



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:46 AM GMT

PDB ID : 4DHC
Title : Crystal structure of YAEJ bound to the 70S ribosome
Authors : Gagnon, M.G.; Seetharaman, S.V.; Bulkley, D.P.; Steitz, T.A.
Deposited on : 2012-01-27
Resolution : 3.20 Å(reported)

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

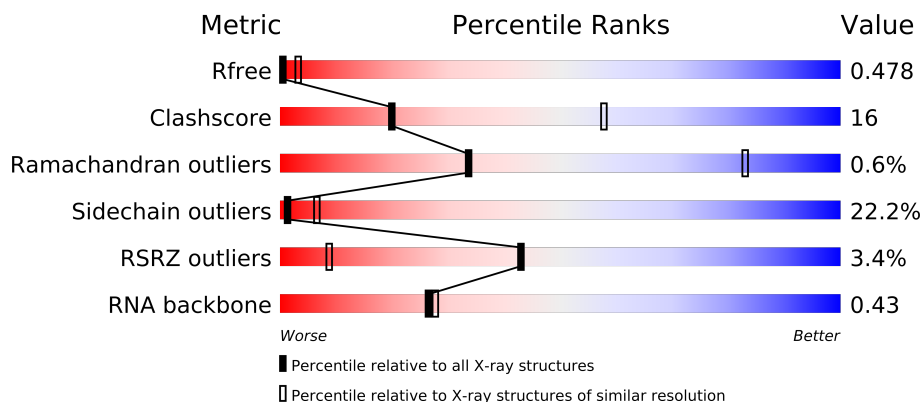
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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

Mol	Chain	Length	Quality of chain
1	A	2915	
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 89631 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	2722	Total	C	N	O	P	0	0	0
			58627	26093	10971	18843	2720			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1578	1007	297	272	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	180	Total	C	N	O	S	0	0	0
			1361	874	241	243	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
			1057	682	182	192	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			
			873	550	174	149	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	130	Total	C	N	O	S			
			1058	663	212	182	1	0	0	0

- 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			
			959	608	201	149	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	100	Total	C	N	O	S			
			770	496	140	133	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	W	111	Total	C	N	O	S			
			877	552	171	152	2	0	0	0

- 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			
			732	477	130	124	1	0	0	0

- 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			
			781	502	145	128	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	189	Total	C	N	O	S	0	0	0
			1451	925	253	270	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	77	Total	C	N	O	S	0	0	0
			607	376	126	104	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	71	Total	C	N	O	S	0	0	0
			584	361	118	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	58	Total	C	N	O	0	0	0
			453	290	86	77			

- 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
			451	283	89	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
			437	272	84	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
			402	248	97	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	35	Total	C	N	O	S	0	0	0
			292	180	65	44	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	0	3	Total	Mg	0	0
			3	3		
32	Q	2	Total	Mg	0	0
			2	2		
32	D	3	Total	Mg	0	0
			3	3		
32	E	4	Total	Mg	0	0
			4	4		
32	B	16	Total	Mg	0	0
			16	16		
32	V	1	Total	Mg	0	0
			1	1		
32	1	1	Total	Mg	0	0
			1	1		
32	7	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	686	Total 686	Mg 686	0	0
32	T	3	Total 3	Mg 3	0	0
32	6	2	Total 2	Mg 2	0	0
32	U	1	Total 1	Mg 1	0	0
32	X	1	Total 1	Mg 1	0	0
32	O	1	Total 1	Mg 1	0	0
32	R	1	Total 1	Mg 1	0	0
32	F	3	Total 3	Mg 3	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	1013	Total 1013	O 1013	0	0
34	B	40	Total 40	O 40	0	0
34	D	7	Total 7	O 7	0	0
34	E	11	Total 11	O 11	0	0

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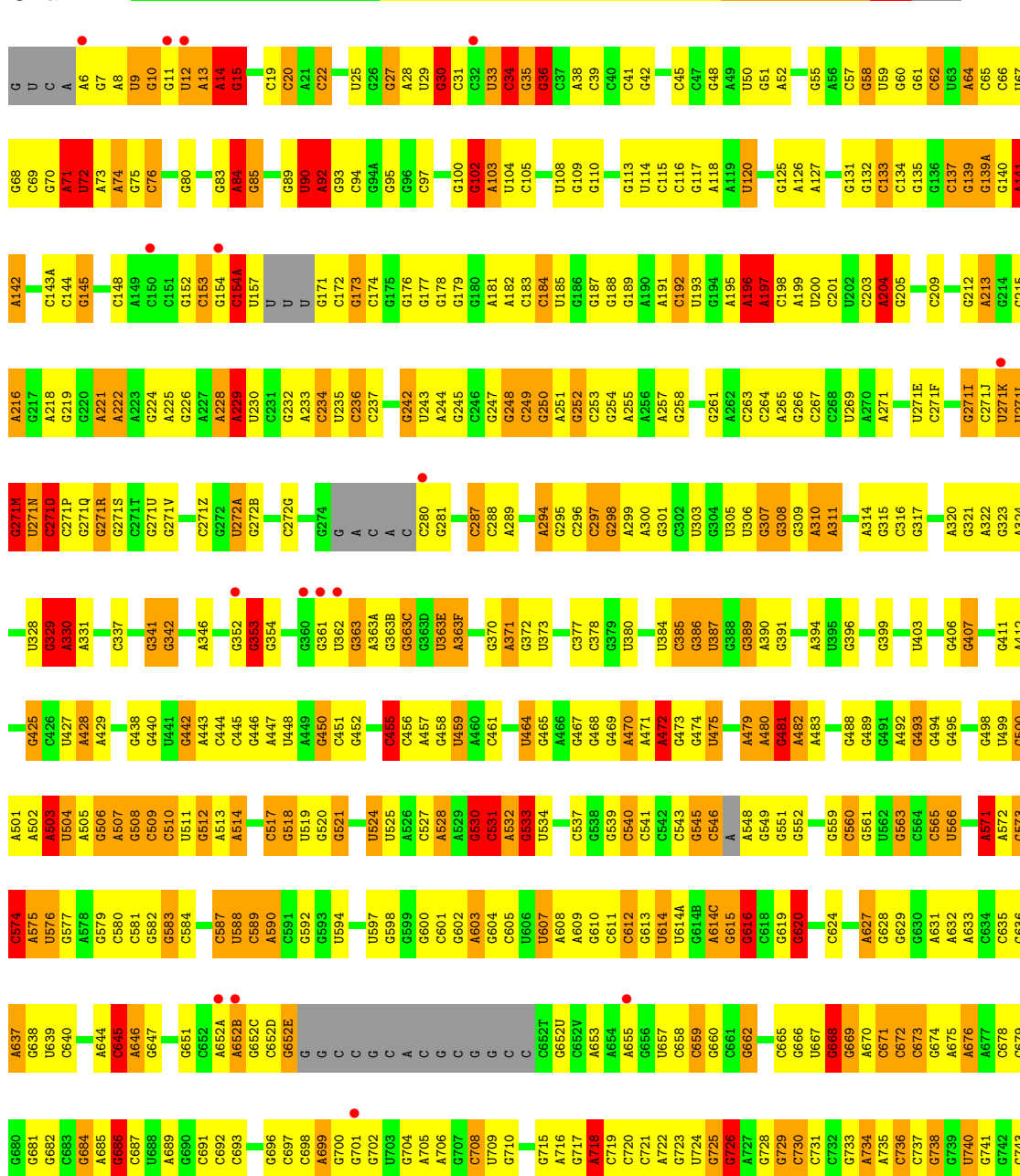
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	F	4	Total 4	O 4	0	0
34	N	2	Total 2	O 2	0	0
34	O	4	Total 4	O 4	0	0
34	P	4	Total 4	O 4	0	0
34	R	6	Total 6	O 6	0	0
34	T	2	Total 2	O 2	0	0
34	V	1	Total 1	O 1	0	0
34	W	1	Total 1	O 1	0	0
34	1	2	Total 2	O 2	0	0
34	3	1	Total 1	O 1	0	0
34	6	2	Total 2	O 2	0	0
34	7	2	Total 2	O 2	0	0
34	8	4	Total 4	O 4	0	0

3 Residue-property plots

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

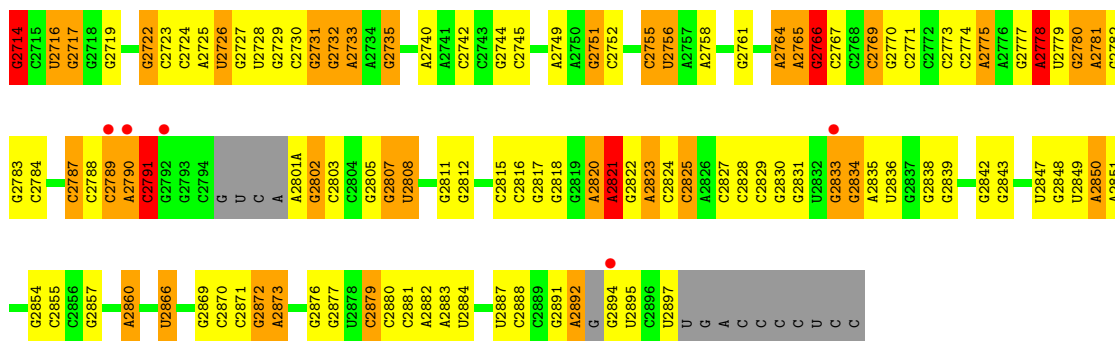
• Molecule 1: 23S Ribosomal RNA

Chain A:



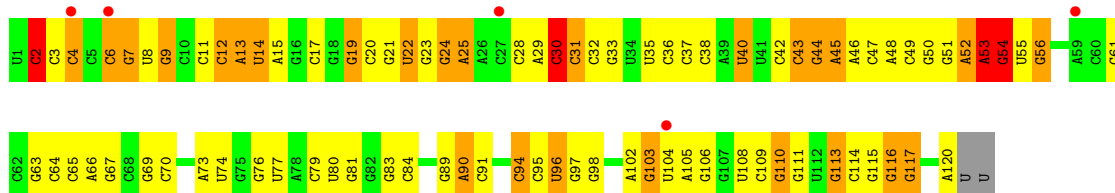
C1600	C1601	C1602	A1603	C1607	A1608	A1609	A1610	C1611	A1614	C1615	A1616	C1617	A1618	C1619	G1620	A1621	C1622	G1623	C1624	C1625	G1626	U1629	G1630	C1631	A1631A	A1632	G1635	C1636	A1637	C1638	U1639	C1640	A1641	G1642	C1643	G1644	G1645	G1646	G1647	C1648	G1649	G1650	G1651	A1652	G1653	A1654	C1655	C1656	C1657	C1658	U1659	G1659	C1660	G1661	C1662	C1663	
G1526	G1527	G1528	A1528A	G1529	C1530	C1531	C1532	G1533	U	A	G1536	G1537	G1538	G1539	U1540	G1541	A1542	C1543	A1544	A1545	C1546	C1547	C1551	G1552	A1553	C1556	C1557	A1558	G1559	G1560	G1561	A1566	A1567	G1568	A1569	C1574	C1577	U1578	A1579	A1580	G1581	C1584	A1586	A1587	C1588	C1589	U1590	C1593	G1594	C1598	C1599	G1599	C1600				
G1455	G1461	C1462	C1463	C1464	G1465	G1466	C1467	C1468	A1469	G1470	A1471	A1472	G1473	G1474	G1475	C1476	A1477	G1478	G1479	G1480	U1481	G1482	A1486	G1487	G1488	U1489	G1492	C1493	A1494	A1495	A1496	U1497	C1498	U1503	C1504	C1505	C1506	A1507	A1508	C1509	A1509A	G1510	C1511	U1512	C1513	U1514	G1515	C1516	G1517	U1518	G1519	C1520	C1525	C1526			
C1387	G1388	G1389	U1390	A1393	U1394	A1396	U1396	U1397	C1403	C1404	U1405	U1406	C1407	C1408	A1412	G1413	G1414	U1415	G1416	C1417	G1418	G1419	U1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	G1428	G1429	C1430	U1431	C1432	U1433	A1434	C1437	U1438	A1439	G1440	G1441	G1442	A1445	C1446	A1447	G1448	A1449	G1450	C1450A	C1451	A1452	U1453				
C1320	A1321	A1322	C1327	G1328	U1329	C1330	A1331	C1333	A1336	G1337	G1338	G1339	U1340	U1341	G1344	C1345	G1346	G1347	G1348	A1349	C1350	C1351	U1352	A1353	C1354	G1355	G1356	U1357	C1358	A1359	A1360	C1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	A1373	C1374	C1375	C1376	G1377	A1378	A1379	G1380	A1384	G1385	C1386				
U1255	G1256	C1257	U1258	G1259	C1260	C1261	A1262	U1263	G1264	A1265	G1266	U1267	A1268	A1269	C1270	G1271	U1272	U1273	A1274	A1275	A1276	G1277	A1278	G1279	G1280	U1281	U1282	C1283	A1284	G1285	A1286	U1287	U1288	U1292	C1293	U1294	C1295	C1297	C1298	U1299	U1300	A1301	A1302	C1305	C1306	A1307	A1308	G1309	U1313	C1314	C1315	U1316	A1317	C1318	G1319		
A1194	G1195	U1198	U1199	C1200	C1201	G1202	C1203	A1204	U1205	G1206	C1207	G1208	C1209	A1210	U1211	G1212	A1213	G1214	G1215	G1216	C1217	G1218	G1219	A1220	C1221	C1222	G1223	C1224	G1225	A1226	G1227	G1228	G1229	C1230	G1231	G1232	C1233	U1234	G1235	G1236	A1237	G1238	U1240	A1241	A1242	G1243	G1244	A1246	A1247	G1250	C1251	G1252	A1253	A1254			
A1127	A1128	A1129	U1130	G1131	C1135	G1136	G1137	G1138	U1139	C1140	U1141	U1142	A1142A	A1143	G1144	G1149	C1150	G1151	C1152	C1153	G1154	A1155	A1156	G1157	G1160	C1161	G1162	G1163	G1164	U1165	U1167	C1168	G1169	G1170	G1171	G	A	G	U	U	C	A	C1178	C1179	C1180	C1181	A1182	G1183	G1186	C1187	U1188	A1189	G1190	G1191	G1193		
U	A	G	A	A	C	C	A	G	A	U	C	U	C	U	U	A	A	A	G	A	G	C	U	G	G	U	A	A	U	U	C	C	A	G	A	G	U	U	C	A	G	C	C	A	U	U	G	C	U	U	G	C	U				
G940	A941	G944	A945	G946	G947	G948	C949	G950	C951	G952	A953	C954	C955	G956	A957	U958	A959	A960	C961	G962	C965	G968	U969	C970	C971	C972	A973	G974	C975	G976	C977	G978	C979	A980	A981	C982	A983	A984	C985	C986	G987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001		
G1002	G1003	C1004	C1005	C1006	C1007	C1008	A1009	G1010	G1011	U1012	C1013	G1017	U1018	U1019	A1020	A1021	U1022	A1023	G1024	G1025	A1026	A1027	A1028	G1031	A1032	U1033	G1034	U1035	C1038	G1039	C1040	C1041	G1042	C1043	G	A	A	G	G	A	C	A	G	C	C	A	G	C	U	U	G	C	U				
C805	C806	U807	G808	G809	U810	U811	C812	C817	C818	C819	A820	A821	U822	C825	U826	C827	U828	A829	C830	G831	G832	U833	C834	A835	C836	C837	C838	U839	C840	A841	A842	G843	C844	G845	C846	U847	G848	A849	C850	U851	G852	G853	G854	C855	C856	C857	U858	G859	U860	A861	G862	A863	G864	C865	A866	G869	
A870	U871	A872	G873	G874	G875	U876	C880	C884	C885	C886	A887	C888	C889	G892	C893	C894	U895	C896	C897	C898	A899	A900	A901	C902	C903	C904	U905	G906	U907	C908	A909	G910	A911	C912	U913	C914	C915	A916	A917	A918	G921	U922	C923	C924	C925	A926	G927	G928	U930	G931	G932	A933	G934	G938	G939		
G744	G745	A746	U747	G748	G749	A752	A753	C754	C755	C756	U757	C758	A759	C760	A761	U762	G763	A764	C765	U766	G767	G768	U769	G770	G771	C772	U773	A774	C775	G776	G777	A778	C779	A781	A782	A783	A784	C785	C786	U787	A788	A789	C790	C791	G792	A793	G794	C795	G796	C797	G798	G799	A800	G801	A802	U803	A804





