18	104.33	106.40
1	A	1128	A	N1-C2-N3	5.18	131.89	129.30
1	A	1553	A	C8-N9-C4	-5.18	103.73	105.80
1	A	2040	C	N1-C2-N3	-5.18	115.57	119.20
1	A	2451	A	N9-C4-C5	5.18	107.87	105.80
5	F	16	GLY	N-CA-C	5.18	126.06	113.10
1	A	610	G	N9-C4-C5	-5.18	103.33	105.40
1	A	1865	G	N1-C6-O6	5.18	123.01	119.90
1	A	579	G	C5-C6-N1	-5.17	108.91	111.50
1	A	2250	G	C5-C6-O6	5.17	131.70	128.60
1	A	2705	A	N7-C8-N9	-5.17	111.21	113.80
1	A	750	A	N1-C2-N3	5.17	131.89	129.30
1	A	1181	C	C6-N1-C2	5.17	122.37	120.30
1	A	488	G	N1-C6-O6	-5.17	116.80	119.90
1	A	1932	A	N1-C6-N6	5.17	121.70	118.60
1	A	102	G	C6-C5-N7	-5.17	127.30	130.40
1	A	526	A	N9-C4-C5	5.17	107.87	105.80
1	A	530	G	N1-C2-N2	5.17	120.85	116.20
1	A	729	G	N3-C2-N2	-5.17	116.28	119.90
1	A	2251	G	C2-N3-C4	5.17	114.48	111.90
2	B	54	G	N1-C6-O6	5.17	123.00	119.90
1	A	494	G	N3-C2-N2	-5.17	116.28	119.90
1	A	590	A	C8-N9-C4	-5.17	103.73	105.80
1	A	1882	C	C2-N1-C1'	5.17	124.48	118.80
1	A	2251	G	C4-N9-C1'	5.17	133.22	126.50
1	A	809	G	C5-C6-O6	5.17	131.70	128.60
1	A	1359	A	C8-N9-C4	-5.17	103.73	105.80
1	A	99	U	C5-C6-N1	-5.16	120.12	122.70
2	B	1	U	C2-N1-C1'	5.16	123.90	117.70
1	A	2090	G	C8-N9-C4	5.16	108.47	106.40
1	A	841	A	N1-C6-N6	-5.16	115.50	118.60
1	A	2842	G	C5-C6-O6	-5.16	125.50	128.60
1	A	242	G	C4-N9-C1'	-5.16	119.80	126.50
1	A	652(B)	A	C2-N3-C4	5.16	113.18	110.60
1	A	2489	G	N3-C4-N9	5.16	129.09	126.00
1	A	562	U	C6-N1-C2	-5.16	117.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	732	C	C5-C4-N4	-5.16	116.59	120.20
1	A	2026	C	C4-C5-C6	5.16	119.98	117.40
2	B	43	C	C6-N1-C2	-5.16	118.24	120.30
1	A	1184	G	C5-C6-N1	-5.15	108.92	111.50
1	A	2763	G	C8-N9-C4	-5.15	104.34	106.40
1	A	2856	C	C5-C6-N1	5.15	123.58	121.00
1	A	2010	G	C5-C6-O6	-5.15	125.51	128.60
1	A	2086	U	C4-C5-C6	5.15	122.79	119.70
1	A	178	G	C8-N9-C4	5.15	108.46	106.40
1	A	2322	A	C2-N3-C4	5.15	113.17	110.60
1	A	1029	A	C8-N9-C4	5.15	107.86	105.80
1	A	2191	G	N1-C6-O6	5.15	122.99	119.90
1	A	2522	U	C2-N1-C1'	5.15	123.88	117.70
1	A	2669	G	N1-C6-O6	5.15	122.99	119.90
1	A	686	G	C5-C6-O6	-5.15	125.51	128.60
1	A	1243	G	C5-N7-C8	-5.15	101.73	104.30
1	A	1325	G	C6-C5-N7	-5.14	127.31	130.40
1	A	541	C	N3-C2-O2	-5.14	118.30	121.90
1	A	602	G	N9-C4-C5	-5.14	103.34	105.40
1	A	2088	G	N1-C6-O6	5.14	122.98	119.90
1	A	2700	C	C5-C4-N4	-5.14	116.60	120.20
1	A	2769	C	C2-N3-C4	-5.14	117.33	119.90
1	A	234	C	C6-N1-C2	-5.14	118.24	120.30
1	A	281	G	C8-N9-C4	5.14	108.46	106.40
1	A	975	C	N1-C2-N3	5.14	122.80	119.20
1	A	1340	U	C2-N3-C4	-5.14	123.92	127.00
1	A	1417	C	N3-C4-C5	-5.14	119.84	121.90
1	A	1957	C	N3-C4-C5	5.14	123.96	121.90
1	A	2056	G	N3-C4-N9	5.14	129.08	126.00
1	A	2116	G	P-O3'-C3'	5.14	125.86	119.70
1	A	2370	G	N1-C2-N2	-5.14	111.58	116.20
1	A	792	G	C4-N9-C1'	5.14	133.18	126.50
1	A	1307	A	C2-N3-C4	-5.14	108.03	110.60
1	A	1932	A	C5-N7-C8	-5.14	101.33	103.90
2	B	12	C	N3-C4-C5	5.14	123.95	121.90
1	A	893	C	N3-C2-O2	-5.13	118.31	121.90
1	A	1278	A	C6-N1-C2	-5.13	115.52	118.60
1	A	2607	G	C4-N9-C1'	5.13	133.17	126.50
2	B	29	A	C5-N7-C8	-5.13	101.33	103.90
1	A	826	U	N1-C2-N3	5.13	117.98	114.90
1	A	2572	A	N1-C6-N6	-5.13	115.52	118.60
1	A	1269	A	C2-N3-C4	-5.13	108.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2310	A	N1-C6-N6	5.13	121.68	118.60
1	A	2362	G	N3-C4-C5	5.13	131.16	128.60
1	A	272(I)	U	C6-N1-C2	-5.12	117.92	121.00
1	A	330	A	C4-C5-N7	5.12	113.26	110.70
1	A	1669	A	C5-N7-C8	-5.12	101.34	103.90
1	A	1047	G	C2-N3-C4	5.12	114.46	111.90
1	A	1688	U	N1-C2-O2	-5.12	119.21	122.80
1	A	1826	G	C5-C6-O6	5.12	131.67	128.60
1	A	2182	G	C5-C6-N1	-5.12	108.94	111.50
1	A	2259	G	C5-C6-N1	-5.12	108.94	111.50
1	A	2330	G	N1-C2-N3	5.12	126.97	123.90
1	A	2497	A	N3-C4-N9	5.12	131.50	127.40
1	A	2597	G	C4-N9-C1'	5.12	133.16	126.50
1	A	154(A)	C	N3-C4-C5	5.12	123.95	121.90
1	A	2370	G	C5-C6-N1	5.12	114.06	111.50
1	A	2819	G	N7-C8-N9	-5.12	110.54	113.10
1	A	636	G	C4-N9-C1'	5.12	133.16	126.50
1	A	1216	G	C2-N3-C4	-5.12	109.34	111.90
1	A	1626	G	C2-N3-C4	-5.12	109.34	111.90
1	A	1687	G	N7-C8-N9	5.12	115.66	113.10
1	A	513	A	C8-N9-C4	-5.12	103.75	105.80
1	A	676	A	N1-C2-N3	5.12	131.86	129.30
1	A	1781	C	C6-N1-C2	5.12	122.35	120.30
1	A	1816	G	N3-C4-N9	5.12	129.07	126.00
1	A	2351	G	C6-C5-N7	-5.12	127.33	130.40
1	A	2712(A)	A	C5-C6-N1	-5.12	115.14	117.70
1	A	774	A	N7-C8-N9	5.12	116.36	113.80
1	A	1214	A	C5-C6-N6	-5.12	119.61	123.70
1	A	1914	C	C6-N1-C1'	5.12	126.94	120.80
1	A	2327	A	N7-C8-N9	-5.12	111.24	113.80
1	A	117	G	N3-C2-N2	5.12	123.48	119.90
1	A	1123	C	C2-N1-C1'	-5.12	113.17	118.80
1	A	2768	C	N3-C4-N4	-5.12	114.42	118.00
1	A	1291	C	N3-C4-N4	-5.11	114.42	118.00
1	A	2791	C	C2-N3-C4	5.11	122.46	119.90
1	A	286	C	N1-C2-O2	5.11	121.97	118.90
1	A	773	U	C5-C6-N1	-5.11	120.14	122.70
1	A	1498	C	N3-C2-O2	5.11	125.48	121.90
1	A	1941	C	N1-C2-O2	-5.11	115.83	118.90
1	A	2296	U	C3'-C2'-C1'	-5.11	97.41	101.50
1	A	2613	U	N1-C2-O2	5.11	126.38	122.80
1	A	1043	C	C6-N1-C2	-5.11	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	G	N1-C6-O6	-5.11	116.84	119.90
1	A	799	G	C4-C5-N7	-5.11	108.76	110.80
1	A	1658	C	C6-N1-C2	-5.11	118.26	120.30
1	A	1827	C	N3-C2-O2	-5.11	118.32	121.90
1	A	652(E)	G	C5-C6-N1	-5.11	108.95	111.50
1	A	886	C	C2-N3-C4	5.11	122.45	119.90
1	A	2356	C	C5-C6-N1	-5.10	118.45	121.00
1	A	2574	G	C4-C5-N7	5.10	112.84	110.80
1	A	411	G	C5-C6-O6	5.10	131.66	128.60
1	A	2346	A	C4-C5-C6	5.10	119.55	117.00
1	A	1790	C	N3-C4-N4	5.10	121.57	118.00
1	A	1819	A	C6-N1-C2	-5.10	115.54	118.60
1	A	1364	G	N9-C4-C5	-5.10	103.36	105.40
1	A	2053	G	C8-N9-C4	5.10	108.44	106.40
1	A	2706	G	C6-N1-C2	-5.10	122.04	125.10
1	A	591	C	N3-C4-C5	-5.10	119.86	121.90
2	B	9	G	C2-N3-C4	5.10	114.45	111.90
1	A	389	G	C8-N9-C4	5.09	108.44	106.40
1	A	420	C	N1-C2-O2	5.09	121.96	118.90
1	A	208	C	C5-C4-N4	-5.09	116.64	120.20
1	A	633	A	C4-C5-C6	5.09	119.55	117.00
1	A	1327	C	N1-C2-O2	-5.09	115.84	118.90
1	A	2519	U	N3-C2-O2	5.09	125.76	122.20
1	A	2557	G	C4-C5-N7	5.09	112.84	110.80
1	A	627	A	C8-N9-C4	5.09	107.84	105.80
1	A	1334	G	C4-C5-N7	-5.09	108.76	110.80
1	A	122	G	C4-C5-C6	5.09	121.85	118.80
1	A	1229	G	C6-C5-N7	-5.09	127.35	130.40
1	A	131	G	C5-C6-N1	5.09	114.04	111.50
1	A	676	A	C6-C5-N7	-5.09	128.74	132.30
1	A	801	G	N1-C2-N3	5.09	126.95	123.90
1	A	2370	G	N3-C4-C5	-5.09	126.06	128.60
1	A	2851	A	C4-C5-C6	5.09	119.54	117.00
1	A	2354	G	C4-C5-N7	5.08	112.83	110.80
1	A	2495	G	C8-N9-C4	-5.08	104.37	106.40
1	A	2552	U	N1-C2-O2	-5.08	119.24	122.80
1	A	955	C	N3-C2-O2	5.08	125.46	121.90
1	A	989	G	N1-C6-O6	5.08	122.95	119.90
1	A	1372	U	N1-C2-O2	5.08	126.36	122.80
1	A	2610	C	C2-N3-C4	-5.08	117.36	119.90
1	A	975(A)	G	C5-C6-N1	5.08	114.04	111.50
1	A	2230	G	N3-C2-N2	-5.08	116.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2440	C	C5-C6-N1	-5.08	118.46	121.00
1	A	1020	A	C5-C6-N1	-5.08	115.16	117.70
1	A	1990	C	C4-C5-C6	5.08	119.94	117.40
1	A	2225	A	C2-N3-C4	5.08	113.14	110.60
1	A	2242	G	N1-C2-N2	5.08	120.77	116.20
1	A	847	U	N3-C2-O2	-5.08	118.65	122.20
1	A	1204	A	C1'-O4'-C4'	-5.08	105.84	109.90
1	A	2038	G	C8-N9-C4	-5.08	104.37	106.40
1	A	555	U	N1-C2-O2	-5.08	119.25	122.80
1	A	738	G	N7-C8-N9	5.08	115.64	113.10
1	A	1672	C	C2-N3-C4	-5.08	117.36	119.90
1	A	2556	C	C5-C4-N4	-5.08	116.65	120.20
1	A	2689	U	C2-N3-C4	-5.08	123.95	127.00
1	A	100	G	C8-N9-C4	5.07	108.43	106.40
1	A	2285	C	N3-C2-O2	-5.07	118.35	121.90
1	A	2315	G	C8-N9-C4	5.07	108.43	106.40
1	A	1414	G	N7-C8-N9	5.07	115.64	113.10
1	A	116	C	N1-C2-N3	5.07	122.75	119.20
1	A	196	A	C5-C6-N6	-5.07	119.64	123.70
1	A	1489	U	C5-C4-O4	5.07	128.94	125.90
1	A	1974	C	C2-N3-C4	-5.07	117.36	119.90
3	D	60	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	187	G	C6-C5-N7	-5.07	127.36	130.40
1	A	934	G	N7-C8-N9	-5.07	110.57	113.10
1	A	1041	C	C2-N3-C4	5.07	122.43	119.90
1	A	1256	G	C6-C5-N7	-5.07	127.36	130.40
1	A	2273	A	C4-C5-N7	5.07	113.23	110.70
1	A	2376	A	C4-C5-C6	5.07	119.53	117.00
1	A	765	G	N1-C2-N2	5.07	120.76	116.20
1	A	989	G	C6-C5-N7	-5.07	127.36	130.40
1	A	1336	A	C2-N3-C4	5.07	113.13	110.60
1	A	1463	C	N1-C2-O2	5.07	121.94	118.90
2	B	27	C	C2-N1-C1'	5.07	124.37	118.80
2	B	57	A	C8-N9-C4	5.07	107.83	105.80
1	A	2107	C	C5-C6-N1	5.06	123.53	121.00
1	A	1597	A	N1-C6-N6	-5.06	115.56	118.60
1	A	2874	C	N3-C4-C5	5.06	123.92	121.90
1	A	1211	U	N1-C2-O2	-5.06	119.26	122.80
1	A	1745	C	N3-C2-O2	5.06	125.44	121.90
1	A	2330	G	C2-N3-C4	-5.06	109.37	111.90
1	A	211	A	N7-C8-N9	-5.06	111.27	113.80
1	A	2755	C	C2-N3-C4	5.06	122.43	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2853	C	C6-N1-C2	5.06	122.32	120.30
1	A	2743	C	N1-C2-N3	5.06	122.74	119.20
1	A	614(B)	G	N1-C6-O6	-5.05	116.87	119.90
1	A	2053	G	C5-C6-O6	-5.05	125.57	128.60
1	A	2291	U	N1-C2-N3	5.05	117.93	114.90
1	A	2646	C	C5-C6-N1	-5.05	118.47	121.00
1	A	435	C	C6-N1-C2	5.05	122.32	120.30
1	A	1824	G	N7-C8-N9	-5.05	110.57	113.10
1	A	559	G	C8-N9-C4	-5.05	104.38	106.40
1	A	607	U	C2-N1-C1'	-5.05	111.64	117.70
1	A	2050	C	C2-N3-C4	-5.05	117.37	119.90
1	A	2382	G	C8-N9-C4	5.05	108.42	106.40
1	A	1042	G	C2-N3-C4	5.05	114.42	111.90
1	A	1358	G	C5-C6-O6	5.05	131.63	128.60
1	A	1368	G	C2-N3-C4	5.05	114.42	111.90
1	A	2129	C	C5-C4-N4	5.05	123.73	120.20
1	A	686	G	C8-N9-C4	5.05	108.42	106.40
1	A	1422	G	C4-C5-N7	-5.05	108.78	110.80
1	A	2025	C	N1-C2-O2	-5.05	115.87	118.90
1	A	2042	A	C8-N9-C4	-5.05	103.78	105.80
1	A	2601	C	N3-C4-C5	-5.05	119.88	121.90
1	A	1256	G	C6-N1-C2	-5.05	122.07	125.10
1	A	2603	G	C5-C6-O6	-5.05	125.57	128.60
1	A	179	G	C2-N3-C4	-5.04	109.38	111.90
1	A	124	G	N1-C6-O6	5.04	122.93	119.90
1	A	465	G	C5-C6-N1	-5.04	108.98	111.50
1	A	1603	A	C8-N9-C4	-5.04	103.78	105.80
1	A	48	G	C8-N9-C4	5.04	108.42	106.40
1	A	1472	A	N1-C6-N6	-5.04	115.58	118.60
2	B	6	C	C6-N1-C2	5.04	122.32	120.30
1	A	729	G	C6-C5-N7	-5.04	127.38	130.40
1	A	2237	G	C8-N9-C4	5.04	108.42	106.40
1	A	2510	C	C6-N1-C2	-5.04	118.28	120.30
1	A	2182	G	N3-C4-C5	5.04	131.12	128.60
1	A	2563	U	N3-C4-C5	-5.04	111.58	114.60
1	A	745	G	C4-C5-N7	5.04	112.81	110.80
1	A	1901	A	C5-C6-N6	5.04	127.73	123.70
1	A	2751	G	N1-C6-O6	-5.04	116.88	119.90
1	A	425	G	N7-C8-N9	-5.03	110.58	113.10
1	A	844	C	C2-N3-C4	-5.03	117.38	119.90
1	A	988	A	N7-C8-N9	5.03	116.32	113.80
1	A	1298	C	C6-N1-C2	5.03	122.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2842	G	N1-C6-O6	5.03	122.92	119.90
2	B	61	G	C8-N9-C4	-5.03	104.39	106.40
1	A	1427	A	N1-C2-N3	5.03	131.81	129.30
1	A	908	C	C5-C4-N4	-5.03	116.68	120.20
1	A	48	G	N3-C4-C5	5.03	131.11	128.60
1	A	272(A)	U	P-O3'-C3'	5.03	125.73	119.70
1	A	735	A	C5-N7-C8	5.03	106.41	103.90
1	A	748	G	C6-N1-C2	-5.03	122.08	125.10
1	A	1221(A)	C	N3-C4-C5	5.03	123.91	121.90
1	A	1617	C	N3-C4-N4	5.03	121.52	118.00
1	A	393	C	N1-C2-N3	5.03	122.72	119.20
1	A	1815	A	N9-C4-C5	5.03	107.81	105.80
1	A	848	G	N3-C4-N9	5.02	129.01	126.00
1	A	1283	G	C4-C5-N7	-5.02	108.79	110.80
1	A	2713	A	N1-C6-N6	-5.02	115.58	118.60
1	A	108	U	N3-C2-O2	-5.02	118.69	122.20
1	A	179	G	C6-C5-N7	-5.02	127.39	130.40
1	A	1970	A	N9-C4-C5	-5.02	103.79	105.80
1	A	2623	G	C4-N9-C1'	5.02	133.03	126.50
1	A	1330	C	C5-C4-N4	-5.02	116.69	120.20
1	A	265	A	C4-N9-C1'	5.02	135.33	126.30
1	A	928	G	C5-N7-C8	-5.02	101.79	104.30
1	A	1754	C	N1-C2-N3	5.02	122.71	119.20
1	A	1963	U	C6-N1-C1'	-5.02	114.17	121.20
1	A	2028	U	C4-C5-C6	-5.02	116.69	119.70
1	A	2762	G	C5-C6-N1	5.02	114.01	111.50
1	A	102	G	P-O3'-C3'	5.02	125.72	119.70
1	A	767	U	C6-N1-C2	-5.02	117.99	121.00
1	A	1348	G	C5-C6-O6	-5.02	125.59	128.60
1	A	983	A	C8-N9-C4	5.02	107.81	105.80
1	A	1808	U	N1-C2-O2	5.02	126.31	122.80
1	A	1914	C	C2-N1-C1'	-5.02	113.28	118.80
1	A	205	G	C4-C5-N7	5.01	112.81	110.80
1	A	607	U	N3-C4-O4	-5.01	115.89	119.40
1	A	77	C	C2-N1-C1'	5.01	124.31	118.80
1	A	1452	A	N1-C2-N3	5.01	131.81	129.30
1	A	1539	G	C4-N9-C1'	5.01	133.01	126.50
1	A	2778	A	N1-C2-N3	5.01	131.81	129.30
1	A	225	A	C8-N9-C4	5.01	107.80	105.80
1	A	267	C	N3-C4-C5	5.01	123.90	121.90
1	A	652(R)	C	C5-C6-N1	5.01	123.50	121.00
1	A	2070	G	N1-C2-N2	-5.01	111.69	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2148	G	C6-C5-N7	5.01	133.41	130.40
1	A	2573	C	C6-N1-C2	5.01	122.30	120.30
2	B	103	G	N3-C2-N2	-5.01	116.39	119.90
1	A	1233	C	C6-N1-C2	-5.01	118.30	120.30
1	A	2425	A	N7-C8-N9	5.01	116.30	113.80
1	A	334	C	N1-C2-O2	-5.01	115.90	118.90
1	A	723	G	C4-C5-N7	5.01	112.80	110.80
1	A	754	C	C2-N3-C4	-5.01	117.40	119.90
1	A	1121	C	N1-C2-O2	-5.01	115.90	118.90
1	A	1752	C	C2-N1-C1'	-5.01	113.29	118.80
1	A	1777	U	C5-C6-N1	-5.01	120.20	122.70
1	A	1896	G	C5-C6-O6	-5.01	125.60	128.60
1	A	2201	C	C5-C6-N1	-5.01	118.50	121.00
1	A	2038	G	C5-N7-C8	-5.00	101.80	104.30
1	A	570	G	C5-C6-N1	5.00	114.00	111.50
1	A	975(A)	G	C2-N3-C4	5.00	114.40	111.90
1	A	1938	A	N3-C4-C5	-5.00	123.30	126.80
1	A	33	U	N3-C4-O4	-5.00	115.90	119.40
1	A	569	U	C5-C4-O4	-5.00	122.90	125.90
1	A	1606	G	N1-C6-O6	-5.00	116.90	119.90
1	A	2303	G	N3-C2-N2	-5.00	116.40	119.90

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	1	83	GLU	Peptide
26	4	43	TYR	Peptide
1	A	2335	A	Sidechain
4	E	72	VAL	Peptide
12	Q	18	LYS	Peptide
14	S	82	ILE	Peptide
19	X	93	GLU	Peptide
21	Z	159	PRO	Peptide
21	Z	191	VAL	Peptide
21	Z	199	LYS	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61112	0	30809	1206	1
2	B	2573	0	1306	56	0
3	D	2135	0	2214	73	0
4	E	1555	0	1607	52	0
5	F	1580	0	1621	63	0
6	G	1368	0	1324	74	0
7	H	1317	0	1376	35	0
8	I	1037	0	1036	54	0
9	N	1112	0	1180	33	0
10	O	923	0	981	24	0
11	P	1131	0	1201	45	0
12	Q	1122	0	1179	46	0
13	R	968	0	1033	32	0
14	S	865	0	905	50	0
15	T	1063	0	1103	35	0
16	U	959	0	1019	34	0
17	V	771	0	830	23	0
18	W	881	0	935	21	0
19	X	742	0	799	23	0
20	Y	785	0	828	23	0
21	Z	1536	0	1518	52	0
22	0	594	0	604	16	0
23	1	745	0	804	21	0
24	2	588	0	643	16	0
25	3	458	0	503	8	0
26	4	349	0	336	23	0
27	5	455	0	472	13	0
28	6	449	0	462	18	0
29	7	418	0	467	14	0
30	8	509	0	565	18	0
31	9	297	0	316	9	0
32	0	1	0	0	0	0
32	1	1	0	0	0	0
32	2	1	0	0	0	0
32	5	2	0	0	0	0
32	8	2	0	0	0	0
32	9	1	0	0	0	0
32	A	658	0	0	0	0
32	B	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	D	3	0	0	0	0
32	E	5	0	0	0	0
32	F	2	0	0	0	0
32	G	1	0	0	0	0
32	P	1	0	0	0	0
32	Q	4	0	0	0	0
32	R	1	0	0	0	0
32	S	1	0	0	0	0
32	T	2	0	0	0	0
32	V	1	0	0	0	0
32	W	2	0	0	0	0
32	Z	1	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	6	1	0	0	0	0
33	9	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	8	0	0	0	0
34	1	2	0	0	0	0
34	3	1	0	0	0	0
34	5	5	0	0	0	0
34	6	1	0	0	1	0
34	7	3	0	0	0	0
34	8	11	0	0	1	0
34	9	1	0	0	1	0
34	A	1678	0	0	168	0
34	B	58	0	0	3	1
34	D	18	0	0	3	0
34	E	10	0	0	0	0
34	F	7	0	0	1	0
34	H	1	0	0	0	0
34	N	2	0	0	0	0
34	O	1	0	0	0	0
34	P	10	0	0	1	0
34	Q	4	0	0	0	0
34	R	6	0	0	1	0
34	T	1	0	0	0	0
34	U	4	0	0	0	0
34	V	3	0	0	0	0
34	W	2	0	0	0	0
34	X	2	0	0	0	0
34	Y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	92957	0	59976	2000	1