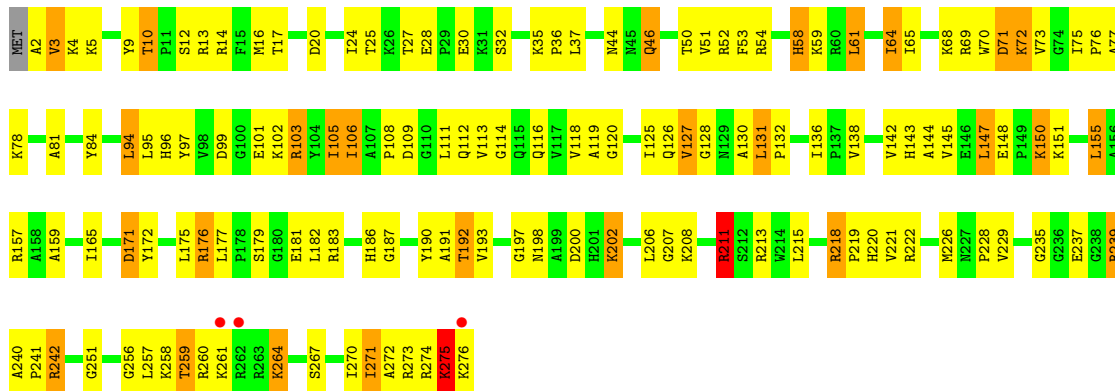
• Molecule 2: 5S Ribosomal RNA

Chain B:



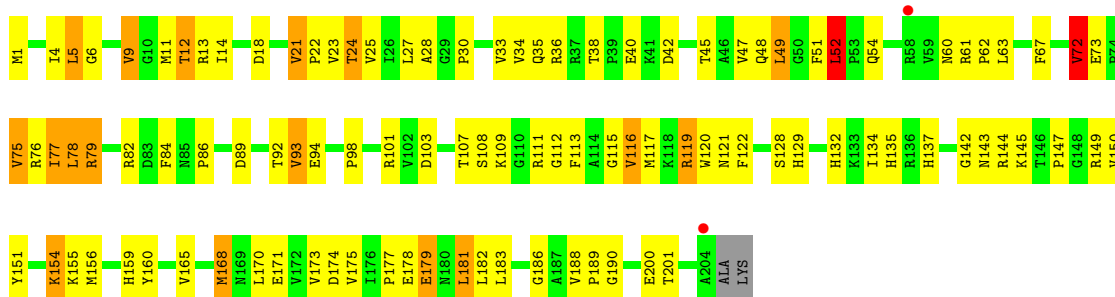
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



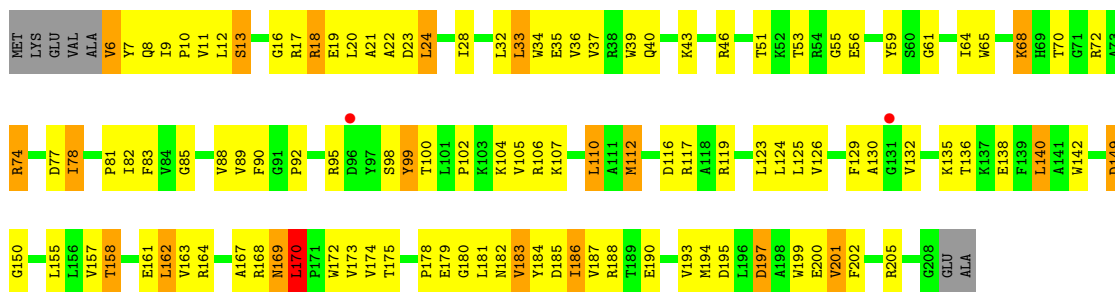
• Molecule 4: 50S Ribosomal Protein L3

Chain E:



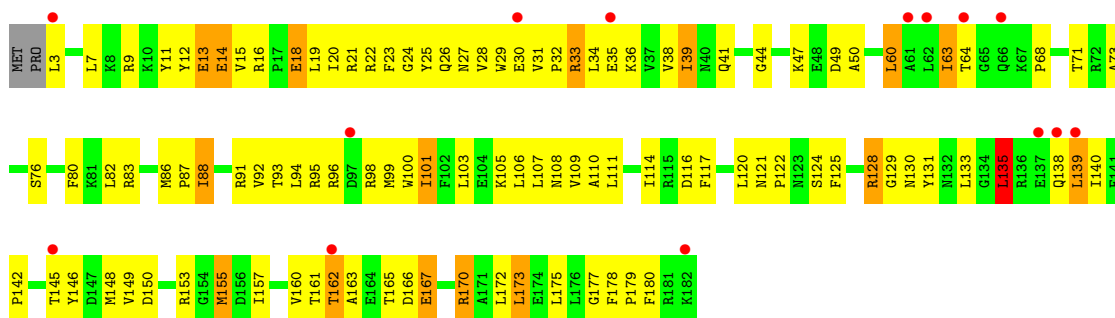
• Molecule 5: 50S Ribosomal Protein L4

Chain F:



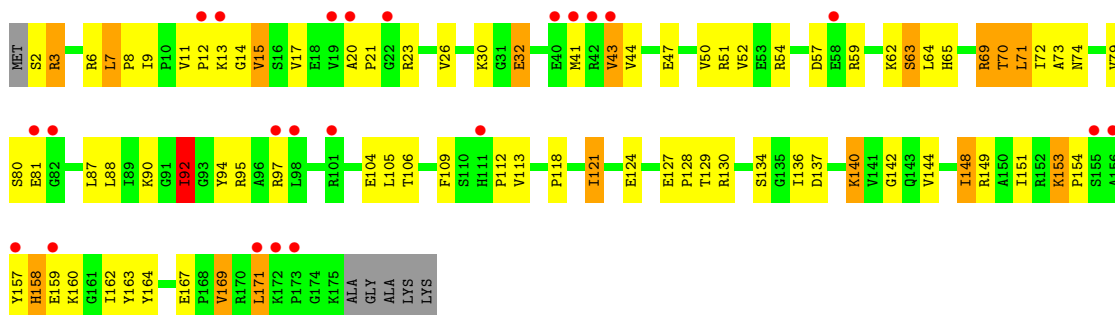
• Molecule 6: 50S Ribosomal Protein L5

Chain G:



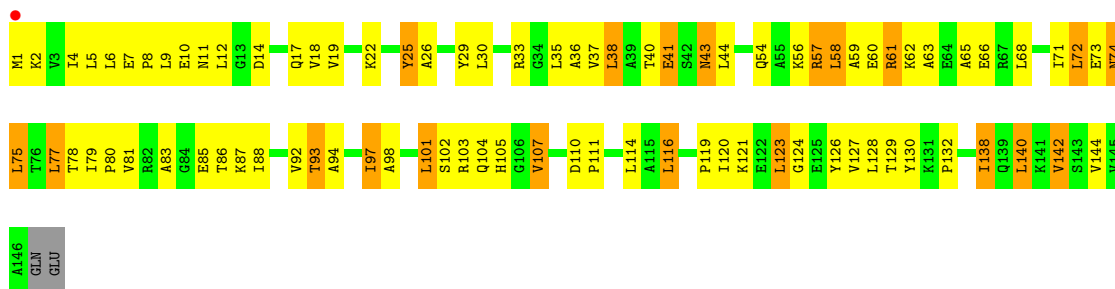
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



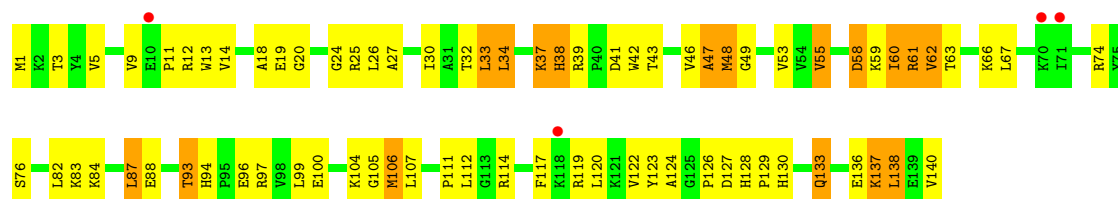
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



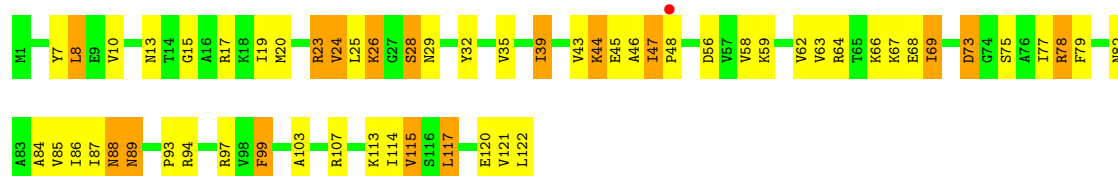
• Molecule 9: 50S Ribosomal Protein L13

Chain N:



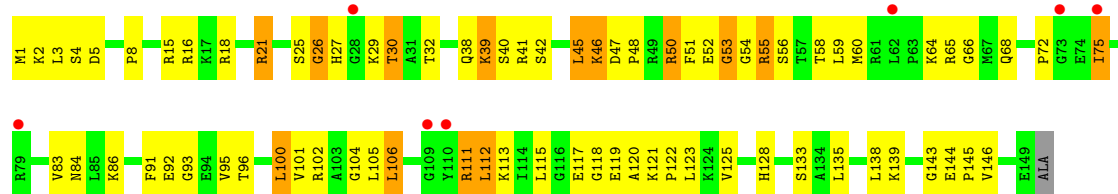
- Molecule 10: 50S Ribosomal Protein L14