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

All (2000) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2296:U:O4	1:A:2335:A:N6	1.76	1.19
1:A:885:C:C4	1:A:890:A:N6	2.20	1.10
1:A:885:C:N4	1:A:890:A:C6	2.22	1.08
1:A:2820:A:OP2	13:R:2:ARG:NH2	1.87	1.07
1:A:2036:C:OP1	34:A:4545:HOH:O	1.77	1.02
1:A:847:U:O4	1:A:933:A:N6	1.92	1.02
1:A:463:G:OP1	34:A:3931:HOH:O	1.79	0.97
1:A:2122:U:H3	1:A:2176:A:H61	1.00	0.97
1:A:631:A:OP1	11:P:65:ARG:NH1	1.98	0.96
1:A:450:G:O6	34:A:4564:HOH:O	1.84	0.96
1:A:1359:A:N6	1:A:1372:U:O4	1.99	0.94
1:A:2228:G:OP1	3:D:261:LYS:NZ	2.01	0.93
26:4:42:PHE:HB3	26:4:43:TYR:HB2	1.48	0.93
1:A:1689:A:H62	1:A:1698:A:H2	1.14	0.93
1:A:271(I):G:H1	1:A:271(O):C:H42	0.97	0.92
1:A:583:G:N7	34:A:5058:HOH:O	2.03	0.90
1:A:676:A:H8	1:A:2069:G:H21	1.17	0.90
1:A:1533:G:H21	1:A:1536:C:H5	1.19	0.90
1:A:271(I):G:H1	1:A:271(O):C:N4	1.69	0.90
11:P:39:LYS:HB2	11:P:45:LEU:HG	1.53	0.90
6:G:63:ILE:HA	6:G:143:GLU:HG3	1.54	0.90
1:A:2322:A:H61	1:A:2335:A:N6	1.70	0.90
1:A:1210:A:H5''	1:A:1210:A:H8	1.35	0.90
1:A:1189:A:OP2	34:A:4511:HOH:O	1.88	0.89
1:A:2406:U:OP1	34:A:4484:HOH:O	1.90	0.89
15:T:16:ARG:NH2	15:T:83:ILE:O	2.05	0.88
1:A:2366:A:OP1	34:A:4088:HOH:O	1.90	0.88
23:1:82:LEU:HA	23:1:85:LEU:HD23	1.53	0.88
1:A:974:G:N7	34:A:4191:HOH:O	2.08	0.87
1:A:2122:U:H3	1:A:2176:A:N6	1.71	0.87
1:A:2304:G:H1	1:A:2312:U:H3	1.22	0.87
1:A:1284:A:N7	34:A:5004:HOH:O	2.06	0.86
1:A:883:G:H2'	1:A:884:C:H5''	1.57	0.86
1:A:1530:C:O2'	1:A:1531:C:O5'	1.94	0.86
1:A:558:G:N7	34:A:4932:HOH:O	2.09	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:745:G:O6	34:A:5268:HOH:O	1.94	0.85
1:A:1474:C:N4	34:A:4405:HOH:O	2.10	0.85
1:A:2639:A:OP2	34:A:4103:HOH:O	1.94	0.85
1:A:885:C:N4	1:A:890:A:N6	2.22	0.85
5:F:101:LEU:O	5:F:106:ARG:NH1	2.10	0.85
1:A:2317:C:H2'	1:A:2318:G:H5'	1.58	0.84
1:A:1177:A:O2'	1:A:1178:C:O4'	1.95	0.84
11:P:126:VAL:HG12	11:P:148:LEU:HD22	1.60	0.84
1:A:242:G:OP1	34:A:4226:HOH:O	1.94	0.84
8:I:3:VAL:HG12	8:I:38:LEU:HA	1.57	0.84
1:A:510:C:OP1	34:A:3878:HOH:O	1.94	0.84
1:A:2036:C:H6	1:A:2036:C:H5'	1.42	0.83
1:A:330:A:H2	1:A:1210:A:H2'	1.43	0.83
1:A:805:G:OP1	34:A:4490:HOH:O	1.95	0.83
3:D:118:VAL:H	3:D:129:ASN:HD22	1.25	0.83
1:A:1210:A:C8	1:A:1210:A:H5''	2.13	0.83
1:A:2134:A:O2'	1:A:2159:G:N2	2.12	0.83
9:N:20:GLY:HA2	9:N:61:ARG:HG3	1.60	0.82
1:A:624:C:OP1	34:A:4227:HOH:O	1.96	0.82
1:A:1667:G:O6	34:A:4974:HOH:O	1.95	0.82
1:A:922:U:O4	34:A:4354:HOH:O	1.98	0.82
9:N:130:HIS:HB3	9:N:133:GLN:HE21	1.43	0.81
1:A:578:A:OP2	34:A:4040:HOH:O	1.97	0.81
6:G:41:GLN:HB3	6:G:43:LEU:HD13	1.60	0.81
16:U:28:ARG:NH1	16:U:38:THR:OG1	2.12	0.81
1:A:2033:A:OP1	34:A:4582:HOH:O	1.97	0.81
1:A:1320:C:OP2	34:A:5001:HOH:O	1.99	0.81
17:V:62:LEU:HD11	17:V:95:LEU:HB2	1.63	0.81
1:A:1173:G:N1	1:A:1176:G:OP2	2.11	0.80
6:G:15:VAL:HG13	6:G:175:LEU:HB3	1.63	0.80
1:A:2287:A:N6	1:A:2344:U:H3	1.80	0.80
1:A:300:A:N6	34:A:3906:HOH:O	2.13	0.80
1:A:1541:G:O6	34:A:4721:HOH:O	1.98	0.80
1:A:2161:C:C5	1:A:2161:C:OP2	2.34	0.80
1:A:561:G:N7	34:A:5343:HOH:O	2.15	0.79
1:A:1517:G:O6	34:A:4405:HOH:O	2.00	0.79
1:A:1888:G:N7	34:A:4823:HOH:O	2.15	0.79
1:A:1607:C:N4	1:A:1622:G:OP2	2.16	0.79
1:A:2296:U:O4	1:A:2335:A:C6	2.36	0.79
1:A:885:C:C4	1:A:890:A:C6	2.69	0.79
3:D:239:ARG:N	34:D:408:HOH:O	2.15	0.79
1:A:2298:A:H62	1:A:2318:G:H8	1.27	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:105:LYS:NZ	26:4:25:TYR:O	2.16	0.79
1:A:1664:A:OP1	34:A:4759:HOH:O	2.00	0.78
1:A:1019:U:H3	1:A:1142(A):A:H62	1.29	0.78
1:A:784:A:OP1	34:A:4411:HOH:O	2.00	0.78
1:A:1639:U:H2'	1:A:1640:C:H5''	1.64	0.78
1:A:1970:A:N1	34:A:5030:HOH:O	2.16	0.78
21:Z:82:ARG:HB3	21:Z:82:ARG:HH21	1.48	0.78
1:A:778:G:O6	34:A:3892:HOH:O	2.02	0.78
1:A:1022:G:H22	1:A:1142(A):A:H2	1.31	0.78
1:A:31:C:OP1	34:A:3865:HOH:O	2.01	0.78
1:A:154(A):C:N4	1:A:171:G:H1	1.83	0.77
1:A:2161:C:C6	1:A:2161:C:OP2	2.38	0.77
18:W:25:ARG:NH2	18:W:74:ALA:O	2.16	0.77
1:A:2285:C:OP2	28:6:6:ARG:NH1	2.17	0.77
1:A:1468:C:OP1	34:A:4156:HOH:O	2.02	0.77
1:A:2472:G:H5'	1:A:2473:U:H5''	1.66	0.77
1:A:1840:G:N7	34:A:4626:HOH:O	2.17	0.77
1:A:1535:A:OP2	1:A:1535:A:H3'	1.84	0.76
3:D:118:VAL:H	3:D:129:ASN:ND2	1.83	0.76
1:A:2439:A:O2'	34:A:4412:HOH:O	2.03	0.76
1:A:2408:U:OP2	34:A:4483:HOH:O	2.04	0.76
1:A:2070:G:OP2	34:A:3845:HOH:O	2.04	0.76
1:A:2206:G:H5'	1:A:2207:G:N7	2.01	0.76
1:A:2365:G:OP1	34:A:4086:HOH:O	2.03	0.75
1:A:744:G:OP1	34:A:4590:HOH:O	2.03	0.75
1:A:1790:C:N3	34:A:3720:HOH:O	2.18	0.75
1:A:990:A:OP2	34:A:4504:HOH:O	2.04	0.75
1:A:188:G:N7	34:A:4287:HOH:O	2.18	0.75
1:A:1319:G:OP2	34:A:3788:HOH:O	2.04	0.75
1:A:380:U:OP1	34:A:4323:HOH:O	2.05	0.75
1:A:942:G:O6	34:A:4947:HOH:O	2.04	0.75
1:A:2147:G:H2'	1:A:2148:G:O4'	1.86	0.75
1:A:1980:G:O2'	1:A:1982:C:OP2	2.04	0.75
1:A:1900:A:OP2	34:A:4613:HOH:O	2.05	0.75
2:B:31:C:O2'	2:B:53:A:N6	2.20	0.75
28:6:22:ALA:O	34:6:201:HOH:O	2.05	0.75
1:A:2371:G:O6	34:A:4861:HOH:O	2.05	0.74
1:A:71:A:C2	19:X:31:HIS:HE1	2.05	0.74
1:A:1190:G:N7	34:A:4511:HOH:O	2.20	0.74
3:D:234:GLY:O	34:D:413:HOH:O	2.04	0.74
1:A:910:A:OP2	34:A:4342:HOH:O	2.04	0.74
1:A:833:U:O2	11:P:55:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1030:G:OP1	34:A:4396:HOH:O	2.05	0.73
2:B:60:C:N4	34:B:316:HOH:O	2.19	0.73
1:A:883:G:H1	1:A:893:C:H42	1.35	0.73
1:A:1171:G:H1'	1:A:1173:G:H5'	1.69	0.73
1:A:2296:U:OP2	14:S:9:ARG:NH2	2.21	0.73
1:A:1047:G:H2'	1:A:1110:G:H22	1.53	0.73
2:B:86:G:O6	34:B:340:HOH:O	2.06	0.73
1:A:271(A):A:N7	1:A:271(W):G:N2	2.35	0.73
30:8:33:ASN:HA	30:8:36:LYS:HD2	1.69	0.73
1:A:2109:U:H3	1:A:2180:U:H3	1.36	0.73
1:A:1913:A:OP2	1:A:1913:A:H3'	1.88	0.73
15:T:95:ARG:HG2	15:T:95:ARG:HH11	1.53	0.73
1:A:531:C:OP1	1:A:561:G:N2	2.20	0.73
1:A:1845:G:N7	34:A:5132:HOH:O	2.22	0.73
1:A:2534:A:N7	34:A:5049:HOH:O	2.21	0.73
1:A:2136:C:H42	1:A:2155:G:H1	1.36	0.72
1:A:2706:G:O6	34:A:4840:HOH:O	2.06	0.72
1:A:2287:A:H62	1:A:2344:U:H3	1.36	0.72
21:Z:10:ARG:NH2	21:Z:26:GLY:O	2.22	0.72
1:A:1817:G:OP1	3:D:88:ARG:NH2	2.23	0.72
1:A:674:G:OP2	34:A:3852:HOH:O	2.07	0.72
1:A:1022:G:O2'	34:A:3713:HOH:O	2.05	0.72
1:A:1721:G:H8	1:A:1741:A:H62	1.37	0.72
6:G:76:SER:HA	6:G:83:ARG:HA	1.71	0.72
1:A:1429:G:H2'	1:A:1430:C:C6	2.25	0.72
8:I:83:ALA:HB2	8:I:88:ILE:HA	1.70	0.72
1:A:607:U:OP1	5:F:102:PRO:HA	1.90	0.72
1:A:2117:A:H61	1:A:2166:G:H22	1.38	0.72
1:A:243:U:OP1	30:8:6:THR:OG1	2.08	0.71
1:A:882:G:H1	1:A:894:C:H42	1.38	0.71
1:A:1324:G:O6	34:A:4942:HOH:O	2.07	0.71
8:I:130:TYR:HB3	8:I:138:ILE:HB	1.70	0.71
1:A:2322:A:N6	1:A:2335:A:H61	1.87	0.71
1:A:1634:A:N1	34:A:4310:HOH:O	2.23	0.71
1:A:1370:C:OP1	34:A:4681:HOH:O	2.08	0.71
1:A:1045:A:N3	1:A:1045:A:H2'	2.04	0.71
1:A:1235:G:OP1	34:A:4211:HOH:O	2.08	0.71
1:A:269:U:OP1	34:A:5061:HOH:O	2.07	0.71
1:A:1665:A:OP2	34:A:4759:HOH:O	2.09	0.71
1:A:1204:A:H2	1:A:1241:A:H62	1.37	0.71
1:A:2126:A:N6	1:A:2163:C:H5'	2.06	0.71
17:V:72:VAL:HG13	17:V:85:LYS:HB3	1.71	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:56:ALA:HB2	6:G:153:ARG:HE	1.56	0.70
12:Q:58:PHE:HB3	12:Q:61:GLY:HA3	1.74	0.70
5:F:178:PRO:HB2	5:F:201:VAL:HG11	1.72	0.70
12:Q:111:GLU:OE1	12:Q:133:ARG:NH2	2.24	0.70
4:E:47:VAL:HG11	4:E:86:PRO:HD2	1.73	0.70
6:G:16:ARG:HE	6:G:31:VAL:HG21	1.57	0.70
7:H:154:PRO:HB3	7:H:163:TYR:CZ	2.27	0.70
1:A:2600:A:OP2	34:A:4412:HOH:O	2.09	0.70
18:W:13:SER:HB3	18:W:16:LYS:HD2	1.72	0.70
1:A:453:C:OP1	34:A:4564:HOH:O	2.09	0.70
8:I:1:MET:N	8:I:21:VAL:O	2.24	0.70
1:A:2322:A:H61	1:A:2335:A:H61	1.39	0.69
1:A:2637:U:H5''	4:E:82:ARG:HH21	1.57	0.69
1:A:1997:G:OP2	34:A:4604:HOH:O	2.10	0.69
3:D:17:THR:O	3:D:211:ARG:NH2	2.23	0.69
1:A:2781:A:H5''	1:A:2782:G:H5'	1.74	0.69
1:A:1507:A:O2'	1:A:1508:A:H8	1.74	0.69
1:A:517:C:OP1	27:5:16:ARG:NH2	2.24	0.69
1:A:29:U:H2'	1:A:30:G:C8	2.27	0.69
8:I:83:ALA:HA	8:I:89:TYR:CE2	2.27	0.69
1:A:1364:G:OP2	23:1:3:LYS:HG2	1.91	0.69
21:Z:110:GLY:HA3	21:Z:174:VAL:HG11	1.72	0.69
1:A:278:A:O2'	1:A:279:C:OP1	2.04	0.69
1:A:2306:C:H3'	1:A:2307:G:C8	2.27	0.69
1:A:956:G:OP2	12:Q:14:ARG:NH2	2.25	0.69
20:Y:23:ARG:HG2	20:Y:42:VAL:HG22	1.75	0.69
1:A:1914:C:H2'	1:A:1915:U:C6	2.28	0.69
29:7:24:THR:HG23	29:7:27:GLY:H	1.55	0.69
1:A:1359:A:N6	1:A:1372:U:C4	2.58	0.69
1:A:2115:G:H4'	1:A:2167:U:H4'	1.74	0.69
1:A:94:C:H5'	1:A:94(A):G:OP2	1.93	0.69
1:A:438:G:O6	34:A:4801:HOH:O	2.09	0.69
1:A:580:C:H2'	1:A:581:C:H6	1.57	0.69
1:A:2588:G:OP1	34:A:4411:HOH:O	2.10	0.69
1:A:392:C:OP1	34:A:3943:HOH:O	2.11	0.69
1:A:1226:A:OP1	17:V:84:LYS:NZ	2.25	0.69
1:A:1266:G:O5'	18:W:15:ARG:NH2	2.26	0.68
22:0:53:MET:HG3	22:0:59:LEU:HD23	1.76	0.68
1:A:1529:G:C6	1:A:1530:C:N4	2.61	0.68
1:A:804:A:OP1	34:A:4491:HOH:O	2.10	0.68
6:G:101:ILE:HD13	26:4:25:TYR:HB2	1.76	0.68
5:F:185:ASP:HA	5:F:188:ARG:HD3	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271(V):G:N7	34:A:4895:HOH:O	2.26	0.68
1:A:2010:G:N7	34:A:5213:HOH:O	2.27	0.68
1:A:450:G:OP2	34:A:4568:HOH:O	2.12	0.68
1:A:975:C:OP2	34:A:4189:HOH:O	2.10	0.68
1:A:1250:G:N7	11:P:18:ARG:NH2	2.42	0.68
8:I:93:THR:HG23	8:I:96:ASP:H	1.58	0.68
1:A:2786:U:O2'	4:E:62:PRO:O	2.07	0.68
1:A:379:G:O6	34:A:4385:HOH:O	2.11	0.68
27:5:16:ARG:NH1	27:5:17:ASP:OD1	2.26	0.68
28:6:13:CYS:SG	28:6:47:THR:HG21	2.33	0.68
1:A:271(I):G:N2	1:A:271(O):C:N3	2.38	0.68
1:A:1157:G:OP1	34:A:4180:HOH:O	2.12	0.68
1:A:1484:G:N7	34:A:4149:HOH:O	2.26	0.68
1:A:2712(A):A:H5''	1:A:2713:A:OP2	1.93	0.68
1:A:2833:G:H3'	1:A:2834:G:H5'	1.75	0.68
1:A:1352:U:OP2	34:A:3896:HOH:O	2.12	0.67
1:A:821:A:N1	34:A:5231:HOH:O	2.27	0.67
14:S:11:LYS:HG3	14:S:91:PRO:HD3	1.75	0.67
1:A:271(F):C:H2'	1:A:271(G):C:H6	1.59	0.67
15:T:118:ARG:HA	15:T:118:ARG:CZ	2.25	0.67
1:A:2336:A:H61	22:0:43:THR:HG22	1.60	0.67
1:A:885:C:C5	1:A:890:A:N6	2.61	0.67
1:A:1403:C:H5''	1:A:1471:A:H1'	1.77	0.67
1:A:2249:U:O2'	34:A:4473:HOH:O	2.13	0.67
1:A:620:G:H5''	1:A:620:G:N3	2.10	0.67
1:A:271(M):G:OP2	8:I:57:ARG:NH2	2.28	0.67
1:A:885:C:OP1	1:A:885:C:H4'	1.92	0.67
7:H:86:GLU:OE2	7:H:132:ARG:NH1	2.28	0.67
1:A:2243:U:H2'	1:A:2244:U:C6	2.30	0.67
1:A:1186:G:OP2	34:A:4504:HOH:O	2.11	0.67
1:A:2134:A:C2	1:A:2159:G:H1'	2.30	0.66
6:G:138:GLN:HG3	6:G:144:ILE:HG21	1.75	0.66
1:A:862:G:OP2	34:A:4337:HOH:O	2.13	0.66
18:W:4:LYS:HB2	18:W:106:ILE:HG12	1.77	0.66
1:A:1434:A:H61	1:A:1558:A:N6	1.93	0.66
5:F:7:TYR:H	5:F:22:ALA:HB3	1.60	0.66
1:A:587:C:OP2	11:P:21:ARG:NH2	2.28	0.66
1:A:885:C:C2	1:A:886:C:H1'	2.31	0.66
15:T:24:PRO:HA	15:T:49:VAL:HG22	1.75	0.66
9:N:47:ALA:HB2	9:N:112:LEU:HD11	1.76	0.66
1:A:105:C:OP1	34:A:3758:HOH:O	2.13	0.66
1:A:1265:A:OP2	34:A:4981:HOH:O	2.12	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1026:U:O2'	1:A:1027:A:O5'	2.13	0.66
1:A:2318:G:N2	14:S:3:ARG:HD3	2.10	0.66
17:V:35:LEU:HB2	17:V:57:VAL:HG13	1.77	0.66
2:B:66:A:H61	2:B:109:C:H5'	1.60	0.66
1:A:1171:G:O2'	1:A:1173:G:OP2	2.06	0.66
1:A:1379:A:H4'	1:A:1380:G:OP2	1.95	0.66
1:A:1561:G:OP2	34:A:4347:HOH:O	2.14	0.66
6:G:122:PRO:HG3	6:G:180:PHE:HB3	1.78	0.66
1:A:1778:U:H2'	1:A:1784:A:N6	2.10	0.66
1:A:631:A:OP2	30:8:47:LYS:NZ	2.22	0.66
1:A:563:G:OP2	34:A:4452:HOH:O	2.14	0.66
1:A:2705:A:OP2	34:A:4842:HOH:O	2.13	0.66
1:A:1016:G:N7	34:A:5110:HOH:O	2.28	0.66
14:S:10:ARG:HH21	14:S:91:PRO:HB2	1.60	0.65
12:Q:54:MET:HE3	12:Q:64:ILE:HD13	1.77	0.65
1:A:376:C:OP2	34:A:3944:HOH:O	2.13	0.65
1:A:2319:G:N2	14:S:3:ARG:HD2	2.11	0.65
25:3:23:LEU:HD13	25:3:50:VAL:HG11	1.78	0.65
1:A:639:U:H2'	1:A:640:C:C6	2.32	0.65
1:A:856:C:H5'	22:0:27:GLU:OE2	1.96	0.65
1:A:2712:U:O2'	1:A:2712(A):A:OP2	2.14	0.65
1:A:2533:A:OP2	34:A:5046:HOH:O	2.14	0.65
29:7:34:ARG:NH1	29:7:41:ARG:O	2.30	0.65
15:T:60:THR:HG22	15:T:77:PRO:HA	1.79	0.65
6:G:11:TYR:CE2	6:G:16:ARG:HD3	2.31	0.65
1:A:504:U:OP2	34:A:4923:HOH:O	2.13	0.65
1:A:1423:G:H2'	1:A:1424:G:H8	1.62	0.65
1:A:606:U:H4'	1:A:658:C:H4'	1.79	0.65
15:T:64:ARG:NH1	15:T:103:ARG:HA	2.11	0.65
21:Z:45:ASP:OD2	21:Z:49:ARG:NH1	2.29	0.65
1:A:2887:U:H2'	1:A:2888:C:C6	2.32	0.65
1:A:1587:A:H2'	1:A:1588:C:C6	2.31	0.65
1:A:154(A):C:N4	1:A:171:G:N1	2.44	0.65
1:A:1833:U:H2'	1:A:1834:U:H6	1.60	0.65
1:A:1174:A:H5'	1:A:1177:A:H62	1.61	0.65
1:A:1560:G:OP1	34:A:4347:HOH:O	2.13	0.65
1:A:696:G:N7	34:A:5330:HOH:O	2.29	0.65
1:A:886:C:H2'	1:A:889:C:H41	1.62	0.64
1:A:1174:A:H4'	1:A:1175:U:OP1	1.97	0.64
1:A:314:A:N6	34:A:5250:HOH:O	2.21	0.64
1:A:2721:A:OP2	34:A:4059:HOH:O	2.14	0.64
20:Y:23:ARG:HH11	20:Y:23:ARG:HB2	1.61	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:53:THR:HG23	5:F:55:GLY:H	1.62	0.64
1:A:2305:A:H5''	6:G:134:GLY:HA3	1.80	0.64
1:A:674:G:H1'	5:F:74:ARG:HD3	1.78	0.64
26:4:16:CYS:SG	26:4:20:ASN:HB3	2.38	0.64
1:A:2526:G:H21	31:9:2:LYS:HG2	1.63	0.64
1:A:459:U:H5''	29:7:40:TRP:CD2	2.33	0.64
1:A:2322:A:N6	1:A:2335:A:N6	2.42	0.64
18:W:18:ARG:HG3	18:W:76:VAL:HB	1.80	0.64
16:U:44:ASN:ND2	17:V:75:PHE:O	2.24	0.64
4:E:28:ALA:HB3	4:E:93:VAL:HG12	1.78	0.64
1:A:1176:G:H1'	1:A:1177:A:OP1	1.96	0.64
1:A:2808:U:H5'	1:A:2891:G:O6	1.97	0.64
1:A:90:U:H2'	1:A:92:A:C8	2.32	0.64
3:D:71:ASP:HB3	3:D:103:ARG:HH22	1.63	0.64
14:S:58:LEU:HB2	14:S:59:LYS:HB2	1.78	0.64
1:A:492:A:OP2	34:A:4847:HOH:O	2.15	0.64
1:A:787:U:OP1	34:A:4555:HOH:O	2.15	0.64
1:A:2492:U:H2'	1:A:2493:U:C6	2.32	0.64
1:A:1176:G:H21	1:A:1178:C:P	2.21	0.64
11:P:25:SER:O	34:P:303:HOH:O	2.15	0.64
1:A:2122:U:H2'	1:A:2123:G:C8	2.32	0.64
1:A:271(J):C:O2'	1:A:271(K):U:H5'	1.98	0.64
5:F:123:LEU:HD13	5:F:192:LEU:HD13	1.80	0.64
8:I:12:LEU:HD22	8:I:19:VAL:HG21	1.79	0.64
1:A:2206:G:O2'	1:A:2207:G:OP1	2.13	0.64
1:A:89:G:H3'	1:A:90:U:H5''	1.79	0.64
4:E:128:SER:OG	4:E:129:HIS:N	2.27	0.64
1:A:1288:U:C2	1:A:1327:C:O2	2.51	0.64
3:D:142:VAL:HG23	3:D:193:VAL:HA	1.79	0.64
1:A:1019:U:HO2'	1:A:1021:A:H2	1.44	0.63
1:A:1639:U:C2'	1:A:1640:C:H5''	2.28	0.63
1:A:994:C:H3'	16:U:54:LYS:HE3	1.81	0.63
1:A:2115:G:C2	1:A:2117:A:N7	2.66	0.63
28:6:3:SER:OG	28:6:4:GLU:N	2.28	0.63
8:I:62:LYS:HG2	8:I:133:HIS:CE1	2.33	0.63
1:A:1536:C:H4'	1:A:1537:G:OP1	1.97	0.63
1:A:301:G:OP2	20:Y:84:ARG:NH2	2.31	0.63
6:G:56:ALA:HA	6:G:153:ARG:HH21	1.63	0.63
21:Z:82:ARG:HB3	21:Z:82:ARG:NH2	2.14	0.63
10:O:25:LEU:HD21	10:O:40:VAL:HG23	1.81	0.63
11:P:127:ALA:O	11:P:148:LEU:HD23	1.98	0.63
1:A:910:A:H62	12:Q:12:GLN:HA	1.63	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:314:A:C2'	1:A:315:G:H5'	2.28	0.63
1:A:1968:G:OP1	34:A:3881:HOH:O	2.15	0.63
27:5:16:ARG:HH11	27:5:16:ARG:HG2	1.62	0.63
1:A:249:C:OP1	34:A:4488:HOH:O	2.15	0.63
31:9:4:ARG:NH1	34:9:201:HOH:O	2.32	0.63
1:A:1278:A:OP1	13:R:36:THR:HG23	1.98	0.63
1:A:570:G:H5''	34:A:4128:HOH:O	1.98	0.63
1:A:484:C:H2'	1:A:485:C:C6	2.34	0.63
7:H:3:ARG:CZ	7:H:4:ILE:H	2.12	0.63
1:A:1532:C:H2'	1:A:1533:G:O4'	1.99	0.63
1:A:1566:A:OP1	3:D:211:ARG:NH1	2.32	0.63
7:H:70:THR:HA	7:H:73:ALA:HB3	1.81	0.63
1:A:240:G:O6	34:A:4230:HOH:O	2.12	0.63
1:A:2646:C:OP2	1:A:2732:G:O2'	2.15	0.63
1:A:1171:G:O2'	1:A:1173:G:H2'	2.00	0.62
1:A:1047:G:H2'	1:A:1110:G:H1	1.64	0.62
1:A:2562:U:H1'	10:O:23:ARG:HH11	1.63	0.62
1:A:1405:U:H2'	1:A:1406:U:C6	2.35	0.62
1:A:2567:G:H2'	1:A:2568:C:C6	2.34	0.62
4:E:175:VAL:HG23	4:E:177:PRO:HD3	1.80	0.62
1:A:1858:G:O6	34:A:3991:HOH:O	2.13	0.62
11:P:59:LEU:HD11	30:8:10:ALA:HB2	1.81	0.62
1:A:2327:A:H2'	1:A:2328:A:C8	2.34	0.62
1:A:83:G:OP1	20:Y:95:LYS:NZ	2.32	0.62
1:A:1763:G:OP1	1:A:1763:G:H4'	1.99	0.62
1:A:1914:C:H2'	1:A:1915:U:H6	1.65	0.62
15:T:11:GLU:OE1	15:T:57:PHE:HB3	2.00	0.62
1:A:2127:G:H21	1:A:2173:A:H1'	1.64	0.62
1:A:1049:C:H4'	1:A:1050:A:OP1	1.99	0.62
12:Q:27:VAL:N	12:Q:138:ASP:OD1	2.33	0.62
1:A:1560:G:H3'	34:A:4346:HOH:O	1.99	0.62
1:A:2104:G:N7	1:A:2186:G:N2	2.48	0.62
16:U:92:ARG:HA	16:U:95:LEU:HB2	1.81	0.62
1:A:2760:C:H2'	1:A:2761:G:H5''	1.81	0.62
1:A:580:C:H2'	1:A:581:C:C6	2.35	0.62
1:A:2318:G:O2'	1:A:2319:G:OP1	2.15	0.62
1:A:2206:G:H5'	1:A:2207:G:C5	2.35	0.62
1:A:1721:G:H2'	1:A:1740:G:O6	2.00	0.62
5:F:65:TRP:HH2	5:F:72:ARG:HH21	1.48	0.62
1:A:188:G:H1	1:A:208:C:H42	1.48	0.62
5:F:185:ASP:HA	5:F:188:ARG:CD	2.30	0.62
1:A:1153:C:OP1	16:U:92:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2602:A:H4'	1:A:2603:G:OP1	2.00	0.62
1:A:307:G:N2	1:A:309:G:H3'	2.15	0.61
2:B:49:C:OP1	14:S:97:ARG:N	2.33	0.61
1:A:1165:U:H2'	1:A:1166:C:C6	2.35	0.61
1:A:2119:A:C2	1:A:2170:A:H2'	2.35	0.61
1:A:2394:C:OP1	30:8:30:ARG:NH1	2.33	0.61
1:A:250:G:OP2	30:8:13:ARG:NH2	2.33	0.61
15:T:53:ARG:NH1	15:T:60:THR:OG1	2.33	0.61
3:D:222:ARG:NH1	34:D:418:HOH:O	2.32	0.61
9:N:15:LEU:HB2	9:N:135:PRO:HB2	1.82	0.61
1:A:467:G:OP1	29:7:33:ARG:NH1	2.32	0.61
1:A:2162:G:H1'	1:A:2173:A:H1'	1.82	0.61
1:A:1972:A:OP2	34:A:4856:HOH:O	2.16	0.61
1:A:668:G:H5''	1:A:669:G:OP2	2.01	0.61
15:T:56:GLY:O	15:T:59:THR:HG22	2.00	0.61
23:1:50:ARG:HG2	23:1:59:THR:HG22	1.83	0.61
1:A:1534:U:H3'	1:A:1535:A:C2	2.36	0.61
1:A:910:A:C5	12:Q:13:GLN:HG3	2.35	0.61
1:A:1030:G:OP2	12:Q:128:LYS:NZ	2.32	0.61
1:A:2306:C:H5'	1:A:2307:G:H2'	1.81	0.61
14:S:14:VAL:O	14:S:18:ILE:HG12	2.01	0.61
1:A:271(E):U:H2'	1:A:271(F):C:C6	2.36	0.61
1:A:1584:C:H2'	1:A:1586:A:H5'	1.82	0.61
1:A:1047:G:H2'	1:A:1110:G:N2	2.16	0.60
8:I:139:GLN:HA	8:I:139:GLN:HE21	1.65	0.60
1:A:1187:G:O6	34:A:4418:HOH:O	2.13	0.60
1:A:1784:A:OP1	34:A:4592:HOH:O	2.16	0.60
21:Z:158:PRO:O	21:Z:161:VAL:HB	2.02	0.60
3:D:108:PRO:HG2	3:D:111:LEU:HG	1.83	0.60
21:Z:48:PHE:HE2	21:Z:71:VAL:HG11	1.65	0.60
1:A:387:U:OP1	34:A:3939:HOH:O	2.16	0.60
1:A:644:A:H4'	1:A:645:C:C5	2.36	0.60
15:T:53:ARG:HH11	15:T:53:ARG:HB3	1.66	0.60
1:A:1131:G:H21	9:N:73:THR:HG21	1.65	0.60
1:A:527:C:OP1	34:A:4542:HOH:O	2.15	0.60
1:A:2318:G:H22	14:S:3:ARG:HH11	1.48	0.60
1:A:1819:A:H4'	1:A:1820:U:O5'	2.01	0.60
1:A:9:U:H3	1:A:2629:A:H2	1.48	0.60
1:A:430:G:OP1	34:A:4235:HOH:O	2.16	0.60
6:G:106:LEU:HD12	6:G:110:ALA:HB3	1.81	0.60
1:A:747:U:O2	1:A:2014:A:H1'	2.01	0.60
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.37	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:110:G:H2'	2:B:111:G:C8	2.36	0.60
8:I:145:VAL:HG12	8:I:146:ALA:H	1.67	0.60
6:G:77:ILE:N	6:G:82:LEU:O	2.30	0.60
1:A:2845:G:O2'	1:A:2846:G:H5'	2.02	0.60
1:A:887:A:H5'	1:A:889:C:H41	1.67	0.60
1:A:2136:C:N4	1:A:2155:G:H1	2.00	0.60
5:F:184:TYR:O	5:F:188:ARG:HG3	2.02	0.60
2:B:110:G:H2'	2:B:111:G:H8	1.67	0.60
1:A:1796:U:H2'	1:A:1797:C:C6	2.37	0.60
20:Y:76:CYS:HB3	20:Y:79:CYS:HB2	1.82	0.60
1:A:1177:A:OP1	1:A:1177:A:H3'	2.02	0.60
1:A:1607:C:H4'	1:A:1608:A:O5'	2.02	0.60
8:I:83:ALA:HA	8:I:89:TYR:CD2	2.36	0.60
15:T:53:ARG:NH1	15:T:53:ARG:HB3	2.16	0.60
8:I:115:ALA:HB2	8:I:129:THR:OG1	2.01	0.60
1:A:2199:A:H3'	1:A:2200:C:H6	1.65	0.60
19:X:36:LYS:HG2	19:X:54:VAL:HB	1.83	0.60
1:A:71:A:H2	19:X:31:HIS:HE1	1.47	0.60
1:A:1048:A:H4'	1:A:1049:C:OP1	2.00	0.60
1:A:1277:G:OP1	34:A:3709:HOH:O	2.17	0.60
5:F:129:PHE:CD2	5:F:163:VAL:HG21	2.37	0.59
28:6:9:LEU:HD13	28:6:51:GLU:HG3	1.84	0.59
26:4:42:PHE:CB	26:4:43:TYR:HB2	2.27	0.59
19:X:27:THR:HG23	19:X:80:ILE:HG13	1.84	0.59
1:A:2612:C:O5'	27:5:2:ALA:HB3	2.02	0.59
22:0:27:GLU:HG3	22:0:68:GLU:HA	1.84	0.59
1:A:1449:A:H5'	1:A:1450:G:OP2	2.03	0.59
1:A:2773:C:H5''	4:E:164:ARG:HG2	1.84	0.59
1:A:2406:U:H2'	1:A:2406:U:OP2	2.02	0.59
18:W:84:ARG:HG3	18:W:98:LYS:HD2	1.84	0.59
1:A:652(B):A:H2'	1:A:652(B):A:N3	2.18	0.59
1:A:2820:A:OP1	13:R:4:LEU:HD23	2.01	0.59
1:A:61:G:H1	1:A:94:C:H42	1.49	0.59
16:U:76:TYR:CE2	16:U:80:ILE:HG13	2.37	0.59
14:S:96:GLY:HA2	14:S:97:ARG:C	2.22	0.59
1:A:196:A:O4'	11:P:46:LYS:HE2	2.03	0.59
1:A:1049:C:H2'	1:A:1050:A:H8	1.68	0.59
6:G:124:SER:HB2	6:G:131:TYR:CE1	2.37	0.59
1:A:253:C:OP2	30:8:5:LYS:NZ	2.30	0.59
1:A:2867:G:OP2	15:T:119:LYS:NZ	2.31	0.59
7:H:117:PRO:HB3	7:H:123:PHE:CE2	2.37	0.59
5:F:85:GLY:O	34:F:403:HOH:O	2.15	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:50:SER:HB2	5:F:94:PRO:HD3	1.84	0.59
19:X:8:ILE:O	24:2:36:ARG:NH2	2.35	0.59
1:A:2272:U:H5''	1:A:2273:A:OP1	2.02	0.59
1:A:203:C:H3'	1:A:204:A:H5''	1.85	0.59
1:A:784:A:H5'	1:A:785:G:OP1	2.02	0.59
1:A:1047:G:H21	1:A:1111:A:N6	2.01	0.59
1:A:546:C:H2'	1:A:547:A:H5'	1.83	0.59
1:A:2406:U:OP1	34:A:4482:HOH:O	2.17	0.58
1:A:1790:C:H5''	1:A:1791:A:OP1	2.02	0.58
23:1:3:LYS:HB2	23:1:61:ARG:HH11	1.68	0.58
1:A:1865:G:H5'	1:A:1866:C:OP2	2.03	0.58
9:N:120:LEU:HD22	9:N:122:VAL:HG23	1.83	0.58
1:A:2196:C:OP2	34:A:4400:HOH:O	2.17	0.58
1:A:1426:G:N7	3:D:31:LYS:NZ	2.51	0.58
1:A:226:G:H21	1:A:228:A:H62	1.50	0.58
1:A:8:A:OP1	9:N:121:LYS:NZ	2.36	0.58
1:A:588:U:H2'	1:A:589:C:C6	2.38	0.58
1:A:581:C:H2'	1:A:582:G:H8	1.69	0.58
1:A:184:C:H2'	1:A:185:U:C6	2.38	0.58
6:G:150:ASP:CG	6:G:151:ALA:H	2.07	0.58
3:D:148:GLU:HB2	3:D:151:LYS:HD2	1.86	0.58
1:A:581:C:H2'	1:A:582:G:C8	2.39	0.58
6:G:11:TYR:CZ	6:G:16:ARG:HD3	2.38	0.58
8:I:77:LEU:HB3	8:I:142:VAL:HG12	1.85	0.58
1:A:2610:C:H4'	1:A:2611:U:OP2	2.04	0.58
1:A:1021:A:H62	1:A:1141:U:H3	1.52	0.58
1:A:1351:C:H3'	34:A:3896:HOH:O	2.03	0.58
1:A:1352:U:P	34:A:3896:HOH:O	2.60	0.58
25:3:10:LYS:NZ	25:3:15:TYR:OH	2.37	0.58
1:A:662:G:OP1	34:A:4527:HOH:O	2.17	0.58
1:A:2892:A:H2'	1:A:2893:G:H5'	1.84	0.58
2:B:14:U:O3'	2:B:108:U:O2'	2.20	0.58
1:A:1429:G:H2'	1:A:1430:C:H6	1.67	0.58
1:A:2002:G:OP2	13:R:9:LYS:NZ	2.37	0.58
1:A:1899:G:N3	1:A:1899:G:H2'	2.18	0.58
19:X:32:PRO:HA	19:X:77:LYS:HB2	1.84	0.58
1:A:2593:U:H2'	1:A:2594:C:C6	2.39	0.58
1:A:883:G:H1	1:A:893:C:N4	2.02	0.57
1:A:885:C:N3	1:A:886:C:H1'	2.19	0.57
1:A:1689:A:N6	1:A:1698:A:H2	1.93	0.57
2:B:52:A:O2'	2:B:53:A:H5''	2.03	0.57
1:A:83:G:N2	1:A:102:G:H2'	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2161:C:H2'	1:A:2162:G:C8	2.38	0.57
2:B:103:G:OP2	34:B:314:HOH:O	2.18	0.57
1:A:2377:A:H2'	1:A:2378:A:C8	2.39	0.57
1:A:2294:C:P	14:S:89:ARG:HH22	2.27	0.57
1:A:647:G:N7	34:A:5352:HOH:O	2.32	0.57
1:A:2318:G:N2	14:S:3:ARG:HH11	2.02	0.57
1:A:769:G:O6	34:A:4247:HOH:O	2.13	0.57
1:A:1014:U:H2'	1:A:1015:G:H8	1.69	0.57
1:A:2184:G:H2'	1:A:2185:C:O4'	2.03	0.57
12:Q:122:GLY:HA2	12:Q:125:LEU:HD12	1.86	0.57
1:A:2853:C:H2'	1:A:2854:G:H8	1.69	0.57
21:Z:125:LEU:HG	21:Z:164:ALA:HB3	1.87	0.57
17:V:56:SER:H	17:V:100:ARG:HB2	1.67	0.57
1:A:2275:C:H5'	1:A:2275:C:H6	1.69	0.57
1:A:2299:G:O6	34:A:4992:HOH:O	2.14	0.57
1:A:1833:U:H2'	1:A:1834:U:C6	2.39	0.57
15:T:26:ASP:OD2	15:T:91:ARG:NH1	2.38	0.57
1:A:1669:A:H5''	1:A:2550:G:OP1	2.04	0.57
1:A:543:C:H3'	1:A:545:G:O4'	2.05	0.57
1:A:530:G:N3	1:A:530:G:O4'	2.32	0.57
1:A:1495:A:H2'	1:A:1496:A:C8	2.39	0.57
1:A:2335:A:N7	1:A:2337:G:C5	2.72	0.57
1:A:1045:A:H4'	1:A:1047:G:C4	2.40	0.57
1:A:1014:U:H2'	1:A:1015:G:C8	2.40	0.57
1:A:602:G:O2'	1:A:655:A:N6	2.37	0.57
22:O:40:GLN:OE1	22:O:44:ARG:N	2.31	0.57
29:7:23:ARG:HB3	29:7:23:ARG:HH11	1.70	0.57
1:A:2790:A:H3'	1:A:2790:A:N3	2.19	0.57
21:Z:33:LEU:HD23	21:Z:90:VAL:HG21	1.87	0.57
11:P:84:ASN:HB2	11:P:86:LYS:HD3	1.85	0.57
1:A:1174:A:H1'	1:A:1175:U:H5''	1.87	0.57
13:R:11:ASN:ND2	34:R:303:HOH:O	2.38	0.57
1:A:2321:G:N3	1:A:2321:G:H2'	2.20	0.57
2:B:52:A:N6	14:S:33:LYS:HG2	2.20	0.56
1:A:1329:U:H5''	1:A:1330:C:H5	1.69	0.56
21:Z:179:ASP:HB2	21:Z:182:LYS:HD3	1.87	0.56
1:A:2461:C:H2'	1:A:2462:U:C6	2.39	0.56
1:A:558:G:C5	34:A:4932:HOH:O	2.57	0.56
3:D:5:LYS:HA	3:D:17:THR:HG22	1.88	0.56
1:A:1882:C:H5'	1:A:1883:G:OP2	2.06	0.56
1:A:1991:U:H2'	1:A:1992:G:H5''	1.87	0.56
2:B:40:U:H1'	2:B:45:A:H61	1.70	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2322:A:H2'	1:A:2323:G:O4'	2.05	0.56
1:A:71:A:H5'	1:A:71:A:C8	2.40	0.56
1:A:2023:G:H5'	1:A:2617:C:H4'	1.87	0.56
4:E:11:MET:HG2	4:E:24:THR:HB	1.87	0.56
1:A:908:C:OP1	12:Q:22:LYS:HB3	2.06	0.56
5:F:28:ILE:HD13	5:F:119:ARG:HE	1.69	0.56
6:G:72:ARG:HH12	6:G:87:PRO:HG3	1.69	0.56
1:A:1762:A:H8	1:A:1762:A:O5'	1.88	0.56
1:A:2350:C:O2	1:A:2367:G:N2	2.29	0.56
1:A:1935:G:H1'	1:A:1964:G:N2	2.20	0.56
1:A:1963:U:H4'	1:A:1964:G:OP1	2.06	0.56
1:A:690:G:O6	34:A:5163:HOH:O	2.15	0.56
7:H:7:LEU:HD12	7:H:8:PRO:HD2	1.87	0.56
29:7:47:ARG:HH11	29:7:47:ARG:HG3	1.70	0.56
1:A:2615:U:C2	27:5:7:PRO:HA	2.40	0.56
11:P:39:LYS:CB	11:P:45:LEU:HG	2.32	0.56
1:A:1049:C:O2'	1:A:1050:A:O5'	2.22	0.56
1:A:1786:A:H1'	1:A:1938:A:N6	2.19	0.56
13:R:28:LEU:HD12	13:R:48:VAL:HG21	1.87	0.56
4:E:9:VAL:HG22	4:E:25:VAL:HB	1.88	0.56
3:D:175:LEU:HD12	3:D:185:VAL:HG21	1.87	0.56
1:A:1430:C:H2'	1:A:1431:U:C6	2.39	0.56
22:0:53:MET:HG3	22:0:59:LEU:CD2	2.35	0.56
4:E:174:ASP:OD2	4:E:175:VAL:N	2.39	0.56
1:A:185:U:H4'	1:A:218:A:H4'	1.88	0.56
1:A:252:G:OP2	11:P:50:ARG:NH1	2.39	0.56
6:G:133:LEU:HG	6:G:157:ILE:HB	1.86	0.56
13:R:50:HIS:CE1	13:R:54:LEU:HD21	2.41	0.56
1:A:559:G:H22	16:U:49:HIS:CD2	2.23	0.56
20:Y:86:ARG:HD2	20:Y:100:ALA:HA	1.88	0.56
1:A:1173:G:H1'	1:A:1177:A:H61	1.70	0.56
1:A:1140:C:O3'	9:N:25:ARG:NH1	2.38	0.56
1:A:2199:A:H3'	1:A:2200:C:C6	2.41	0.56
1:A:1494:A:H2'	1:A:1495:A:C8	2.41	0.56
10:O:64:ARG:NH1	10:O:81:ASP:OD2	2.38	0.56
1:A:1510:G:H2'	1:A:1511:C:C6	2.41	0.56
1:A:1488:G:N2	1:A:1502:C:C2	2.73	0.56
1:A:1587:A:H2'	1:A:1588:C:H6	1.68	0.56
1:A:1268:A:H2'	1:A:1269:A:O4'	2.06	0.56
18:W:80:PRO:O	18:W:100:THR:HB	2.06	0.56
3:D:118:VAL:N	3:D:129:ASN:ND2	2.53	0.56
1:A:546:C:H6	1:A:547:A:H5'	1.70	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:8:U:O3'	14:S:25:ARG:NH2	2.39	0.56
1:A:2298:A:N6	1:A:2318:G:H8	2.02	0.55
1:A:2591:C:OP2	3:D:239:ARG:HB3	2.06	0.55
1:A:2690:C:OP2	13:R:14:S:SER:HB3	2.06	0.55
1:A:1357:U:OP2	34:A:4673:HOH:O	2.18	0.55
2:B:20:C:C2'	2:B:21:G:H5'	2.36	0.55
1:A:1050:A:C4	1:A:1051:G:C8	2.95	0.55
6:G:86:MET:O	6:G:88:ILE:HG13	2.06	0.55
15:T:106:S:SER:O	15:T:110:ILE:HG12	2.06	0.55
13:R:117:VAL:HG12	13:R:118:GLU:H	1.71	0.55
20:Y:15:VAL:HG21	20:Y:42:VAL:HG11	1.89	0.55
1:A:2562:U:H1'	10:O:23:ARG:HD3	1.87	0.55
11:P:50:ARG:HD3	30:8:7:HIS:CD2	2.41	0.55
1:A:2096:U:H3	1:A:2193:G:H1	1.54	0.55
23:1:94:LEU:O	23:1:97:LEU:HB2	2.06	0.55
15:T:20:PRO:HG2	15:T:86:ILE:O	2.05	0.55
1:A:652(S):C:H2'	1:A:652(T):C:O4'	2.06	0.55
1:A:1018:C:O2'	1:A:1019:U:H5'	2.07	0.55
1:A:1509(A):A:H3'	1:A:1509(B):A:H8	1.71	0.55
1:A:511:U:C5	1:A:512:G:C5	2.94	0.55
1:A:536:A:H2'	1:A:537:C:C6	2.40	0.55
1:A:674:G:C1'	5:F:74:ARG:HD3	2.37	0.55
1:A:1889:A:H2'	1:A:1890:A:C8	2.41	0.55
1:A:1419:A:O2'	1:A:1421:G:N7	2.32	0.55
1:A:443:A:N7	5:F:45:ARG:HG2	2.21	0.55
1:A:2732:G:H3'	1:A:2733:A:O4'	2.07	0.55
8:I:74:ASN:HD22	8:I:75:LEU:HD13	1.70	0.55
24:2:50:ILE:C	24:2:52:ASP:H	2.07	0.55
1:A:71:A:H2	19:X:31:HIS:CE1	2.24	0.55
8:I:81:VAL:O	8:I:146:ALA:HA	2.06	0.55
1:A:548:A:N6	17:V:19:LYS:H	2.04	0.55
11:P:38:GLN:O	11:P:40:S:SER:N	2.40	0.55
18:W:18:ARG:NH1	18:W:76:VAL:O	2.39	0.55
1:A:2629:A:O2'	1:A:2630:G:OP2	2.17	0.55
1:A:272:G:N7	1:A:421:U:H2'	2.22	0.55
14:S:49:VAL:HG13	14:S:76:LYS:HD2	1.89	0.55
1:A:885:C:N4	1:A:890:A:C5	2.71	0.55
6:G:60:LEU:HD23	6:G:63:ILE:HD12	1.89	0.55
1:A:1406:U:H2'	1:A:1407:C:C6	2.42	0.55
1:A:1858:G:H1'	1:A:1884:A:N6	2.22	0.55
1:A:1279:G:H4'	13:R:31:HIS:CD2	2.42	0.55
4:E:52:LEU:HB3	4:E:76:ARG:HG2	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2753:A:N3	31:9:15:LYS:NZ	2.54	0.55
3:D:274:ARG:HA	3:D:275:LYS:HB3	1.88	0.55
8:I:21:VAL:HG23	8:I:22:LYS:O	2.07	0.54
1:A:530:G:N1	34:A:4461:HOH:O	2.16	0.54
26:4:18:CYS:SG	26:4:39:CYS:HB3	2.47	0.54
1:A:2577:A:OP1	34:A:4585:HOH:O	2.18	0.54
1:A:275:G:C2'	1:A:276:A:H5'	2.37	0.54
1:A:2110:G:OP2	1:A:2110:G:H8	1.89	0.54
23:1:23:LYS:HB3	23:1:29:GLY:HA3	1.89	0.54
5:F:46:ARG:HG2	5:F:46:ARG:HH11	1.72	0.54
9:N:15:LEU:HD12	9:N:137:LYS:HG2	1.90	0.54
12:Q:43:THR:N	12:Q:46:GLN:OE1	2.40	0.54
1:A:2319:G:C2	14:S:3:ARG:HA	2.42	0.54
4:E:32:PRO:HA	4:E:90:THR:HG22	1.89	0.54
22:0:55:ARG:CZ	22:0:55:ARG:HB3	2.37	0.54
16:U:58:ARG:HA	16:U:61:TRP:CE3	2.43	0.54
1:A:2880:C:O3'	13:R:90:ARG:NH1	2.40	0.54
1:A:271(M):G:O2'	1:A:271(N):U:OP1	2.16	0.54
15:T:51:ARG:HG3	15:T:98:LYS:HE3	1.89	0.54
14:S:67:ARG:HG2	14:S:71:ARG:NH2	2.23	0.54
1:A:2307:G:H5'	1:A:2308:G:N2	2.21	0.54
1:A:2492:U:H2'	1:A:2493:U:H6	1.73	0.54
1:A:630:G:N2	1:A:633:A:OP2	2.38	0.54
6:G:116:ASP:H	6:G:136:ARG:HH22	1.54	0.54
1:A:1019:U:O2'	1:A:1021:A:H2	1.91	0.54
1:A:1833:U:O2'	1:A:1969:A:N1	2.29	0.54
1:A:2463:C:C2'	1:A:2464:C:H5'	2.37	0.54
8:I:92:VAL:HG13	8:I:120:ILE:HB	1.90	0.54
1:A:1912:A:O2'	1:A:1913:A:OP2	2.25	0.54
1:A:493:G:O6	34:A:4846:HOH:O	2.18	0.54
24:2:51:ARG:O	24:2:55:ARG:HB2	2.06	0.54
4:E:112:GLY:O	4:E:159:HIS:HA	2.08	0.54
13:R:103:ARG:HH12	13:R:110:PRO:HD3	1.72	0.54
1:A:1534:U:H3'	1:A:1535:A:N1	2.23	0.54
5:F:126:VAL:HG21	5:F:129:PHE:CE1	2.43	0.54
1:A:141:A:H8	1:A:1408:C:HO2'	1.48	0.54
1:A:1693:U:O2'	3:D:14:ARG:NH2	2.40	0.54
25:3:7:LYS:HG3	25:3:34:GLU:HG2	1.90	0.54
20:Y:92:ASN:N	20:Y:93:GLY:HA2	2.22	0.54
1:A:1774:C:H6	1:A:1774:C:O5'	1.91	0.54
21:Z:52:SER:OG	21:Z:53:ILE:N	2.41	0.54
1:A:1485:G:H1	1:A:1504:C:H42	1.56	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:T:109:GLU:O	15:T:113:LYS:N	2.36	0.54
1:A:1173:G:O2'	1:A:1174:A:O5'	2.26	0.54
1:A:975(A):G:H1'	1:A:990:A:C2	2.43	0.54
1:A:1050:A:H2'	1:A:1051:G:H8	1.72	0.54
1:A:1586:A:O5'	1:A:1586:A:H8	1.90	0.54
5:F:64:ILE:HD12	5:F:65:TRP:CE3	2.42	0.54
6:G:44:GLY:HA2	6:G:88:ILE:HG22	1.90	0.54
26:4:36:CYS:N	26:4:39:CYS:SG	2.76	0.54
5:F:11:VAL:O	5:F:17:ARG:HA	2.08	0.54
1:A:1815:A:OP2	3:D:54:ARG:NH2	2.41	0.54
1:A:322:A:OP1	5:F:168:ARG:NH1	2.41	0.54
1:A:1364:G:C8	23:1:3:LYS:HD3	2.43	0.53
14:S:10:ARG:NH2	14:S:91:PRO:HB2	2.23	0.53
1:A:1427:A:H4'	1:A:1428:C:O5'	2.06	0.53
1:A:1812:A:O2'	3:D:45:ASN:N	2.40	0.53
1:A:2513:G:N2	4:E:143:ASN:HD21	2.06	0.53
9:N:56:ASN:H	9:N:125:GLY:HA3	1.73	0.53
1:A:1948:G:O6	34:A:4978:HOH:O	2.18	0.53
1:A:603:A:H4'	1:A:604:G:H5'	1.90	0.53
1:A:445:C:OP1	16:U:2:PRO:HA	2.08	0.53
12:Q:27:VAL:HG11	12:Q:134:ARG:HG2	1.89	0.53
1:A:271(E):U:H3	1:A:271(S):G:H1	1.57	0.53
4:E:201:THR:OG1	4:E:202:LYS:N	2.41	0.53
5:F:68:LYS:HB3	5:F:69:HIS:ND1	2.23	0.53
1:A:2884:U:O2	27:5:53:ALA:HB2	2.08	0.53
1:A:2296:U:N3	1:A:2333:A:N3	2.56	0.53
1:A:459:U:H4'	29:7:40:TRP:CZ3	2.44	0.53
1:A:994:C:OP2	16:U:54:LYS:NZ	2.34	0.53
26:4:40:HIS:CE1	26:4:42:PHE:HB2	2.44	0.53
3:D:101:GLU:OE1	3:D:103:ARG:NH1	2.40	0.53
6:G:145:THR:OG1	6:G:146:TYR:N	2.40	0.53
1:A:1914:C:OP2	1:A:1914:C:H6	1.91	0.53
5:F:116:ASP:OD1	5:F:119:ARG:NH2	2.42	0.53
1:A:1040:C:H2'	1:A:1041:C:C1'	2.39	0.53
8:I:98:ALA:O	8:I:101:LEU:N	2.38	0.53
1:A:2320:A:N3	1:A:2320:A:H2'	2.23	0.53
2:B:87:G:N2	2:B:90:A:OP2	2.36	0.53
8:I:110:ASP:N	8:I:130:TYR:OH	2.35	0.53
1:A:528:A:N1	1:A:2042:A:H2'	2.23	0.53
7:H:124:GLU:HB2	7:H:132:ARG:HB3	1.90	0.53
1:A:2104:G:O6	1:A:2185:C:N3	2.41	0.53
6:G:19:LEU:HD22	6:G:23:PHE:HE1	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:130:ALA:HB2	3:D:192:THR:HB	1.90	0.53
1:A:2849:U:H4'	1:A:2868:A:C2	2.43	0.53
23:1:82:LEU:O	23:1:83:GLU:HG3	2.08	0.53
1:A:303:U:O4	34:A:4537:HOH:O	2.19	0.53
13:R:36:THR:HG22	13:R:37:THR:H	1.73	0.53
1:A:1297:C:OP1	1:A:2710:C:H4'	2.08	0.53
16:U:82:GLY:HA3	16:U:113:ALA:HB1	1.90	0.53
1:A:2661:G:H2'	1:A:2662:A:C8	2.44	0.53
1:A:1358:G:OP2	34:A:4674:HOH:O	2.19	0.53
11:P:38:GLN:HA	11:P:41:ARG:HG2	1.91	0.53
1:A:2126:A:H4'	1:A:2127:G:O5'	2.09	0.53
20:Y:9:LYS:NZ	20:Y:28:LYS:O	2.41	0.53
8:I:5:LEU:HD12	8:I:5:LEU:H	1.74	0.53
2:B:15:A:H1'	2:B:110:G:C5	2.44	0.53
1:A:2516:G:O6	1:A:2517:C:N4	2.42	0.53
5:F:164:ARG:HD2	5:F:175:THR:HG23	1.90	0.53
1:A:2865:U:O4	34:A:4099:HOH:O	2.14	0.53
1:A:821:A:H2'	1:A:946:G:H5''	1.90	0.52
1:A:2741:A:H2'	1:A:2742:C:O4'	2.09	0.52
1:A:83:G:N2	1:A:103:A:OP2	2.38	0.52
1:A:1301:A:C8	1:A:1303:G:C8	2.96	0.52
12:Q:24:GLY:O	12:Q:102:VAL:HG23	2.08	0.52
1:A:2250:G:C5	12:Q:83:MET:HB2	2.44	0.52
2:B:40:U:H1'	2:B:45:A:N6	2.25	0.52
1:A:2469:A:H5'	1:A:2470:G:OP2	2.09	0.52
1:A:2564:A:C2	1:A:2647:U:H4'	2.44	0.52
28:6:8:LYS:HD3	30:8:34:TRP:CD2	2.44	0.52
20:Y:23:ARG:HB2	20:Y:23:ARG:NH1	2.25	0.52
1:A:975:C:H6	34:A:4740:HOH:O	1.89	0.52
1:A:1156:A:C8	16:U:51:LYS:HD2	2.44	0.52
6:G:32:PRO:HB2	6:G:172:LEU:HD22	1.91	0.52
1:A:2580:U:O4	34:A:4277:HOH:O	2.14	0.52
21:Z:43:GLU:O	21:Z:47:VAL:HG23	2.09	0.52
1:A:2699:C:H2'	1:A:2700:C:O4'	2.09	0.52
1:A:2572:A:N7	4:E:144:ARG:HD2	2.24	0.52
1:A:2296:U:H4'	1:A:2297:C:OP1	2.09	0.52
1:A:911:A:H2'	12:Q:9:TYR:OH	2.08	0.52
1:A:315:G:H2'	1:A:316:C:C6	2.44	0.52
16:U:76:TYR:OH	16:U:92:ARG:NH1	2.41	0.52
18:W:82:LEU:HD22	18:W:84:ARG:NH2	2.23	0.52
21:Z:152:ALA:HA	21:Z:155:LEU:HD13	1.92	0.52
3:D:206:LEU:HD22	3:D:211:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:511:U:O4	1:A:512:G:N1	2.43	0.52
3:D:131:LEU:HD22	3:D:136:ILE:HG12	1.91	0.52
8:I:125:GLU:OE1	8:I:143:SER:HB3	2.09	0.52
9:N:24:GLY:HA2	9:N:27:ALA:HB3	1.91	0.52
1:A:2850:A:C2	1:A:2851:A:C4	2.97	0.52
1:A:2180:U:H2'	1:A:2181:G:C8	2.45	0.52
14:S:15:ARG:O	14:S:19:LYS:HG2	2.09	0.52
21:Z:160:GLY:HA2	21:Z:161:VAL:HB	1.91	0.52
1:A:1971:A:C4	3:D:241:PRO:HD3	2.44	0.52
1:A:2319:G:N2	14:S:3:ARG:HA	2.25	0.52
2:B:61:G:C6	2:B:62:C:C4	2.98	0.52
1:A:1818:U:O4	3:D:154:LYS:HE3	2.10	0.52
13:R:55:ALA:HB2	13:R:79:LEU:HD13	1.91	0.52
21:Z:40:ASP:OD1	21:Z:42:VAL:HG13	2.09	0.52
1:A:1403:C:C5'	1:A:1471:A:H1'	2.38	0.52
1:A:492:A:H2'	1:A:493:G:O4'	2.10	0.52
1:A:993:G:OP1	16:U:50:ARG:NH2	2.43	0.52
1:A:102:G:O2'	1:A:103:A:O5'	2.27	0.52
1:A:218:A:C2	1:A:235:U:H4'	2.45	0.52
1:A:498:G:O2'	1:A:499:U:H5'	2.10	0.52
25:3:18:ASP:OD1	25:3:18:ASP:N	2.42	0.52
1:A:2672:G:H5''	1:A:2672:G:H8	1.73	0.52
1:A:2117:A:N6	1:A:2171:A:C6	2.78	0.52
21:Z:98:MET:O	21:Z:125:LEU:HD12	2.09	0.52
1:A:878:A:H2'	1:A:879:G:H5'	1.92	0.52
1:A:1335:U:O4	34:A:4435:HOH:O	2.17	0.52
14:S:35:ILE:HG12	14:S:101:LEU:HD12	1.91	0.52
1:A:229:A:H3'	1:A:229:A:C8	2.45	0.52
1:A:582:G:H2'	1:A:583:G:C8	2.44	0.52
1:A:2319:G:H22	14:S:3:ARG:HD2	1.75	0.52
1:A:2364:C:H2'	1:A:2365:G:O4'	2.10	0.52
1:A:2109:U:H1'	1:A:2181:G:N2	2.24	0.52
1:A:335:C:H2'	1:A:336:C:H6	1.75	0.52
25:3:40:THR:HG23	25:3:43:ILE:HD12	1.92	0.52
1:A:1173:G:H1'	1:A:1177:A:N6	2.24	0.51
1:A:2308:G:H4'	1:A:2309:A:OP2	2.10	0.51
14:S:95:HIS:C	14:S:99:LYS:HB3	2.31	0.51
2:B:48:A:H4'	14:S:95:HIS:HD2	1.75	0.51
1:A:2755:C:HO2'	1:A:2756:U:H6	1.58	0.51
6:G:22:ARG:HH21	6:G:175:LEU:HD11	1.74	0.51
8:I:83:ALA:HA	8:I:89:TYR:HE2	1.74	0.51
20:Y:28:LYS:HG3	20:Y:40:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1040:C:H2'	1:A:1041:C:H1'	1.91	0.51
10:O:77:ILE:HG13	15:T:74:ARG:HG2	1.92	0.51
6:G:111:LEU:HB2	6:G:112:PRO:HD3	1.92	0.51
1:A:1530:C:O2'	1:A:1531:C:P	2.68	0.51
14:S:99:LYS:O	14:S:103:GLU:HG3	2.10	0.51
1:A:2200:C:H5'	1:A:2201:C:OP2	2.09	0.51
3:D:130:ALA:C	3:D:131:LEU:HD12	2.31	0.51
10:O:73:ASP:OD1	15:T:32:TYR:OH	2.22	0.51
1:A:1593:G:H2'	1:A:1594:G:C8	2.46	0.51
8:I:4:ILE:HG21	8:I:47:LEU:HG	1.92	0.51
1:A:143(A):C:H2'	1:A:144:C:H6	1.75	0.51
9:N:99:LEU:HD22	9:N:103:VAL:HG23	1.91	0.51
1:A:2097:C:H2'	1:A:2098:U:O4'	2.10	0.51
5:F:34:TRP:HE3	5:F:35:GLU:HG2	1.74	0.51
7:H:24:VAL:HG13	7:H:37:VAL:HG21	1.92	0.51
1:A:1792:G:O2'	1:A:1830:C:OP1	2.28	0.51
1:A:2169:A:H3'	1:A:2170:A:H8	1.75	0.51
1:A:2572:A:N7	4:E:145:LYS:HB2	2.26	0.51
1:A:1782:C:H2'	1:A:2608:G:O2'	2.11	0.51
12:Q:42:ILE:HD13	12:Q:97:VAL:HG21	1.91	0.51
1:A:774:A:H2'	1:A:774:A:N3	2.26	0.51
6:G:41:GLN:HG3	6:G:60:LEU:HD11	1.92	0.51
1:A:271(D):G:H2'	1:A:271(E):U:O4'	2.11	0.51
8:I:16:GLY:O	8:I:47:LEU:HD11	2.10	0.51
30:8:61:LEU:O	30:8:63:PRO:HD3	2.10	0.51
1:A:2872:G:O2'	1:A:2873:A:H5'	2.09	0.51
2:B:2:C:H2'	2:B:3:C:C6	2.45	0.51
15:T:18:ASP:N	15:T:18:ASP:OD1	2.37	0.51
4:E:135:HIS:H	4:E:135:HIS:CD2	2.26	0.51
1:A:2036:C:C6	1:A:2036:C:H5'	2.33	0.51
1:A:26:G:H1'	1:A:515:A:H61	1.76	0.51
6:G:105:LYS:NZ	26:4:26:SER:HB2	2.26	0.51
1:A:2116:G:H4'	1:A:2117:A:OP1	2.11	0.51
7:H:46:GLU:HB2	7:H:49:VAL:HG12	1.93	0.51
2:B:7:G:H5''	2:B:7:G:H8	1.75	0.51
21:Z:69:THR:HG22	21:Z:90:VAL:HA	1.93	0.51
10:O:64:ARG:HG2	10:O:79:PHE:CG	2.46	0.51
7:H:137:ASP:HB3	7:H:140:LYS:HE2	1.93	0.51
1:A:1252:G:C2	1:A:1253:A:C2	2.99	0.51
1:A:1999:C:H5''	1:A:2723:C:O2'	2.11	0.51
1:A:288:C:H2'	1:A:289:A:H8	1.75	0.51
20:Y:102:CYS:O	20:Y:104:GLY:N	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:25:TYR:CD1	8:I:30:LEU:HD11	2.46	0.51
5:F:101:LEU:HB3	5:F:106:ARG:HD3	1.92	0.51
1:A:2134:A:N6	1:A:2157:G:H1'	2.26	0.51
13:R:36:THR:HG22	13:R:37:THR:N	2.25	0.51
28:6:23:THR:OG1	28:6:24:GLU:N	2.44	0.51
1:A:1654:A:OP1	13:R:1:MET:HA	2.11	0.51
1:A:71:A:OP2	1:A:71:A:H3'	2.11	0.51
4:E:7:VAL:HG13	4:E:27:LEU:HB3	1.93	0.51
1:A:187:G:N3	1:A:1365:A:H2	2.09	0.51
1:A:1927:A:H2'	1:A:1928:A:C8	2.46	0.51
1:A:1858:G:H1'	1:A:1884:A:H61	1.76	0.50
5:F:158:THR:O	5:F:164:ARG:NH1	2.44	0.50
2:B:37:C:C5	2:B:38:C:C5	2.98	0.50
1:A:2173:A:OP2	1:A:2174:C:H5	1.93	0.50
9:N:23:LEU:HB2	9:N:60:ILE:HG12	1.92	0.50
1:A:2782:G:N7	34:A:4071:HOH:O	2.35	0.50
16:U:76:TYR:HH	16:U:92:ARG:HH11	1.57	0.50
1:A:543:C:H42	1:A:549:G:H1	1.60	0.50
1:A:141:A:C8	1:A:1408:C:O2'	2.60	0.50
3:D:137:PRO:O	3:D:140:THR:HG23	2.12	0.50
5:F:34:TRP:CE3	5:F:35:GLU:HG2	2.45	0.50
1:A:2839:G:H5'	13:R:46:GLY:HA2	1.92	0.50
1:A:2839:G:C5'	13:R:46:GLY:HA2	2.40	0.50
1:A:748:G:C8	18:W:89:ALA:HB1	2.46	0.50
21:Z:101:PRO:O	21:Z:102:LEU:HD12	2.11	0.50
1:A:314:A:O2'	1:A:315:G:H5'	2.10	0.50
1:A:1977:A:OP2	34:A:4891:HOH:O	2.18	0.50
1:A:796:C:H2'	1:A:797:C:C6	2.46	0.50
1:A:80:G:O6	34:A:4421:HOH:O	2.18	0.50
1:A:769:G:N7	34:A:4252:HOH:O	2.35	0.50
1:A:530:G:C6	1:A:2022:U:H5''	2.46	0.50
2:B:17:C:H2'	2:B:18:G:O4'	2.11	0.50
1:A:2523:G:O6	34:A:5188:HOH:O	2.19	0.50
1:A:2130:U:O2'	1:A:2133:G:O2'	2.11	0.50
1:A:2206:G:HO2'	1:A:2207:G:P	2.34	0.50
1:A:2638:G:P	4:E:82:ARG:HH22	2.34	0.50
1:A:1558:A:N3	1:A:1558:A:O4'	2.45	0.50
26:4:35:VAL:HA	26:4:39:CYS:SG	2.52	0.50
1:A:2286:A:OP1	28:6:29:ASN:ND2	2.44	0.50
1:A:649:G:H2'	1:A:650:C:C6	2.46	0.50
1:A:1177:A:P	1:A:1177:A:H3'	2.51	0.50
12:Q:134:ARG:O	12:Q:138:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:C:H42	1:A:361:G:H1	1.59	0.50
14:S:11:LYS:O	14:S:15:ARG:HG3	2.12	0.50
1:A:1026:U:HO2'	1:A:1027:A:P	2.33	0.50
6:G:98:ARG:NH1	6:G:98:ARG:HB2	2.26	0.50
1:A:1651:G:H2'	1:A:1652:A:O4'	2.12	0.50
1:A:481:G:H1'	1:A:507:A:N1	2.27	0.50
8:I:29:TYR:O	8:I:32:PRO:HD2	2.11	0.50
1:A:2144:U:H2'	1:A:2146:C:N4	2.26	0.50
1:A:1178:C:H2'	1:A:1179:C:C6	2.46	0.50
1:A:1021:A:H3'	1:A:1021:A:C8	2.47	0.50
1:A:485:C:H2'	1:A:486:C:H6	1.76	0.50
1:A:187:G:N7	34:A:4284:HOH:O	2.35	0.50
1:A:95:G:O2'	24:2:46:GLN:HA	2.12	0.50
1:A:576:U:H6	1:A:576:U:O5'	1.95	0.50
7:H:171:LEU:H	7:H:171:LEU:HD23	1.76	0.50
11:P:38:GLN:C	11:P:40:SER:H	2.14	0.50
9:N:132:ALA:HB3	9:N:133:GLN:NE2	2.27	0.50
1:A:1026:U:O2	1:A:1026:U:H5''	2.12	0.50
1:A:1300:U:H4'	1:A:1301:A:C5'	2.41	0.50
1:A:2251:G:C6	1:A:2252:G:C5	3.00	0.50
1:A:860:U:C2	1:A:2268:A:C8	3.00	0.50
1:A:980:A:N3	1:A:2037:G:O2'	2.36	0.50
1:A:286:C:H42	1:A:355:G:H1	1.60	0.50
10:O:35:VAL:HG21	10:O:103:ALA:HB3	1.93	0.50
1:A:413:C:H6	1:A:413:C:O5'	1.95	0.50
1:A:2158:A:H1'	1:A:2159:G:C8	2.47	0.50
14:S:96:GLY:N	14:S:99:LYS:H	2.10	0.50
1:A:2275:C:C6	1:A:2275:C:H5'	2.47	0.50
1:A:534:U:H5'	16:U:42:ALA:HB1	1.93	0.50
1:A:979:G:H3'	1:A:980:A:C5'	2.42	0.50
1:A:1339:G:H5''	19:X:16:LYS:HD3	1.94	0.50
19:X:61:GLY:HA3	19:X:73:ARG:O	2.11	0.50
8:I:123:LEU:HD23	8:I:123:LEU:H	1.76	0.50
1:A:330:A:C2	1:A:1210:A:H2'	2.34	0.49
5:F:22:ALA:HB1	5:F:24:LEU:HD22	1.94	0.49
1:A:1419:A:C8	1:A:1421:G:C6	3.00	0.49
1:A:960:A:C8	1:A:962:G:C8	3.00	0.49
1:A:216:A:C4	1:A:432:A:C2	3.00	0.49
1:A:725:G:C6	1:A:726:G:N1	2.80	0.49
1:A:30:G:H2'	1:A:31:C:C6	2.47	0.49
1:A:1174:A:H5'	1:A:1177:A:N6	2.25	0.49
1:A:2033:A:P	34:A:4582:HOH:O	2.69	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:X:31:HIS:CD2	19:X:33:LYS:H	2.30	0.49
1:A:2165:G:H2'	1:A:2166:G:C8	2.47	0.49
1:A:2782:G:OP2	34:A:4074:HOH:O	2.18	0.49
3:D:108:PRO:HB3	3:D:143:HIS:HE1	1.75	0.49
1:A:2853:C:H2'	1:A:2854:G:C8	2.47	0.49
1:A:2350:C:H2'	1:A:2351:G:O4'	2.12	0.49
18:W:86:LEU:HD22	18:W:96:ILE:HD11	1.94	0.49
10:O:10:VAL:HG13	10:O:17:ARG:O	2.12	0.49
1:A:686:G:OP1	29:7:11:LYS:NZ	2.30	0.49
19:X:50:LYS:HB3	19:X:84:ALA:HB2	1.93	0.49
1:A:1506:C:H2'	1:A:1507:A:H5'	1.94	0.49
1:A:1434:A:H61	1:A:1558:A:H62	1.59	0.49
1:A:2516:G:C6	1:A:2517:C:N4	2.80	0.49
1:A:1028:A:N6	1:A:1125:G:H2'	2.28	0.49
9:N:58:ASP:N	9:N:58:ASP:OD1	2.43	0.49
1:A:2406:U:C2	11:P:72:PRO:HG2	2.48	0.49
1:A:2133:G:C2'	1:A:2158:A:H61	2.26	0.49
1:A:2602:A:H1'	1:A:2603:G:C5'	2.41	0.49
15:T:91:ARG:HH11	15:T:120:ARG:NH1	2.09	0.49
24:2:13:ALA:HA	24:2:16:LEU:HD12	1.93	0.49
1:A:1171:G:OP2	1:A:1171:G:H8	1.96	0.49
1:A:2892:A:H2'	1:A:2893:G:C5'	2.42	0.49
2:B:106:G:H5'	21:Z:31:ARG:HG2	1.94	0.49
6:G:11:TYR:HA	6:G:15:VAL:HB	1.93	0.49
1:A:784:A:C5	3:D:229:VAL:HG21	2.47	0.49
1:A:1840:G:C6	1:A:1841:U:C4	3.01	0.49
2:B:31:C:N4	14:S:32:LEU:HD13	2.28	0.49
1:A:2580:U:C5	1:A:2581:G:C6	3.01	0.49
2:B:43:C:H5''	26:4:1:MET:HG2	1.93	0.49
1:A:1688:U:H1'	1:A:1701:A:C6	2.48	0.49
16:U:59:ARG:O	16:U:63:VAL:HG23	2.12	0.49
1:A:1952:A:C6	1:A:1953:A:N1	2.80	0.49
20:Y:6:HIS:CD2	20:Y:6:HIS:H	2.30	0.49
1:A:2335:A:O2'	1:A:2336:A:OP2	2.28	0.49
1:A:886:C:H2'	1:A:887:A:H5'	1.95	0.49
1:A:885:C:H5'	1:A:886:C:OP2	2.13	0.49
1:A:826:U:C4'	11:P:55:ARG:HB2	2.43	0.49
1:A:2114:A:O2'	1:A:2168:G:H5'	2.12	0.49
1:A:1364:G:OP1	23:1:2:SER:HA	2.13	0.49
1:A:528:A:C2	1:A:2043:C:H4'	2.47	0.49
21:Z:48:PHE:O	21:Z:52:SER:N	2.45	0.49
1:A:2150:U:H2'	1:A:2151:G:H8	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2648:C:H2'	1:A:2649:U:C6	2.47	0.49
1:A:2203:U:O2'	1:A:2205:C:H5'	2.12	0.49
1:A:1533:G:N2	1:A:1536:C:H5	2.00	0.49
23:1:2:SER:HB3	23:1:46:LEU:HD11	1.95	0.49
1:A:1799:G:H5'	1:A:1819:A:H61	1.77	0.49
20:Y:90:LEU:C	20:Y:92:ASN:H	2.15	0.49
2:B:105:A:OP1	21:Z:72:ARG:NH1	2.37	0.49
1:A:96:G:H4'	24:2:48:HIS:CD2	2.48	0.49
4:E:2:LYS:HG3	4:E:200:GLU:HB2	1.95	0.49
18:W:14:PRO:HG2	18:W:78:GLU:HG2	1.94	0.49
11:P:138:LEU:HD23	11:P:145:PRO:HG3	1.94	0.49
20:Y:68:HIS:ND1	20:Y:70:SER:HB3	2.28	0.49
1:A:2322:A:N6	1:A:2335:A:C6	2.72	0.49
1:A:2593:U:H2'	1:A:2594:C:H6	1.76	0.49
1:A:1356:G:C6	1:A:1357:U:C4	3.01	0.49
1:A:1796:U:H2'	1:A:1797:C:H6	1.77	0.49
1:A:2461:C:H2'	1:A:2462:U:H6	1.77	0.49
1:A:2648:C:H2'	1:A:2649:U:H6	1.78	0.49
2:B:96:U:H2'	2:B:97:G:H8	1.78	0.49
1:A:751:A:H5'	18:W:90:ARG:HA	1.95	0.49
1:A:1657:C:H2'	1:A:1658:C:C6	2.48	0.49
9:N:39:ARG:NH2	9:N:41:ASP:OD2	2.44	0.49
1:A:1140:C:OP1	9:N:23:LEU:O	2.30	0.48
1:A:826:U:H4'	11:P:55:ARG:HB2	1.95	0.48
1:A:1866:C:H2'	1:A:1876:A:O4'	2.13	0.48
1:A:226:G:H21	1:A:228:A:N6	2.10	0.48
1:A:1509(B):A:H3'	1:A:1510:G:H8	1.77	0.48
1:A:1419:A:O2'	1:A:1420:U:H5''	2.13	0.48
1:A:1638:C:O2	1:A:2698:U:O2'	2.28	0.48
1:A:1794:U:H2'	1:A:1795:C:H6	1.78	0.48
1:A:1632:A:C6	1:A:1633:G:C6	3.01	0.48
1:A:127:A:H5''	1:A:128:C:C6	2.48	0.48
21:Z:180:VAL:O	21:Z:183:LEU:HB2	2.12	0.48
1:A:2130:U:H2'	1:A:2131:G:N7	2.27	0.48
1:A:784:A:C8	1:A:792:G:C5	3.01	0.48
14:S:96:GLY:N	14:S:99:LYS:HB3	2.28	0.48
1:A:1664:A:OP1	34:A:4761:HOH:O	2.19	0.48
1:A:1047:G:H2'	1:A:1110:G:N1	2.26	0.48
5:F:197:ASP:O	5:F:201:VAL:HG12	2.12	0.48
19:X:9:LEU:HA	24:2:36:ARG:HH21	1.79	0.48
1:A:2205:C:O2	1:A:2220:G:C2	2.66	0.48
2:B:96:U:H2'	2:B:97:G:C8	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:67:LEU:O	7:H:71:LEU:HB2	2.13	0.48
27:5:20:ARG:HG2	27:5:23:HIS:CD2	2.48	0.48
1:A:955:C:OP1	12:Q:87:LYS:HE2	2.13	0.48
4:E:119:ARG:HG2	4:E:160:TYR:HB2	1.94	0.48
1:A:573:G:O2'	1:A:574:C:H3'	2.13	0.48
1:A:729:G:OP2	3:D:13:ARG:NH1	2.45	0.48
6:G:59:GLU:O	6:G:63:ILE:HG13	2.13	0.48
1:A:2318:G:N3	1:A:2318:G:H2'	2.28	0.48
11:P:52:GLU:OE1	11:P:55:ARG:NH1	2.47	0.48
15:T:95:ARG:HG2	15:T:95:ARG:NH1	2.26	0.48
1:A:1366:A:OP1	23:1:3:LYS:NZ	2.46	0.48
28:6:14:THR:HG21	28:6:48:VAL:HG13	1.95	0.48
1:A:83:G:H22	1:A:102:G:H2'	1.77	0.48