Chain O:



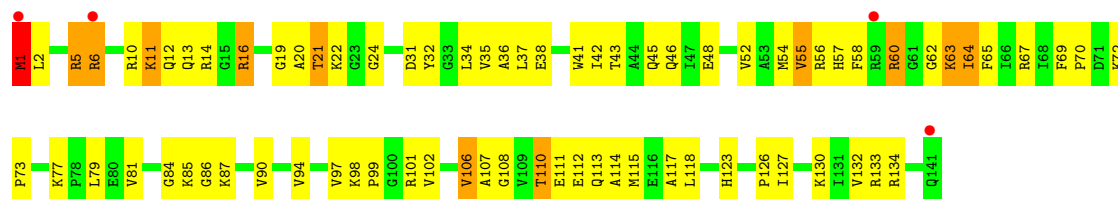
- Molecule 11: 50S Ribosomal Protein L15

Chain P:



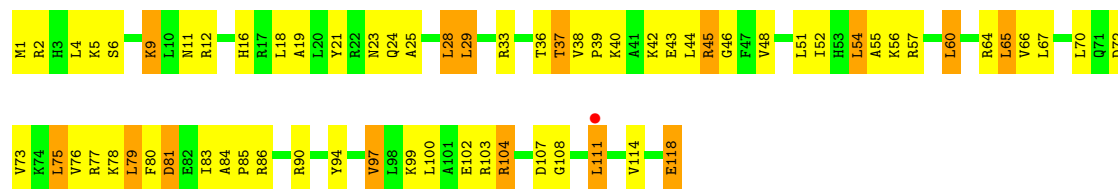
- Molecule 12: 50S Ribosomal Protein L16

Chain Q:



- Molecule 13: 50S Ribosomal Protein L17

Chain R:



- Molecule 14: 50S Ribosomal Protein L18

Chain S:

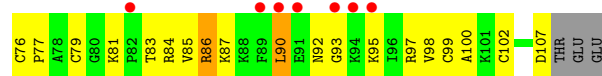
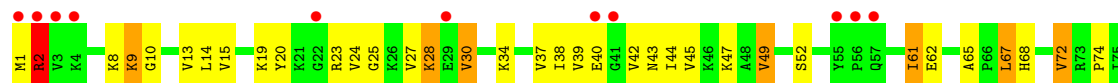






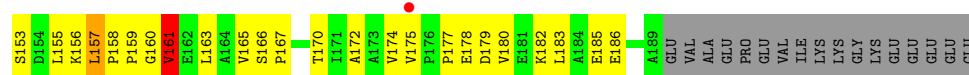
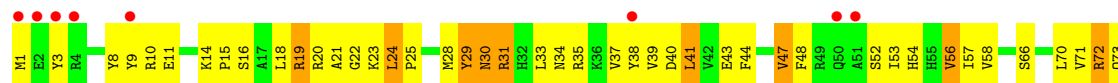
• Molecule 20: 50S Ribosomal Protein L24

Chain Y:



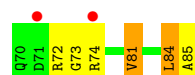
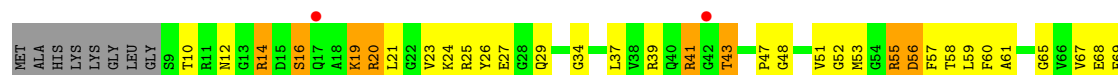
• Molecule 21: 50S Ribosomal Protein L25

Chain Z:



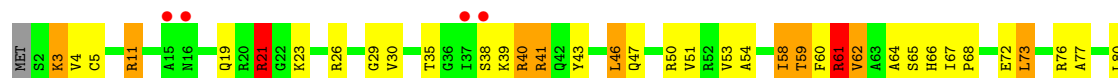
• Molecule 22: 50S Ribosomal Protein L27

Chain 0:



• Molecule 23: 50S Ribosomal Protein L28

Chain 1:



• Molecule 24: 50S Ribosomal Protein L29

Chain 2:



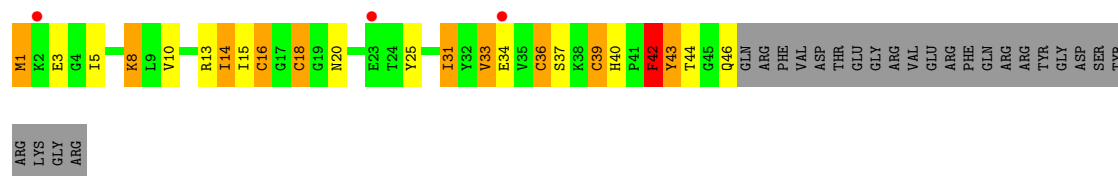
• Molecule 25: 50S Ribosomal Protein L30

Chain 3:



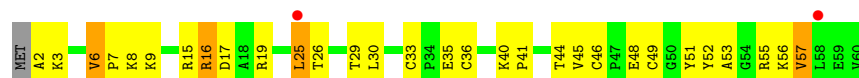
• Molecule 26: 50S Ribosomal Protein L31

Chain 4:



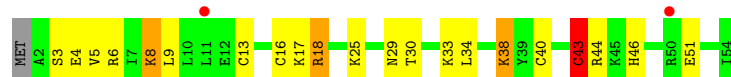
• Molecule 27: 50S Ribosomal Protein L32

Chain 5:



• Molecule 28: 50S Ribosomal Protein L33

Chain 6:



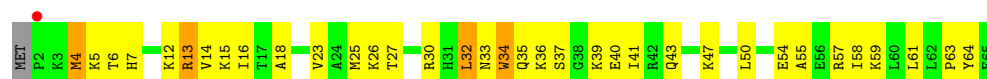
• Molecule 29: 50S Ribosomal Protein L34

Chain 7:



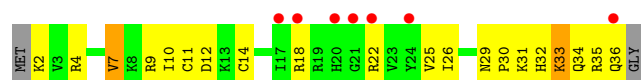
• Molecule 30: 50S Ribosomal Protein L35

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, α , β , γ	209.96Å 448.86Å 624.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 – 3.20 34.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.91-3.20) 99.8 (34.91-3.20)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.188 , 0.245 0.474 , 0.478	Depositor DCC
R_{free} test set	48022 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 956750 reflections	Xtriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	89631	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.06	69/65653 (0.1%)	1.63	1707/102473 (1.7%)
2	B	0.88	1/2878 (0.0%)	1.42	35/4490 (0.8%)
3	D	0.83	3/2186 (0.1%)	0.98	2/2944 (0.1%)
4	E	0.72	0/1588	0.90	1/2145 (0.0%)
5	F	0.64	0/1611	0.87	2/2180 (0.1%)
6	G	0.53	0/1385	0.83	1/1881 (0.1%)
7	H	0.53	0/1343	0.76	1/1820 (0.1%)
8	I	0.59	0/1072	0.85	1/1465 (0.1%)
9	N	0.63	0/1139	0.83	0/1538
10	O	0.74	0/933	0.93	2/1257 (0.2%)
11	P	0.65	0/1148	0.91	2/1529 (0.1%)
12	Q	0.67	0/1143	0.89	1/1527 (0.1%)
13	R	0.65	0/982	0.90	0/1312
14	S	0.55	0/883	0.87	0/1176
15	T	0.68	0/1072	0.81	0/1437
16	U	0.70	0/977	0.87	0/1301
17	V	0.67	0/781	0.86	1/1048 (0.1%)
18	W	0.77	0/887	0.90	2/1192 (0.2%)
19	X	0.75	0/746	0.88	1/1005 (0.1%)
20	Y	0.64	0/794	0.87	0/1067
21	Z	0.58	0/1483	0.80	0/2023
22	0	0.64	0/615	0.89	0/820
23	1	0.70	0/752	0.92	2/1003 (0.2%)
24	2	0.63	0/586	0.79	1/779 (0.1%)
25	3	0.57	0/458	0.79	0/616
26	4	0.66	0/358	0.82	1/487 (0.2%)
27	5	0.69	0/465	0.90	0/630
28	6	0.73	0/444	0.87	0/595
29	7	0.78	0/410	0.88	0/543
30	8	0.75	0/516	0.93	0/679
31	9	0.68	0/295	0.87	0/390
All	All	0.96	73/95583 (0.1%)	1.47	1763/143352 (1.2%)

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
4	E	0	1
5	F	0	1
6	G	0	3
7	H	0	1
10	O	0	1
11	P	0	1
12	Q	0	1
14	S	0	1
15	T	0	1
23	1	0	1
24	2	0	1
26	4	0	1
28	6	0	1
All	All	0	15

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	A	N9-C4	-9.93	1.31	1.37
1	A	590	A	N9-C4	-7.79	1.33	1.37
3	D	28	GLU	CG-CD	7.75	1.63	1.51
1	A	1332	G	N9-C4	-7.64	1.31	1.38
1	A	2565	A	N9-C4	-7.27	1.33	1.37
1	A	761	A	N7-C5	-7.20	1.34	1.39
1	A	2057	A	N3-C4	-7.13	1.30	1.34
1	A	2287	A	N9-C4	-7.08	1.33	1.37
1	A	271(M)	G	N9-C4	6.73	1.43	1.38
3	D	237	GLU	CB-CG	6.57	1.64	1.52
1	A	1698	A	N9-C4	-6.54	1.33	1.37
3	D	28	GLU	CB-CG	6.53	1.64	1.52
1	A	2207	G	N7-C5	-6.46	1.35	1.39
1	A	1689	A	N7-C5	-6.38	1.35	1.39
1	A	1782	C	N1-C6	-6.27	1.33	1.37
1	A	571	A	N9-C4	-6.26	1.34	1.37
1	A	1021	A	N9-C4	-6.25	1.34	1.37
1	A	945	A	C5-C6	-6.13	1.35	1.41
1	A	528	A	N3-C4	-6.07	1.31	1.34
1	A	2733	A	N9-C4	6.07	1.41	1.37
1	A	955	C	N3-C4	-5.96	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1785	A	N7-C5	-5.95	1.35	1.39
1	A	861	A	N9-C4	5.92	1.41	1.37
1	A	2207	G	N9-C8	-5.89	1.33	1.37
1	A	1332	G	C2-N3	-5.84	1.28	1.32
1	A	2451	A	N9-C4	-5.81	1.34	1.37
1	A	2598	A	C5-C6	-5.81	1.35	1.41
1	A	1625	C	N1-C6	-5.81	1.33	1.37
1	A	733	G	N7-C5	-5.74	1.35	1.39
1	A	1773	A	N3-C4	-5.71	1.31	1.34
1	A	753	C	N1-C6	-5.70	1.33	1.37
1	A	2689	U	C3'-O3'	5.69	1.50	1.42
1	A	1142(A)	A	N9-C4	-5.67	1.34	1.37
1	A	756	C	N1-C6	-5.65	1.33	1.37
1	A	2429	G	N7-C5	-5.59	1.35	1.39
1	A	1678	G	C6-N1	-5.54	1.35	1.39
1	A	141	A	C5-C6	-5.52	1.36	1.41
1	A	191	A	N7-C5	-5.50	1.35	1.39
1	A	265	A	N7-C5	-5.49	1.35	1.39
1	A	2581	G	C6-N1	-5.49	1.35	1.39
1	A	1698	A	C5-C6	-5.46	1.36	1.41
1	A	1776	G	N7-C5	-5.46	1.35	1.39
1	A	1332	G	N3-C4	-5.44	1.31	1.35
1	A	1669	A	N3-C4	-5.44	1.31	1.34
1	A	450	G	C6-O6	5.41	1.29	1.24
1	A	394	A	N7-C5	-5.34	1.36	1.39
1	A	1996	C	N1-C6	-5.31	1.33	1.37
1	A	1246	A	N9-C4	-5.30	1.34	1.37
1	A	2001	A	N9-C4	-5.30	1.34	1.37
1	A	1670	C	N1-C6	-5.29	1.33	1.37
1	A	733	G	C8-N7	-5.29	1.27	1.30
1	A	838	C	N3-C4	-5.24	1.30	1.33
1	A	188	G	N9-C4	-5.22	1.33	1.38
1	A	465	G	N7-C5	-5.18	1.36	1.39
1	A	676	A	C5-C4	5.18	1.42	1.38
1	A	204	A	N3-C4	-5.16	1.31	1.34
1	A	213	A	N9-C4	-5.16	1.34	1.37
1	A	2765	A	N7-C5	-5.16	1.36	1.39
1	A	1959	G	N3-C4	-5.14	1.31	1.35
2	B	53	A	N9-C4	5.13	1.41	1.37
1	A	509	C	N3-C4	-5.11	1.30	1.33
1	A	2821	A	N9-C4	-5.09	1.34	1.37
1	A	734	A	N9-C4	-5.09	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2897	U	N1-C2	5.08	1.43	1.38
1	A	699	A	C5-C4	-5.07	1.35	1.38
1	A	1790	C	N1-C6	-5.07	1.34	1.37
1	A	1638	C	N3-C4	-5.06	1.30	1.33
1	A	1675	C	N3-C4	-5.06	1.30	1.33
1	A	84	A	N9-C4	-5.04	1.34	1.37
1	A	191	A	C5-C6	-5.02	1.36	1.41
1	A	530	G	N9-C8	5.02	1.41	1.37
1	A	1992	G	C3'-O3'	5.02	1.49	1.42
1	A	754	C	N1-C6	-5.01	1.34	1.37