20:Y:79:CYS:HB3	20:Y:81:LYS:H	1.77	0.48
1:A:535:C:O3'	16:U:53:ARG:NH1	2.46	0.48
26:4:14:ILE:HG22	26:4:33:VAL:HG23	1.95	0.48
4:E:72:VAL:HA	4:E:73:GLU:OE2	2.13	0.48
1:A:848:G:H2'	1:A:849:A:C8	2.49	0.48
1:A:271(I):G:H2'	1:A:271(J):C:C6	2.48	0.48
1:A:2069:G:OP2	34:A:3844:HOH:O	2.20	0.48
1:A:71:A:H5'	1:A:71:A:H8	1.75	0.48
1:A:2807:G:N1	1:A:2808:U:C2	2.82	0.48
12:Q:63:LYS:HD2	12:Q:65:PHE:CZ	2.49	0.48
11:P:95:VAL:HG22	11:P:125:VAL:HB	1.96	0.48
1:A:828:U:H4'	1:A:831:G:N1	2.28	0.48
8:I:5:LEU:HD12	8:I:17:GLN:O	2.13	0.48
13:R:37:THR:OG1	13:R:40:LYS:HG3	2.13	0.48
1:A:7:G:H2'	1:A:8:A:C8	2.48	0.48
6:G:132:ASN:OD1	6:G:158:ALA:HA	2.13	0.48
18:W:71:VAL:HA	18:W:107:LEU:HD12	1.94	0.48
6:G:104:GLU:O	6:G:108:ASN:ND2	2.47	0.48
4:E:92:THR:O	4:E:95:ILE:HG23	2.12	0.48
1:A:2324:C:H5''	1:A:2325:G:H5'	1.95	0.48
1:A:12:U:H2'	1:A:12:U:O2	2.14	0.48
1:A:2175:C:H2'	1:A:2176:A:O4'	2.14	0.48
1:A:2127:G:N2	1:A:2173:A:H1'	2.28	0.48
3:D:101:GLU:OE1	3:D:103:ARG:HD3	2.14	0.48
1:A:1494:A:H2'	1:A:1495:A:H8	1.78	0.48
29:7:9:ARG:HB3	29:7:46:VAL:HG23	1.96	0.48
24:2:50:ILE:O	24:2:51:ARG:HB3	2.13	0.48
22:0:23:VAL:HG13	22:0:38:VAL:HG23	1.95	0.48
10:O:107:ARG:CZ	15:T:36:GLU:HG3	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:102:SER:HA	8:I:106:GLY:HA3	1.95	0.48
1:A:2751:G:C4	7:H:2:SER:N	2.82	0.48
1:A:2315:G:H2'	1:A:2316:C:C6	2.49	0.48
1:A:171:G:H2'	1:A:172:C:O4'	2.13	0.48
1:A:1113:U:H2'	1:A:1114:G:C8	2.49	0.48
14:S:14:VAL:HG11	14:S:90:GLY:O	2.14	0.48
14:S:62:LYS:HB3	14:S:97:ARG:HD2	1.95	0.48
1:A:2001:A:H2'	1:A:2002:G:C8	2.49	0.48
1:A:646:A:H2'	1:A:647:G:O4'	2.14	0.48
1:A:363(A):A:H2'	1:A:363(B):G:H8	1.78	0.48
1:A:1001:A:H2'	1:A:1002:G:O4'	2.13	0.48
9:N:36:GLY:HA2	9:N:38:HIS:CE1	2.49	0.48
4:E:21:VAL:HG23	4:E:185:LYS:HG3	1.96	0.48
1:A:1359:A:N6	1:A:1372:U:C5	2.82	0.48
1:A:2312:U:O2'	6:G:40:ASN:ND2	2.41	0.48
1:A:2173:A:H2'	1:A:2174:C:H5'	1.96	0.48
18:W:4:LYS:HE2	18:W:6:ILE:HD11	1.96	0.48
1:A:1433:U:O2	1:A:1561:G:C2	2.67	0.48
1:A:1423:G:H2'	1:A:1424:G:C8	2.47	0.48
15:T:123:GLN:O	15:T:126:ALA:HB3	2.14	0.48
11:P:101:VAL:HA	11:P:106:LEU:O	2.13	0.48
1:A:1388:G:H4'	1:A:1525:G:O2'	2.14	0.48
6:G:3:LEU:HD11	6:G:97:ASP:HB3	1.95	0.48
1:A:528:A:O2'	1:A:529:A:H5'	2.14	0.48
1:A:2110:G:O2'	1:A:2120:G:H5'	2.14	0.48
1:A:1925:C:O2'	1:A:1926:U:H5'	2.14	0.48
19:X:24:GLY:O	19:X:83:VAL:HG22	2.14	0.47
28:6:11:LEU:HB3	28:6:49:HIS:HB3	1.96	0.47
1:A:2208:A:H1'	1:A:2219:G:C5	2.49	0.47
1:A:1011:G:OP2	16:U:66:ASN:ND2	2.44	0.47
16:U:109:LEU:HD23	16:U:109:LEU:HA	1.67	0.47
1:A:31:C:N4	34:A:5258:HOH:O	2.46	0.47
12:Q:43:THR:OG1	12:Q:45:GLN:HG2	2.13	0.47
10:O:98:VAL:HG13	10:O:117:LEU:HB3	1.97	0.47
5:F:183:VAL:O	5:F:187:VAL:HG23	2.14	0.47
1:A:863:A:H2'	1:A:864:G:C8	2.49	0.47
9:N:34:LEU:O	9:N:49:GLY:HA3	2.14	0.47
21:Z:108:PRO:HB2	21:Z:111:VAL:HG23	1.96	0.47
1:A:330:A:HO2'	1:A:331:A:H8	1.62	0.47
1:A:2119:A:H2'	1:A:2119:A:OP1	2.15	0.47
1:A:2713:A:H2'	1:A:2713:A:N3	2.30	0.47
1:A:645:C:H2'	1:A:645:C:O2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:229:A:H8	1:A:229:A:H3'	1.77	0.47
1:A:2091:U:O2'	23:1:47:GLN:HG3	2.14	0.47
1:A:789:A:H5''	34:A:4554:HOH:O	2.14	0.47
17:V:52:VAL:CG2	17:V:55:ALA:HB3	2.44	0.47
1:A:1246:A:OP1	5:F:38:ARG:NH1	2.45	0.47
17:V:76:LYS:HB2	17:V:81:TYR:HB3	1.96	0.47
19:X:5:TYR:CZ	24:2:30:ARG:HB2	2.48	0.47
6:G:38:VAL:HG22	6:G:93:THR:HG23	1.95	0.47
11:P:65:ARG:HD3	11:P:66:GLY:N	2.29	0.47
1:A:1320:C:P	34:A:5001:HOH:O	2.67	0.47
28:6:14:THR:HB	28:6:48:VAL:O	2.13	0.47
1:A:1513:C:H2'	1:A:1514:U:H6	1.78	0.47
1:A:2094:G:H5'	8:I:25:TYR:CD2	2.50	0.47
3:D:10:THR:OG1	3:D:13:ARG:HB2	2.15	0.47
12:Q:11:LYS:HE2	12:Q:88:GLY:O	2.15	0.47
1:A:1628:G:H2'	1:A:1629:U:C6	2.49	0.47
1:A:495:G:H21	18:W:61:ASN:HD21	1.61	0.47
1:A:2133:G:H21	1:A:2158:A:H62	1.61	0.47
6:G:5:VAL:HG12	26:4:25:TYR:CE1	2.49	0.47
8:I:130:TYR:HD2	8:I:132:PRO:HD3	1.79	0.47
1:A:528:A:C2	1:A:2042:A:H2'	2.49	0.47
1:A:830:G:H4'	1:A:831:G:OP2	2.15	0.47
23:1:51:VAL:HG11	23:1:74:VAL:HG21	1.95	0.47
1:A:1321:A:H2'	1:A:1322:A:O4'	2.14	0.47
1:A:244:A:C2	1:A:255:A:C4	3.02	0.47
11:P:65:ARG:HB3	34:8:207:HOH:O	2.14	0.47
1:A:2126:A:H1'	1:A:2127:G:OP2	2.14	0.47
1:A:2243:U:H2'	1:A:2244:U:H6	1.79	0.47
1:A:993:G:C6	1:A:994:C:C4	3.03	0.47
28:6:25:LYS:HE3	28:6:30:THR:O	2.15	0.47
1:A:2462:U:H1'	1:A:2491:U:O4	2.15	0.47
1:A:322:A:OP2	5:F:169:ASN:HB2	2.14	0.47
1:A:1545:A:H2'	1:A:1546:C:O4'	2.15	0.47
1:A:1578:U:H2'	1:A:1579:A:H5'	1.96	0.47
1:A:2505:G:H2'	1:A:2576:G:O6	2.13	0.47
9:N:96:GLU:H	9:N:96:GLU:CD	2.18	0.47
1:A:885:C:H3'	1:A:886:C:H6	1.79	0.47
1:A:1358:G:O2'	1:A:1359:A:H5'	2.14	0.47
1:A:975:C:C6	34:A:4740:HOH:O	2.56	0.47
21:Z:126:VAL:HG21	21:Z:161:VAL:HG13	1.95	0.47
2:B:110:G:C2	2:B:111:G:C5	3.02	0.47
6:G:81:LYS:CB	6:G:82:LEU:HD12	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1695:G:H2'	1:A:1696:G:O4'	2.15	0.47
9:N:55:VAL:HG22	9:N:125:GLY:HA3	1.96	0.47
1:A:2469:A:C2	1:A:2482:G:C8	3.03	0.47
1:A:1794:U:H2'	1:A:1795:C:C6	2.49	0.47
1:A:2505:G:O6	1:A:2576:G:H2'	2.14	0.47
3:D:33:LEU:O	3:D:64:ILE:HG13	2.14	0.47
21:Z:151:HIS:HD2	21:Z:168:GLU:O	1.98	0.47
1:A:1810:A:H2'	1:A:1811:G:O4'	2.14	0.47
1:A:652(O):C:H2'	1:A:652(P):G:C8	2.50	0.47
10:O:4:PRO:O	10:O:5:GLN:HB2	2.14	0.47
4:E:10:GLY:HA2	4:E:192:ASN:OD1	2.14	0.47
1:A:2674:G:H2'	1:A:2675:A:C8	2.49	0.47
10:O:70:LYS:HB3	10:O:70:LYS:HE2	1.70	0.47
5:F:117:ARG:HD3	5:F:117:ARG:HA	1.56	0.47
1:A:301:G:C4	1:A:302:C:C5	3.03	0.47
1:A:2516:G:C6	1:A:2517:C:C4	3.02	0.47
21:Z:151:HIS:N	21:Z:154:ASP:OD1	2.46	0.47
17:V:60:GLU:HB2	17:V:97:LYS:HE2	1.96	0.47
1:A:34:C:H5''	1:A:35:G:OP2	2.15	0.47
1:A:1641:A:H2'	1:A:1642:G:O4'	2.14	0.47
1:A:1529:G:O2'	1:A:1530:C:H5'	2.15	0.47
13:R:20:LEU:HD21	13:R:40:LYS:HD3	1.96	0.47
8:I:72:LEU:C	8:I:74:ASN:H	2.17	0.47
1:A:576:U:H2'	1:A:577:G:C8	2.49	0.47
1:A:2536:G:C6	1:A:2537:U:C4	3.03	0.47
30:8:54:GLU:O	30:8:58:ILE:HG12	2.15	0.47
1:A:2176:A:H5'	1:A:2177:C:OP2	2.15	0.47
1:A:819:A:C4	1:A:1189:A:C2	3.03	0.47
1:A:184:C:H2'	1:A:185:U:H6	1.79	0.47
4:E:52:LEU:O	4:E:76:ARG:HG2	2.15	0.47
1:A:1649:G:N1	1:A:2009:G:C6	2.83	0.47
1:A:2008:C:OP2	34:A:4700:HOH:O	2.20	0.47
6:G:37:VAL:HG23	6:G:99:MET:HG3	1.96	0.47
22:O:24:LYS:O	22:O:25:ARG:HD3	2.15	0.47
15:T:93:ARG:HH11	15:T:93:ARG:HG2	1.79	0.47
7:H:154:PRO:HB3	7:H:163:TYR:CE2	2.51	0.46
16:U:76:TYR:CZ	16:U:80:ILE:HG13	2.50	0.46
1:A:879:G:H2'	1:A:880:G:O4'	2.15	0.46
12:Q:26:TYR:CE1	12:Q:28:ALA:HB2	2.50	0.46
1:A:414:C:H2'	1:A:415:A:C8	2.51	0.46
8:I:127:VAL:HA	8:I:140:LEU:O	2.15	0.46
7:H:40:GLU:OE2	7:H:60:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2472:G:H5'	1:A:2473:U:C5'	2.40	0.46
4:E:47:VAL:CG1	4:E:86:PRO:HD2	2.42	0.46
8:I:9:LEU:HB3	8:I:12:LEU:HB2	1.97	0.46
14:S:96:GLY:H	14:S:99:LYS:H	1.64	0.46
8:I:73:GLU:HG2	8:I:139:GLN:O	2.15	0.46
1:A:443:A:H1'	1:A:1201:C:O4'	2.14	0.46
1:A:143(A):C:H2'	1:A:144:C:C6	2.50	0.46
19:X:35:THR:O	19:X:39:ILE:HG13	2.16	0.46
21:Z:138:GLU:HG2	21:Z:156:LYS:NZ	2.30	0.46
1:A:709:U:H2'	1:A:710:G:C8	2.51	0.46
1:A:896:A:N1	12:Q:60:ARG:NH2	2.63	0.46
16:U:36:ARG:HD2	16:U:40:PHE:CZ	2.50	0.46
1:A:207:A:H2'	1:A:208:C:O4'	2.15	0.46
14:S:59:LYS:HE2	14:S:60:GLY:HA2	1.98	0.46
1:A:1450:G:H2'	1:A:1450(A):C:H6	1.80	0.46
1:A:118:A:C8	1:A:119:A:C8	3.03	0.46
11:P:82:GLY:HA2	11:P:113:LYS:O	2.15	0.46
12:Q:2:LEU:HB3	12:Q:70:PRO:HG3	1.97	0.46
1:A:54:G:O6	34:A:3978:HOH:O	2.20	0.46
2:B:46:A:C5	2:B:47:C:C5	3.03	0.46
1:A:944:G:H2'	34:A:4970:HOH:O	2.15	0.46
1:A:27:G:O2'	1:A:28:A:OP2	2.26	0.46
1:A:2319:G:H1'	1:A:2320:A:H5''	1.98	0.46
1:A:1534:U:O2'	1:A:1535:A:P	2.73	0.46
1:A:188:G:H1	1:A:208:C:N4	2.13	0.46
1:A:1505:C:H2'	1:A:1506:C:H6	1.80	0.46
1:A:228:A:H2'	1:A:230:U:O4'	2.15	0.46
1:A:2463:C:O2'	1:A:2464:C:H5'	2.16	0.46
3:D:13:ARG:HD2	3:D:16:MET:HE3	1.96	0.46
1:A:2729:G:H2'	1:A:2730:C:O4'	2.16	0.46
1:A:706:A:H2'	1:A:707:G:O4'	2.16	0.46
1:A:265:A:N6	1:A:427:U:O2'	2.43	0.46
1:A:1907:G:C6	1:A:1908:C:C4	3.04	0.46
21:Z:39:VAL:HG21	21:Z:44:PHE:HB2	1.98	0.46
1:A:2774:C:H2'	1:A:2775:A:O4'	2.15	0.46
1:A:2117:A:N6	1:A:2166:G:H22	2.10	0.46
1:A:1557:C:H5''	1:A:1558:A:OP2	2.16	0.46
1:A:534:U:O2'	16:U:49:HIS:CD2	2.68	0.46
1:A:143:G:H2'	1:A:143(A):C:C6	2.50	0.46
13:R:12:ARG:HG2	13:R:16:HIS:CG	2.50	0.46
7:H:90:LYS:O	7:H:160:LYS:HA	2.16	0.46
1:A:2223:G:H2'	1:A:2224:G:H5'	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:A:HO2'	1:A:279:C:P	2.33	0.46
29:7:9:ARG:HH21	29:7:47:ARG:HD3	1.80	0.46
3:D:112:GLN:HA	3:D:112:GLN:NE2	2.31	0.46
21:Z:24:LEU:HD12	21:Z:24:LEU:C	2.36	0.46
14:S:36:TYR:N	14:S:36:TYR:CD1	2.84	0.46
29:7:8:ASN:OD1	29:7:8:ASN:C	2.53	0.46
1:A:807:U:OP2	11:P:41:ARG:NH2	2.49	0.46
1:A:1142(A):A:C5	1:A:1144:G:C5	3.03	0.46
1:A:2137:C:H42	1:A:2154:G:H1	1.64	0.46
1:A:213:A:H2'	1:A:214:G:O4'	2.15	0.46
1:A:1259:G:H2'	1:A:1260:G:C8	2.51	0.46
1:A:1829:A:P	34:A:5028:HOH:O	2.73	0.46
1:A:1932:A:H2'	1:A:1933:G:O4'	2.16	0.46
2:B:91:C:C2'	2:B:92:C:H5'	2.46	0.46
8:I:133:HIS:HD2	8:I:134:PRO:HD2	1.80	0.46
1:A:2186:G:H2'	1:A:2186:G:N3	2.30	0.46
1:A:2273:A:H2'	1:A:2274:A:C8	2.50	0.46
3:D:172:TYR:CD1	3:D:186:HIS:HA	2.50	0.46
1:A:333:G:H5''	1:A:334:C:OP2	2.14	0.46
1:A:257:A:H2'	1:A:258:G:O4'	2.16	0.46
23:1:86:SER:HB3	23:1:89:GLU:OE2	2.16	0.46
1:A:470:A:OP1	5:F:59:TYR:HE2	1.99	0.46
1:A:859:G:O2'	1:A:916:G:O6	2.28	0.46
9:N:13:TRP:O	9:N:135:PRO:HA	2.16	0.46
1:A:2464:C:O2'	1:A:2465:C:P	2.74	0.46
26:4:22:ILE:HG22	26:4:24:THR:HG23	1.97	0.46
17:V:52:VAL:HG21	17:V:55:ALA:HB3	1.98	0.46
1:A:212:G:O2'	1:A:213:A:H5'	2.16	0.46
1:A:2836:U:H2'	1:A:2837:G:C8	2.51	0.46
27:5:41:PRO:O	27:5:44:THR:OG1	2.34	0.46
1:A:64:A:O3'	19:X:71:GLY:HA3	2.15	0.46
19:X:60:ARG:HE	19:X:60:ARG:HB3	1.43	0.46
1:A:2846:G:H2'	1:A:2847:U:O4'	2.16	0.46
1:A:2193:G:H2'	1:A:2194:G:C8	2.51	0.46
1:A:2233:U:H2'	1:A:2234:G:C8	2.50	0.46
15:T:105:LEU:HB3	15:T:109:GLU:HB2	1.98	0.46
1:A:2850:A:OP2	1:A:2866:U:C5	2.69	0.46
1:A:2836:U:C4	1:A:2883:A:N6	2.84	0.46
1:A:1188:U:H4'	17:V:79:VAL:HG22	1.97	0.46
1:A:2685:G:H2'	1:A:2686:G:H5''	1.97	0.46
1:A:652(Q):G:H2'	1:A:652(R):C:C6	2.51	0.46
14:S:74:ALA:HB2	14:S:105:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2304:G:H21	6:G:156:ASP:CG	2.19	0.45
1:A:2526:G:H5'	1:A:2742:C:O2'	2.16	0.45
1:A:2022:U:O2'	1:A:2617:C:H5'	2.16	0.45
1:A:2850:A:OP2	1:A:2866:U:H5	1.98	0.45
30:8:61:LEU:C	30:8:63:PRO:HD3	2.37	0.45
1:A:1652:A:OP1	13:R:8:ARG:NH1	2.49	0.45
3:D:112:GLN:HB2	3:D:115:GLN:OE1	2.15	0.45
1:A:2282:G:OP1	1:A:2283:C:H1'	2.16	0.45
5:F:39:TRP:O	5:F:43:LYS:HG2	2.15	0.45
1:A:448:U:H1'	5:F:84:VAL:HG11	1.98	0.45
1:A:581:C:OP1	16:U:33:ARG:HG3	2.16	0.45
1:A:2293:C:H2'	1:A:2294:C:C6	2.51	0.45
18:W:79:GLY:HA3	18:W:100:THR:HG22	1.98	0.45
3:D:166:GLN:HB2	3:D:174:ILE:HG22	1.97	0.45
19:X:11:PRO:HD3	24:2:37:PHE:CE2	2.52	0.45
1:A:2190:G:H2'	1:A:2191:G:O4'	2.15	0.45
24:2:9:GLN:HE22	24:2:56:GLN:HG2	1.82	0.45
22:0:51:VAL:N	22:0:62:LEU:HD12	2.31	0.45
1:A:2287:A:C5	1:A:2289:G:C5	3.04	0.45
1:A:2711:A:OP1	1:A:2712(A):A:OP1	2.34	0.45
1:A:2833:G:C3'	1:A:2834:G:H5'	2.44	0.45
1:A:2567:G:H2'	1:A:2568:C:H6	1.81	0.45
1:A:2387:U:OP1	22:0:55:ARG:NH2	2.49	0.45
1:A:1512:U:H2'	1:A:1513:C:C6	2.51	0.45
7:H:37:VAL:HG12	7:H:38:SER:O	2.15	0.45
4:E:195:LEU:HG	4:E:196:VAL:N	2.30	0.45
1:A:909:A:C6	1:A:912:C:C2	3.05	0.45
27:5:36:CYS:O	27:5:37:LYS:HD3	2.16	0.45
3:D:96:HIS:NE2	3:D:102:LYS:HE2	2.31	0.45
1:A:1292:U:H2'	1:A:1293:C:C6	2.51	0.45
1:A:2140:C:H2'	1:A:2141:G:H8	1.80	0.45
1:A:2115:G:H4'	1:A:2167:U:C4'	2.45	0.45
1:A:1328:G:O5'	1:A:1328:G:H8	1.99	0.45
3:D:71:ASP:HB3	3:D:103:ARG:NH2	2.28	0.45
1:A:485:C:H2'	1:A:486:C:C6	2.51	0.45
12:Q:103:MET:CE	12:Q:125:LEU:HD13	2.46	0.45
15:T:120:ARG:HA	15:T:123:GLN:HG2	1.97	0.45
1:A:1903:G:OP1	3:D:241:PRO:HB2	2.16	0.45
9:N:67:LEU:HA	9:N:87:LEU:HD12	1.98	0.45
1:A:2777:G:H5''	1:A:2778:A:H5'	1.98	0.45
6:G:89:GLY:C	6:G:90:LEU:HD23	2.36	0.45
1:A:2054:A:H5''	1:A:2055:C:O5'	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1320:C:O2'	34:A:4938:HOH:O	2.21	0.45
6:G:72:ARG:HD3	6:G:85:GLY:HA2	1.98	0.45
8:I:4:ILE:HD11	8:I:44:LEU:HD12	1.99	0.45
1:A:858:U:O2	1:A:2268:A:H2'	2.17	0.45
21:Z:35:ARG:HA	21:Z:35:ARG:HD2	1.63	0.45
1:A:2154:G:H2'	1:A:2155:G:C8	2.52	0.45
6:G:56:ALA:CA	6:G:153:ARG:HH21	2.29	0.45
1:A:2309:A:N6	1:A:2310:A:N1	2.65	0.45
1:A:1418:G:OP1	1:A:1588:C:O2'	2.31	0.45
5:F:123:LEU:HD11	5:F:194:MET:HE2	1.97	0.45
11:P:59:LEU:HD11	30:8:10:ALA:CB	2.46	0.45
2:B:111:G:H2'	2:B:112:U:H6	1.81	0.45
1:A:2870:C:H2'	1:A:2871:C:O4'	2.16	0.45
1:A:2854:G:H2'	1:A:2855:C:C6	2.51	0.45
7:H:7:LEU:HD12	7:H:8:PRO:CD	2.47	0.45
1:A:2464:C:O2'	1:A:2465:C:OP2	2.30	0.45
11:P:101:VAL:HG23	11:P:106:LEU:HB3	1.97	0.45
12:Q:37:LEU:HD21	12:Q:130:LYS:HB2	1.98	0.45
1:A:2064:C:H2'	1:A:2065:C:C6	2.51	0.45
27:5:45:VAL:HA	27:5:52:TYR:HB2	1.98	0.45
2:B:89:G:H8	2:B:89:G:OP2	2.00	0.45
1:A:26:G:C6	1:A:27:G:N1	2.85	0.45
1:A:1540:U:H2'	1:A:1541:G:O4'	2.16	0.45
2:B:20:C:H2'	2:B:21:G:H5'	1.97	0.45
1:A:1287:A:C6	1:A:1288:U:C4	3.05	0.45
1:A:570:G:H2'	1:A:2030:A:C5	2.52	0.45
1:A:323:G:H1'	1:A:1205:U:O2	2.17	0.45
16:U:43:GLY:HA3	17:V:73:SER:OG	2.15	0.45
1:A:247:G:H4'	1:A:386:G:C5	2.52	0.45
1:A:2056:G:C2	1:A:2057:A:C8	3.05	0.45
16:U:5:LYS:HB2	16:U:5:LYS:HE3	1.74	0.45
5:F:188:ARG:HG3	5:F:188:ARG:H	1.48	0.45
1:A:2742:C:OP1	31:9:35:ARG:HD3	2.17	0.45
1:A:1287:A:C5	1:A:1288:U:C4	3.05	0.45
4:E:111:ARG:HD3	4:E:160:TYR:CD1	2.52	0.45
12:Q:60:ARG:NH1	21:Z:177:PRO:HG3	2.31	0.45
31:9:11:CYS:HB3	31:9:32:HIS:CE1	2.52	0.45
1:A:363(D):G:O2'	1:A:363(E):U:H5'	2.16	0.45
1:A:272(E):G:C2	1:A:364:C:N3	2.85	0.45
16:U:17:ILE:HD13	16:U:17:ILE:HA	1.81	0.45
1:A:29:U:H2'	1:A:30:G:H8	1.77	0.45
1:A:30:G:H2'	1:A:31:C:H6	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:307:G:H21	1:A:330:A:H62	1.65	0.45
1:A:2130:U:OP2	1:A:2132:U:H5	2.00	0.45
1:A:1046:A:O2'	1:A:1047:G:OP2	2.34	0.45
1:A:1164:G:H2'	1:A:1165:U:C6	2.52	0.45
15:T:19:LEU:HA	15:T:20:PRO:HD3	1.81	0.45
1:A:1814:G:H2'	1:A:1815:A:C8	2.52	0.45
1:A:2607:G:H2'	1:A:2608:G:O4'	2.17	0.45
1:A:2252:G:H2'	1:A:2253:G:O4'	2.17	0.45
2:B:104:U:O3'	21:Z:72:ARG:NH1	2.50	0.45
1:A:1025:G:C4	1:A:1135:C:H1'	2.52	0.45
25:3:44:ARG:O	25:3:48:GLU:HG3	2.17	0.45
10:O:87:ILE:HG22	10:O:93:PRO:HA	1.98	0.45
12:Q:109:VAL:HG22	12:Q:113:GLN:OE1	2.17	0.45
1:A:396:G:O3'	23:1:44:PRO:HA	2.16	0.45
11:P:147:LEU:HA	11:P:147:LEU:HD22	1.83	0.45
1:A:1328:G:H2'	1:A:1330:C:C5	2.52	0.45
23:1:3:LYS:HB2	23:1:61:ARG:NH1	2.32	0.45
28:6:4:GLU:HG3	28:6:5:VAL:N	2.31	0.45
11:P:64:LYS:HA	30:8:13:ARG:HB3	1.98	0.45
21:Z:182:LYS:O	21:Z:186:GLU:HG2	2.16	0.45
20:Y:85:VAL:HG23	20:Y:86:ARG:O	2.17	0.45
12:Q:2:LEU:HB3	12:Q:70:PRO:CG	2.47	0.45
9:N:128:HIS:H	9:N:128:HIS:CD2	2.34	0.45
21:Z:94:GLU:HB2	21:Z:95:PRO:HD2	1.99	0.45
1:A:455:C:N3	1:A:472:A:H2'	2.32	0.45
4:E:178:GLU:CD	4:E:178:GLU:H	2.21	0.45
16:U:74:LEU:H	16:U:74:LEU:HD12	1.82	0.45
30:8:23:VAL:HG12	30:8:47:LYS:HB3	1.99	0.44
1:A:1319:G:C2	1:A:1334:G:C5	3.04	0.44
16:U:83:LEU:HD12	16:U:113:ALA:HB2	1.99	0.44
1:A:979:G:H3'	1:A:980:A:H5''	1.98	0.44
27:5:36:CYS:HB3	27:5:49:CYS:HB3	1.99	0.44
1:A:195:A:H4'	1:A:251:A:O2'	2.17	0.44
21:Z:100:VAL:HG11	21:Z:134:PRO:HG2	2.00	0.44
1:A:2318:G:O2'	1:A:2319:G:H5''	2.17	0.44
1:A:1845:G:C2'	1:A:1846:G:H5'	2.47	0.44
1:A:996:A:C2	1:A:997:G:C8	3.05	0.44
1:A:997:G:OP1	16:U:92:ARG:HG2	2.18	0.44
1:A:2378:A:H4'	14:S:23:ARG:HH11	1.82	0.44
1:A:1300:U:H4'	1:A:1301:A:H5'	1.99	0.44
6:G:111:LEU:HA	6:G:114:ILE:HG13	1.99	0.44
7:H:144:VAL:O	7:H:148:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:84:GLY:C	8:I:86:THR:H	2.21	0.44
1:A:1464:C:H2'	1:A:1465:G:C8	2.52	0.44
2:B:32:C:C2	2:B:51:G:N2	2.85	0.44
2:B:60:C:C2	2:B:61:G:C8	3.06	0.44
1:A:2306:C:N3	1:A:2307:G:O6	2.50	0.44
1:A:271(F):C:H2'	1:A:271(G):C:C6	2.46	0.44
8:I:33:ARG:HB2	8:I:35:LEU:HD12	1.99	0.44
1:A:545:G:OP1	1:A:545:G:H4'	2.17	0.44
1:A:2491:U:O2'	1:A:2570:G:OP1	2.27	0.44
1:A:2208:A:H1'	1:A:2219:G:C4	2.52	0.44
31:9:10:ILE:HD12	31:9:32:HIS:HA	1.99	0.44
16:U:106:PHE:O	16:U:110:VAL:HG23	2.18	0.44
1:A:2391:G:O6	1:A:2425:A:H8	2.00	0.44
6:G:9:ARG:NH1	6:G:13:GLU:OE1	2.46	0.44
1:A:1161:C:O2'	17:V:8:GLY:HA2	2.18	0.44
1:A:1282:U:H2'	1:A:1283:G:O4'	2.17	0.44
1:A:566:U:H5''	11:P:29:LYS:HE3	1.98	0.44
1:A:428:A:H8	1:A:428:A:OP2	2.00	0.44
5:F:101:LEU:HD12	5:F:101:LEU:HA	1.74	0.44
1:A:2319:G:H22	14:S:3:ARG:CD	2.30	0.44
26:4:26:SER:OG	26:4:27:THR:N	2.43	0.44
1:A:1049:C:H1'	1:A:1113:U:H4'	1.99	0.44
2:B:90:A:C5	2:B:91:C:H1'	2.53	0.44
1:A:2306:C:H3'	1:A:2307:G:H8	1.77	0.44
14:S:88:ASP:OD1	14:S:90:GLY:N	2.47	0.44
6:G:178:PHE:HB3	6:G:180:PHE:CE1	2.53	0.44
1:A:504:U:H2'	34:A:4212:HOH:O	2.18	0.44
20:Y:76:CYS:HA	20:Y:77:PRO:HD3	1.87	0.44
15:T:27:THR:HB	15:T:89:VAL:HG23	1.98	0.44
1:A:1949:G:C6	1:A:1950:G:C6	3.06	0.44
1:A:868:U:H2'	1:A:869:G:O4'	2.17	0.44
1:A:2058:A:H5''	1:A:2059:A:OP2	2.17	0.44
12:Q:7:MET:HB2	12:Q:7:MET:HE3	1.66	0.44
1:A:1171:G:HO2'	1:A:1173:G:P	2.30	0.44
1:A:993:G:C6	1:A:994:C:N4	2.85	0.44
3:D:107:ALA:HA	3:D:108:PRO:HD2	1.90	0.44
1:A:1799:G:H5'	1:A:1819:A:N6	2.32	0.44
6:G:39:ILE:HG23	6:G:157:ILE:HD13	2.00	0.44
5:F:168:ARG:HH11	5:F:168:ARG:CB	2.31	0.44
26:4:14:ILE:HD11	26:4:24:THR:OG1	2.16	0.44
1:A:1547:C:H2'	1:A:1548:C:C6	2.53	0.44
1:A:2282:G:H4'	1:A:2389:G:O2'	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:G:C6	29:7:10:ARG:HG3	2.52	0.44
1:A:2496:C:OP1	12:Q:82:ARG:HB3	2.18	0.44
3:D:145:VAL:HG12	3:D:146:GLU:O	2.18	0.44
16:U:39:LEU:HA	16:U:39:LEU:HD23	1.74	0.44
1:A:1530:C:HO2'	1:A:1531:C:P	2.35	0.44
1:A:1488:G:N1	1:A:1489:U:O2	2.50	0.44
1:A:2698:U:H2'	1:A:2699:C:C6	2.52	0.44
1:A:2150:U:H2'	1:A:2151:G:C8	2.53	0.44
1:A:1525:G:H2'	1:A:1526:G:O4'	2.17	0.44
3:D:69:ARG:NH2	3:D:128:GLY:O	2.50	0.44
30:8:62:LEU:HB3	30:8:65:GLU:HG2	1.99	0.44
12:Q:57:HIS:CD2	12:Q:117:ALA:HB2	2.52	0.44
2:B:13:A:N1	2:B:69:G:O2'	2.40	0.44
1:A:272(H):C:H5''	1:A:272(H):C:H6	1.82	0.44
1:A:2031:A:C6	1:A:2498:C:H1'	2.53	0.44
6:G:143:GLU:H	6:G:143:GLU:HG2	1.55	0.44
6:G:59:GLU:O	6:G:63:ILE:N	2.46	0.44
11:P:71:VAL:HG23	11:P:72:PRO:HA	2.00	0.44
1:A:1530:C:H1'	1:A:1531:C:OP1	2.18	0.44
26:4:9:LEU:HD22	26:4:26:SER:HA	2.00	0.44
1:A:2309:A:C6	1:A:2310:A:C2	3.05	0.44
28:6:47:THR:HG22	28:6:48:VAL:N	2.31	0.44
5:F:64:ILE:HG13	5:F:65:TRP:N	2.32	0.44
1:A:2601:C:H3'	1:A:2602:A:C8	2.53	0.44
4:E:9:VAL:HB	15:T:3:ARG:HG2	1.99	0.44
1:A:2032:G:O2'	4:E:145:LYS:NZ	2.50	0.44
1:A:335:C:H2'	1:A:336:C:C6	2.52	0.44
10:O:17:ARG:HD2	10:O:47:ILE:HG23	1.99	0.44
21:Z:72:ARG:HA	21:Z:72:ARG:HD3	1.58	0.44
31:9:32:HIS:O	31:9:34:GLN:HG3	2.18	0.44
1:A:1965:C:H3'	1:A:1966:A:H2'	1.99	0.44
1:A:2478:A:H5'	31:9:31:LYS:HD3	2.00	0.44
1:A:2881:C:H2'	1:A:2882:A:O4'	2.18	0.44
18:W:36:LEU:HA	18:W:36:LEU:HD23	1.71	0.44
21:Z:144:LEU:HD12	21:Z:144:LEU:HA	1.76	0.44
1:A:2336:A:H61	22:0:43:THR:CG2	2.29	0.44
1:A:36:G:O2'	1:A:450:G:H2'	2.18	0.44
11:P:38:GLN:HG3	11:P:45:LEU:HD23	1.99	0.44
1:A:1142(A):A:C4	1:A:1144:G:C8	3.05	0.44
1:A:1790:C:H2'	1:A:1791:A:C5	2.53	0.44
1:A:2169:A:H3'	1:A:2170:A:C8	2.51	0.44
5:F:129:PHE:O	5:F:132:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:P:46:LYS:HE3	11:P:51:PHE:CD1	2.53	0.44
26:4:34:GLU:CD	26:4:35:VAL:H	2.21	0.44
1:A:2463:C:H2'	1:A:2464:C:H5'	2.00	0.44
1:A:141:A:H8	1:A:1408:C:O2'	1.99	0.44
1:A:1040:C:H6	1:A:1040:C:O5'	2.00	0.44
1:A:1952:A:N3	10:O:22:ILE:HD12	2.33	0.44
4:E:111:ARG:HD3	4:E:160:TYR:CE1	2.52	0.44
10:O:117:LEU:HD23	10:O:117:LEU:HA	1.71	0.44
10:O:63:VAL:HG12	10:O:106:LEU:HD11	2.00	0.44
21:Z:150:LEU:O	21:Z:171:ILE:HG13	2.18	0.44
1:A:1039:G:H1'	1:A:1117:G:N2	2.32	0.44
1:A:1910:G:O2'	1:A:1911:U:H5'	2.17	0.44
1:A:1108:U:O2	1:A:1108:U:H2'	2.17	0.44
1:A:63:U:OP2	34:A:4998:HOH:O	2.21	0.44
29:7:43:THR:HA	29:7:44:PRO:HD2	1.74	0.44
1:A:2296:U:C4	1:A:2333:A:H1'	2.53	0.44
1:A:1357:U:H2'	1:A:1358:G:O4'	2.18	0.44
1:A:1185:C:H5''	1:A:1186:G:OP1	2.18	0.44
12:Q:12:GLN:HG2	12:Q:73:PRO:HD2	1.99	0.44
20:Y:40:GLU:O	20:Y:42:VAL:HG23	2.17	0.44
1:A:528:A:O2'	34:A:4469:HOH:O	1.85	0.44
1:A:493:G:H2'	1:A:494:G:O4'	2.17	0.44
1:A:570:G:H2'	1:A:2030:A:N7	2.33	0.44
1:A:102:G:O2'	1:A:103:A:P	2.76	0.44
1:A:2199:A:H5''	1:A:2200:C:OP2	2.18	0.44
1:A:2572:A:C8	4:E:144:ARG:HD2	2.52	0.44
1:A:1648:C:H2'	1:A:1649:G:O5'	2.18	0.44
8:I:47:LEU:HA	8:I:47:LEU:HD23	1.88	0.44
2:B:7:G:C8	2:B:7:G:H5''	2.52	0.44
1:A:973:A:O4'	1:A:1188:U:C6	2.71	0.44
1:A:885:C:C4	1:A:886:C:H1'	2.53	0.43
1:A:102:G:HO2'	1:A:103:A:P	2.40	0.43
1:A:275:G:O2'	1:A:276:A:H5'	2.18	0.43
21:Z:151:HIS:C	21:Z:153:SER:H	2.22	0.43
1:A:1956:U:H2'	1:A:1957:C:H5'	2.01	0.43
30:8:39:LYS:HA	30:8:42:ARG:NH1	2.33	0.43
7:H:13:LYS:HA	7:H:14:GLY:HA2	1.60	0.43
9:N:115:ARG:O	9:N:118:LYS:HB2	2.18	0.43
1:A:1740:G:H2'	1:A:1741:A:H8	1.83	0.43
1:A:2119:A:N6	1:A:2168:G:H1'	2.33	0.43
5:F:64:ILE:HG13	5:F:65:TRP:H	1.83	0.43
1:A:1786:A:OP1	34:A:4745:HOH:O	2.20	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1814:G:H4'	3:D:51:VAL:HG21	2.01	0.43
1:A:62:C:OP1	34:A:4998:HOH:O	2.21	0.43
1:A:296:C:O2'	1:A:297:C:H5'	2.18	0.43
1:A:2789:C:N3	1:A:2894:G:O6	2.51	0.43
1:A:300:A:H3'	20:Y:84:ARG:NH2	2.33	0.43
1:A:1535:A:P	1:A:1535:A:H3'	2.58	0.43
12:Q:71:ASP:O	12:Q:73:PRO:HD3	2.18	0.43
1:A:1050:A:H2'	1:A:1051:G:C8	2.52	0.43
14:S:56:LEU:C	14:S:58:LEU:HD22	2.38	0.43
1:A:1003:G:N2	1:A:1153:C:C2	2.86	0.43
1:A:652(B):A:O2'	1:A:652(C):G:H5'	2.18	0.43
1:A:652(E):G:O6	1:A:652(T):C:N3	2.51	0.43
13:R:103:ARG:NH1	13:R:103:ARG:HG2	2.33	0.43
1:A:1632:A:N6	1:A:1633:G:C6	2.87	0.43
1:A:265:A:H1'	1:A:266:G:O4'	2.19	0.43
27:5:45:VAL:HG11	27:5:58:LEU:HD13	1.99	0.43
1:A:2261:C:O2'	1:A:2262:U:H5'	2.18	0.43
1:A:1518:U:H2'	1:A:1519:G:O4'	2.18	0.43
11:P:77:ARG:HB2	11:P:78:PRO:HD2	2.01	0.43
13:R:72:ASP:O	13:R:76:VAL:HG23	2.18	0.43
1:A:1142(A):A:C4	1:A:1144:G:N7	2.87	0.43
1:A:2306:C:C4	1:A:2307:G:O6	2.72	0.43
1:A:2309:A:C6	1:A:2310:A:N1	2.86	0.43
7:H:70:THR:HA	7:H:73:ALA:CB	2.47	0.43
19:X:54:VAL:HG13	19:X:81:VAL:HG12	2.01	0.43
17:V:76:LYS:HD2	17:V:81:TYR:CD1	2.54	0.43
1:A:503:A:O2'	34:A:4921:HOH:O	2.20	0.43
23:1:52:ARG:HA	23:1:56:GLN:O	2.18	0.43
1:A:2590:A:OP2	3:D:238:GLY:HA2	2.18	0.43
19:X:15:GLU:CD	19:X:15:GLU:H	2.21	0.43
1:A:895:U:H6	1:A:895:U:H5''	1.84	0.43
1:A:885:C:H3'	1:A:886:C:O4'	2.19	0.43
6:G:76:SER:CA	6:G:83:ARG:HA	2.45	0.43
1:A:2165:G:H2'	1:A:2166:G:H8	1.83	0.43
1:A:94:C:O2	1:A:94:C:H2'	2.17	0.43
1:A:769:G:H5'	1:A:1379:A:N6	2.33	0.43
1:A:316:C:N4	34:A:5247:HOH:O	2.50	0.43
1:A:729:G:H2'	1:A:1775:U:H1'	1.99	0.43
11:P:106:LEU:HD23	11:P:106:LEU:HA	1.83	0.43
3:D:33:LEU:HA	3:D:33:LEU:HD23	1.63	0.43
1:A:2125:G:N2	1:A:2126:A:H62	2.17	0.43
1:A:744:G:OP1	4:E:132:HIS:ND1	2.50	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:154:LYS:HG2	3:D:154:LYS:H	1.70	0.43
3:D:155:LEU:HD23	3:D:177:LEU:HD22	1.99	0.43
3:D:5:LYS:HB3	3:D:5:LYS:HE3	1.77	0.43
9:N:67:LEU:HA	9:N:67:LEU:HD22	1.73	0.43
1:A:1954:G:O2'	1:A:1956:U:O4	2.19	0.43
1:A:2290:G:C2	1:A:2343:C:O2	2.72	0.43
1:A:2360:A:H2'	1:A:2361:A:O4'	2.19	0.43
5:F:32:LEU:HD21	5:F:105:VAL:HG13	2.01	0.43
1:A:1655:A:H3'	1:A:1656:C:H6	1.84	0.43
10:O:21:CYS:HB2	10:O:39:ILE:HD12	1.99	0.43
1:A:1842:G:C5	1:A:1843:C:C4	3.06	0.43
1:A:1049:C:H41	1:A:1111:A:H2	1.63	0.43
14:S:10:ARG:O	14:S:14:VAL:HG12	2.18	0.43
1:A:1693:U:O2'	1:A:1695:G:O6	2.29	0.43
1:A:857:C:N4	1:A:858:U:O4	2.52	0.43
10:O:98:VAL:HG22	10:O:118:ALA:HA	2.01	0.43
1:A:1042:G:C6	1:A:1043:C:C4	3.07	0.43
15:T:80:SER:HA	15:T:81:PRO:HD2	1.74	0.43
1:A:1169:G:H1	1:A:1180:C:H42	1.64	0.43
1:A:2356:C:O3'	22:O:20:ARG:HD3	2.18	0.43
6:G:122:PRO:HG3	6:G:180:PHE:HD2	1.84	0.43
8:I:59:ALA:HA	8:I:62:LYS:HB2	2.01	0.43
1:A:527:C:C4	1:A:2779:U:H2'	2.54	0.43
17:V:52:VAL:O	17:V:52:VAL:HG23	2.18	0.43
21:Z:137:ILE:HG23	21:Z:156:LYS:HD2	2.01	0.43
2:B:28:C:OP1	14:S:36:TYR:OH	2.23	0.43
1:A:2801(A):A:H1'	1:A:2895:U:H1'	2.00	0.43
1:A:1341:U:OP2	1:A:1394:U:O2'	2.26	0.43
1:A:219:G:C6	34:A:3956:HOH:O	2.72	0.43
1:A:451:C:H5'	34:A:4566:HOH:O	2.19	0.43
1:A:2028:U:H2'	1:A:2029:G:O4'	2.18	0.43
1:A:757:U:H2'	1:A:758:C:O4'	2.19	0.43
1:A:760:G:H2'	1:A:761:A:O4'	2.19	0.43
26:4:40:HIS:HA	26:4:41:PRO:HD3	1.81	0.43
1:A:557:U:H2'	1:A:558:G:H8	1.84	0.43
1:A:2133:G:H2'	1:A:2158:A:H61	1.83	0.43
7:H:3:ARG:HG3	7:H:3:ARG:NH1	2.34	0.43
4:E:9:VAL:HG13	4:E:25:VAL:O	2.19	0.43
1:A:548:A:H61	17:V:19:LYS:H	1.67	0.43
1:A:223:A:O2'	1:A:420:C:O2	2.35	0.43
6:G:10:LYS:O	6:G:14:GLU:HB3	2.19	0.43
1:A:903:C:H2'	1:A:904:C:C6	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:V:65:GLY:HA3	17:V:91:TYR:CZ	2.54	0.43
3:D:159:ALA:HB1	3:D:198:ASN:O	2.19	0.43
1:A:2296:U:C4	1:A:2333:A:N3	2.87	0.43
1:A:2307:G:H5'	1:A:2308:G:C2	2.53	0.43
1:A:658:C:H2'	1:A:659:C:C6	2.54	0.43
1:A:1586:A:H2'	1:A:1587:A:H5'	2.01	0.43
7:H:69:ARG:HG3	7:H:70:THR:N	2.33	0.43
1:A:1163:G:O2'	1:A:1164:G:H5'	2.18	0.43
21:Z:128:VAL:HG23	21:Z:161:VAL:HG22	2.00	0.43
6:G:124:SER:HB2	6:G:131:TYR:CZ	2.53	0.43
1:A:1425:G:H2'	1:A:1426:G:C8	2.54	0.43
15:T:90:GLN:HG3	15:T:91:ARG:N	2.34	0.43
1:A:1011:G:C4	1:A:1151:G:N2	2.87	0.43
3:D:112:GLN:O	3:D:115:GLN:HG2	2.19	0.43
1:A:1957:C:H2'	1:A:1958:C:C6	2.54	0.43
1:A:272(H):C:H5'	1:A:272(I):U:OP2	2.18	0.43
21:Z:124:ILE:HD11	21:Z:165:VAL:HG11	2.00	0.43
1:A:1804:C:H6	1:A:1804:C:O5'	2.01	0.43
1:A:1804:C:H2'	1:A:1805:U:H6	1.83	0.43
1:A:2793:G:N2	1:A:2804:C:H1'	2.34	0.43
5:F:12:LEU:HA	5:F:12:LEU:HD22	1.73	0.43
31:9:6:SER:O	31:9:6:SER:OG	2.37	0.43
1:A:271(K):U:H6	1:A:271(K):U:H2'	1.60	0.42
3:D:118:VAL:N	3:D:129:ASN:HD22	2.03	0.42
6:G:16:ARG:HB2	6:G:17:PRO:HD3	2.01	0.42
1:A:1047:G:H2'	1:A:1110:G:C2	2.54	0.42
3:D:85:ASP:OD2	3:D:88:ARG:NH1	2.49	0.42
7:H:3:ARG:NH2	7:H:5:GLY:H	2.17	0.42
28:6:30:THR:O	28:6:30:THR:OG1	2.37	0.42
1:A:1205:U:H4'	1:A:1206:G:OP2	2.19	0.42
6:G:146:TYR:O	6:G:149:VAL:HG12	2.19	0.42
1:A:1546:C:H5'	1:A:1547:C:H5'	2.00	0.42
12:Q:70:PRO:HA	12:Q:94:VAL:O	2.19	0.42
24:2:56:GLN:O	24:2:60:LEU:HG	2.19	0.42
1:A:968:G:H2'	1:A:969:U:O4'	2.19	0.42
8:I:40:THR:C	8:I:42:SER:N	2.73	0.42
3:D:223:GLY:HA3	3:D:231:HIS:CE1	2.54	0.42
7:H:54:ARG:HA	7:H:55:PRO:HD2	1.87	0.42
5:F:140:LEU:HA	5:F:140:LEU:HD13	1.61	0.42
4:E:134:ILE:HG13	4:E:134:ILE:H	1.71	0.42
5:F:106:ARG:HG2	5:F:106:ARG:H	1.37	0.42
1:A:302:C:O2'	1:A:303:U:H5'	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:154:LYS:HB2	3:D:155:LEU:HD12	2.01	0.42
1:A:1488:G:H5''	1:A:1489:U:OP2	2.18	0.42
1:A:686:G:N2	1:A:788:A:H61	2.17	0.42
8:I:140:LEU:HD23	8:I:140:LEU:HA	1.82	0.42
1:A:2079:U:O3'	23:I:35:THR:OG1	2.35	0.42
1:A:2302:G:O2'	6:G:126:ASP:O	2.32	0.42
9:N:62:VAL:CG1	9:N:66:LYS:HB2	2.49	0.42
25:3:8:LEU:HD13	25:3:31:LEU:HD23	2.00	0.42
1:A:39:C:H2'	1:A:40:C:H6	1.83	0.42
5:F:88:VAL:HG21	5:F:91:GLY:HA3	2.01	0.42
1:A:673:C:H5''	5:F:81:PRO:HD2	2.01	0.42
4:E:170:LEU:HA	4:E:170:LEU:HD12	1.77	0.42
1:A:1891:G:H8	1:A:1891:G:O5'	2.03	0.42
24:2:61:LEU:HA	24:2:61:LEU:HD23	1.76	0.42
1:A:2298:A:H2'	1:A:2299:G:O4'	2.19	0.42
1:A:2791:C:N4	1:A:2893:G:O4'	2.52	0.42
2:B:9:G:OP1	14:S:25:ARG:NH2	2.52	0.42
4:E:52:LEU:HA	4:E:53:PRO:HD2	1.83	0.42
13:R:103:ARG:HH11	13:R:103:ARG:HG2	1.85	0.42
3:D:136:ILE:HA	3:D:137:PRO:HD3	1.92	0.42
26:4:14:ILE:HG23	26:4:31:ILE:HB	2.01	0.42
9:N:36:GLY:O	9:N:42:TRP:HD1	2.03	0.42
10:O:3:GLN:HB2	10:O:4:PRO:HD2	2.01	0.42
21:Z:24:LEU:HD22	21:Z:41:LEU:HD23	2.01	0.42
1:A:1031:G:H1	1:A:1123:C:H42	1.66	0.42
4:E:40:GLU:H	4:E:40:GLU:CD	2.22	0.42
21:Z:61:LEU:HA	21:Z:61:LEU:HD13	1.72	0.42
1:A:674:G:H1'	5:F:74:ARG:CD	2.48	0.42
1:A:528:A:C2'	1:A:529:A:H5'	2.49	0.42
1:A:1352:U:O2	1:A:1570:A:H2	2.02	0.42
1:A:1434:A:O2'	1:A:1435:G:H5'	2.19	0.42
1:A:2065:C:H2'	1:A:2066:C:C6	2.54	0.42
1:A:340:A:H2'	1:A:341:G:O4'	2.19	0.42
1:A:362:U:O2'	1:A:363:G:H5''	2.19	0.42
1:A:2584:U:H2'	1:A:2585:U:H2'	2.00	0.42
9:N:12:ARG:HD3	9:N:50:ASP:OD2	2.19	0.42
15:T:13:ARG:HG2	15:T:13:ARG:H	1.27	0.42
23:1:82:LEU:CA	23:1:85:LEU:HD23	2.36	0.42
1:A:2070:G:C2	1:A:2442:C:C2	3.08	0.42
1:A:1912:A:HO2'	1:A:1913:A:P	2.43	0.42
1:A:2632:A:O2'	1:A:2811:G:O2'	2.21	0.42
8:I:5:LEU:HD11	8:I:19:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:571:A:H5'	1:A:2030:A:N7	2.35	0.42
5:F:64:ILE:HD11	5:F:75:HIS:HB2	2.02	0.42
6:G:47:LYS:HA	6:G:88:ILE:HG22	2.01	0.42
1:A:322:A:H4'	1:A:323:G:OP2	2.20	0.42
8:I:39:ALA:HB1	8:I:44:LEU:HD11	2.01	0.42
1:A:2065:C:H2'	1:A:2066:C:H6	1.85	0.42
12:Q:110:THR:HG23	12:Q:113:GLN:HB2	2.00	0.42
1:A:1107:G:N7	1:A:1108:U:C5	2.88	0.42
1:A:705:A:C2	1:A:727:A:H1'	2.55	0.42
1:A:1441:G:H2'	1:A:1442:G:C8	2.55	0.42
1:A:824:A:H1'	1:A:2358:G:N7	2.34	0.42
1:A:479:A:H4'	1:A:480:A:OP1	2.20	0.42
25:3:4:LEU:HD23	25:3:4:LEU:HA	1.88	0.42
20:Y:51:VAL:HG12	20:Y:51:VAL:O	2.20	0.42
1:A:1166:C:O2	1:A:1184:G:C2	2.73	0.42
1:A:248:G:H5'	1:A:250:G:N7	2.34	0.42
6:G:110:ALA:HA	6:G:140:ILE:O	2.19	0.42
1:A:2273:A:O2'	1:A:2274:A:H5'	2.18	0.42
1:A:1489:U:H6	1:A:1489:U:H3'	1.83	0.42
1:A:2464:C:O2'	1:A:2465:C:H5''	2.19	0.42
3:D:130:ALA:HA	3:D:192:THR:HA	2.01	0.42
12:Q:39:PRO:HA	12:Q:97:VAL:O	2.19	0.42
1:A:1259:G:O2'	1:A:1260:G:H5'	2.20	0.42
3:D:146:GLU:HB2	3:D:189:CYS:HB3	2.02	0.42
10:O:115:VAL:HG13	10:O:121:VAL:HG21	2.02	0.42
1:A:2821:A:H2'	1:A:2822:G:O4'	2.19	0.42
1:A:764:A:OP1	3:D:208:LYS:HE2	2.19	0.42
1:A:853:G:H1	1:A:924:C:H42	1.67	0.42
1:A:1747(A):G:N7	34:A:5098:HOH:O	2.36	0.42
1:A:1749:A:N6	34:A:5357:HOH:O	2.53	0.42
1:A:586:A:C2	1:A:1254:A:C2	3.08	0.42
2:B:79:C:O5'	2:B:79:C:H6	2.02	0.42
7:H:94:TYR:CD1	7:H:94:TYR:N	2.87	0.42
1:A:928:G:O5'	1:A:928:G:H8	2.03	0.42
1:A:1356:G:C5	1:A:1357:U:C5	3.07	0.42
1:A:2304:G:O6	1:A:2312:U:O4	2.37	0.42
1:A:804:A:H5''	1:A:805:G:OP1	2.20	0.42
1:A:2161:C:C5	1:A:2162:G:N7	2.88	0.42
6:G:138:GLN:HE22	6:G:153:ARG:NH2	2.18	0.42
15:T:64:ARG:HB2	15:T:73:GLU:HG2	2.00	0.42
1:A:1153:C:H2'	1:A:1154:G:O4'	2.19	0.42
7:H:137:ASP:HB3	7:H:140:LYS:CB	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:P:101:VAL:HG12	11:P:102:ARG:N	2.34	0.42
21:Z:27:VAL:HA	21:Z:35:ARG:O	2.19	0.42
1:A:219:G:O6	34:A:3956:HOH:O	2.22	0.42
2:B:75:G:H5''	2:B:76:G:OP2	2.20	0.42
2:B:78:A:C2	2:B:100:A:C4	3.08	0.42
1:A:1717:G:C2	1:A:1718:G:C8	3.08	0.42
1:A:27:G:HO2'	1:A:28:A:P	2.42	0.42
1:A:330:A:H2	1:A:1210:A:C2'	2.24	0.42
2:B:21:G:H2'	2:B:22:U:O4'	2.20	0.42
1:A:2117:A:H61	1:A:2166:G:N2	2.12	0.42
1:A:2741:A:H61	1:A:2763:G:H1'	1.85	0.42
8:I:9:LEU:HD21	8:I:35:LEU:CD2	2.50	0.42
7:H:5:GLY:HA2	7:H:69:ARG:HB3	2.01	0.42
8:I:77:LEU:HA	8:I:77:LEU:HD22	1.78	0.42
1:A:1488:G:C6	1:A:1489:U:N3	2.87	0.42
7:H:38:SER:HB2	7:H:64:LEU:HD22	2.02	0.42
1:A:1011:G:C2	1:A:1151:G:C2	3.07	0.42
1:A:1467:C:C5	1:A:1546:C:H2'	2.54	0.42
7:H:80:SER:OG	7:H:81:GLU:N	2.53	0.42
30:8:8:LYS:HB3	30:8:12:LYS:HE3	2.02	0.42
9:N:18:ALA:O	9:N:19:GLU:HB3	2.18	0.42
1:A:2279:G:O6	22:O:14:ARG:HD2	2.20	0.42
1:A:1376:C:N4	1:A:1377:G:C6	2.88	0.42
1:A:839:U:H2'	1:A:840:C:C6	2.54	0.42
5:F:179:GLU:CD	5:F:179:GLU:H	2.23	0.42
1:A:1324:G:C5	1:A:1328:G:O6	2.73	0.42
1:A:2791:C:H3'	1:A:2791:C:OP2	2.19	0.42
1:A:2782:G:C8	34:A:4071:HOH:O	2.70	0.42
1:A:627:A:H62	11:P:84:ASN:HD21	1.68	0.42
13:R:50:HIS:O	13:R:54:LEU:HD22	2.20	0.42
24:2:50:ILE:O	24:2:52:ASP:N	2.45	0.42
1:A:2838:G:C6	1:A:2839:G:C5	3.08	0.42
1:A:1952:A:C2	10:O:22:ILE:HD12	2.55	0.42
1:A:863:A:H2'	1:A:864:G:H8	1.83	0.42
1:A:2178:C:H2'	1:A:2179:C:O4'	2.19	0.42
1:A:2565:A:H5''	1:A:2566:A:OP2	2.19	0.42
1:A:900:A:H2'	1:A:901:A:H8	1.85	0.42
1:A:1138:G:O2'	9:N:105:GLY:HA3	2.19	0.42
4:E:181:LEU:HA	4:E:181:LEU:HD13	1.74	0.42
1:A:2121:G:O6	1:A:2176:A:N6	2.53	0.42
2:B:91:C:O2'	2:B:92:C:H5'	2.19	0.42
1:A:635:C:O2'	1:A:639:U:OP1	2.33	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:6:9:LEU:CD2	28:6:25:LYS:HB3	2.50	0.42
1:A:1889:A:N1	1:A:2234:G:H1'	2.35	0.42
1:A:19:C:H2'	1:A:20:C:H6	1.84	0.42
8:I:121:LYS:HD3	8:I:121:LYS:HA	1.91	0.42
5:F:7:TYR:N	5:F:22:ALA:HB3	2.30	0.41
1:A:1405:U:H2'	1:A:1406:U:H6	1.80	0.41
1:A:1797:C:C2'	1:A:1798:U:H5'	2.50	0.41
1:A:1814:G:O3'	3:D:54:ARG:NH2	2.53	0.41
1:A:2574:G:O2'	4:E:143:ASN:HB3	2.20	0.41
6:G:19:LEU:HD22	6:G:23:PHE:CE1	2.53	0.41
1:A:907:U:O2'	12:Q:101:ARG:NH2	2.45	0.41
1:A:12:U:O2	1:A:12:U:C2'	2.68	0.41
4:E:14:ILE:HG13	4:E:21:VAL:HG13	2.02	0.41
4:E:4:ILE:HG12	4:E:5:LEU:O	2.20	0.41
1:A:593:G:N2	1:A:665:C:C2	2.87	0.41
28:6:40:CYS:HA	28:6:41:PRO:HD3	1.68	0.41
23:1:32:LYS:HB3	23:1:32:LYS:HE2	1.93	0.41
24:2:35:LEU:HA	24:2:35:LEU:HD23	1.71	0.41
12:Q:34:LEU:HA	12:Q:34:LEU:HD12	1.86	0.41
7:H:87:LEU:HD23	7:H:87:LEU:HA	1.84	0.41
1:A:2193:G:H2'	1:A:2194:G:H8	1.85	0.41
4:E:32:PRO:HD2	4:E:50:GLY:O	2.21	0.41
1:A:857:C:H4'	22:0:23:VAL:HG21	2.02	0.41
18:W:107:LEU:HD12	18:W:107:LEU:HA	1.85	0.41
1:A:1925:C:C2'	1:A:1926:U:H5'	2.49	0.41
2:B:46:A:C5	2:B:47:C:C4	3.08	0.41
1:A:916:G:H5'	1:A:917:A:OP1	2.20	0.41
1:A:236:C:H2'	1:A:237:C:C6	2.54	0.41
1:A:817:C:O2'	1:A:839:U:H5''	2.20	0.41
1:A:1313:U:H3'	1:A:1314:C:H5'	2.02	0.41
5:F:150:GLY:HA2	5:F:172:TRP:CD2	2.55	0.41
1:A:656:G:H2'	1:A:657:U:O4'	2.21	0.41
1:A:666:G:O2'	1:A:667:U:H5'	2.20	0.41
16:U:32:PHE:O	16:U:35:ALA:HB3	2.21	0.41
1:A:2811:G:N2	1:A:2891:G:H1'	2.36	0.41
1:A:1488:G:C2	1:A:1489:U:O2	2.73	0.41
13:R:94:TYR:O	13:R:117:VAL:HG23	2.20	0.41
1:A:141:A:OP2	34:A:3964:HOH:O	2.22	0.41
17:V:91:TYR:C	17:V:91:TYR:CD1	2.94	0.41
1:A:2435:A:H2'	1:A:2436:G:O5'	2.21	0.41
11:P:38:GLN:HA	11:P:41:ARG:CG	2.50	0.41
1:A:2126:A:C2	1:A:2162:G:N3	2.88	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1740:G:H2'	1:A:1741:A:C8	2.55	0.41
1:A:1759:A:H1'	1:A:2711:A:C2	2.55	0.41
1:A:1040:C:H2'	1:A:1041:C:O4'	2.20	0.41
1:A:229:A:OP1	1:A:229:A:C8	2.73	0.41
21:Z:28:MET:HG3	21:Z:35:ARG:HB2	2.02	0.41
1:A:541:C:O2'	1:A:542:C:H5'	2.21	0.41
1:A:1453:U:O2'	1:A:1455:G:N7	2.46	0.41
1:A:1368:G:C2	1:A:1369:G:C8	3.08	0.41
1:A:1742:G:H2'	1:A:1743:C:O4'	2.21	0.41
2:B:33:G:C2	2:B:50:G:C2	3.09	0.41
8:I:61:ARG:HH11	8:I:61:ARG:HA	1.85	0.41
1:A:1536:C:C5	1:A:1537:G:C5	3.09	0.41
5:F:101:LEU:HD12	5:F:102:PRO:HD2	2.02	0.41
1:A:2161:C:H5	1:A:2161:C:OP2	1.97	0.41
1:A:910:A:C6	1:A:911:A:C6	3.09	0.41
12:Q:32:TYR:HE2	12:Q:133:ARG:HE	1.69	0.41
14:S:7:TYR:CE1	14:S:91:PRO:HG3	2.55	0.41
3:D:275:LYS:O	3:D:275:LYS:HG3	2.21	0.41
1:A:962:G:C6	1:A:963:U:C4	3.08	0.41
1:A:1028:A:H61	1:A:1125:G:H2'	1.86	0.41
19:X:11:PRO:HG2	19:X:13:LEU:HD21	2.02	0.41
9:N:28:THR:HG22	9:N:29:LYS:N	2.35	0.41
1:A:2415:G:H2'	1:A:2416:C:C6	2.55	0.41
19:X:21:PHE:CZ	19:X:92:LEU:HD12	2.56	0.41
11:P:6:LEU:HD23	11:P:6:LEU:HA	1.61	0.41
17:V:70:ILE:HA	17:V:70:ILE:HD13	1.78	0.41
17:V:82:ARG:HD2	17:V:82:ARG:N	2.36	0.41
26:4:40:HIS:O	26:4:42:PHE:N	2.49	0.41
1:A:1319:G:C6	1:A:1320:C:N4	2.89	0.41
1:A:1832:C:N4	1:A:1833:U:C4	2.88	0.41
14:S:99:LYS:HE2	14:S:103:GLU:OE2	2.20	0.41
8:I:139:GLN:NE2	8:I:139:GLN:HA	2.31	0.41
3:D:111:LEU:HA	3:D:111:LEU:HD23	1.67	0.41
3:D:148:GLU:CB	3:D:151:LYS:HD2	2.49	0.41
1:A:2516:G:O2'	1:A:2517:C:H5'	2.20	0.41
1:A:2537:U:H2'	1:A:2538:C:C6	2.55	0.41
10:O:106:LEU:HD23	10:O:106:LEU:HA	1.84	0.41
18:W:10:VAL:HG21	18:W:103:ILE:HD12	2.03	0.41
6:G:129:GLY:HA2	6:G:166:ASP:HA	2.02	0.41
1:A:1686:C:C2'	1:A:1687:G:H5'	2.50	0.41
1:A:2051:A:C6	1:A:2614:A:C5	3.08	0.41
28:6:19:ARG:H	28:6:19:ARG:HD2	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:303:U:H2'	1:A:304:G:C8	2.56	0.41
1:A:2114:A:H3'	1:A:2115:G:C8	2.55	0.41
1:A:2117:A:H2'	1:A:2118:U:H3'	2.02	0.41
1:A:269:U:C5	1:A:271(Y):U:C5	3.08	0.41
8:I:77:LEU:HB3	8:I:142:VAL:CG1	2.50	0.41
1:A:2321:G:N3	1:A:2321:G:C2'	2.84	0.41
7:H:137:ASP:HB3	7:H:140:LYS:HB3	2.02	0.41
26:4:1:MET:HB3	26:4:6:HIS:CD2	2.56	0.41
1:A:54:G:O2'	29:7:35:ARG:HD3	2.21	0.41
1:A:2099:U:H3	1:A:2190:G:H1	1.69	0.41
1:A:1106:G:H2'	1:A:1107:G:H21	1.85	0.41
1:A:1453:U:OP1	13:R:77:ARG:NH1	2.53	0.41
2:B:77:U:OP1	21:Z:19:ARG:NH2	2.53	0.41
8:I:94:ALA:HA	8:I:97:ILE:HG13	2.03	0.41
4:E:120:TRP:CD1	4:E:155:LYS:HB3	2.56	0.41
1:A:1936:A:C8	1:A:1940:U:O2	2.74	0.41
1:A:28:A:C5	1:A:29:U:C5	3.09	0.41
1:A:1537:G:O2'	1:A:1538:G:H5'	2.21	0.41
1:A:2172:U:H4'	1:A:2173:A:OP2	2.21	0.41
6:G:5:VAL:HG11	6:G:101:ILE:HG12	2.02	0.41
1:A:1022:G:C6	1:A:1140:C:C4	3.09	0.41
4:E:36:ARG:NH1	4:E:86:PRO:O	2.37	0.41
14:S:27:SER:HA	14:S:88:ASP:HB3	2.02	0.41
1:A:1827:C:OP2	3:D:222:ARG:HD2	2.21	0.41
12:Q:26:TYR:HE1	12:Q:28:ALA:HB2	1.85	0.41
16:U:74:LEU:HD12	16:U:74:LEU:N	2.36	0.41
7:H:12:PRO:O	7:H:14:GLY:HA2	2.20	0.41
1:A:1947:C:N3	1:A:1960:A:C2	2.89	0.41
13:R:38:VAL:HB	13:R:39:PRO:HD3	2.02	0.41
1:A:65:C:O2'	1:A:456:C:O2	2.38	0.41
14:S:78:LEU:HA	14:S:78:LEU:HD13	1.82	0.41
1:A:2335:A:N6	1:A:2337:G:H1'	2.35	0.41
1:A:890:A:H3'	1:A:892:G:C8	2.56	0.41
1:A:330:A:O2'	1:A:331:A:H8	2.04	0.41
1:A:1473:G:H2'	1:A:1474:C:O4'	2.21	0.41
3:D:147:LEU:HD13	3:D:155:LEU:HD11	2.03	0.41
1:A:1224:C:O2'	17:V:85:LYS:HA	2.21	0.41
12:Q:133:ARG:HG2	12:Q:134:ARG:N	2.36	0.41
1:A:606:U:H4'	1:A:658:C:C4'	2.49	0.41
1:A:2887:U:O2'	1:A:2888:C:H5'	2.21	0.41
7:H:5:GLY:HA3	7:H:65:HIS:CD2	2.56	0.41
11:P:59:LEU:HA	11:P:59:LEU:HD23	1.73	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:S:99:LYS:O	14:S:102:ALA:HB3	2.20	0.41
1:A:2869:G:H2'	1:A:2870:C:O4'	2.20	0.41
1:A:2615:U:N1	27:5:7:PRO:HA	2.35	0.41
13:R:103:ARG:HH11	13:R:103:ARG:CG	2.33	0.41
12:Q:101:ARG:HG3	12:Q:102:VAL:N	2.36	0.41
1:A:2872:G:HO2'	1:A:2873:A:H5'	1.85	0.41
6:G:98:ARG:HE	26:4:1:MET:HE3	1.85	0.41
20:Y:6:HIS:H	20:Y:6:HIS:HD2	1.68	0.41
1:A:2202:C:H2'	1:A:2203:U:O4'	2.20	0.41
1:A:2278:A:OP1	12:Q:11:LYS:HD2	2.20	0.41
9:N:128:HIS:O	9:N:131:GLN:NE2	2.40	0.41
14:S:82:ILE:HA	14:S:83:LYS:CB	2.51	0.41
1:A:2695:C:H2'	1:A:2696:U:H6	1.86	0.41
14:S:77:ALA:O	14:S:80:LEU:N	2.48	0.41
1:A:116:C:H2'	1:A:117:G:O4'	2.21	0.41
18:W:64:MET:HE3	18:W:109:GLU:HG3	2.02	0.41
1:A:2108:C:H42	1:A:2181:G:H1	1.69	0.41
1:A:2893:G:N3	1:A:2893:G:H2'	2.36	0.41
6:G:139:LEU:HB3	6:G:144:ILE:HG22	2.03	0.41
6:G:174:GLU:HG2	6:G:180:PHE:CD1	2.56	0.41
21:Z:152:ALA:HA	21:Z:155:LEU:HB2	2.02	0.41
22:O:25:ARG:HD2	22:O:29:GLN:NE2	2.36	0.41
12:Q:72:LYS:HB3	12:Q:94:VAL:HG23	2.03	0.41
1:A:1257:C:O2'	5:F:84:VAL:HG23	2.20	0.41
1:A:2330:G:H2'	1:A:2331:G:O4'	2.21	0.41
1:A:1336:A:H2'	1:A:1337:G:C8	2.56	0.41
4:E:37:ARG:HB2	4:E:46:ALA:N	2.36	0.41
6:G:169:ALA:O	6:G:173:LEU:HG	2.21	0.41
6:G:128:ARG:HE	6:G:128:ARG:HB2	1.55	0.41
5:F:196:LEU:HA	5:F:196:LEU:HD23	1.72	0.41
5:F:112:MET:HB2	5:F:112:MET:HE2	1.91	0.41
17:V:18:LEU:HD23	17:V:18:LEU:HA	1.84	0.41
1:A:883:G:H8	1:A:883:G:O5'	2.04	0.40
1:A:2125:G:N2	1:A:2126:A:N6	2.69	0.40
1:A:2791:C:C4	1:A:2893:G:O4'	2.73	0.40
1:A:652(T):C:H2'	1:A:652(U):G:C8	2.56	0.40
1:A:288:C:H2'	1:A:289:A:C8	2.56	0.40
1:A:2251:G:C6	1:A:2252:G:C6	3.09	0.40
12:Q:59:ARG:HB3	12:Q:60:ARG:H	1.73	0.40
1:A:19:C:H2'	1:A:20:C:C6	2.57	0.40
1:A:224:G:H2'	1:A:225:A:O4'	2.22	0.40
6:G:36:LYS:HE3	6:G:160:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:103:LYS:H	5:F:103:LYS:HG3	1.74	0.40
1:A:2228:G:C5	1:A:2229:C:C4	3.09	0.40
1:A:271(H):G:O2'	1:A:271(I):G:P	2.79	0.40
11:P:127:ALA:C	11:P:148:LEU:HD23	2.40	0.40
2:B:90:A:N7	2:B:91:C:H1'	2.36	0.40
1:A:1817:G:H2'	1:A:1818:U:H5'	2.03	0.40
1:A:2892:A:C2'	1:A:2893:G:H5'	2.51	0.40
1:A:1224:C:H6	1:A:1224:C:O5'	2.04	0.40
1:A:2561:A:H2'	1:A:2562:U:O4'	2.21	0.40
1:A:1450:G:H2'	1:A:1450(A):C:C6	2.56	0.40
1:A:1876:A:H8	1:A:1876:A:OP2	2.04	0.40
1:A:7:G:H2'	1:A:8:A:O4'	2.20	0.40
3:D:180:GLY:HA3	3:D:275:LYS:HG2	2.03	0.40
21:Z:44:PHE:CE2	21:Z:86:VAL:HG11	2.56	0.40
1:A:2349:G:OP1	34:A:3915:HOH:O	2.22	0.40
1:A:2241:A:N7	34:A:4278:HOH:O	2.37	0.40
1:A:1247:A:OP1	5:F:95:ARG:NH2	2.46	0.40
1:A:2342:C:O2'	1:A:2374:C:H5''	2.21	0.40
3:D:67:PHE:HB3	3:D:153:ALA:H	1.86	0.40
1:A:1194:A:N7	34:A:5292:HOH:O	2.37	0.40
7:H:35:VAL:HA	7:H:36:PRO:HD2	1.74	0.40
2:B:24:G:N7	2:B:56:G:H2'	2.36	0.40
1:A:2709:G:N2	34:A:4836:HOH:O	2.54	0.40
1:A:719:C:H6	1:A:719:C:O5'	2.04	0.40
1:A:2296:U:N3	1:A:2333:A:C2	2.89	0.40
1:A:884:C:H2'	1:A:885:C:O4'	2.22	0.40
1:A:2317:C:C2'	1:A:2318:G:H5'	2.39	0.40
1:A:1022:G:C5	1:A:1140:C:C4	3.09	0.40
14:S:32:LEU:HD23	14:S:32:LEU:HA	1.85	0.40
1:A:1996:C:H4'	1:A:1997:G:OP1	2.21	0.40
1:A:530:G:O6	1:A:2023:G:OP1	2.39	0.40
2:B:8:U:H5'	2:B:9:G:OP2	2.21	0.40
24:2:50:ILE:C	24:2:52:ASP:N	2.73	0.40
5:F:34:TRP:NE1	11:P:8:PRO:HD3	2.36	0.40
1:A:704:G:H1'	1:A:726:G:N2	2.37	0.40
19:X:84:ALA:HB3	19:X:87:GLN:CD	2.41	0.40
1:A:2301:C:H2'	1:A:2302:G:H8	1.86	0.40
1:A:1213:A:N3	1:A:1238:G:O2'	2.45	0.40
6:G:20:ILE:O	6:G:24:GLY:N	2.46	0.40
13:R:53:HIS:O	13:R:56:LYS:HB2	2.20	0.40
3:D:183:ARG:HG3	3:D:270:ILE:HG12	2.03	0.40
15:T:99:LEU:HD22	15:T:101:PHE:HE1	1.85	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:76:LEU:HD12	21:Z:76:LEU:HA	1.64	0.40
1:A:1647:G:H3'	1:A:1647:G:P	2.60	0.40
13:R:2:ARG:CZ	13:R:2:ARG:HB3	2.46	0.40
1:A:921:G:H2'	1:A:922:U:C6	2.57	0.40
6:G:97:ASP:O	6:G:101:ILE:HG13	2.22	0.40
1:A:528:A:N1	1:A:2043:C:O5'	2.55	0.40
1:A:563:G:H5'	1:A:572:A:H4'	2.04	0.40
1:A:2628:C:H5''	1:A:2629:A:O5'	2.21	0.40
1:A:2818:G:O2'	1:A:2819:G:H5'	2.21	0.40
1:A:2466:C:C2	1:A:2485:G:C2	3.09	0.40
1:A:1448:G:H5''	1:A:1542:A:OP1	2.21	0.40
1:A:2409:G:C6	1:A:2410:G:C5	3.09	0.40
21:Z:70:LEU:HD23	21:Z:70:LEU:HA	1.93	0.40
1:A:515:A:H1'	1:A:581:C:H1'	2.04	0.40
8:I:37:VAL:HG12	8:I:38:LEU:N	2.36	0.40
1:A:1019:U:H3	1:A:1142(A):A:N6	2.06	0.40
34:A:4323:HOH:O	23:1:18:ILE:N	2.48	0.40
1:A:2791:C:H2'	1:A:2792:G:C8	2.57	0.40
20:Y:14:LEU:HD12	20:Y:23:ARG:O	2.21	0.40
1:A:271(S):G:C6	1:A:271(T):C:C4	3.09	0.40
1:A:314:A:H2'	1:A:315:G:H5'	2.03	0.40
1:A:2762:G:H2'	1:A:2763:G:H5'	2.04	0.40
1:A:1406:U:H2'	1:A:1407:C:H6	1.83	0.40
1:A:1154:G:H8	1:A:1154:G:O5'	2.04	0.40
1:A:646:A:H5'	34:A:5350:HOH:O	2.21	0.40
1:A:2291:U:H2'	1:A:2292:C:C6	2.57	0.40
1:A:1260:G:C6	1:A:1261:C:C4	3.10	0.40
2:B:77:U:H4'	21:Z:84:GLU:OE1	2.22	0.40
4:E:38:THR:O	4:E:42:ASP:N	2.51	0.40
6:G:125:PHE:CE1	6:G:170:ARG:HG2	2.57	0.40
4:E:203:LYS:CB	4:E:204:ALA:HA	2.52	0.40
4:E:97:LYS:HA	4:E:98:PRO:HD3	1.96	0.40
2:B:117:G:H8	2:B:117:G:O5'	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1594:G:OP1	34:B:323:HOH:O[1_455]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	43	84
4	E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	22	68
5	F	201/210 (96%)	195 (97%)	6 (3%)	0	100	100
6	G	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	33	78
7	H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	33	78
8	I	144/148 (97%)	121 (84%)	21 (15%)	2 (1%)	16	58
9	N	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	10	46
10	O	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
11	P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
12	Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	30	76
13	R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	T	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
16	U	114/118 (97%)	114 (100%)	0	0	100	100
17	V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	W	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	25	71
19	X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	22	68
21	Z	199/206 (97%)	183 (92%)	14 (7%)	2 (1%)	22	68
22	0	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
23	1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	65
24	2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	4	44/71 (62%)	36 (82%)	8 (18%)	0	100	100
27	5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	10	46
30	8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	3376/3526 (96%)	3167 (94%)	192 (6%)	17 (0%)	38	81