All (1763) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1332	G	C2-N3-C4	-18.31	102.74	111.90
1	A	1332	G	N3-C4-C5	16.91	137.05	128.60
1	A	1332	G	N3-C4-N9	-16.60	116.04	126.00
1	A	528	A	C2-N3-C4	-15.85	102.67	110.60
1	A	945	A	N1-C6-N6	15.56	127.94	118.60
1	A	141	A	N7-C8-N9	14.62	121.11	113.80
1	A	141	A	C5-N7-C8	-13.66	97.07	103.90
1	A	141	A	N1-C6-N6	13.62	126.77	118.60
1	A	856	C	C6-N1-C2	-12.94	115.12	120.30
1	A	2286	A	N1-C6-N6	12.83	126.30	118.60
1	A	1698	A	C2-N3-C4	-12.49	104.36	110.60
1	A	450	G	C5-C6-N1	-12.47	105.26	111.50
1	A	141	A	C6-C5-N7	-12.21	123.75	132.30
1	A	1558	A	C2-N3-C4	-12.18	104.51	110.60
1	A	271(M)	G	N3-C4-N9	12.07	133.24	126.00
1	A	975	C	C2-N1-C1'	11.84	131.82	118.80
2	B	115	G	C8-N9-C4	11.40	110.96	106.40
1	A	2829	C	C6-N1-C2	11.37	124.85	120.30
1	A	1653	G	N3-C4-N9	11.25	132.75	126.00
1	A	450	G	C4-C5-N7	-11.20	106.32	110.80
1	A	1021	A	C2-N3-C4	-11.18	105.01	110.60
1	A	1607	C	N1-C2-O2	11.02	125.51	118.90
1	A	945	A	C6-C5-N7	-10.97	124.62	132.30
1	A	2326	C	N3-C4-C5	-10.95	117.52	121.90
2	B	6	C	C6-N1-C2	10.95	124.68	120.30
1	A	2286	A	C6-C5-N7	-10.84	124.71	132.30
1	A	141	A	C4-C5-N7	10.75	116.08	110.70
1	A	994	C	C6-N1-C1'	-10.61	108.07	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1210	A	N1-C6-N6	10.55	124.93	118.60
1	A	2628	C	C6-N1-C2	10.54	124.52	120.30
1	A	2587	A	N1-C6-N6	10.46	124.87	118.60
1	A	932	G	N3-C4-N9	-10.45	119.73	126.00
1	A	141	A	C8-N9-C4	-10.33	101.67	105.80
1	A	676	A	C2-N3-C4	-10.30	105.45	110.60
1	A	748	G	N1-C6-O6	-10.28	113.73	119.90
1	A	1653	G	C8-N9-C1'	-10.14	113.81	127.00
1	A	1703	G	N1-C6-O6	10.14	125.99	119.90
1	A	945	A	N9-C4-C5	-10.04	101.78	105.80
1	A	1979	C	C6-N1-C2	-10.03	116.29	120.30
1	A	566	U	C5-C6-N1	-9.97	117.72	122.70
1	A	994	C	C2-N1-C1'	9.97	129.76	118.80
1	A	1332	G	N3-C2-N2	-9.95	112.94	119.90
1	A	945	A	C4-C5-N7	9.95	115.67	110.70
1	A	1204	A	C2-N3-C4	-9.91	105.65	110.60
1	A	1204	A	N1-C6-N6	9.89	124.53	118.60
1	A	271(M)	G	N3-C4-C5	-9.86	123.67	128.60
1	A	668	G	C2-N3-C4	-9.85	106.97	111.90
1	A	2791	C	C6-N1-C2	-9.82	116.37	120.30
1	A	528	A	N1-C2-N3	9.81	134.21	129.30
1	A	945	A	C2-N3-C4	-9.81	105.70	110.60
1	A	2751	G	N3-C4-N9	9.79	131.88	126.00
1	A	1932	A	C8-N9-C4	-9.79	101.89	105.80
1	A	2056	G	N1-C6-O6	9.78	125.77	119.90
1	A	1332	G	C8-N9-C1'	9.76	139.69	127.00
1	A	676	A	C5-N7-C8	-9.74	99.03	103.90
1	A	271(M)	G	C8-N9-C1'	-9.72	114.37	127.00
1	A	1914	C	N3-C2-O2	-9.71	115.10	121.90
1	A	480	A	C8-N9-C4	-9.71	101.92	105.80
1	A	271(M)	G	C4-N9-C1'	9.70	139.12	126.50
1	A	459	U	N3-C4-O4	-9.63	112.66	119.40
1	A	330	A	N1-C6-N6	9.58	124.35	118.60
1	A	1698	A	C5-N7-C8	-9.53	99.14	103.90
1	A	504	U	C2-N1-C1'	9.49	129.09	117.70
1	A	2502	G	C6-C5-N7	-9.47	124.72	130.40
1	A	1807	G	C8-N9-C4	9.45	110.18	106.40
1	A	1269	A	N1-C6-N6	9.36	124.22	118.60
1	A	2447	G	C5-C6-O6	-9.36	122.99	128.60
1	A	1899	G	C5-C6-O6	-9.34	122.99	128.60
1	A	1269	A	C8-N9-C4	9.33	109.53	105.80
1	A	1327	C	C6-N1-C2	-9.31	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1269	A	N9-C4-C5	-9.30	102.08	105.80
1	A	236	C	C6-N1-C2	9.29	124.02	120.30
1	A	1252	G	C5-C6-O6	-9.27	123.04	128.60
1	A	975	C	C6-N1-C1'	-9.24	109.72	120.80
1	A	2599	G	C4-C5-N7	-9.22	107.11	110.80
1	A	736	C	N3-C2-O2	9.22	128.35	121.90
1	A	337	C	C5-C6-N1	-9.20	116.40	121.00
1	A	1558	A	C5-C6-N1	-9.20	113.10	117.70
1	A	772	C	N3-C4-C5	9.19	125.58	121.90
1	A	22	C	C6-N1-C2	9.18	123.97	120.30
1	A	1813	G	C5-C6-O6	-9.17	123.10	128.60
1	A	2689	U	C5-C6-N1	-9.15	118.12	122.70
1	A	2686	G	C8-N9-C4	-9.12	102.75	106.40
1	A	2058	A	C8-N9-C4	-9.12	102.15	105.80
1	A	2056	G	C5-C6-O6	-9.12	123.13	128.60
1	A	2575	C	N1-C2-O2	9.12	124.37	118.90
1	A	298	G	N1-C6-O6	9.06	125.34	119.90
1	A	2598	A	N1-C6-N6	9.05	124.03	118.60
1	A	530	G	C8-N9-C4	-9.05	102.78	106.40
1	A	1332	G	N1-C2-N3	9.04	129.32	123.90
1	A	1999	C	C6-N1-C2	9.03	123.91	120.30
1	A	2447	G	N1-C6-O6	9.00	125.30	119.90
1	A	2751	G	C4-N9-C1'	8.99	138.19	126.50
1	A	1827	C	N3-C2-O2	-8.99	115.61	121.90
1	A	265	A	C6-C5-N7	-8.98	126.02	132.30
1	A	1210	A	C5-N7-C8	-8.96	99.42	103.90
1	A	1698	A	C4-C5-N7	8.96	115.18	110.70
1	A	461	C	N1-C2-O2	-8.95	113.53	118.90
1	A	1645	G	N1-C6-O6	-8.93	114.55	119.90
1	A	71	A	N7-C8-N9	8.91	118.26	113.80
1	A	912	C	C6-N1-C2	-8.90	116.74	120.30
1	A	962	G	C8-N9-C4	-8.87	102.85	106.40
1	A	2253	G	N9-C4-C5	-8.86	101.85	105.40
1	A	145	G	C8-N9-C4	8.86	109.94	106.40
1	A	528	A	N3-C4-N9	-8.82	120.35	127.40
1	A	933	A	N7-C8-N9	8.76	118.18	113.80
1	A	2828	C	C6-N1-C2	8.74	123.80	120.30
2	B	54	G	C8-N9-C4	-8.74	102.91	106.40
1	A	1653	G	C4-N9-C1'	8.67	137.78	126.50
1	A	1830	C	N3-C4-C5	8.65	125.36	121.90
1	A	1332	G	C4-N9-C1'	-8.62	115.30	126.50
1	A	2457	U	N3-C2-O2	-8.60	116.18	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2356	C	N1-C2-O2	-8.60	113.74	118.90
1	A	2023	G	N3-C4-C5	-8.59	124.31	128.60
1	A	1703	G	C5-C6-O6	-8.58	123.45	128.60
1	A	994	C	N1-C2-O2	8.55	124.03	118.90
1	A	991	C	C6-N1-C2	-8.55	116.88	120.30
1	A	760	G	C8-N9-C4	-8.54	102.98	106.40
1	A	1353	A	C8-N9-C4	-8.53	102.39	105.80
1	A	2387	U	C5-C6-N1	-8.50	118.45	122.70
1	A	2751	G	C8-N9-C1'	-8.50	115.95	127.00
1	A	733	G	C6-C5-N7	-8.48	125.31	130.40
1	A	528	A	N3-C4-C5	8.46	132.72	126.80
1	A	92	A	N7-C8-N9	8.45	118.03	113.80
1	A	706	A	C8-N9-C4	8.43	109.17	105.80
1	A	765	G	N1-C6-O6	8.42	124.95	119.90
1	A	1142	U	C2-N1-C1'	8.42	127.80	117.70
1	A	1698	A	N3-C4-C5	8.42	132.69	126.80
1	A	1966	A	N1-C6-N6	-8.42	113.55	118.60
1	A	2396	G	N1-C6-O6	8.41	124.95	119.90
1	A	2253	G	N1-C6-O6	8.41	124.94	119.90
1	A	528	A	C5-N7-C8	-8.41	99.70	103.90
1	A	1332	G	C5-N7-C8	-8.40	100.10	104.30
1	A	1769	G	N1-C6-O6	8.39	124.94	119.90
1	A	2259	G	N1-C6-O6	8.38	124.92	119.90
1	A	265	A	N7-C8-N9	8.37	117.99	113.80
1	A	337	C	N3-C4-N4	-8.37	112.14	118.00
1	A	250	G	C8-N9-C4	-8.37	103.05	106.40
1	A	590	A	C2-N3-C4	-8.36	106.42	110.60
1	A	945	A	C5-C6-N6	-8.36	117.02	123.70
1	A	566	U	C6-N1-C2	8.35	126.01	121.00
1	A	1558	A	N1-C6-N6	8.35	123.61	118.60
1	A	1653	G	N9-C4-C5	-8.35	102.06	105.40
1	A	481	G	C8-N9-C4	-8.35	103.06	106.40
1	A	1914	C	N1-C2-O2	8.34	123.90	118.90
1	A	2563	U	C5-C6-N1	-8.34	118.53	122.70
1	A	1767	C	C5-C6-N1	-8.33	116.83	121.00
1	A	71	A	C5-N7-C8	-8.31	99.75	103.90
1	A	1313	U	C6-N1-C2	-8.30	116.02	121.00
1	A	2286	A	C5-N7-C8	-8.27	99.77	103.90
1	A	1558	A	N1-C2-N3	8.27	133.43	129.30
1	A	583	G	N1-C6-O6	8.26	124.86	119.90
1	A	1558	A	C6-C5-N7	-8.26	126.52	132.30
1	A	2286	A	C4-C5-C6	8.25	121.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	C	N3-C2-O2	-8.23	116.14	121.90
1	A	645	C	C2-N1-C1'	8.23	127.86	118.80
1	A	1776	G	N1-C6-O6	8.22	124.83	119.90
1	A	1257	C	C6-N1-C2	-8.22	117.01	120.30
1	A	330	A	C4-C5-N7	8.20	114.80	110.70
1	A	467	G	C8-N9-C4	8.18	109.67	106.40
1	A	2286	A	C5-C6-N1	-8.18	113.61	117.70
1	A	2206	G	C8-N9-C4	8.16	109.66	106.40
1	A	1252	G	N1-C6-O6	8.14	124.79	119.90
1	A	1813	G	N1-C6-O6	8.14	124.79	119.90
1	A	932	G	C6-C5-N7	8.14	135.28	130.40
1	A	1998	G	N7-C8-N9	-8.14	109.03	113.10
1	A	216	A	C2-N3-C4	-8.13	106.54	110.60
1	A	329	G	N3-C4-C5	-8.12	124.54	128.60
1	A	1314	C	C2-N1-C1'	8.11	127.72	118.80
1	A	2538	C	C6-N1-C2	8.10	123.54	120.30
1	A	127	A	N1-C6-N6	8.10	123.46	118.60
1	A	1210	A	C6-C5-N7	-8.09	126.64	132.30
1	A	1307	A	N1-C6-N6	-8.08	113.75	118.60
1	A	236	C	N3-C4-C5	8.08	125.13	121.90
1	A	1204	A	C4-C5-N7	8.08	114.74	110.70