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	5	VAL
12	Q	135	ASP
8	I	86	THR
9	N	4	TYR
21	Z	192	ALA
23	1	3	LYS
29	7	46	VAL
7	H	170	ARG
9	N	18	ALA
8	I	107	VAL
4	E	52	LEU
4	E	72	VAL
3	D	3	VAL
18	W	80	PRO
20	Y	3	VAL
6	G	87	PRO
21	Z	161	VAL

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	215/218 (99%)	182 (85%)	33 (15%)	4	15
4	E	163/166 (98%)	135 (83%)	28 (17%)	3	11
5	F	159/166 (96%)	135 (85%)	24 (15%)	4	16
6	G	128/156 (82%)	109 (85%)	19 (15%)	4	17
7	H	141/148 (95%)	123 (87%)	18 (13%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	98/124 (79%)	81 (83%)	17 (17%)	3	11
9	N	117/119 (98%)	98 (84%)	19 (16%)	3	13
10	O	98/100 (98%)	82 (84%)	16 (16%)	3	12
11	P	114/116 (98%)	99 (87%)	15 (13%)	6	23
12	Q	111/111 (100%)	96 (86%)	15 (14%)	6	22
13	R	101/101 (100%)	79 (78%)	22 (22%)	1	6
14	S	84/88 (96%)	67 (80%)	17 (20%)	2	8
15	T	110/127 (87%)	98 (89%)	12 (11%)	9	34
16	U	93/94 (99%)	82 (88%)	11 (12%)	8	29
17	V	80/82 (98%)	63 (79%)	17 (21%)	1	7
18	W	89/92 (97%)	81 (91%)	8 (9%)	14	47
19	X	75/78 (96%)	71 (95%)	4 (5%)	32	72
20	Y	80/91 (88%)	64 (80%)	16 (20%)	2	8
21	Z	159/179 (89%)	137 (86%)	22 (14%)	5	21
22	0	59/67 (88%)	51 (86%)	8 (14%)	5	21
23	1	78/83 (94%)	63 (81%)	15 (19%)	2	9
24	2	65/67 (97%)	54 (83%)	11 (17%)	3	11
25	3	49/52 (94%)	44 (90%)	5 (10%)	11	37
26	4	39/63 (62%)	33 (85%)	6 (15%)	4	15
27	5	50/52 (96%)	42 (84%)	8 (16%)	3	13
28	6	50/52 (96%)	39 (78%)	11 (22%)	1	6
29	7	41/42 (98%)	34 (83%)	7 (17%)	3	11
30	8	52/55 (94%)	42 (81%)	10 (19%)	2	9
31	9	32/34 (94%)	28 (88%)	4 (12%)	7	25
All	All	2730/2923 (93%)	2312 (85%)	418 (15%)	4	15

All (418) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	12	SER
3	D	13	ARG
3	D	18	VAL
3	D	24	ILE
3	D	27	THR

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Mol	Chain	Res	Type
3	D	54	ARG
3	D	83	GLU
3	D	94	LEU
3	D	103	ARG
3	D	106	ILE
3	D	111	LEU
3	D	117	VAL
3	D	126	GLN
3	D	141	VAL
3	D	150	LYS
3	D	154	LYS
3	D	157	ARG
3	D	173	VAL
3	D	192	THR
3	D	200	ASP
3	D	211	ARG
3	D	212	SER
3	D	217	ARG
3	D	218	ARG
3	D	221	VAL
3	D	229	VAL
3	D	254	THR
3	D	257	LEU
3	D	259	THR
3	D	260	ARG
3	D	271	ILE
3	D	273	ARG
3	D	274	ARG
4	E	7	VAL
4	E	12	THR
4	E	21	VAL
4	E	24	THR
4	E	33	VAL
4	E	34	VAL
4	E	40	GLU
4	E	47	VAL
4	E	49	LEU
4	E	52	LEU
4	E	61	ARG
4	E	69	LYS
4	E	72	VAL
4	E	75	VAL

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Mol	Chain	Res	Type
4	E	77	ILE
4	E	82	ARG
4	E	92	THR
4	E	111	ARG
4	E	116	VAL
4	E	119	ARG
4	E	128	SER
4	E	144	ARG
4	E	154	LYS
4	E	167	VAL
4	E	170	LEU
4	E	179	GLU
4	E	181	LEU
4	E	195	LEU
5	F	12	LEU
5	F	18	ARG
5	F	20	LEU
5	F	24	LEU
5	F	33	LEU
5	F	38	ARG
5	F	41	LEU
5	F	50	SER
5	F	57	VAL
5	F	69	HIS
5	F	77	ASP
5	F	88	VAL
5	F	106	ARG
5	F	110	LEU
5	F	112	MET
5	F	132	VAL
5	F	137	LYS
5	F	140	LEU
5	F	158	THR
5	F	168	ARG
5	F	170	LEU
5	F	175	THR
5	F	188	ARG
5	F	192	LEU
6	G	3	LEU
6	G	5	VAL
6	G	7	LEU
6	G	21	ARG

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Mol	Chain	Res	Type
6	G	28	VAL
6	G	35	GLU
6	G	47	LYS
6	G	98	ARG
6	G	128	ARG
6	G	136	ARG
6	G	139	LEU
6	G	140	ILE
6	G	143	GLU
6	G	146	TYR
6	G	149	VAL
6	G	155	MET
6	G	161	THR
6	G	170	ARG
6	G	175	LEU
7	H	3	ARG
7	H	6	ARG
7	H	7	LEU
7	H	15	VAL
7	H	24	VAL
7	H	41	MET
7	H	44	VAL
7	H	49	VAL
7	H	51	ARG
7	H	58	GLU
7	H	68	THR
7	H	69	ARG
7	H	98	LEU
7	H	113	VAL
7	H	122	THR
7	H	134	SER
7	H	139	GLN
7	H	169	VAL
8	I	1	MET
8	I	9	LEU
8	I	47	LEU
8	I	51	ILE
8	I	54	GLN
8	I	61	ARG
8	I	68	LEU
8	I	75	LEU
8	I	77	LEU

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Mol	Chain	Res	Type
8	I	78	THR
8	I	81	VAL
8	I	92	VAL
8	I	117	GLU
8	I	123	LEU
8	I	140	LEU
8	I	142	VAL
8	I	144	VAL
9	N	1	MET
9	N	5	VAL
9	N	12	ARG
9	N	28	THR
9	N	33	LEU
9	N	34	LEU
9	N	38	HIS
9	N	46	VAL
9	N	48	MET
9	N	62	VAL
9	N	67	LEU
9	N	68	GLU
9	N	85	ILE
9	N	99	LEU
9	N	112	LEU
9	N	120	LEU
9	N	130	HIS
9	N	133	GLN
9	N	140	VAL
10	O	8	LEU
10	O	10	VAL
10	O	17	ARG
10	O	21	CYS
10	O	24	VAL
10	O	25	LEU
10	O	26	LYS
10	O	29	ASN
10	O	32	TYR
10	O	52	VAL
10	O	53	LYS
10	O	58	VAL
10	O	94	ARG
10	O	98	VAL
10	O	104	ARG

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Mol	Chain	Res	Type
10	O	113	LYS
11	P	21	ARG
11	P	32	THR
11	P	40	SER
11	P	42	SER
11	P	45	LEU
11	P	55	ARG
11	P	59	LEU
11	P	65	ARG
11	P	71	VAL
11	P	83	VAL
11	P	86	LYS
11	P	95	VAL
11	P	106	LEU
11	P	112	LEU
11	P	125	VAL
12	Q	1	MET
12	Q	5	ARG
12	Q	7	MET
12	Q	16	ARG
12	Q	45	GLN
12	Q	55	VAL
12	Q	56	ARG
12	Q	59	ARG
12	Q	63	LYS
12	Q	75	THR
12	Q	81	VAL
12	Q	109	VAL
12	Q	110	THR
12	Q	134	ARG
12	Q	138	ASP
13	R	1	MET
13	R	2	ARG
13	R	6	SER
13	R	15	SER
13	R	18	LEU
13	R	24	GLN
13	R	28	LEU
13	R	29	LEU
13	R	33	ARG
13	R	44	LEU
13	R	54	LEU

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Mol	Chain	Res	Type
13	R	60	LEU
13	R	65	LEU
13	R	67	LEU
13	R	79	LEU
13	R	86	ARG
13	R	100	LEU
13	R	103	ARG
13	R	111	LEU
13	R	113	LEU
13	R	114	VAL
13	R	117	VAL
14	S	3	ARG
14	S	8	GLU
14	S	12	PHE
14	S	13	ARG
14	S	20	ARG
14	S	30	ARG
14	S	36	TYR
14	S	50	SER
14	S	52	SER
14	S	57	LYS
14	S	58	LEU
14	S	69	VAL
14	S	75	GLU
14	S	78	LEU
14	S	84	GLN
14	S	85	VAL
14	S	95	HIS
15	T	13	ARG
15	T	16	ARG
15	T	17	THR
15	T	36	GLU
15	T	39	ARG
15	T	49	VAL
15	T	64	ARG
15	T	74	ARG
15	T	82	LEU
15	T	96	ARG
15	T	107	ASP
15	T	118	ARG
16	U	5	LYS
16	U	8	VAL

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Mol	Chain	Res	Type
16	U	30	LYS
16	U	31	SER
16	U	36	ARG
16	U	59	ARG
16	U	60	LEU
16	U	74	LEU
16	U	85	LYS
16	U	104	GLN
16	U	108	GLU
17	V	7	THR
17	V	12	TYR
17	V	18	LEU
17	V	21	ARG
17	V	28	GLU
17	V	32	THR
17	V	33	VAL
17	V	57	VAL
17	V	61	VAL
17	V	62	LEU
17	V	72	VAL
17	V	73	SER
17	V	79	VAL
17	V	85	LYS
17	V	89	GLN
17	V	95	LEU
17	V	100	ARG
18	W	4	LYS
18	W	11	ARG
18	W	19	LEU
18	W	23	LEU
18	W	27	LYS
18	W	51	LEU
18	W	100	THR
18	W	107	LEU
19	X	15	GLU
19	X	57	LEU
19	X	65	ARG
19	X	76	ARG
20	Y	2	ARG
20	Y	3	VAL
20	Y	6	HIS
20	Y	9	LYS

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Mol	Chain	Res	Type
20	Y	23	ARG
20	Y	45	VAL
20	Y	49	VAL
20	Y	55	TYR
20	Y	72	VAL
20	Y	90	LEU
20	Y	91	GLU
20	Y	92	ASN
20	Y	97	ARG
20	Y	101	LYS
20	Y	102	CYS
20	Y	107	ASP
21	Z	5	LEU
21	Z	10	ARG
21	Z	11	GLU
21	Z	19	ARG
21	Z	24	LEU
21	Z	37	VAL
21	Z	42	VAL
21	Z	52	SER
21	Z	56	VAL
21	Z	66	SER
21	Z	72	ARG
21	Z	76	LEU
21	Z	82	ARG
21	Z	91	LEU
21	Z	97	GLU
21	Z	118	GLN
21	Z	126	VAL
21	Z	155	LEU
21	Z	156	LYS
21	Z	165	VAL
21	Z	179	ASP
21	Z	185	GLU
22	0	9	SER
22	0	10	THR
22	0	20	ARG
22	0	38	VAL
22	0	55	ARG
22	0	74	ARG
22	0	77	ARG
22	0	83	PRO

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Mol	Chain	Res	Type
23	1	4	VAL
23	1	5	CYS
23	1	14	VAL
23	1	21	ARG
23	1	39	LYS
23	1	40	ARG
23	1	46	LEU
23	1	51	VAL
23	1	58	ILE
23	1	59	THR
23	1	76	ARG
23	1	82	LEU
23	1	83	GLU
23	1	86	SER
23	1	95	LEU
24	2	17	SER
24	2	28	LYS
24	2	32	LEU
24	2	34	GLU
24	2	43	GLN
24	2	44	LEU
24	2	47	ASN
24	2	53	LEU
24	2	55	ARG
24	2	68	ARG
24	2	70	GLN
25	3	8	LEU
25	3	18	ASP
25	3	23	LEU
25	3	31	LEU
25	3	40	THR
26	4	14	ILE
26	4	16	CYS
26	4	27	THR
26	4	34	GLU
26	4	43	TYR
26	4	46	GLN
27	5	6	VAL
27	5	8	LYS
27	5	9	LYS
27	5	23	HIS
27	5	29	THR

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Mol	Chain	Res	Type
27	5	37	LYS
27	5	40	LYS
27	5	58	LEU
28	6	4	GLU
28	6	6	ARG
28	6	13	CYS
28	6	14	THR
28	6	23	THR
28	6	28	ARG
28	6	30	THR
28	6	34	LEU
28	6	38	LYS
28	6	40	CYS
28	6	44	ARG
29	7	1	MET
29	7	4	THR
29	7	8	ASN
29	7	9	ARG
29	7	23	ARG
29	7	32	LYS
29	7	47	ARG
30	8	6	THR
30	8	11	LYS
30	8	14	VAL
30	8	23	VAL
30	8	31	HIS
30	8	32	LEU
30	8	34	TRP
30	8	35	GLN
30	8	41	ILE
30	8	49	VAL
31	9	6	SER
31	9	7	VAL
31	9	17	ILE
31	9	26	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	112	GLN
3	D	129	ASN
3	D	143	HIS

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Mol	Chain	Res	Type
4	E	143	ASN
5	F	75	HIS
6	G	40	ASN
6	G	66	GLN
6	G	108	ASN
6	G	138	GLN
7	H	74	ASN
7	H	111	HIS
8	I	74	ASN
8	I	133	HIS
8	I	139	GLN
9	N	128	HIS
9	N	133	GLN
10	O	3	GLN
11	P	84	ASN
12	Q	12	GLN
14	S	68	GLN
16	U	49	HIS
16	U	72	HIS
17	V	80	GLN
18	W	60	ASN
18	W	61	ASN
19	X	31	HIS
24	2	9	GLN
26	4	46	GLN
28	6	20	ASN
28	6	49	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2833/2913 (97%)	609 (21%)	60 (2%)
2	B	119/122 (97%)	25 (21%)	0
All	All	2952/3035 (97%)	634 (21%)	60 (2%)

All (634) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	12	U
1	A	15	G

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Mol	Chain	Res	Type
1	A	34	C
1	A	36	G
1	A	45	C
1	A	55	G
1	A	69	C
1	A	71	A
1	A	72	U
1	A	74	A
1	A	75	G
1	A	82	G
1	A	84	A
1	A	90	U
1	A	94	C
1	A	95	G
1	A	100	G
1	A	102	G
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	131	G
1	A	141	A
1	A	154	G
1	A	154(A)	C
1	A	157	U
1	A	181	A
1	A	182	A
1	A	188	G
1	A	196	A
1	A	199	A
1	A	200	U
1	A	201	C
1	A	204	A
1	A	205	G
1	A	214	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	225	A
1	A	229	A
1	A	233	A

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Mol	Chain	Res	Type
1	A	248	G
1	A	250	G
1	A	266	G
1	A	269	U
1	A	271(I)	G
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	271(N)	U
1	A	271(Y)	U
1	A	272(B)	G
1	A	272(G)	C
1	A	272(H)	C
1	A	272(I)	U
1	A	272(J)	C
1	A	276	A
1	A	277	C
1	A	278	A
1	A	279	C
1	A	280	C
1	A	286	C
1	A	311	A
1	A	315	G
1	A	316	C
1	A	324	A
1	A	329	G
1	A	330	A
1	A	331	A
1	A	332	A
1	A	333	G
1	A	335	C
1	A	342	G
1	A	352	G
1	A	353	G
1	A	363	G
1	A	363(C)	G
1	A	363(F)	A
1	A	386	G
1	A	404	C
1	A	405	U
1	A	407	G
1	A	411	G

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Mol	Chain	Res	Type
1	A	412	A
1	A	428	A
1	A	444	C
1	A	448	U
1	A	457	A
1	A	460	A
1	A	470	A
1	A	471	A
1	A	481	G
1	A	482	A
1	A	505	A
1	A	509	C
1	A	512	G
1	A	513	A
1	A	529	A
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	543	C
1	A	545	G
1	A	546	C
1	A	547	A
1	A	548	A
1	A	563	G
1	A	573	G
1	A	575	A
1	A	586	A
1	A	587	C
1	A	588	U
1	A	602	G
1	A	603	A
1	A	604	G
1	A	607	U
1	A	614(A)	U
1	A	614(B)	G
1	A	614(C)	A
1	A	615	G
1	A	620	G
1	A	627	A
1	A	632	A
1	A	637	A

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Mol	Chain	Res	Type
1	A	645	C
1	A	646	A
1	A	647	G
1	A	652(A)	A
1	A	652(B)	A
1	A	652(C)	G
1	A	652(E)	G
1	A	652(F)	G
1	A	652(J)	G
1	A	652(Q)	G
1	A	652(R)	C
1	A	652(T)	C
1	A	652(U)	G
1	A	668	G
1	A	669	G
1	A	686	G
1	A	701	G
1	A	708	C
1	A	709	U
1	A	715	G
1	A	717	G
1	A	730	C
1	A	752	A
1	A	753	C
1	A	762	U
1	A	764	A
1	A	765	G
1	A	771	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	A
1	A	785	G
1	A	792	G
1	A	805	G
1	A	810	U
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	857	C

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Mol	Chain	Res	Type
1	A	859	G
1	A	879	G
1	A	882	G
1	A	884	C
1	A	885	C
1	A	886	C
1	A	888	C
1	A	889	C
1	A	890	A
1	A	895	U
1	A	896	A
1	A	897	C
1	A	900	A
1	A	901	A
1	A	910	A
1	A	914	C
1	A	917	A
1	A	932	G
1	A	938	G
1	A	941	A
1	A	945	A
1	A	946	G
1	A	953	A
1	A	958	U
1	A	959	A
1	A	961	C
1	A	974	G
1	A	975	C
1	A	975(A)	G
1	A	983	A
1	A	990	A
1	A	991	C
1	A	994	C
1	A	996	A
1	A	1005	C
1	A	1012	U
1	A	1013	C
1	A	1020	A
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	U

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Mol	Chain	Res	Type
1	A	1027	A
1	A	1033	U
1	A	1038	C
1	A	1039	G
1	A	1040	C
1	A	1041	C
1	A	1042	G
1	A	1043	C
1	A	1045	A
1	A	1046	A
1	A	1047	G
1	A	1048	A
1	A	1049	C
1	A	1050	A
1	A	1052	C
1	A	1107	G
1	A	1109	C
1	A	1110	G
1	A	1112	G
1	A	1115	G
1	A	1128	A
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1141	U
1	A	1154	G
1	A	1155	A
1	A	1170	G
1	A	1171	G
1	A	1173	G
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1177	A
1	A	1188	U
1	A	1210	A
1	A	1211	U
1	A	1224	C
1	A	1244	G
1	A	1252	G

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Mol	Chain	Res	Type
1	A	1253	A
1	A	1256	G
1	A	1267	U
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1292	U
1	A	1300	U
1	A	1301	A
1	A	1305	C
1	A	1314	C
1	A	1320	C
1	A	1321	A
1	A	1329	U
1	A	1345	C
1	A	1352	U
1	A	1359	A
1	A	1360	A
1	A	1365	A
1	A	1368	G
1	A	1370	C
1	A	1373	A
1	A	1374	G
1	A	1378	A
1	A	1379	A
1	A	1380	G
1	A	1383	C
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1395	A
1	A	1405	U
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	U
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1437	C
1	A	1445	A

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Mol	Chain	Res	Type
1	A	1449	A
1	A	1455	G
1	A	1459	G
1	A	1467	C
1	A	1471	A
1	A	1482	G
1	A	1488	G
1	A	1490	A
1	A	1493	C
1	A	1497	U
1	A	1507	A
1	A	1508	A
1	A	1509	C
1	A	1509(A)	A
1	A	1510	G
1	A	1520	G
1	A	1531	C
1	A	1533	G
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1539	G
1	A	1540	U
1	A	1542	A
1	A	1543	C
1	A	1545	A
1	A	1548	C
1	A	1554	A
1	A	1558	A
1	A	1559	G
1	A	1560	G
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1579	A
1	A	1580	A
1	A	1581	G
1	A	1584	C
1	A	1586	A
1	A	1598	C
1	A	1608	A

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Mol	Chain	Res	Type
1	A	1609	A
1	A	1610	A
1	A	1617	C
1	A	1635	G
1	A	1640	C
1	A	1647	G
1	A	1648	C
1	A	1652	A
1	A	1654	A
1	A	1674	G
1	A	1675	C
1	A	1696	G
1	A	1698	A
1	A	1700	A
1	A	1701	A
1	A	1703	G
1	A	1721	G
1	A	1722	A
1	A	1746	G
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1780	A
1	A	1782	C
1	A	1791	A
1	A	1799	G
1	A	1800	C
1	A	1801	G
1	A	1812	A
1	A	1816	G
1	A	1819	A
1	A	1820	U
1	A	1826	G
1	A	1828	G
1	A	1829	A
1	A	1835	G
1	A	1838	C
1	A	1840	G
1	A	1847	A
1	A	1848	A
1	A	1858	G
1	A	1865	G

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Mol	Chain	Res	Type
1	A	1866	C
1	A	1877	A
1	A	1878	G
1	A	1881	C
1	A	1882	C
1	A	1896	G
1	A	1900	A
1	A	1905	C
1	A	1906	G
1	A	1912	A
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	U
1	A	1952	A
1	A	1955	U
1	A	1963	U
1	A	1964	G
1	A	1967	C
1	A	1969	A
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1982	C
1	A	1991	U
1	A	1993	U
1	A	1997	G
1	A	2005	A
1	A	2020	A
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2036	C
1	A	2043	C
1	A	2049	G
1	A	2055	C

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Mol	Chain	Res	Type
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2099	U
1	A	2100	G
1	A	2103	C
1	A	2104	G
1	A	2108	C
1	A	2110	G
1	A	2111	C
1	A	2112	G
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2119	A
1	A	2123	G
1	A	2126	A
1	A	2127	G
1	A	2128	C
1	A	2131	G
1	A	2133	G
1	A	2134	A
1	A	2135	A
1	A	2136	C
1	A	2146	C
1	A	2147	G
1	A	2150	U
1	A	2159	G
1	A	2160	G
1	A	2161	C
1	A	2162	G
1	A	2164	C
1	A	2169	A
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2174	C
1	A	2176	A
1	A	2179	C
1	A	2180	U

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Mol	Chain	Res	Type
1	A	2183	C
1	A	2185	C
1	A	2186	G
1	A	2187	G
1	A	2188	C
1	A	2191	G
1	A	2192	G
1	A	2193	G
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2225	A
1	A	2234	G
1	A	2238	G
1	A	2239	G
1	A	2240	C
1	A	2248	C
1	A	2249	U
1	A	2252	G
1	A	2268	A
1	A	2273	A
1	A	2275	C
1	A	2278	A
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2289	G
1	A	2291	U
1	A	2294	C
1	A	2305	A
1	A	2306	C
1	A	2308	G
1	A	2309	A
1	A	2311	A
1	A	2316	C
1	A	2319	G
1	A	2320	A
1	A	2321	G
1	A	2325	G

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Mol	Chain	Res	Type
1	A	2334	G
1	A	2336	A
1	A	2343	C
1	A	2347	C
1	A	2350	C
1	A	2354	G
1	A	2379	G
1	A	2383	G
1	A	2385	C
1	A	2388	A
1	A	2400	G
1	A	2406	U
1	A	2410	G
1	A	2414	G
1	A	2418	A
1	A	2422	A
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2439	A
1	A	2441	C
1	A	2448	A
1	A	2465	C
1	A	2469	A
1	A	2470	G
1	A	2472	G
1	A	2474	C
1	A	2476	A
1	A	2477	C
1	A	2486	G
1	A	2487	G
1	A	2502	G
1	A	2504	U
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2520	C
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2554	U

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Mol	Chain	Res	Type
1	A	2564	A
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2582	G
1	A	2585	U
1	A	2586	C
1	A	2602	A
1	A	2603	G
1	A	2604	U
1	A	2608	G
1	A	2609	U
1	A	2610	C
1	A	2611	U
1	A	2612	C
1	A	2615	U
1	A	2628	C
1	A	2629	A
1	A	2630	G
1	A	2654	A
1	A	2663	G
1	A	2672	G
1	A	2674	G
1	A	2686	G
1	A	2690	C
1	A	2691	C
1	A	2702	U
1	A	2703	C
1	A	2707	G
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2739	U
1	A	2744	G
1	A	2758	A
1	A	2761	G
1	A	2765	A
1	A	2766	G
1	A	2778	A
1	A	2790	A

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Mol	Chain	Res	Type
1	A	2791	C
1	A	2802	G
1	A	2803	C
1	A	2808	U
1	A	2820	A
1	A	2821	A
1	A	2833	G
1	A	2834	G
1	A	2835	A
1	A	2847	U
1	A	2872	G
1	A	2873	A
1	A	2880	C
1	A	2892	A
1	A	2893	G
1	A	2894	G
1	A	2895	U
1	A	2897	U
2	B	2	C
2	B	8	U
2	B	9	G
2	B	12	C
2	B	13	A
2	B	15	A
2	B	19	G
2	B	21	G
2	B	24	G
2	B	25	A
2	B	28	C
2	B	33	G
2	B	40	U
2	B	53	A
2	B	54	G
2	B	56	G
2	B	73	A
2	B	74	U
2	B	75	G
2	B	84	C
2	B	85	G
2	B	88	C
2	B	89	G
2	B	106	G

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Mol	Chain	Res	Type
2	B	110	G

All (60) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	71	A
1	A	102	G
1	A	196	A
1	A	249	C
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	278	A
1	A	363(E)	U
1	A	481	G
1	A	542	C
1	A	547	A
1	A	587	C
1	A	669	G
1	A	685	A
1	A	746	A
1	A	752	A
1	A	764	A
1	A	827	U
1	A	856	C
1	A	900	A
1	A	945	A
1	A	974	G
1	A	1026	U
1	A	1047	G
1	A	1049	C
1	A	1106	G
1	A	1108	U
1	A	1110	G
1	A	1155	A
1	A	1174	A
1	A	1175	U
1	A	1176	G
1	A	1210	A
1	A	1300	U
1	A	1378	A
1	A	1419	A

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Mol	Chain	Res	Type
1	A	1427	A
1	A	1507	A
1	A	1530	C
1	A	1536	C
1	A	1538	G
1	A	1558	A
1	A	1608	A
1	A	1653	G
1	A	1799	G
1	A	1819	A
1	A	1992	G
1	A	2116	G
1	A	2126	A
1	A	2172	U
1	A	2308	G
1	A	2318	G
1	A	2406	U
1	A	2439	A
1	A	2602	A
1	A	2610	C
1	A	2689	U
1	A	2778	A
1	A	2802	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 718 ligands modelled in this entry, 718 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2837/2913 (97%)	-0.29	44 (1%) 68 15	26, 47, 132, 176	0
2	B	120/122 (98%)	-0.13	0 100 100	43, 72, 93, 110	0
3	D	275/276 (99%)	-0.08	1 (0%) 90 45	29, 45, 63, 113	0
4	E	204/206 (99%)	-0.20	1 (0%) 88 39	28, 49, 72, 95	0
5	F	203/210 (96%)	-0.22	0 100 100	29, 54, 88, 111	0
6	G	181/182 (99%)	0.13	5 (2%) 50 8	76, 110, 133, 144	0
7	H	174/180 (96%)	-0.10	0 100 100	54, 73, 94, 110	0
8	I	146/148 (98%)	0.01	2 (1%) 72 17	54, 81, 99, 115	0
9	N	140/140 (100%)	-0.14	1 (0%) 84 32	38, 49, 78, 92	0
10	O	122/122 (100%)	-0.22	0 100 100	35, 50, 69, 77	0
11	P	149/150 (99%)	-0.19	0 100 100	30, 58, 89, 105	0
12	Q	141/141 (100%)	-0.02	1 (0%) 84 32	39, 54, 71, 83	0
13	R	118/118 (100%)	-0.04	1 (0%) 83 28	34, 44, 58, 77	0
14	S	110/112 (98%)	-0.06	1 (0%) 81 25	50, 69, 89, 96	0
15	T	131/146 (89%)	-0.13	1 (0%) 83 28	43, 55, 92, 119	0
16	U	116/118 (98%)	-0.20	0 100 100	32, 44, 62, 71	0
17	V	101/101 (100%)	-0.09	1 (0%) 79 23	29, 56, 79, 103	0
18	W	112/113 (99%)	-0.20	0 100 100	33, 40, 62, 103	0
19	X	95/96 (98%)	-0.16	0 100 100	38, 49, 72, 88	0
20	Y	107/110 (97%)	-0.00	1 (0%) 81 25	47, 61, 85, 108	0
21	Z	201/206 (97%)	0.01	4 (1%) 62 12	53, 76, 99, 122	0
22	0	76/85 (89%)	-0.10	0 100 100	39, 48, 64, 91	0
23	1	97/98 (98%)	-0.04	0 100 100	36, 48, 82, 97	0
24	2	70/72 (97%)	0.11	1 (1%) 72 17	46, 60, 76, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	3	59/60 (98%)	-0.10	1 (1%) 67 15	38, 49, 86, 97	0
26	4	46/71 (64%)	0.35	2 (4%) 34 5	101, 129, 144, 148	0
27	5	59/60 (98%)	-0.27	0 100 100	30, 45, 66, 80	0
28	6	53/54 (98%)	-0.37	0 100 100	42, 51, 70, 79	0
29	7	48/49 (97%)	0.20	4 (8%) 11 2	30, 34, 55, 80	0
30	8	64/65 (98%)	-0.04	2 (3%) 47 7	38, 43, 52, 70	0
31	9	36/37 (97%)	0.37	0 100 100	44, 55, 62, 73	0
All	All	6391/6561 (97%)	-0.17	74 (1%) 75 20	26, 51, 115, 176	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	652(B)	A	6.7
6	G	75	LYS	6.2
6	G	74	LYS	5.4
1	A	652(A)	A	5.1
1	A	897	C	5.0
1	A	2897	U	4.8
1	A	2132	U	4.5
1	A	1847	A	4.5
1	A	614(A)	U	4.2
9	N	8	GLN	4.0
1	A	2150	U	3.9
1	A	2107	C	3.9
21	Z	1	MET	3.8
1	A	2149	G	3.7
1	A	2108	C	3.7
1	A	614(B)	G	3.5
21	Z	164	ALA	3.4
1	A	2146	C	3.2
4	E	87	GLU	3.2
1	A	2833	G	3.2
8	I	41	GLU	3.1
21	Z	70	LEU	3.1
29	7	47	ARG	3.0
15	T	111	ARG	3.0
1	A	229	A	3.0
1	A	157	U	2.9
29	7	48	LYS	2.8
29	7	45	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1450	G	2.8
1	A	2338	G	2.8
1	A	405	U	2.8
1	A	2173	A	2.7
1	A	230	U	2.7
1	A	271(N)	U	2.7
1	A	1745(A)	C	2.6
1	A	2175	C	2.6
12	Q	1	MET	2.6
6	G	26	GLN	2.6
1	A	10	G	2.5
1	A	896	A	2.5
1	A	2123	G	2.5
20	Y	92	ASN	2.5
8	I	117	GLU	2.5
1	A	900	A	2.4
1	A	2174	C	2.4
1	A	1115	G	2.4
1	A	2122	U	2.4
1	A	1116	C	2.4
13	R	102	GLU	2.3
21	Z	194	PRO	2.3
1	A	1848	A	2.3
29	7	41	ARG	2.3
3	D	2	ALA	2.3
1	A	1509	C	2.3
17	V	101	GLY	2.3
25	3	57	GLU	2.3
24	2	11	GLU	2.3
1	A	1049	C	2.2
1	A	2801(A)	A	2.2
1	A	9	U	2.2
1	A	34	C	2.2
6	G	137	GLU	2.2
30	8	65	GLU	2.2
1	A	1745	C	2.2
1	A	2145	C	2.1
26	4	21	VAL	2.1
1	A	2165	G	2.1
1	A	1044	G	2.1
26	4	3	GLU	2.1
1	A	2164	C	2.1