1	A	530	G	N1-C6-O6	-8.06	115.06	119.90
1	A	1670	C	C4-C5-C6	8.06	121.43	117.40
1	A	2765	A	C8-N9-C4	-8.06	102.58	105.80
1	A	1210	A	N7-C8-N9	8.06	117.83	113.80
1	A	2103	C	C5-C4-N4	8.06	125.84	120.20
1	A	737	C	C6-N1-C2	8.05	123.52	120.30
1	A	671	C	N3-C4-C5	-8.04	118.68	121.90
1	A	2287	A	C2-N3-C4	-8.01	106.59	110.60
1	A	2751	G	N3-C4-C5	-8.01	124.60	128.60
1	A	1553	A	C8-N9-C4	-8.00	102.60	105.80
1	A	265	A	N1-C6-N6	7.99	123.39	118.60
1	A	1254	A	C8-N9-C4	-7.99	102.61	105.80
1	A	1767	C	C2-N3-C4	-7.98	115.91	119.90
1	A	2897	U	C2-N1-C1'	7.97	127.27	117.70
1	A	1791	A	C8-N9-C4	-7.95	102.62	105.80
1	A	2498	C	C6-N1-C2	7.94	123.48	120.30
2	B	43	C	C6-N1-C2	-7.94	117.12	120.30
1	A	972	G	C5-C6-O6	7.94	133.36	128.60
1	A	788	A	N1-C6-N6	7.93	123.36	118.60
1	A	888	C	C6-N1-C2	-7.93	117.13	120.30
1	A	1302	A	N1-C6-N6	-7.92	113.85	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	A	C5-C6-N1	-7.92	113.74	117.70
1	A	2286	A	N7-C8-N9	7.92	117.76	113.80
1	A	975	C	N1-C2-O2	7.92	123.65	118.90
1	A	2035	G	C4-C5-N7	-7.91	107.64	110.80
1	A	733	G	N1-C6-O6	7.87	124.62	119.90
1	A	1914	C	C6-N1-C2	-7.87	117.15	120.30
1	A	2326	C	C6-N1-C2	-7.87	117.15	120.30
1	A	2412	A	N1-C6-N6	-7.84	113.89	118.60
1	A	2396	G	C4-C5-N7	7.84	113.94	110.80
1	A	811	U	N3-C4-O4	-7.84	113.91	119.40
1	A	2452	C	N3-C4-N4	7.84	123.49	118.00
1	A	676	A	N7-C8-N9	7.83	117.72	113.80
1	A	504	U	C5-C6-N1	7.83	126.61	122.70
1	A	92	A	C8-N9-C4	-7.83	102.67	105.80
1	A	676	A	C4-C5-N7	7.83	114.61	110.70
1	A	2876	G	C5-C6-O6	-7.82	123.91	128.60
1	A	2253	G	C8-N9-C4	7.82	109.53	106.40
1	A	71	A	C6-C5-N7	-7.81	126.83	132.30
1	A	736	C	N1-C2-O2	-7.81	114.21	118.90
1	A	2056	G	C6-C5-N7	-7.81	125.71	130.40
1	A	1998	G	C8-N9-C4	7.80	109.52	106.40
1	A	450	G	N3-C2-N2	-7.80	114.44	119.90
1	A	798	G	N3-C2-N2	-7.80	114.44	119.90
1	A	2439	A	C8-N9-C4	-7.80	102.68	105.80
1	A	533	G	C2-N3-C4	-7.80	108.00	111.90
1	A	2218	U	N1-C2-O2	7.79	128.25	122.80
1	A	102	G	C8-N9-C4	-7.79	103.28	106.40
2	B	54	G	N7-C8-N9	7.79	116.99	113.10
1	A	1653	G	N1-C2-N2	-7.79	109.19	116.20
1	A	1934	C	C6-N1-C2	7.77	123.41	120.30
1	A	686	G	C2-N3-C4	-7.76	108.02	111.90
1	A	1776	G	C5-C6-O6	-7.76	123.94	128.60
1	A	932	G	C5-C6-O6	7.75	133.25	128.60
1	A	2877	G	N1-C6-O6	7.75	124.55	119.90
1	A	1992	G	C8-N9-C4	-7.75	103.30	106.40
1	A	540	C	C6-N1-C2	-7.74	117.21	120.30
1	A	2599	G	N9-C4-C5	7.74	108.49	105.40
1	A	2848	G	C4-C5-N7	-7.74	107.71	110.80
1	A	811	U	C5-C4-O4	7.71	130.53	125.90
1	A	2224	G	C5-C6-N1	-7.71	107.64	111.50
1	A	102	G	N9-C4-C5	7.71	108.48	105.40
1	A	1579	A	N1-C6-N6	7.71	123.22	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	811	U	C5-C6-N1	-7.71	118.85	122.70
1	A	1313	U	C2-N1-C1'	7.70	126.94	117.70
1	A	924	C	C6-N1-C2	7.69	123.38	120.30
1	A	2235	G	N1-C6-O6	7.69	124.51	119.90
1	A	2473	U	C2-N1-C1'	7.69	126.92	117.70
1	A	933	A	C5-N7-C8	-7.68	100.06	103.90
1	A	949	C	N1-C2-O2	-7.68	114.29	118.90
1	A	265	A	C5-N7-C8	-7.66	100.07	103.90
1	A	1294	U	N1-C2-O2	-7.66	117.44	122.80
1	A	1377	G	N3-C4-N9	7.66	130.60	126.00
1	A	298	G	N3-C4-C5	7.66	132.43	128.60
1	A	204	A	N9-C4-C5	7.63	108.85	105.80
1	A	735	A	C8-N9-C4	7.63	108.85	105.80
1	A	1962	C	N3-C2-O2	7.63	127.24	121.90
1	A	1313	U	C5-C6-N1	7.63	126.51	122.70
1	A	1677	A	C8-N9-C4	7.62	108.85	105.80
1	A	1698	A	N1-C6-N6	7.62	123.17	118.60
1	A	676	A	N1-C6-N6	7.61	123.17	118.60
1	A	1327	C	N1-C2-O2	-7.61	114.33	118.90
1	A	2598	A	C4-C5-N7	7.60	114.50	110.70
1	A	22	C	C5-C6-N1	-7.60	117.20	121.00
1	A	1204	A	C5-N7-C8	-7.60	100.10	103.90
1	A	380	U	N3-C4-O4	7.57	124.69	119.40
1	A	330	A	C5-N7-C8	-7.56	100.12	103.90
1	A	1021	A	N1-C2-N3	7.54	133.07	129.30
1	A	2501	C	C6-N1-C2	7.54	123.31	120.30
1	A	1204	A	C6-C5-N7	-7.53	127.03	132.30
1	A	2686	G	N9-C4-C5	7.53	108.41	105.40
1	A	141	A	C2-N3-C4	-7.52	106.84	110.60
1	A	2207	G	N7-C8-N9	7.49	116.84	113.10
1	A	2224	G	N1-C6-O6	7.48	124.39	119.90
1	A	2235	G	N7-C8-N9	7.46	116.83	113.10
1	A	2207	G	C6-C5-N7	-7.46	125.93	130.40
1	A	36	G	N1-C6-O6	7.45	124.37	119.90
1	A	1123	C	C6-N1-C2	7.45	123.28	120.30
1	A	391	G	C6-C5-N7	-7.44	125.94	130.40
1	A	980	A	N1-C6-N6	7.43	123.06	118.60
1	A	1314	C	C6-N1-C1'	-7.43	111.89	120.80
1	A	932	G	C4-N9-C1'	-7.43	116.84	126.50
1	A	594	U	N1-C2-O2	-7.41	117.61	122.80
1	A	932	G	C8-N9-C1'	7.41	136.64	127.00
1	A	645	C	C5-C6-N1	7.41	124.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1552	G	C4-C5-N7	-7.41	107.84	110.80
1	A	972	G	N1-C6-O6	-7.40	115.46	119.90
1	A	90	U	C5-C6-N1	7.40	126.40	122.70
1	A	2207	G	N1-C6-O6	7.40	124.34	119.90
1	A	2599	G	N3-C2-N2	-7.39	114.72	119.90
1	A	1828	G	N3-C4-C5	-7.39	124.91	128.60
1	A	1204	A	N9-C4-C5	-7.38	102.85	105.80
1	A	298	G	C5-C6-O6	-7.37	124.18	128.60
1	A	1937	A	N1-C6-N6	7.36	123.02	118.60
1	A	1293	C	C4-C5-C6	-7.36	113.72	117.40
1	A	837	C	C6-N1-C2	-7.36	117.36	120.30
1	A	337	C	C2-N3-C4	-7.34	116.23	119.90
23	1	61	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	923	C	C6-N1-C2	-7.34	117.36	120.30
1	A	2877	G	C2-N3-C4	-7.34	108.23	111.90
1	A	932	G	N3-C4-C5	7.33	132.27	128.60
1	A	786	C	C6-N1-C2	7.33	123.23	120.30
1	A	2412	A	N9-C4-C5	7.33	108.73	105.80
1	A	2589	A	C8-N9-C4	7.33	108.73	105.80
1	A	265	A	C2-N3-C4	-7.32	106.94	110.60
1	A	2644	G	C5-C6-O6	7.32	132.99	128.60
1	A	2700	C	C6-N1-C2	7.31	123.23	120.30
1	A	2700	C	C5-C6-N1	-7.31	117.34	121.00
1	A	1210	A	C4-C5-N7	7.31	114.36	110.70
1	A	620	G	C8-N9-C4	-7.30	103.48	106.40
1	A	748	G	C5-C6-N1	7.30	115.15	111.50
1	A	1983	C	C5-C6-N1	-7.30	117.35	121.00
1	A	614	U	C5-C4-O4	7.29	130.27	125.90
1	A	178	G	N9-C4-C5	7.27	108.31	105.40
1	A	1926	U	N3-C2-O2	-7.27	117.11	122.20
1	A	2733	A	C8-N9-C4	-7.26	102.89	105.80
19	X	57	LEU	CA-CB-CG	7.26	132.00	115.30
1	A	1293	C	C5-C4-N4	-7.25	115.12	120.20
1	A	80	G	N3-C4-C5	-7.25	124.97	128.60
1	A	2755	C	C5-C6-N1	7.25	124.62	121.00
1	A	303	U	C5-C6-N1	-7.24	119.08	122.70
1	A	2501	C	N3-C4-C5	7.24	124.80	121.90
1	A	188	G	C4-C5-N7	7.24	113.70	110.80
1	A	778	G	C2-N3-C4	-7.24	108.28	111.90
1	A	933	A	C8-N9-C4	-7.23	102.91	105.80
1	A	399	G	C5-C6-O6	-7.23	124.26	128.60
1	A	1618	A	C8-N9-C4	-7.23	102.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	A	C8-N9-C4	-7.22	102.91	105.80
1	A	458	G	N1-C6-O6	-7.22	115.57	119.90
1	A	1965	C	C6-N1-C2	7.22	123.19	120.30
1	A	2624	G	N1-C6-O6	7.21	124.23	119.90
1	A	2609	U	N1-C2-N3	7.20	119.22	114.90
1	A	1960	A	C8-N9-C4	7.20	108.68	105.80
1	A	2058	A	N7-C8-N9	7.19	117.39	113.80
1	A	975	C	N3-C2-O2	-7.19	116.87	121.90
1	A	2595	G	C5-N7-C8	-7.18	100.71	104.30
1	A	1820	U	C6-N1-C2	7.18	125.31	121.00
1	A	1607	C	C6-N1-C2	7.17	123.17	120.30
1	A	728	G	C8-N9-C4	7.17	109.27	106.40
1	A	1970	A	C8-N9-C4	-7.17	102.93	105.80
1	A	1670	C	N3-C4-C5	-7.17	119.03	121.90
1	A	271(O)	C	N1-C2-O2	7.17	123.20	118.90
1	A	1353	A	N9-C4-C5	7.16	108.67	105.80
1	A	1932	A	N7-C8-N9	7.16	117.38	113.80
1	A	2781	A	N1-C6-N6	-7.16	114.31	118.60
1	A	450	G	C4-C5-C6	7.15	123.09	118.80
1	A	1223	G	N3-C4-N9	-7.15	121.71	126.00
1	A	2607	G	N3-C4-N9	7.14	130.29	126.00
1	A	820	A	N1-C6-N6	-7.14	114.32	118.60
1	A	1934	C	N3-C4-C5	7.13	124.75	121.90
1	A	1769	G	C8-N9-C4	-7.12	103.55	106.40
1	A	2373	G	C8-N9-C4	7.12	109.25	106.40
1	A	2755	C	C2-N1-C1'	7.12	126.63	118.80
1	A	1979	C	N3-C4-C5	-7.12	119.05	121.90
1	A	1776	G	C6-C5-N7	-7.12	126.13	130.40
1	A	2423	U	C2-N1-C1'	-7.10	109.18	117.70
1	A	1273	U	C5-C6-N1	-7.10	119.15	122.70
1	A	2286	A	C2-N3-C4	-7.10	107.05	110.60