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Mol	Chain	Res	Type	RSRZ
30	8	28	GLY	2.1
1	A	2176	A	2.0
14	S	103	GLU	2.0
6	G	30	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3275	1/1	0.24	-	30,30,30,30	0
32	MG	A	3303	1/1	0.43	-	55,55,55,55	0
32	MG	A	3294	1/1	0.53	-	46,46,46,46	0
32	MG	A	3658	1/1	0.23	-	104,104,104,104	0
32	MG	A	3278	1/1	0.20	-	24,24,24,24	0
32	MG	A	3455	1/1	0.10	-	27,27,27,27	0
32	MG	A	3113	1/1	0.41	-	53,53,53,53	0
32	MG	A	3358	1/1	0.09	-	59,59,59,59	0
32	MG	A	3496	1/1	0.09	-	32,32,32,32	0
32	MG	A	3161	1/1	0.18	-	50,50,50,50	0
32	MG	A	3242	1/1	0.41	-	23,23,23,23	0
32	MG	A	3042	1/1	0.36	-	35,35,35,35	0
32	MG	A	3383	1/1	0.14	-	63,63,63,63	0
32	MG	A	3421	1/1	0.14	-	33,33,33,33	0
32	MG	A	3379	1/1	0.13	-	66,66,66,66	0
32	MG	A	3348	1/1	0.07	-	60,60,60,60	0
32	MG	A	3149	1/1	0.38	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3534	1/1	0.10	-	68,68,68,68	0
32	MG	A	3304	1/1	0.18	-	44,44,44,44	0
32	MG	A	3332	1/1	0.15	-	66,66,66,66	0
32	MG	B	213	1/1	0.12	-	38,38,38,38	0
32	MG	A	3267	1/1	0.35	-	25,25,25,25	0
32	MG	A	3361	1/1	0.15	-	81,81,81,81	0
32	MG	A	3034	1/1	0.25	-	32,32,32,32	0
32	MG	A	3357	1/1	0.34	-	35,35,35,35	0
32	MG	A	3124	1/1	0.22	-	38,38,38,38	0
32	MG	A	3615	1/1	0.17	-	94,94,94,94	0
32	MG	A	3467	1/1	0.14	-	40,40,40,40	0
32	MG	A	3330	1/1	0.20	-	40,40,40,40	0
32	MG	A	3605	1/1	0.09	-	99,99,99,99	0
32	MG	A	3056	1/1	0.68	-	54,54,54,54	0
32	MG	A	3363	1/1	0.17	-	83,83,83,83	0
32	MG	A	3435	1/1	0.18	-	49,49,49,49	0
32	MG	A	3265	1/1	0.31	-	27,27,27,27	0
32	MG	A	3226	1/1	0.19	-	41,41,41,41	0
32	MG	A	3177	1/1	0.42	-	41,41,41,41	0
32	MG	A	3399	1/1	0.46	-	58,58,58,58	0
32	MG	A	3613	1/1	0.09	-	52,52,52,52	0
32	MG	A	3621	1/1	0.35	-	73,73,73,73	0
32	MG	A	3009	1/1	1.46	-	65,65,65,65	0
32	MG	A	3312	1/1	0.05	-	31,31,31,31	0
32	MG	A	3448	1/1	0.08	-	38,38,38,38	0
32	MG	A	3551	1/1	0.67	-	89,89,89,89	0
32	MG	A	3249	1/1	0.19	-	36,36,36,36	0
32	MG	A	3408	1/1	0.11	-	77,77,77,77	0
32	MG	A	3482	1/1	0.17	-	27,27,27,27	0
32	MG	A	3130	1/1	0.29	-	53,53,53,53	0
32	MG	A	3604	1/1	0.11	-	34,34,34,34	0
32	MG	A	3019	1/1	0.17	-	41,41,41,41	0
32	MG	A	3537	1/1	0.43	-	47,47,47,47	0
32	MG	A	3505	1/1	0.11	-	41,41,41,41	0
32	MG	A	3082	1/1	0.30	-	52,52,52,52	0
32	MG	A	3274	1/1	0.15	-	22,22,22,22	0
32	MG	A	3637	1/1	0.17	-	65,65,65,65	0
32	MG	A	3395	1/1	0.16	-	86,86,86,86	0
32	MG	A	3469	1/1	0.06	-	27,27,27,27	0
32	MG	A	3232	1/1	0.65	-	50,50,50,50	0
32	MG	A	3079	1/1	0.57	-	36,36,36,36	0
32	MG	A	3008	1/1	0.93	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3144	1/1	1.68	-	55,55,55,55	0
32	MG	A	3341	1/1	0.35	-	61,61,61,61	0
32	MG	A	3319	1/1	0.05	-	37,37,37,37	0
32	MG	A	3235	1/1	0.49	-	53,53,53,53	0
32	MG	A	3030	1/1	0.39	-	45,45,45,45	0
32	MG	B	223	1/1	0.14	-	133,133,133,133	0
32	MG	A	3036	1/1	0.21	-	40,40,40,40	0
32	MG	A	3453	1/1	0.10	-	22,22,22,22	0
32	MG	A	3096	1/1	0.13	-	46,46,46,46	0
32	MG	A	3413	1/1	0.24	-	33,33,33,33	0
32	MG	A	3594	1/1	0.10	-	48,48,48,48	0
32	MG	A	3164	1/1	0.21	-	31,31,31,31	0
32	MG	A	3152	1/1	0.22	-	41,41,41,41	0
32	MG	A	3485	1/1	0.06	-	20,20,20,20	0
32	MG	A	3231	1/1	0.37	-	69,69,69,69	0
32	MG	A	3289	1/1	0.58	-	70,70,70,70	0
32	MG	A	3101	1/1	0.30	-	63,63,63,63	0
32	MG	A	3198	1/1	0.23	-	31,31,31,31	0
32	MG	A	3403	1/1	0.20	-	61,61,61,61	0
32	MG	A	3578	1/1	0.30	-	49,49,49,49	0
32	MG	A	3470	1/1	0.10	-	26,26,26,26	0
32	MG	A	3021	1/1	0.34	-	52,52,52,52	0
32	MG	B	218	1/1	0.10	-	45,45,45,45	0
32	MG	A	3507	1/1	0.17	-	50,50,50,50	0
32	MG	A	3150	1/1	0.37	-	51,51,51,51	0
32	MG	A	3648	1/1	0.41	-	88,88,88,88	0
32	MG	A	3103	1/1	0.37	-	52,52,52,52	0
32	MG	A	3549	1/1	0.16	-	82,82,82,82	0
32	MG	A	3240	1/1	0.67	-	42,42,42,42	0
32	MG	A	3063	1/1	0.21	-	43,43,43,43	0
32	MG	A	3378	1/1	0.09	-	26,26,26,26	0
32	MG	A	3098	1/1	0.30	-	37,37,37,37	0
32	MG	A	3517	1/1	0.08	-	64,64,64,64	0
32	MG	A	3481	1/1	0.19	-	28,28,28,28	0
32	MG	A	3431	1/1	0.10	-	55,55,55,55	0
32	MG	A	3172	1/1	0.33	-	43,43,43,43	0
32	MG	A	3536	1/1	0.13	-	66,66,66,66	0
32	MG	A	3458	1/1	0.65	-	61,61,61,61	0
32	MG	A	3390	1/1	0.29	-	110,110,110,110	0
32	MG	A	3472	1/1	0.26	-	37,37,37,37	0
32	MG	A	3540	1/1	0.22	-	83,83,83,83	0
32	MG	A	3465	1/1	0.33	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3268	1/1	0.25	-	30,30,30,30	0
32	MG	A	3440	1/1	0.14	-	76,76,76,76	0
32	MG	A	3027	1/1	0.17	-	40,40,40,40	0
32	MG	A	3449	1/1	0.08	-	28,28,28,28	0
32	MG	A	3371	1/1	0.09	-	44,44,44,44	0
32	MG	A	3095	1/1	0.34	-	40,40,40,40	0
33	ZN	4	101	1/1	0.09	-	199,199,199,199	0
32	MG	B	208	1/1	0.25	-	43,43,43,43	0
32	MG	B	210	1/1	0.37	-	60,60,60,60	0
32	MG	B	217	1/1	0.12	-	67,67,67,67	0
32	MG	A	3550	1/1	0.20	-	82,82,82,82	0
32	MG	A	3529	1/1	0.27	-	89,89,89,89	0
32	MG	A	3653	1/1	0.24	-	104,104,104,104	0
32	MG	A	3165	1/1	0.20	-	28,28,28,28	0
32	MG	A	3237	1/1	0.28	-	71,71,71,71	0
32	MG	A	3502	1/1	0.34	-	65,65,65,65	0
32	MG	A	3439	1/1	0.25	-	56,56,56,56	0
32	MG	B	205	1/1	0.49	-	45,45,45,45	0
32	MG	A	3384	1/1	0.11	-	40,40,40,40	0
32	MG	A	3273	1/1	0.18	-	23,23,23,23	0
32	MG	A	3069	1/1	0.12	-	59,59,59,59	0
32	MG	A	3071	1/1	0.35	-	53,53,53,53	0
32	MG	A	3129	1/1	0.20	-	33,33,33,33	0
32	MG	A	3255	1/1	0.23	-	55,55,55,55	0
32	MG	A	3263	1/1	0.31	-	22,22,22,22	0
32	MG	8	102	1/1	0.33	-	61,61,61,61	0
32	MG	A	3368	1/1	0.25	-	41,41,41,41	0
32	MG	A	3518	1/1	0.23	-	95,95,95,95	0
32	MG	A	3592	1/1	0.26	-	86,86,86,86	0
32	MG	A	3525	1/1	0.07	-	29,29,29,29	0
32	MG	A	3174	1/1	0.14	-	57,57,57,57	0
32	MG	A	3257	1/1	0.23	-	30,30,30,30	0
32	MG	A	3612	1/1	0.14	-	66,66,66,66	0
32	MG	A	3641	1/1	0.19	-	59,59,59,59	0
32	MG	A	3097	1/1	0.22	-	42,42,42,42	0
32	MG	A	3434	1/1	0.15	-	70,70,70,70	0
32	MG	A	3493	1/1	0.12	-	35,35,35,35	0
32	MG	A	3614	1/1	0.40	-	131,131,131,131	0
32	MG	A	3055	1/1	0.53	-	48,48,48,48	0
32	MG	A	3567	1/1	0.07	-	69,69,69,69	0
32	MG	A	3327	1/1	0.09	-	34,34,34,34	0
32	MG	A	3340	1/1	0.51	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3206	1/1	0.13	-	56,56,56,56	0
32	MG	A	3162	1/1	0.68	-	51,51,51,51	0
32	MG	A	3212	1/1	0.28	-	50,50,50,50	0
32	MG	A	3286	1/1	0.18	-	34,34,34,34	0
32	MG	A	3632	1/1	0.18	-	53,53,53,53	0
32	MG	A	3559	1/1	0.23	-	54,54,54,54	0
32	MG	A	3146	1/1	0.28	-	57,57,57,57	0
32	MG	A	3220	1/1	0.45	-	60,60,60,60	0
32	MG	A	3513	1/1	0.44	-	72,72,72,72	0
32	MG	A	3229	1/1	0.12	-	64,64,64,64	0
32	MG	A	3086	1/1	0.57	-	41,41,41,41	0
32	MG	A	3223	1/1	0.38	-	50,50,50,50	0
32	MG	A	3508	1/1	0.14	-	56,56,56,56	0
32	MG	A	3634	1/1	0.07	-	28,28,28,28	0
32	MG	A	3595	1/1	0.34	-	84,84,84,84	0
32	MG	A	3306	1/1	0.13	-	31,31,31,31	0
32	MG	A	3015	1/1	0.16	-	82,82,82,82	0
32	MG	A	3582	1/1	0.14	-	42,42,42,42	0
32	MG	A	3024	1/1	0.20	-	32,32,32,32	0
32	MG	A	3418	1/1	0.27	-	61,61,61,61	0
32	MG	A	3093	1/1	0.19	-	47,47,47,47	0
32	MG	B	204	1/1	0.55	-	52,52,52,52	0
32	MG	2	101	1/1	0.15	-	45,45,45,45	0
32	MG	A	3059	1/1	0.23	-	54,54,54,54	0
32	MG	A	3259	1/1	0.18	-	27,27,27,27	0
32	MG	A	3397	1/1	0.20	-	43,43,43,43	0
32	MG	A	3329	1/1	0.15	-	50,50,50,50	0
32	MG	A	3193	1/1	0.72	-	46,46,46,46	0
32	MG	A	3299	1/1	0.26	-	47,47,47,47	0
32	MG	A	3520	1/1	0.22	-	74,74,74,74	0
32	MG	A	3423	1/1	0.17	-	53,53,53,53	0
32	MG	A	3524	1/1	0.09	-	22,22,22,22	0
32	MG	A	3480	1/1	0.16	-	27,27,27,27	0
32	MG	A	3236	1/1	0.37	-	67,67,67,67	0
32	MG	A	3102	1/1	0.19	-	28,28,28,28	0
32	MG	A	3562	1/1	0.09	-	59,59,59,59	0
32	MG	A	3483	1/1	0.09	-	32,32,32,32	0
32	MG	A	3352	1/1	0.05	-	29,29,29,29	0
32	MG	A	3405	1/1	0.09	-	47,47,47,47	0
32	MG	A	3140	1/1	0.44	-	30,30,30,30	0
32	MG	A	3565	1/1	0.05	-	54,54,54,54	0
32	MG	A	3185	1/1	0.22	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3254	1/1	0.25	-	23,23,23,23	0
32	MG	A	3528	1/1	0.23	-	56,56,56,56	0
32	MG	D	303	1/1	0.25	-	35,35,35,35	0
32	MG	G	201	1/1	0.17	-	60,60,60,60	0
32	MG	A	3186	1/1	0.39	-	41,41,41,41	0
32	MG	A	3574	1/1	0.14	-	21,21,21,21	0
32	MG	A	3521	1/1	0.27	-	110,110,110,110	0
32	MG	A	3603	1/1	0.22	-	55,55,55,55	0
32	MG	A	3147	1/1	0.85	-	42,42,42,42	0
32	MG	A	3120	1/1	0.14	-	43,43,43,43	0
32	MG	A	3545	1/1	0.15	-	105,105,105,105	0
32	MG	A	3234	1/1	0.39	-	71,71,71,71	0
32	MG	A	3350	1/1	0.13	-	91,91,91,91	0
32	MG	A	3530	1/1	0.16	-	79,79,79,79	0
32	MG	A	3031	1/1	0.24	-	36,36,36,36	0
32	MG	A	3038	1/1	1.23	-	39,39,39,39	0
32	MG	A	3519	1/1	0.08	-	40,40,40,40	0
32	MG	A	3245	1/1	0.24	-	27,27,27,27	0
32	MG	A	3606	1/1	0.70	-	71,71,71,71	0
32	MG	A	3557	1/1	0.09	-	71,71,71,71	0
32	MG	A	3494	1/1	0.29	-	39,39,39,39	0
32	MG	A	3040	1/1	0.18	-	45,45,45,45	0
32	MG	A	3638	1/1	0.07	-	116,116,116,116	0
32	MG	A	3370	1/1	0.22	-	49,49,49,49	0
32	MG	A	3601	1/1	0.09	-	40,40,40,40	0
32	MG	A	3324	1/1	0.23	-	23,23,23,23	0
32	MG	A	3367	1/1	0.12	-	52,52,52,52	0
32	MG	A	3088	1/1	0.35	-	40,40,40,40	0
32	MG	A	3401	1/1	0.10	-	67,67,67,67	0
32	MG	A	3406	1/1	0.10	-	50,50,50,50	0
32	MG	A	3115	1/1	0.30	-	44,44,44,44	0
32	MG	A	3387	1/1	0.26	-	46,46,46,46	0
32	MG	A	3283	1/1	0.58	-	52,52,52,52	0
32	MG	A	3201	1/1	0.18	-	38,38,38,38	0
32	MG	A	3230	1/1	0.88	-	41,41,41,41	0
32	MG	A	3307	1/1	0.27	-	23,23,23,23	0
32	MG	A	3041	1/1	0.30	-	36,36,36,36	0
32	MG	A	3217	1/1	0.16	-	31,31,31,31	0
32	MG	B	222	1/1	0.34	-	80,80,80,80	0
32	MG	A	3219	1/1	1.11	-	60,60,60,60	0
32	MG	A	3553	1/1	0.42	-	47,47,47,47	0
32	MG	A	3081	1/1	0.23	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3649	1/1	0.18	-	87,87,87,87	0
32	MG	A	3138	1/1	0.27	-	36,36,36,36	0
32	MG	B	220	1/1	0.26	-	60,60,60,60	0
32	MG	A	3420	1/1	0.14	-	76,76,76,76	0
32	MG	A	3192	1/1	0.36	-	60,60,60,60	0
32	MG	A	3460	1/1	0.15	-	43,43,43,43	0
32	MG	A	3478	1/1	0.14	-	31,31,31,31	0
32	MG	A	3512	1/1	0.10	-	61,61,61,61	0
32	MG	A	3558	1/1	0.28	-	74,74,74,74	0
32	MG	A	3179	1/1	0.29	-	37,37,37,37	0
32	MG	A	3025	1/1	0.20	-	48,48,48,48	0
32	MG	A	3650	1/1	0.15	-	97,97,97,97	0
32	MG	A	3080	1/1	0.21	-	43,43,43,43	0
32	MG	A	3646	1/1	0.33	-	91,91,91,91	0
32	MG	A	3336	1/1	0.13	-	70,70,70,70	0
32	MG	A	3173	1/1	0.24	-	60,60,60,60	0
32	MG	A	3048	1/1	0.37	-	52,52,52,52	0
32	MG	A	3122	1/1	0.15	-	45,45,45,45	0
32	MG	A	3560	1/1	0.21	-	59,59,59,59	0
32	MG	A	3438	1/1	0.14	-	46,46,46,46	0
32	MG	A	3222	1/1	0.21	-	44,44,44,44	0
32	MG	A	3239	1/1	0.20	-	38,38,38,38	0
32	MG	A	3292	1/1	0.73	-	54,54,54,54	0
32	MG	A	3261	1/1	0.33	-	41,41,41,41	0
32	MG	5	102	1/1	0.28	-	52,52,52,52	0
32	MG	A	3583	1/1	0.09	-	52,52,52,52	0
32	MG	A	3090	1/1	0.22	-	42,42,42,42	0
32	MG	A	3013	1/1	0.23	-	40,40,40,40	0
32	MG	A	3584	1/1	0.12	-	63,63,63,63	0
32	MG	A	3369	1/1	0.09	-	33,33,33,33	0
32	MG	A	3154	1/1	0.29	-	48,48,48,48	0
32	MG	A	3091	1/1	0.30	-	54,54,54,54	0
32	MG	A	3542	1/1	0.10	-	46,46,46,46	0
32	MG	A	3626	1/1	0.12	-	35,35,35,35	0
32	MG	A	3555	1/1	0.12	-	78,78,78,78	0
32	MG	A	3167	1/1	0.19	-	29,29,29,29	0
32	MG	A	3495	1/1	0.54	-	61,61,61,61	0
32	MG	A	3617	1/1	0.13	-	64,64,64,64	0
32	MG	A	3318	1/1	0.24	-	32,32,32,32	0
32	MG	A	3347	1/1	0.09	-	40,40,40,40	0
32	MG	A	3012	1/1	0.15	-	31,31,31,31	0
32	MG	A	3137	1/1	0.33	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3392	1/1	0.17	-	50,50,50,50	0
32	MG	A	3207	1/1	0.22	-	40,40,40,40	0
32	MG	A	3188	1/1	0.30	-	40,40,40,40	0
32	MG	A	3314	1/1	0.17	-	34,34,34,34	0
32	MG	A	3409	1/1	0.36	-	63,63,63,63	0
32	MG	A	3345	1/1	0.07	-	59,59,59,59	0
32	MG	A	3074	1/1	0.20	-	42,42,42,42	0
32	MG	A	3200	1/1	1.32	-	55,55,55,55	0
32	MG	A	3633	1/1	0.07	-	23,23,23,23	0
32	MG	A	3280	1/1	0.41	-	21,21,21,21	0
32	MG	A	3105	1/1	0.33	-	51,51,51,51	0
32	MG	9	102	1/1	0.24	-	28,28,28,28	0
32	MG	B	214	1/1	0.16	-	40,40,40,40	0
32	MG	Q	202	1/1	0.30	-	34,34,34,34	0
32	MG	A	3568	1/1	0.24	-	78,78,78,78	0
33	ZN	5	101	1/1	0.06	-	45,45,45,45	0
32	MG	A	3083	1/1	0.67	-	57,57,57,57	0
32	MG	A	3264	1/1	0.28	-	36,36,36,36	0
32	MG	A	3054	1/1	0.72	-	32,32,32,32	0
32	MG	A	3277	1/1	0.27	-	46,46,46,46	0
32	MG	A	3506	1/1	0.13	-	29,29,29,29	0
32	MG	A	3410	1/1	0.17	-	78,78,78,78	0
32	MG	A	3209	1/1	0.36	-	68,68,68,68	0
32	MG	A	3258	1/1	0.31	-	34,34,34,34	0
32	MG	A	3532	1/1	0.10	-	25,25,25,25	0
32	MG	A	3033	1/1	0.28	-	76,76,76,76	0
32	MG	A	3298	1/1	0.62	-	75,75,75,75	0
32	MG	A	3253	1/1	0.32	-	23,23,23,23	0
32	MG	A	3526	1/1	0.12	-	39,39,39,39	0
32	MG	A	3504	1/1	0.11	-	30,30,30,30	0
32	MG	A	3600	1/1	0.10	-	56,56,56,56	0
32	MG	A	3046	1/1	0.76	-	35,35,35,35	0
32	MG	A	3444	1/1	0.10	-	30,30,30,30	0
32	MG	0	101	1/1	0.19	-	89,89,89,89	0
32	MG	A	3077	1/1	0.45	-	39,39,39,39	0
32	MG	A	3486	1/1	0.10	-	24,24,24,24	0
32	MG	A	3163	1/1	0.29	-	36,36,36,36	0
32	MG	A	3199	1/1	0.58	-	48,48,48,48	0
32	MG	A	3644	1/1	0.20	-	142,142,142,142	0
32	MG	A	3377	1/1	0.17	-	22,22,22,22	0
32	MG	A	3620	1/1	0.16	-	45,45,45,45	0
32	MG	A	3210	1/1	0.47	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3515	1/1	0.19	-	26,26,26,26	0
32	MG	A	3183	1/1	0.16	-	26,26,26,26	0
32	MG	A	3611	1/1	0.26	-	65,65,65,65	0
32	MG	A	3353	1/1	0.08	-	29,29,29,29	0
32	MG	A	3311	1/1	0.16	-	37,37,37,37	0
32	MG	A	3351	1/1	0.08	-	37,37,37,37	0
32	MG	A	3011	1/1	0.20	-	47,47,47,47	0
32	MG	A	3320	1/1	0.11	-	23,23,23,23	0
32	MG	A	3543	1/1	0.11	-	43,43,43,43	0
32	MG	A	3100	1/1	0.10	-	29,29,29,29	0
32	MG	A	3588	1/1	0.12	-	31,31,31,31	0
32	MG	A	3051	1/1	0.32	-	53,53,53,53	0
32	MG	A	3251	1/1	0.19	-	25,25,25,25	0
32	MG	A	3238	1/1	0.21	-	65,65,65,65	0
32	MG	A	3454	1/1	0.17	-	32,32,32,32	0
32	MG	A	3608	1/1	0.12	-	63,63,63,63	0
32	MG	A	3523	1/1	0.28	-	35,35,35,35	0
32	MG	A	3645	1/1	0.29	-	70,70,70,70	0
32	MG	A	3308	1/1	0.13	-	24,24,24,24	0
32	MG	A	3426	1/1	0.14	-	56,56,56,56	0
32	MG	E	304	1/1	0.06	-	25,25,25,25	0
32	MG	A	3061	1/1	0.36	-	41,41,41,41	0
32	MG	R	201	1/1	0.18	-	29,29,29,29	0
32	MG	A	3425	1/1	0.20	-	89,89,89,89	0
32	MG	A	3585	1/1	0.43	-	60,60,60,60	0
32	MG	A	3474	1/1	0.55	-	49,49,49,49	0
32	MG	A	3323	1/1	0.10	-	49,49,49,49	0
32	MG	A	3616	1/1	0.45	-	52,52,52,52	0
32	MG	A	3067	1/1	0.17	-	51,51,51,51	0
32	MG	A	3652	1/1	0.10	-	126,126,126,126	0
32	MG	A	3028	1/1	0.24	-	36,36,36,36	0
32	MG	A	3373	1/1	0.16	-	34,34,34,34	0
32	MG	A	3301	1/1	0.46	-	54,54,54,54	0
32	MG	A	3195	1/1	0.33	-	44,44,44,44	0
32	MG	A	3224	1/1	0.14	-	32,32,32,32	0
32	MG	A	3068	1/1	0.34	-	34,34,34,34	0
32	MG	A	3487	1/1	0.13	-	23,23,23,23	0
32	MG	A	3552	1/1	0.23	-	88,88,88,88	0
32	MG	A	3375	1/1	0.16	-	32,32,32,32	0
32	MG	A	3194	1/1	0.93	-	41,41,41,41	0
32	MG	A	3216	1/1	0.19	-	46,46,46,46	0
32	MG	A	3598	1/1	0.41	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	Q	201	1/1	0.56	-	51,51,51,51	0
32	MG	A	3499	1/1	0.10	-	29,29,29,29	0
32	MG	A	3354	1/1	0.08	-	25,25,25,25	0
32	MG	A	3477	1/1	0.17	-	32,32,32,32	0
32	MG	A	3407	1/1	0.08	-	68,68,68,68	0
32	MG	A	3022	1/1	0.22	-	38,38,38,38	0
32	MG	A	3117	1/1	0.16	-	51,51,51,51	0
32	MG	A	3344	1/1	0.16	-	94,94,94,94	0
32	MG	A	3356	1/1	0.10	-	70,70,70,70	0
32	MG	A	3586	1/1	0.13	-	64,64,64,64	0
32	MG	A	3287	1/1	1.11	-	63,63,63,63	0
32	MG	A	3572	1/1	0.18	-	33,33,33,33	0
32	MG	A	3131	1/1	0.29	-	41,41,41,41	0
32	MG	A	3374	1/1	0.14	-	26,26,26,26	0
32	MG	A	3317	1/1	0.13	-	42,42,42,42	0
32	MG	A	3640	1/1	0.14	-	139,139,139,139	0
32	MG	B	219	1/1	0.93	-	105,105,105,105	0
32	MG	A	3338	1/1	0.09	-	44,44,44,44	0
32	MG	A	3462	1/1	0.07	-	39,39,39,39	0
32	MG	A	3309	1/1	0.14	-	51,51,51,51	0
32	MG	A	3631	1/1	0.12	-	43,43,43,43	0
32	MG	A	3057	1/1	0.49	-	54,54,54,54	0
32	MG	A	3622	1/1	0.06	-	36,36,36,36	0
32	MG	A	3159	1/1	0.37	-	42,42,42,42	0
32	MG	5	103	1/1	0.21	-	57,57,57,57	0
32	MG	A	3430	1/1	0.08	-	67,67,67,67	0
32	MG	A	3414	1/1	0.06	-	25,25,25,25	0
32	MG	A	3573	1/1	0.09	-	41,41,41,41	0
32	MG	A	3214	1/1	0.52	-	41,41,41,41	0
32	MG	A	3143	1/1	0.81	-	65,65,65,65	0
32	MG	A	3166	1/1	0.40	-	31,31,31,31	0
32	MG	A	3208	1/1	0.41	-	26,26,26,26	0
32	MG	A	3135	1/1	0.44	-	42,42,42,42	0
32	MG	A	3488	1/1	0.10	-	28,28,28,28	0
32	MG	A	3221	1/1	0.28	-	50,50,50,50	0
32	MG	A	3293	1/1	0.21	-	43,43,43,43	0
32	MG	A	3035	1/1	0.39	-	30,30,30,30	0
32	MG	A	3471	1/1	0.23	-	30,30,30,30	0
32	MG	A	3593	1/1	0.30	-	27,27,27,27	0
32	MG	A	3132	1/1	0.26	-	45,45,45,45	0
32	MG	A	3066	1/1	0.15	-	37,37,37,37	0
32	MG	A	3400	1/1	0.32	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3625	1/1	0.15	-	50,50,50,50	0
32	MG	A	3451	1/1	0.09	-	46,46,46,46	0
32	MG	A	3155	1/1	0.12	-	40,40,40,40	0
32	MG	A	3516	1/1	0.11	-	50,50,50,50	0
32	MG	A	3243	1/1	0.18	-	20,20,20,20	0
32	MG	A	3256	1/1	0.14	-	27,27,27,27	0
32	MG	A	3391	1/1	0.15	-	37,37,37,37	0
32	MG	A	3402	1/1	0.14	-	45,45,45,45	0
32	MG	A	3514	1/1	0.43	-	63,63,63,63	0
32	MG	A	3157	1/1	0.17	-	39,39,39,39	0
32	MG	A	3114	1/1	0.36	-	39,39,39,39	0
32	MG	A	3281	1/1	0.23	-	24,24,24,24	0
32	MG	A	3510	1/1	1.24	-	109,109,109,109	0
32	MG	A	3005	1/1	0.19	-	39,39,39,39	0
32	MG	E	305	1/1	0.29	-	60,60,60,60	0
32	MG	A	3629	1/1	0.13	-	26,26,26,26	0
32	MG	A	3563	1/1	0.18	-	68,68,68,68	0
32	MG	A	3045	1/1	0.59	-	53,53,53,53	0
32	MG	A	3085	1/1	0.26	-	33,33,33,33	0
32	MG	A	3579	1/1	0.14	-	86,86,86,86	0
32	MG	T	202	1/1	0.50	-	52,52,52,52	0
32	MG	A	3092	1/1	0.23	-	48,48,48,48	0
32	MG	A	3388	1/1	0.11	-	62,62,62,62	0
32	MG	A	3065	1/1	0.27	-	42,42,42,42	0
32	MG	A	3017	1/1	0.54	-	46,46,46,46	0
32	MG	A	3142	1/1	0.27	-	44,44,44,44	0
32	MG	A	3463	1/1	0.10	-	44,44,44,44	0
32	MG	A	3014	1/1	0.72	-	34,34,34,34	0
32	MG	A	3581	1/1	0.17	-	34,34,34,34	0
32	MG	A	3006	1/1	0.23	-	26,26,26,26	0
32	MG	A	3498	1/1	0.17	-	44,44,44,44	0
32	MG	A	3291	1/1	0.20	-	39,39,39,39	0
32	MG	A	3424	1/1	0.31	-	37,37,37,37	0
32	MG	A	3272	1/1	0.22	-	26,26,26,26	0
32	MG	A	3433	1/1	0.13	-	48,48,48,48	0
32	MG	A	3181	1/1	0.29	-	40,40,40,40	0
32	MG	A	3087	1/1	0.16	-	62,62,62,62	0
32	MG	A	3247	1/1	0.31	-	26,26,26,26	0
32	MG	A	3211	1/1	1.15	-	52,52,52,52	0
32	MG	A	3241	1/1	0.63	-	30,30,30,30	0
32	MG	1	101	1/1	0.56	-	45,45,45,45	0
32	MG	A	3325	1/1	0.15	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3296	1/1	0.42	-	66,66,66,66	0
32	MG	A	3260	1/1	0.38	-	36,36,36,36	0
32	MG	A	3076	1/1	0.19	-	50,50,50,50	0
32	MG	A	3331	1/1	0.09	-	51,51,51,51	0
32	MG	A	3382	1/1	0.14	-	88,88,88,88	0
32	MG	A	3548	1/1	0.11	-	87,87,87,87	0
32	MG	W	202	1/1	0.84	-	33,33,33,33	0
32	MG	A	3609	1/1	0.19	-	44,44,44,44	0
32	MG	A	3262	1/1	0.14	-	29,29,29,29	0
32	MG	A	3647	1/1	0.19	-	125,125,125,125	0
32	MG	A	3037	1/1	0.29	-	40,40,40,40	0
32	MG	A	3050	1/1	0.28	-	34,34,34,34	0
32	MG	A	3569	1/1	0.27	-	44,44,44,44	0
32	MG	A	3531	1/1	0.16	-	61,61,61,61	0
32	MG	A	3360	1/1	0.14	-	64,64,64,64	0
32	MG	A	3343	1/1	0.28	-	52,52,52,52	0
32	MG	A	3284	1/1	0.46	-	44,44,44,44	0
32	MG	A	3228	1/1	0.16	-	47,47,47,47	0
32	MG	A	3064	1/1	0.69	-	50,50,50,50	0
32	MG	A	3366	1/1	0.20	-	54,54,54,54	0
32	MG	A	3466	1/1	0.12	-	24,24,24,24	0
32	MG	A	3302	1/1	1.95	-	69,69,69,69	0
32	MG	A	3029	1/1	0.25	-	41,41,41,41	0
32	MG	A	3189	1/1	0.21	-	51,51,51,51	0
32	MG	A	3018	1/1	0.22	-	52,52,52,52	0
32	MG	B	221	1/1	0.29	-	50,50,50,50	0
32	MG	A	3204	1/1	0.16	-	33,33,33,33	0
32	MG	A	3372	1/1	0.12	-	34,34,34,34	0
32	MG	A	3575	1/1	0.21	-	77,77,77,77	0
32	MG	A	3007	1/1	0.21	-	27,27,27,27	0
32	MG	A	3443	1/1	0.15	-	31,31,31,31	0
32	MG	A	3602	1/1	0.48	-	50,50,50,50	0
32	MG	A	3654	1/1	1.55	-	68,68,68,68	0
32	MG	B	216	1/1	0.30	-	82,82,82,82	0
32	MG	B	207	1/1	0.21	-	52,52,52,52	0
32	MG	A	3297	1/1	0.50	-	48,48,48,48	0
32	MG	A	3627	1/1	0.11	-	24,24,24,24	0
32	MG	A	3109	1/1	0.23	-	55,55,55,55	0
32	MG	A	3010	1/1	0.34	-	48,48,48,48	0
32	MG	A	3564	1/1	0.12	-	44,44,44,44	0
32	MG	A	3476	1/1	0.18	-	41,41,41,41	0
32	MG	A	3145	1/1	0.21	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3527	1/1	0.18	-	65,65,65,65	0
32	MG	A	3554	1/1	0.40	-	57,57,57,57	0
32	MG	A	3127	1/1	0.27	-	43,43,43,43	0
32	MG	A	3151	1/1	0.52	-	50,50,50,50	0
32	MG	A	3541	1/1	0.45	-	119,119,119,119	0
32	MG	A	3456	1/1	0.09	-	35,35,35,35	0
32	MG	E	302	1/1	0.17	-	41,41,41,41	0
32	MG	A	3544	1/1	0.09	-	73,73,73,73	0
32	MG	8	101	1/1	0.32	-	51,51,51,51	0
32	MG	A	3073	1/1	0.21	-	44,44,44,44	0
32	MG	A	3282	1/1	0.53	-	38,38,38,38	0
32	MG	A	3269	1/1	0.25	-	31,31,31,31	0
32	MG	A	3125	1/1	0.36	-	49,49,49,49	0
32	MG	A	3511	1/1	0.12	-	86,86,86,86	0
32	MG	A	3509	1/1	0.08	-	32,32,32,32	0
32	MG	A	3346	1/1	0.08	-	36,36,36,36	0
32	MG	A	3630	1/1	0.13	-	54,54,54,54	0
32	MG	A	3039	1/1	0.11	-	33,33,33,33	0
32	MG	A	3411	1/1	0.14	-	57,57,57,57	0
32	MG	A	3432	1/1	0.21	-	62,62,62,62	0
32	MG	A	3290	1/1	0.67	-	48,48,48,48	0
32	MG	A	3380	1/1	0.12	-	100,100,100,100	0
32	MG	A	3381	1/1	0.14	-	70,70,70,70	0
32	MG	A	3205	1/1	0.58	-	38,38,38,38	0
32	MG	A	3170	1/1	0.53	-	32,32,32,32	0
32	MG	A	3556	1/1	0.17	-	28,28,28,28	0
32	MG	A	3197	1/1	0.14	-	31,31,31,31	0
32	MG	A	3339	1/1	0.10	-	32,32,32,32	0
32	MG	A	3547	1/1	0.09	-	55,55,55,55	0
32	MG	A	3270	1/1	0.54	-	37,37,37,37	0
32	MG	A	3112	1/1	0.17	-	45,45,45,45	0
32	MG	A	3364	1/1	0.20	-	71,71,71,71	0
32	MG	A	3393	1/1	0.24	-	60,60,60,60	0
32	MG	A	3111	1/1	0.34	-	63,63,63,63	0
32	MG	A	3628	1/1	0.09	-	34,34,34,34	0
32	MG	A	3651	1/1	0.32	-	104,104,104,104	0
32	MG	A	3468	1/1	0.24	-	60,60,60,60	0
32	MG	A	3576	1/1	0.12	-	44,44,44,44	0
32	MG	A	3047	1/1	0.22	-	48,48,48,48	0
32	MG	Q	204	1/1	0.08	-	43,43,43,43	0
32	MG	A	3355	1/1	0.07	-	55,55,55,55	0
32	MG	B	215	1/1	0.17	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3279	1/1	0.23	-	27,27,27,27	0
32	MG	A	3422	1/1	0.21	-	72,72,72,72	0
32	MG	A	3315	1/1	0.08	-	35,35,35,35	0
32	MG	A	3461	1/1	0.10	-	28,28,28,28	0
32	MG	B	211	1/1	0.34	-	47,47,47,47	0
32	MG	A	3450	1/1	0.09	-	64,64,64,64	0
32	MG	A	3642	1/1	0.35	-	88,88,88,88	0
32	MG	A	3656	1/1	0.28	-	114,114,114,114	0
32	MG	A	3133	1/1	0.23	-	45,45,45,45	0
32	MG	A	3072	1/1	0.35	-	46,46,46,46	0
32	MG	A	3108	1/1	0.43	-	56,56,56,56	0
32	MG	A	3337	1/1	0.39	-	79,79,79,79	0
32	MG	A	3276	1/1	0.17	-	27,27,27,27	0
32	MG	A	3126	1/1	0.30	-	37,37,37,37	0
32	MG	A	3026	1/1	0.29	-	44,44,44,44	0
32	MG	A	3490	1/1	0.14	-	27,27,27,27	0
32	MG	A	3271	1/1	0.20	-	26,26,26,26	0
32	MG	A	3252	1/1	0.31	-	25,25,25,25	0
32	MG	A	3187	1/1	0.10	-	27,27,27,27	0
32	MG	F	301	1/1	0.53	-	33,33,33,33	0
32	MG	A	3546	1/1	0.13	-	29,29,29,29	0
32	MG	D	301	1/1	0.73	-	49,49,49,49	0
32	MG	A	3587	1/1	0.28	-	94,94,94,94	0
32	MG	A	3313	1/1	0.04	-	45,45,45,45	0
32	MG	A	3062	1/1	0.22	-	39,39,39,39	0
32	MG	A	3492	1/1	0.13	-	34,34,34,34	0
32	MG	A	3246	1/1	0.18	-	25,25,25,25	0
32	MG	A	3104	1/1	0.30	-	60,60,60,60	0
32	MG	A	3571	1/1	0.10	-	23,23,23,23	0
32	MG	A	3619	1/1	0.30	-	52,52,52,52	0
32	MG	A	3566	1/1	0.08	-	39,39,39,39	0
32	MG	A	3032	1/1	0.14	-	75,75,75,75	0
32	MG	A	3452	1/1	0.07	-	25,25,25,25	0
32	MG	A	3190	1/1	0.52	-	35,35,35,35	0
32	MG	W	201	1/1	0.11	-	32,32,32,32	0
32	MG	A	3442	1/1	0.15	-	53,53,53,53	0
32	MG	A	3412	1/1	0.14	-	29,29,29,29	0
32	MG	A	3459	1/1	0.32	-	79,79,79,79	0
32	MG	A	3300	1/1	0.17	-	64,64,64,64	0
32	MG	A	3333	1/1	0.24	-	45,45,45,45	0
32	MG	A	3213	1/1	0.70	-	43,43,43,43	0
32	MG	A	3427	1/1	0.20	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	B	209	1/1	0.18	-	60,60,60,60	0
32	MG	V	201	1/1	2.21	-	67,67,67,67	0
32	MG	A	3657	1/1	0.12	-	81,81,81,81	0
32	MG	A	3610	1/1	0.30	-	59,59,59,59	0
32	MG	A	3334	1/1	0.35	-	49,49,49,49	0
32	MG	A	3227	1/1	0.16	-	30,30,30,30	0
32	MG	A	3475	1/1	0.12	-	53,53,53,53	0
32	MG	A	3175	1/1	0.43	-	43,43,43,43	0
32	MG	A	3049	1/1	0.29	-	57,57,57,57	0
32	MG	S	201	1/1	0.76	-	49,49,49,49	0
32	MG	A	3635	1/1	0.14	-	108,108,108,108	0
32	MG	A	3134	1/1	0.17	-	38,38,38,38	0
32	MG	E	301	1/1	0.45	-	34,34,34,34	0
32	MG	A	3589	1/1	0.12	-	34,34,34,34	0
32	MG	A	3596	1/1	0.09	-	65,65,65,65	0
32	MG	D	302	1/1	0.32	-	28,28,28,28	0
32	MG	A	3136	1/1	0.40	-	46,46,46,46	0
32	MG	A	3169	1/1	0.31	-	47,47,47,47	0
32	MG	E	303	1/1	0.06	-	26,26,26,26	0
32	MG	A	3570	1/1	0.10	-	63,63,63,63	0
32	MG	A	3396	1/1	0.57	-	52,52,52,52	0
32	MG	A	3023	1/1	0.16	-	22,22,22,22	0
32	MG	A	3590	1/1	0.25	-	47,47,47,47	0
32	MG	A	3316	1/1	0.12	-	54,54,54,54	0
32	MG	A	3365	1/1	0.28	-	53,53,53,53	0
32	MG	A	3158	1/1	0.18	-	40,40,40,40	0
32	MG	A	3202	1/1	0.11	-	54,54,54,54	0
32	MG	A	3002	1/1	0.32	-	28,28,28,28	0
32	MG	A	3577	1/1	0.23	-	100,100,100,100	0
32	MG	A	3491	1/1	0.11	-	40,40,40,40	0
32	MG	A	3089	1/1	0.14	-	26,26,26,26	0
32	MG	B	201	1/1	0.29	-	57,57,57,57	0
32	MG	A	3404	1/1	0.06	-	66,66,66,66	0
32	MG	A	3285	1/1	0.37	-	66,66,66,66	0
32	MG	A	3417	1/1	0.25	-	21,21,21,21	0
32	MG	A	3250	1/1	0.25	-	19,19,19,19	0
33	ZN	9	101	1/1	0.04	-	50,50,50,50	0
32	MG	A	3539	1/1	0.08	-	42,42,42,42	0
32	MG	A	3110	1/1	0.15	-	60,60,60,60	0
32	MG	A	3107	1/1	1.18	-	66,66,66,66	0
32	MG	A	3160	1/1	0.15	-	23,23,23,23	0
32	MG	A	3153	1/1	0.34	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3196	1/1	0.25	-	41,41,41,41	0
32	MG	A	3094	1/1	0.97	-	47,47,47,47	0
32	MG	A	3624	1/1	0.23	-	64,64,64,64	0
32	MG	A	3501	1/1	0.10	-	64,64,64,64	0
32	MG	A	3305	1/1	0.23	-	52,52,52,52	0
32	MG	A	3457	1/1	0.17	-	38,38,38,38	0
32	MG	A	3266	1/1	0.44	-	35,35,35,35	0
32	MG	Z	301	1/1	0.67	-	55,55,55,55	0
32	MG	A	3215	1/1	0.20	-	55,55,55,55	0
32	MG	A	3052	1/1	0.20	-	57,57,57,57	0
32	MG	A	3119	1/1	0.79	-	49,49,49,49	0
32	MG	A	3128	1/1	0.47	-	62,62,62,62	0
32	MG	A	3295	1/1	0.33	-	54,54,54,54	0
32	MG	A	3184	1/1	0.44	-	42,42,42,42	0
32	MG	A	3078	1/1	0.21	-	42,42,42,42	0
32	MG	A	3321	1/1	0.09	-	42,42,42,42	0
32	MG	B	206	1/1	0.19	-	57,57,57,57	0
32	MG	A	3349	1/1	0.21	-	81,81,81,81	0
32	MG	A	3389	1/1	0.10	-	39,39,39,39	0
32	MG	A	3500	1/1	0.14	-	34,34,34,34	0
32	MG	F	302	1/1	0.53	-	42,42,42,42	0
32	MG	A	3099	1/1	0.35	-	44,44,44,44	0
32	MG	A	3437	1/1	0.18	-	59,59,59,59	0
32	MG	A	3522	1/1	0.09	-	38,38,38,38	0
32	MG	A	3218	1/1	0.27	-	57,57,57,57	0
32	MG	A	3182	1/1	0.27	-	51,51,51,51	0
32	MG	B	202	1/1	0.75	-	43,43,43,43	0
32	MG	A	3176	1/1	0.26	-	37,37,37,37	0
32	MG	Q	203	1/1	0.28	-	73,73,73,73	0
33	ZN	6	101	1/1	0.03	-	48,48,48,48	0
32	MG	A	3464	1/1	0.11	-	39,39,39,39	0
32	MG	A	3489	1/1	0.12	-	28,28,28,28	0
32	MG	A	3310	1/1	0.12	-	37,37,37,37	0
32	MG	A	3180	1/1	0.19	-	29,29,29,29	0
32	MG	A	3156	1/1	0.37	-	46,46,46,46	0
32	MG	A	3141	1/1	0.88	-	46,46,46,46	0
32	MG	A	3326	1/1	0.13	-	74,74,74,74	0
32	MG	A	3497	1/1	0.15	-	60,60,60,60	0
32	MG	A	3203	1/1	0.21	-	49,49,49,49	0
32	MG	A	3599	1/1	0.40	-	76,76,76,76	0
32	MG	A	3060	1/1	0.28	-	34,34,34,34	0
32	MG	A	3328	1/1	0.06	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3244	1/1	0.43	-	26,26,26,26	0
32	MG	A	3084	1/1	0.12	-	46,46,46,46	0
32	MG	A	3001	1/1	0.11	-	25,25,25,25	0
32	MG	A	3121	1/1	0.35	-	33,33,33,33	0
32	MG	A	3070	1/1	0.44	-	52,52,52,52	0
32	MG	A	3016	1/1	0.51	-	44,44,44,44	0
32	MG	A	3484	1/1	0.46	-	75,75,75,75	0
32	MG	A	3618	1/1	0.20	-	68,68,68,68	0
32	MG	A	3419	1/1	0.10	-	68,68,68,68	0
32	MG	A	3376	1/1	0.23	-	25,25,25,25	0
32	MG	A	3607	1/1	0.31	-	75,75,75,75	0
32	MG	A	3288	1/1	0.24	-	39,39,39,39	0
32	MG	A	3233	1/1	1.67	-	66,66,66,66	0
32	MG	A	3139	1/1	0.23	-	42,42,42,42	0
32	MG	A	3538	1/1	0.26	-	35,35,35,35	0
32	MG	A	3639	1/1	0.14	-	72,72,72,72	0
32	MG	A	3178	1/1	0.24	-	38,38,38,38	0
32	MG	A	3058	1/1	0.60	-	45,45,45,45	0
32	MG	A	3445	1/1	0.15	-	29,29,29,29	0
32	MG	A	3362	1/1	0.13	-	69,69,69,69	0
32	MG	A	3623	1/1	0.14	-	53,53,53,53	0
32	MG	A	3591	1/1	0.31	-	84,84,84,84	0
32	MG	T	201	1/1	0.60	-	53,53,53,53	0
32	MG	A	3503	1/1	0.17	-	41,41,41,41	0
32	MG	A	3416	1/1	0.11	-	49,49,49,49	0
32	MG	A	3118	1/1	0.31	-	36,36,36,36	0
32	MG	A	3123	1/1	0.18	-	41,41,41,41	0
32	MG	A	3597	1/1	0.12	-	30,30,30,30	0
32	MG	A	3580	1/1	0.25	-	79,79,79,79	0
32	MG	A	3106	1/1	0.33	-	62,62,62,62	0
32	MG	P	201	1/1	0.11	-	45,45,45,45	0
32	MG	A	3075	1/1	0.20	-	30,30,30,30	0
32	MG	A	3004	1/1	0.45	-	45,45,45,45	0
32	MG	A	3428	1/1	0.24	-	49,49,49,49	0
32	MG	B	212	1/1	0.25	-	60,60,60,60	0
32	MG	A	3533	1/1	0.14	-	55,55,55,55	0
32	MG	A	3386	1/1	0.16	-	47,47,47,47	0
32	MG	A	3415	1/1	0.09	-	48,48,48,48	0
32	MG	A	3044	1/1	0.42	-	39,39,39,39	0
32	MG	A	3148	1/1	0.25	-	33,33,33,33	0
32	MG	A	3535	1/1	0.21	-	31,31,31,31	0
32	MG	A	3473	1/1	0.18	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3441	1/1	0.30	-	47,47,47,47	0
32	MG	A	3191	1/1	0.11	-	63,63,63,63	0
32	MG	A	3636	1/1	0.14	-	67,67,67,67	0
32	MG	A	3116	1/1	0.34	-	42,42,42,42	0
32	MG	A	3447	1/1	0.20	-	29,29,29,29	0
32	MG	A	3398	1/1	0.08	-	47,47,47,47	0
32	MG	A	3655	1/1	0.77	-	65,65,65,65	0
33	ZN	Y	201	1/1	0.02	-	69,69,69,69	0
32	MG	A	3043	1/1	0.33	-	68,68,68,68	0
32	MG	A	3385	1/1	0.11	-	63,63,63,63	0
32	MG	A	3335	1/1	0.11	-	62,62,62,62	0
32	MG	A	3479	1/1	0.11	-	25,25,25,25	0
32	MG	A	3225	1/1	0.42	-	37,37,37,37	0
32	MG	B	203	1/1	0.70	-	70,70,70,70	0
32	MG	A	3436	1/1	0.35	-	65,65,65,65	0
32	MG	A	3561	1/1	0.85	-	70,70,70,70	0
32	MG	A	3003	1/1	0.27	-	28,28,28,28	0
32	MG	A	3053	1/1	0.40	-	51,51,51,51	0
32	MG	A	3171	1/1	0.28	-	32,32,32,32	0
32	MG	A	3020	1/1	0.24	-	48,48,48,48	0
32	MG	A	3446	1/1	0.09	-	38,38,38,38	0
32	MG	A	3359	1/1	0.07	-	43,43,43,43	0
32	MG	A	3394	1/1	0.15	-	29,29,29,29	0
32	MG	A	3429	1/1	0.34	-	71,71,71,71	0
32	MG	A	3248	1/1	0.40	-	27,27,27,27	0
32	MG	A	3168	1/1	0.39	-	31,31,31,31	0
32	MG	A	3643	1/1	0.33	-	102,102,102,102	0
32	MG	A	3342	1/1	0.16	-	71,71,71,71	0
32	MG	A	3322	1/1	0.08	-	40,40,40,40	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.