1	A	512	G	N9-C4-C5	7.09	108.24	105.40
1	A	1135	C	N1-C2-O2	7.09	123.16	118.90
1	A	1999	C	C5-C6-N1	-7.09	117.45	121.00
1	A	747	U	C2-N1-C1'	7.08	126.20	117.70
1	A	1830	C	C4-C5-C6	-7.08	113.86	117.40
1	A	1355	G	N1-C6-O6	7.07	124.14	119.90
1	A	803	U	N3-C2-O2	-7.07	117.25	122.20
1	A	113	G	N3-C4-C5	7.06	132.13	128.60
1	A	2512	C	N1-C2-O2	-7.06	114.67	118.90
1	A	1201	C	C6-N1-C2	7.05	123.12	120.30
1	A	1531	C	C6-N1-C2	-7.05	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	45	LEU	CA-CB-CG	-7.04	99.10	115.30
1	A	774	A	C8-N9-C4	-7.04	102.98	105.80
1	A	991	C	C5-C6-N1	7.03	124.52	121.00
1	A	12	U	N1-C2-O2	7.03	127.72	122.80
1	A	2023	G	N3-C4-N9	7.03	130.22	126.00
1	A	303	U	C6-N1-C2	7.02	125.21	121.00
1	A	2583	G	N1-C6-O6	-7.02	115.69	119.90
1	A	2033	A	N1-C6-N6	-7.01	114.39	118.60
1	A	2714	G	N1-C6-O6	7.01	124.11	119.90
1	A	2206	G	N3-C4-C5	7.01	132.10	128.60
1	A	265	A	C4-C5-C6	7.00	120.50	117.00
1	A	503	A	N1-C6-N6	-7.00	114.40	118.60
1	A	2624	G	C5-C6-O6	-6.99	124.41	128.60
1	A	1273	U	C2-N3-C4	-6.99	122.81	127.00
1	A	1798	U	C5-C6-N1	-6.98	119.21	122.70
1	A	2326	C	N1-C2-O2	-6.98	114.71	118.90
1	A	2238	G	N1-C6-O6	6.98	124.09	119.90
1	A	1408	C	N3-C4-N4	6.98	122.88	118.00
1	A	1235	G	C5-C6-O6	6.97	132.78	128.60
1	A	1425	G	C5-C6-N1	-6.97	108.01	111.50
1	A	2587	A	C6-C5-N7	-6.97	127.42	132.30
1	A	972	G	C8-N9-C4	-6.97	103.61	106.40
1	A	1553	A	N1-C6-N6	-6.96	114.42	118.60
1	A	1672	C	C6-N1-C2	6.96	123.08	120.30
1	A	51	G	N3-C4-C5	-6.96	125.12	128.60
1	A	783	A	C2-N3-C4	6.95	114.08	110.60
1	A	1558	A	C4-C5-C6	6.95	120.48	117.00
1	A	1926	U	N1-C2-N3	6.95	119.07	114.90
1	A	2253	G	C5-C6-O6	-6.95	124.43	128.60
1	A	271(M)	G	C6-C5-N7	-6.94	126.23	130.40
1	A	2689	U	N1-C2-N3	6.94	119.06	114.90
1	A	2286	A	C4-C5-N7	6.93	114.17	110.70
1	A	2039	C	C2-N1-C1'	6.93	126.43	118.80
1	A	459	U	C5-C4-O4	6.93	130.06	125.90
1	A	1905	C	N3-C2-O2	-6.93	117.05	121.90
1	A	1372	U	C2-N1-C1'	6.92	126.00	117.70
1	A	1531	C	C5-C6-N1	6.91	124.46	121.00
1	A	2732	G	C5-C6-N1	6.91	114.95	111.50
1	A	2695	C	N3-C4-C5	6.91	124.66	121.90
1	A	399	G	N1-C6-O6	6.90	124.04	119.90
1	A	2063	C	N1-C2-O2	-6.90	114.76	118.90
1	A	2622	C	C6-N1-C2	6.89	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2877	G	N3-C4-C5	6.88	132.04	128.60
1	A	2324	C	C6-N1-C2	6.88	123.05	120.30
1	A	71	A	N1-C6-N6	6.87	122.72	118.60
1	A	2039	C	C6-N1-C2	-6.86	117.56	120.30
1	A	932	G	N1-C6-O6	-6.86	115.78	119.90
1	A	1653	G	N3-C4-C5	-6.86	125.17	128.60
2	B	70	C	C6-N1-C2	-6.86	117.56	120.30
1	A	1845	G	N3-C2-N2	-6.85	115.10	119.90
1	A	391	G	C4-N9-C1'	6.84	135.39	126.50
1	A	265	A	C5-C6-N1	-6.84	114.28	117.70
1	A	1026	U	C2-N1-C1'	6.83	125.90	117.70
1	A	2007	C	C6-N1-C2	6.83	123.03	120.30
1	A	2340	G	N3-C4-C5	6.83	132.02	128.60
1	A	2689	U	C2-N3-C4	-6.83	122.90	127.00
1	A	761	A	C4-C5-C6	6.83	120.42	117.00
1	A	1964	G	N3-C4-N9	6.83	130.10	126.00
1	A	1791	A	C2-N3-C4	6.83	114.01	110.60
1	A	1963	U	C2-N1-C1'	6.83	125.89	117.70
1	A	1962	C	N1-C2-O2	-6.83	114.81	118.90
1	A	530	G	N7-C8-N9	6.82	116.51	113.10
1	A	1698	A	C5-C6-N1	-6.82	114.29	117.70
1	A	1552	G	N1-C6-O6	-6.81	115.81	119.90
1	A	972	G	N9-C4-C5	6.81	108.12	105.40
1	A	1703	G	C6-C5-N7	-6.81	126.31	130.40
17	V	35	LEU	CA-CB-CG	6.81	130.96	115.30
1	A	1294	U	N1-C2-N3	6.80	118.98	114.90
1	A	1814	G	C8-N9-C4	-6.80	103.68	106.40
1	A	1377	G	N3-C4-C5	-6.79	125.20	128.60
1	A	2618	G	C5-C6-O6	6.79	132.67	128.60
1	A	461	C	N3-C4-C5	-6.78	119.19	121.90
1	A	429	A	N1-C6-N6	6.78	122.67	118.60
1	A	2848	G	C5-C6-O6	6.78	132.67	128.60
1	A	51	G	N1-C6-O6	-6.77	115.84	119.90
1	A	1377	G	C8-N9-C1'	-6.76	118.20	127.00
1	A	2080	G	C8-N9-C4	-6.76	103.69	106.40
1	A	2103	C	N3-C4-N4	-6.76	113.27	118.00
1	A	530	G	C5-N7-C8	-6.75	100.92	104.30
1	A	668	G	N1-C2-N3	6.75	127.95	123.90
1	A	2628	C	C5-C6-N1	-6.75	117.62	121.00
1	A	2599	G	C5-C6-O6	6.75	132.65	128.60
1	A	1332	G	C5-C6-N1	-6.74	108.13	111.50
1	A	2089	U	N1-C2-O2	-6.74	118.08	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	G	C4-C5-N7	6.74	113.50	110.80
1	A	2519	U	C6-N1-C2	6.74	125.04	121.00
1	A	22	C	N3-C4-C5	6.73	124.59	121.90
1	A	1958	C	C6-N1-C2	6.73	122.99	120.30
1	A	445	C	N1-C2-O2	-6.72	114.87	118.90
1	A	1695	G	N1-C6-O6	6.71	123.93	119.90
1	A	1625	C	N3-C2-O2	-6.71	117.20	121.90
1	A	2023	G	C8-N9-C4	-6.71	103.72	106.40
1	A	733	G	N9-C4-C5	-6.71	102.72	105.40
1	A	2083	G	C2-N3-C4	-6.71	108.55	111.90
1	A	2430	A	C4-C5-C6	6.71	120.35	117.00
1	A	2724	C	N3-C4-N4	-6.71	113.31	118.00
1	A	13	A	C8-N9-C4	-6.70	103.12	105.80
1	A	1624	G	C5-C6-O6	-6.70	124.58	128.60
1	A	204	A	C8-N9-C4	-6.70	103.12	105.80
1	A	962	G	N1-C6-O6	6.69	123.92	119.90
1	A	1992	G	N3-C4-C5	-6.69	125.25	128.60
1	A	2263	C	C6-N1-C2	6.68	122.97	120.30
1	A	2791	C	C5-C6-N1	6.68	124.34	121.00
1	A	833	U	N3-C2-O2	6.68	126.87	122.20
1	A	2396	G	C6-C5-N7	-6.67	126.39	130.40
1	A	2565	A	C8-N9-C4	6.67	108.47	105.80
1	A	1369	G	C6-N1-C2	-6.67	121.10	125.10
1	A	2341	G	C5-C6-O6	-6.67	124.60	128.60
2	B	115	G	N7-C8-N9	-6.67	109.77	113.10
1	A	2224	G	C6-C5-N7	-6.67	126.40	130.40
1	A	1607	C	N1-C2-N3	-6.66	114.54	119.20
1	A	14	A	C8-N9-C4	-6.65	103.14	105.80
1	A	2512	C	C2-N1-C1'	-6.65	111.48	118.80
1	A	2235	G	C6-C5-N7	-6.65	126.41	130.40
1	A	2430	A	C6-C5-N7	-6.64	127.65	132.30
1	A	589	C	N1-C2-O2	-6.64	114.92	118.90
1	A	2680	C	N3-C4-N4	-6.64	113.35	118.00
1	A	2457	U	C6-N1-C2	-6.64	117.02	121.00
1	A	1531	C	C2-N1-C1'	6.63	126.10	118.80
1	A	2253	G	C4-C5-N7	6.63	113.45	110.80
1	A	2200	C	C2-N1-C1'	6.63	126.09	118.80
1	A	450	G	N9-C4-C5	6.62	108.05	105.40
1	A	1259	G	C8-N9-C4	6.62	109.05	106.40
1	A	2387	U	C2-N3-C4	-6.62	123.03	127.00
1	A	1614	A	C5-C6-N6	6.62	129.00	123.70
1	A	25	U	N1-C2-O2	-6.62	118.17	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2607	G	N9-C4-C5	-6.61	102.75	105.40
1	A	620	G	C2-N3-C4	6.61	115.20	111.90
1	A	1906	G	N1-C6-O6	6.61	123.86	119.90
1	A	213	A	C5-N7-C8	-6.60	100.60	103.90
1	A	1841	U	N3-C2-O2	-6.60	117.58	122.20
1	A	778	G	N1-C2-N3	6.60	127.86	123.90
1	A	2587	A	C4-C5-C6	6.60	120.30	117.00
1	A	1663	C	C6-N1-C2	6.60	122.94	120.30
1	A	2476	A	N1-C6-N6	-6.60	114.64	118.60
1	A	2502	G	C4-C5-N7	6.60	113.44	110.80
1	A	1492	G	N1-C6-O6	6.59	123.86	119.90
1	A	1529	G	C8-N9-C4	6.59	109.03	106.40
1	A	1807	G	N9-C4-C5	-6.59	102.77	105.40
1	A	385	C	N1-C2-O2	6.59	122.85	118.90
1	A	489	G	C4-C5-N7	-6.58	108.17	110.80
1	A	450	G	C5-N7-C8	6.58	107.59	104.30
1	A	1974	C	C6-N1-C2	6.58	122.93	120.30
1	A	1908	C	C6-N1-C2	-6.57	117.67	120.30
1	A	1832	C	C2-N1-C1'	-6.57	111.57	118.80
1	A	2440	C	C5-C4-N4	6.57	124.80	120.20
2	B	113	G	N1-C6-O6	6.57	123.84	119.90
1	A	540	C	N3-C2-O2	-6.56	117.31	121.90
1	A	2512	C	N3-C2-O2	6.56	126.49	121.90
2	B	30	C	C6-N1-C2	-6.56	117.67	120.30
1	A	689	A	C2-N3-C4	6.56	113.88	110.60
1	A	504	U	C6-N1-C1'	-6.55	112.02	121.20
1	A	1703	G	C4-C5-N7	6.55	113.42	110.80
1	A	2714	G	C5-C6-O6	-6.55	124.67	128.60
1	A	754	C	C5-C4-N4	-6.55	115.61	120.20
1	A	2007	C	N1-C2-O2	-6.54	114.97	118.90
1	A	1927	A	C8-N9-C4	-6.54	103.18	105.80
1	A	945	A	C5-N7-C8	-6.54	100.63	103.90
1	A	1142(A)	A	N1-C6-N6	6.54	122.52	118.60
1	A	1650	G	C4-C5-N7	6.53	113.41	110.80
1	A	2723	C	C6-N1-C2	-6.53	117.69	120.30
1	A	1367	A	C5-C6-N6	-6.53	118.47	123.70
1	A	2595	G	C4-C5-N7	6.53	113.41	110.80
1	A	271(Z)	C	C2-N1-C1'	6.53	125.98	118.80
1	A	2054	A	C6-N1-C2	-6.53	114.69	118.60
1	A	2430	A	N1-C2-N3	6.52	132.56	129.30
1	A	2023	G	C6-C5-N7	-6.52	126.49	130.40
1	A	1638	C	N3-C4-C5	6.52	124.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	C	N3-C4-N4	6.51	122.56	118.00
1	A	696	G	C8-N9-C4	6.51	109.01	106.40
1	A	1781	C	N3-C4-N4	-6.51	113.44	118.00
1	A	932	G	N9-C4-C5	6.51	108.00	105.40
1	A	139(A)	G	N3-C4-N9	6.50	129.90	126.00
1	A	184	C	C5-C4-N4	-6.50	115.65	120.20
1	A	1805	U	N3-C2-O2	-6.50	117.65	122.20
1	A	141	A	C5-C6-N6	-6.50	118.50	123.70
1	A	391	G	N1-C6-O6	6.50	123.80	119.90
1	A	271(M)	G	N3-C2-N2	6.50	124.45	119.90
1	A	203	C	C5-C6-N1	6.50	124.25	121.00
1	A	776	G	C4-N9-C1'	6.49	134.94	126.50
1	A	1038	C	C6-N1-C2	-6.49	117.70	120.30
1	A	2724	C	C5-C6-N1	-6.49	117.75	121.00
1	A	797	C	N3-C4-N4	6.49	122.54	118.00
1	A	178	G	C8-N9-C4	-6.48	103.81	106.40
1	A	645	C	C6-N1-C1'	-6.48	113.02	120.80
1	A	407	G	C4-N9-C1'	6.47	134.91	126.50
1	A	1142(A)	A	C6-C5-N7	-6.47	127.77	132.30
1	A	1638	C	C6-N1-C2	6.47	122.89	120.30
1	A	429	A	C5-C6-N6	-6.47	118.53	123.70
1	A	450	G	C5-C6-O6	6.46	132.48	128.60
1	A	1266	G	C8-N9-C4	6.46	108.98	106.40
1	A	6	A	C6-N1-C2	-6.46	114.72	118.60
1	A	80	G	N3-C4-N9	6.46	129.87	126.00
1	A	2897	U	C5-C4-O4	-6.45	122.03	125.90
1	A	1959	G	N9-C4-C5	6.45	107.98	105.40
1	A	1559	G	N1-C6-O6	-6.45	116.03	119.90
1	A	710	G	N1-C6-O6	6.45	123.77	119.90
1	A	2058	A	C5-N7-C8	-6.45	100.68	103.90
1	A	2504	U	C6-N1-C2	6.44	124.86	121.00
2	B	56	G	C8-N9-C4	-6.44	103.83	106.40
1	A	2709	G	N1-C6-O6	6.44	123.76	119.90
1	A	706	A	N9-C4-C5	-6.43	103.23	105.80
1	A	1493	C	N3-C2-O2	-6.43	117.40	121.90
24	2	45	SER	N-CA-C	-6.43	93.63	111.00
1	A	2695	C	N3-C4-N4	-6.43	113.50	118.00
1	A	982	C	N3-C4-C5	-6.42	119.33	121.90
1	A	1314	C	C5-C4-N4	-6.42	115.71	120.20
1	A	269	U	N1-C2-O2	6.42	127.29	122.80
1	A	1516	C	C6-N1-C2	6.42	122.87	120.30
1	A	1204	A	C3'-C2'-C1'	-6.41	96.37	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2105	C	C6-N1-C2	-6.41	117.73	120.30
1	A	676	A	C6-C5-N7	-6.41	127.81	132.30
1	A	1260	G	C8-N9-C4	6.41	108.96	106.40
1	A	201	C	C2-N3-C4	-6.41	116.70	119.90
1	A	12	U	N3-C2-O2	-6.41	117.72	122.20
1	A	1552	G	C5-C6-O6	6.41	132.44	128.60
1	A	1654	A	N1-C6-N6	-6.40	114.76	118.60
1	A	2503	A	C2-N3-C4	6.40	113.80	110.60
1	A	480	A	N7-C8-N9	6.39	117.00	113.80
1	A	787	U	N3-C2-O2	-6.39	117.72	122.20
1	A	1488	G	C8-N9-C4	-6.39	103.84	106.40
1	A	659	C	C6-N1-C2	6.39	122.86	120.30
1	A	2206	G	C4-N9-C1'	-6.39	118.20	126.50
10	O	8	LEU	CA-CB-CG	6.38	129.98	115.30
1	A	834	C	C6-N1-C2	-6.38	117.75	120.30
1	A	725	G	C8-N9-C4	-6.38	103.85	106.40
1	A	759	G	N3-C2-N2	-6.38	115.44	119.90
1	A	794	G	C8-N9-C4	6.37	108.95	106.40
1	A	1142	U	N3-C2-O2	-6.37	117.74	122.20
1	A	2080	G	N7-C8-N9	6.37	116.29	113.10
1	A	2031	A	N1-C6-N6	6.37	122.42	118.60
1	A	2695	C	C6-N1-C2	6.37	122.85	120.30
1	A	184	C	N3-C4-N4	6.36	122.45	118.00
1	A	812	C	N3-C4-C5	-6.36	119.35	121.90
1	A	745	G	C8-N9-C4	-6.36	103.86	106.40
1	A	748	G	C2-N3-C4	6.36	115.08	111.90
1	A	1831	G	N1-C2-N3	6.36	127.72	123.90
1	A	2644	G	C8-N9-C4	-6.35	103.86	106.40
1	A	148	C	N3-C4-C5	6.35	124.44	121.90
2	B	115	G	N3-C4-C5	6.34	131.77	128.60
1	A	141	A	C4-C5-C6	6.34	120.17	117.00
1	A	297	C	C6-N1-C2	-6.34	117.76	120.30
1	A	1677	A	N9-C4-C5	-6.34	103.26	105.80
1	A	1246	A	C2-N3-C4	-6.33	107.43	110.60
1	A	1781	C	C6-N1-C2	6.33	122.83	120.30
1	A	154(A)	C	N1-C2-O2	6.33	122.69	118.90
1	A	2723	C	N1-C2-O2	-6.32	115.11	118.90
1	A	1369	G	C5-C6-N1	6.32	114.66	111.50
1	A	391	G	C8-N9-C1'	-6.32	118.79	127.00
1	A	944	G	C5-C6-N1	-6.32	108.34	111.50
1	A	498	G	N1-C2-N3	-6.31	120.11	123.90
1	A	734	A	N1-C6-N6	6.31	122.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2506	U	N3-C2-O2	-6.31	117.78	122.20
1	A	2396	G	N9-C4-C5	-6.31	102.88	105.40
1	A	730	C	C6-N1-C2	6.30	122.82	120.30
1	A	297	C	N3-C2-O2	-6.29	117.49	121.90
1	A	1640	C	N1-C2-O2	6.29	122.67	118.90
1	A	2598	A	C6-C5-N7	-6.29	127.90	132.30
1	A	2709	G	N3-C2-N2	-6.29	115.50	119.90
1	A	265	A	C8-N9-C4	-6.29	103.28	105.80
1	A	455	C	C6-N1-C2	6.29	122.81	120.30
1	A	979	G	C8-N9-C4	-6.29	103.89	106.40
1	A	2423	U	C5-C6-N1	-6.28	119.56	122.70
1	A	915	C	C6-N1-C2	-6.28	117.79	120.30
1	A	2200	C	C5-C6-N1	6.28	124.14	121.00
1	A	533	G	C5-C6-N1	-6.28	108.36	111.50
1	A	1552	G	C6-C5-N7	6.28	134.16	130.40
1	A	1644	C	N1-C2-O2	6.28	122.67	118.90
1	A	90	U	N1-C2-O2	6.27	127.19	122.80
1	A	1359	A	N1-C6-N6	-6.27	114.83	118.60
1	A	494	G	N3-C4-C5	6.27	131.73	128.60
1	A	1005	C	N3-C4-N4	-6.27	113.61	118.00
1	A	2531	A	C8-N9-C4	6.27	108.31	105.80
1	A	1372	U	N3-C4-O4	6.27	123.79	119.40
1	A	2680	C	N3-C4-C5	6.27	124.41	121.90
1	A	1656	C	C5-C6-N1	6.26	124.13	121.00
1	A	2591	C	N1-C2-O2	-6.26	115.14	118.90
1	A	1340	U	C5-C4-O4	-6.26	122.14	125.90
1	A	857	C	C6-N1-C2	-6.26	117.80	120.30
1	A	955	C	N3-C4-N4	-6.26	113.62	118.00
1	A	1631(A)	A	C5-C6-N1	-6.26	114.57	117.70
1	A	481	G	N7-C8-N9	6.26	116.23	113.10
1	A	584	C	C6-N1-C2	6.26	122.80	120.30
1	A	693	C	N3-C4-N4	-6.26	113.62	118.00
1	A	353	G	C8-N9-C4	-6.25	103.90	106.40
1	A	330	A	C2-N3-C4	-6.24	107.48	110.60
1	A	1408	C	N1-C2-O2	-6.24	115.15	118.90
1	A	1650	G	C5-C6-O6	-6.24	124.85	128.60
1	A	2689	U	N3-C4-O4	-6.24	115.03	119.40
1	A	2283	C	C6-N1-C2	6.23	122.79	120.30
1	A	2647	U	C5-C4-O4	6.23	129.64	125.90
1	A	2081	C	N3-C2-O2	6.23	126.26	121.90
1	A	765	G	C5-C6-O6	-6.23	124.86	128.60
1	A	2587	A	C5-C6-N6	-6.23	118.72	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1678	G	C4-N9-C1'	6.23	134.59	126.50
1	A	2005	A	C2-N3-C4	-6.22	107.49	110.60
1	A	1968	G	C5-C6-O6	-6.21	124.87	128.60
1	A	2686	G	N3-C2-N2	-6.21	115.55	119.90
1	A	139	G	C6-C5-N7	-6.21	126.67	130.40
1	A	12	U	C2-N1-C1'	6.20	125.14	117.70
1	A	428	A	C2-N3-C4	6.20	113.70	110.60
1	A	1981	A	C2-N3-C4	-6.20	107.50	110.60
1	A	1997	G	N3-C4-N9	6.20	129.72	126.00
1	A	503	A	N1-C2-N3	6.20	132.40	129.30
1	A	975	C	N3-C4-C5	6.20	124.38	121.90
1	A	1579	A	C6-C5-N7	-6.20	127.96	132.30
1	A	2592	G	C8-N9-C4	-6.20	103.92	106.40
1	A	1631	C	N1-C2-O2	-6.19	115.19	118.90
1	A	127	A	N9-C4-C5	-6.19	103.32	105.80
1	A	2894	G	C4-N9-C1'	6.19	134.55	126.50
1	A	512	G	C4-C5-N7	-6.19	108.32	110.80
1	A	271(M)	G	N1-C2-N2	-6.19	110.63	116.20
1	A	1906	G	C5-C6-O6	-6.19	124.89	128.60
1	A	2238	G	C5-C6-O6	-6.19	124.89	128.60
1	A	2447	G	C4-N9-C1'	-6.19	118.46	126.50
1	A	2765	A	N1-C2-N3	6.19	132.39	129.30
1	A	127	A	C5-C6-N6	-6.19	118.75	123.70
1	A	533	G	N1-C2-N2	-6.19	110.63	116.20
1	A	807	U	N3-C4-O4	6.19	123.73	119.40
1	A	2577	A	N1-C6-N6	6.18	122.31	118.60
1	A	184	C	N1-C2-O2	-6.18	115.19	118.90
1	A	900	A	C8-N9-C4	-6.18	103.33	105.80
1	A	1437	C	N1-C2-O2	6.18	122.61	118.90
1	A	1997	G	N3-C4-C5	-6.18	125.51	128.60
1	A	2510	C	N3-C4-C5	-6.18	119.43	121.90
1	A	2053	G	C5-C6-O6	-6.18	124.89	128.60
1	A	576	U	N3-C2-O2	6.17	126.52	122.20
1	A	2057	A	N1-C2-N3	6.17	132.39	129.30
1	A	2690	C	N1-C2-O2	-6.17	115.19	118.90
1	A	2773	C	C4-C5-C6	6.17	120.49	117.40
1	A	2235	G	C5-N7-C8	-6.17	101.21	104.30
1	A	928	G	N3-C4-C5	-6.17	125.52	128.60
1	A	1115	G	N3-C4-C5	6.17	131.69	128.60
1	A	455	C	N3-C4-N4	-6.17	113.68	118.00
1	A	1663	C	C5-C6-N1	-6.17	117.92	121.00
1	A	90	U	C2-N1-C1'	6.17	125.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1941	C	C2-N1-C1'	6.16	125.58	118.80
1	A	2731	G	N9-C4-C5	-6.16	102.94	105.40
1	A	1022	G	C4-C5-N7	-6.16	108.33	110.80
1	A	975	C	C5-C6-N1	6.16	124.08	121.00
1	A	1807	G	N7-C8-N9	-6.16	110.02	113.10
1	A	2585	U	N3-C2-O2	-6.16	117.89	122.20
1	A	13	A	N9-C4-C5	6.16	108.26	105.80
1	A	1298	C	C6-N1-C2	-6.16	117.84	120.30
1	A	2246	G	N1-C2-N3	6.16	127.59	123.90
1	A	139(A)	G	C5-C6-O6	-6.16	124.91	128.60
1	A	533	G	C8-N9-C4	6.16	108.86	106.40
1	A	827	U	C6-N1-C2	6.16	124.69	121.00
1	A	2437	U	N1-C2-O2	-6.15	118.49	122.80
1	A	788	A	C6-C5-N7	-6.15	127.99	132.30
1	A	1348	G	N1-C6-O6	6.15	123.59	119.90
1	A	2599	G	C6-C5-N7	6.15	134.09	130.40
1	A	385	C	C2-N1-C1'	6.15	125.57	118.80
1	A	2447	G	C8-N9-C1'	6.15	135.00	127.00
1	A	530	G	N3-C4-N9	-6.15	122.31	126.00
1	A	565	C	N1-C2-O2	6.15	122.59	118.90
1	A	371	A	C8-N9-C4	6.14	108.26	105.80
1	A	58	G	C4-N9-C1'	6.14	134.49	126.50
1	A	113	G	N3-C4-N9	-6.14	122.32	126.00
1	A	849	A	N1-C6-N6	-6.14	114.92	118.60
1	A	502	A	C8-N9-C4	6.13	108.25	105.80
1	A	139	G	N1-C6-O6	6.13	123.58	119.90
1	A	2185	C	C5-C6-N1	6.13	124.06	121.00
1	A	962	G	N7-C8-N9	6.13	116.16	113.10
1	A	2440	C	C2-N1-C1'	-6.13	112.06	118.80
1	A	1390	U	C6-N1-C2	-6.12	117.33	121.00
1	A	1966	A	C6-C5-N7	6.12	136.59	132.30
1	A	2423	U	C6-N1-C2	6.12	124.67	121.00
1	A	2505	G	C8-N9-C4	-6.12	103.95	106.40
1	A	2426	A	N1-C6-N6	6.12	122.27	118.60
1	A	2644	G	N9-C4-C5	6.12	107.85	105.40
1	A	1758	G	C4-C5-N7	-6.12	108.35	110.80
1	A	2103	C	C2-N3-C4	6.12	122.96	119.90
1	A	614	U	N3-C2-O2	-6.11	117.92	122.20
1	A	733	G	N3-C4-N9	6.11	129.66	126.00
1	A	893	C	N1-C2-O2	6.10	122.56	118.90
1	A	754	C	N3-C4-N4	6.10	122.27	118.00
1	A	574	C	C5-C4-N4	6.10	124.47	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	A	N1-C6-N6	6.10	122.26	118.60
1	A	1008	C	N1-C2-O2	6.09	122.56	118.90
1	A	1574	C	N3-C4-C5	6.09	124.34	121.90
1	A	1831	G	C4-N9-C1'	6.09	134.42	126.50
1	A	2430	A	N1-C6-N6	6.09	122.26	118.60
1	A	1142(A)	A	C5-N7-C8	-6.09	100.85	103.90
1	A	305	U	N1-C2-O2	-6.09	118.54	122.80
1	A	1445(A)	C	C6-N1-C2	-6.09	117.86	120.30
1	A	828	U	C5-C6-N1	-6.09	119.66	122.70
1	A	1695	G	C6-C5-N7	-6.09	126.75	130.40
1	A	668	G	N3-C4-C5	6.08	131.64	128.60
1	A	1908	C	N3-C4-C5	-6.08	119.47	121.90
1	A	1923	U	C6-N1-C2	-6.08	117.35	121.00
1	A	2492	U	N3-C2-O2	-6.08	117.94	122.20
1	A	675	A	N1-C6-N6	6.08	122.25	118.60
1	A	912	C	C5-C6-N1	6.08	124.04	121.00
1	A	2049	G	C5-N7-C8	-6.08	101.26	104.30
1	A	2104	G	C4-C5-N7	6.08	113.23	110.80
1	A	2318	G	C6-C5-N7	-6.07	126.76	130.40
1	A	2647	U	C2-N1-C1'	-6.07	110.41	117.70
1	A	2439	A	N7-C8-N9	6.07	116.83	113.80
1	A	179	G	N1-C6-O6	6.07	123.54	119.90
1	A	1332	G	N1-C6-O6	6.07	123.54	119.90
1	A	1647	G	C8-N9-C4	6.06	108.82	106.40
1	A	2623	G	N1-C6-O6	6.06	123.54	119.90
1	A	2686	G	N3-C4-N9	-6.06	122.36	126.00
1	A	747	U	N3-C4-O4	6.05	123.64	119.40
2	B	103	G	N1-C6-O6	6.05	123.53	119.90
1	A	735	A	N7-C8-N9	-6.05	110.78	113.80
1	A	752	A	N7-C8-N9	6.04	116.82	113.80
1	A	1561	G	C5-C6-O6	-6.04	124.97	128.60
1	A	1834	U	N3-C2-O2	-6.04	117.97	122.20
1	A	50	U	N1-C2-O2	6.04	127.03	122.80
1	A	696	G	N7-C8-N9	-6.04	110.08	113.10
1	A	856	C	C5-C6-N1	6.04	124.02	121.00
1	A	2361	A	C2-N3-C4	-6.04	107.58	110.60
1	A	1313	U	N3-C4-C5	-6.03	110.98	114.60
1	A	809	G	C8-N9-C4	-6.03	103.99	106.40
1	A	390	A	N1-C2-N3	6.03	132.31	129.30
1	A	1947	C	N3-C4-C5	6.03	124.31	121.90
1	A	1277	G	C8-N9-C4	6.03	108.81	106.40
1	A	2678	C	C6-N1-C2	6.03	122.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	838	C	N3-C4-N4	-6.02	113.78	118.00
1	A	2412	A	C5-C6-N6	6.02	128.52	123.70
1	A	1558	A	P-O3'-C3'	6.02	126.92	119.70
1	A	2399	G	C8-N9-C4	-6.02	103.99	106.40
1	A	2498	C	C5-C6-N1	-6.02	117.99	121.00
1	A	2755	C	N1-C2-O2	6.02	122.51	118.90
1	A	480	A	C2-N3-C4	6.02	113.61	110.60
2	B	14	U	N3-C2-O2	-6.01	117.99	122.20
1	A	1568	G	C5-C6-O6	-6.01	124.99	128.60
1	A	1845	G	C8-N9-C4	-6.01	104.00	106.40
1	A	1987	G	N1-C6-O6	6.01	123.51	119.90
1	A	2238	G	N1-C2-N2	6.01	121.61	116.20
1	A	2647	U	C5-C6-N1	-6.01	119.70	122.70
1	A	1826	G	N3-C4-C5	-6.01	125.60	128.60
1	A	1338	G	C6-C5-N7	-6.00	126.80	130.40
1	A	827	U	N3-C2-O2	6.00	126.40	122.20
2	B	43	C	N3-C2-O2	-6.00	117.70	121.90
1	A	1830	C	N1-C2-N3	-6.00	115.00	119.20
1	A	1769	G	N3-C2-N2	-6.00	115.70	119.90
1	A	2473	U	N3-C2-O2	-5.99	118.00	122.20
1	A	201	C	C5-C6-N1	-5.99	118.00	121.00
1	A	856	C	N3-C4-C5	-5.99	119.50	121.90
1	A	1987	G	N3-C4-C5	5.99	131.60	128.60
1	A	1204	A	C5-C6-N1	-5.99	114.71	117.70
11	P	45	LEU	N-CA-C	5.99	127.17	111.00
1	A	2051	A	N1-C2-N3	5.98	132.29	129.30
1	A	734	A	C2-N3-C4	-5.98	107.61	110.60
1	A	2104	G	N9-C4-C5	-5.98	103.01	105.40
1	A	1698	A	N7-C8-N9	5.98	116.79	113.80
1	A	2654	A	N1-C6-N6	5.98	122.19	118.60
1	A	1607	C	C6-N1-C1'	-5.98	113.63	120.80
1	A	1614	A	N1-C6-N6	-5.98	115.01	118.60
1	A	1653	G	P-O3'-C3'	5.98	126.87	119.70
1	A	1758	G	C5-C6-O6	5.97	132.18	128.60
1	A	576	U	N1-C2-O2	-5.97	118.62	122.80
1	A	645	C	N1-C2-O2	5.97	122.48	118.90
1	A	2447	G	C4-C5-N7	5.97	113.19	110.80
1	A	733	G	C5-C6-O6	-5.96	125.02	128.60
1	A	748	G	N3-C4-C5	-5.96	125.62	128.60
1	A	141	A	C5-C6-N1	-5.96	114.72	117.70
1	A	2281	C	N3-C4-C5	-5.96	119.52	121.90
1	A	2598	A	C5-C6-N6	-5.96	118.94	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	933	A	C6-C5-N7	-5.96	128.13	132.30
1	A	271(F)	C	C6-N1-C2	-5.95	117.92	120.30
1	A	849	A	C5-C6-N6	5.95	128.46	123.70
1	A	2551	C	N3-C2-O2	-5.95	117.73	121.90
1	A	2876	G	C6-C5-N7	-5.95	126.83	130.40
1	A	1616	A	C5-N7-C8	-5.95	100.93	103.90
1	A	1235	G	N3-C4-C5	-5.94	125.63	128.60
1	A	143(A)	C	C6-N1-C2	5.94	122.68	120.30
1	A	329	G	N3-C4-N9	5.94	129.56	126.00
1	A	1377	G	C4-N9-C1'	5.94	134.22	126.50
1	A	330	A	C6-C5-N7	-5.94	128.14	132.30
1	A	1653	G	C6-C5-N7	-5.94	126.83	130.40
1	A	1932	A	N9-C4-C5	5.94	108.18	105.80
1	A	2603	G	C8-N9-C4	5.94	108.78	106.40
1	A	2791	C	C2-N1-C1'	5.94	125.33	118.80
1	A	665	C	N3-C4-C5	5.94	124.28	121.90
1	A	2623	G	C5-C6-O6	-5.94	125.04	128.60
1	A	1949	G	C2-N3-C4	-5.94	108.93	111.90
1	A	133	C	C5-C6-N1	-5.93	118.03	121.00
1	A	1022	G	C6-C5-N7	5.93	133.96	130.40
1	A	1885	A	C8-N9-C4	5.93	108.17	105.80
1	A	2435	A	C8-N9-C4	-5.93	103.43	105.80
1	A	2860	A	N1-C6-N6	5.93	122.16	118.60
1	A	380	U	C5-C4-O4	-5.93	122.34	125.90
1	A	986	C	N1-C2-O2	5.93	122.46	118.90
1	A	188	G	C5-C6-O6	-5.93	125.04	128.60
1	A	271(M)	G	N9-C4-C5	-5.93	103.03	105.40
1	A	72	U	C5-C6-N1	-5.93	119.74	122.70
1	A	1219	G	N3-C4-N9	-5.93	122.44	126.00
1	A	203	C	C4-C5-C6	-5.92	114.44	117.40
1	A	425	G	C6-C5-N7	-5.92	126.85	130.40
1	A	1142	U	N1-C2-O2	5.92	126.94	122.80
1	A	1914	C	C2-N1-C1'	5.92	125.31	118.80
1	A	2468	G	N1-C6-O6	5.92	123.45	119.90
1	A	131	G	C5-C6-O6	-5.92	125.05	128.60
1	A	2452	C	C5-C4-N4	-5.92	116.06	120.20
1	A	972	G	C4-C5-N7	-5.91	108.44	110.80
1	A	1552	G	N9-C4-C5	5.91	107.77	105.40
1	A	1899	G	N1-C6-O6	5.91	123.45	119.90
1	A	614(A)	U	N3-C2-O2	-5.91	118.06	122.20
1	A	1656	C	C2-N1-C1'	5.91	125.30	118.80
1	A	2081	C	C6-N1-C2	5.91	122.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	668	G	C5-C6-N1	-5.91	108.55	111.50
1	A	2035	G	N9-C4-C5	5.91	107.76	105.40
1	A	102	G	N1-C6-O6	-5.90	116.36	119.90
1	A	1822	G	C2-N3-C4	-5.90	108.95	111.90
1	A	1963	U	C5-C6-N1	5.90	125.65	122.70
1	A	1579	A	C4-C5-C6	5.90	119.95	117.00
1	A	1631(A)	A	C8-N9-C4	5.90	108.16	105.80
1	A	1658	C	N1-C2-O2	5.89	122.44	118.90
1	A	1845	G	N9-C4-C5	5.89	107.76	105.40
1	A	781	A	N7-C8-N9	5.89	116.75	113.80
1	A	524	U	N1-C2-N3	5.89	118.43	114.90
1	A	2848	G	N1-C6-O6	-5.89	116.37	119.90
1	A	1830	C	C5-C4-N4	-5.89	116.08	120.20
1	A	399	G	N9-C4-C5	-5.88	103.05	105.40
1	A	697	C	N3-C4-N4	5.88	122.12	118.00
1	A	1678	G	C8-N9-C1'	-5.88	119.35	127.00
1	A	1827	C	N1-C2-N3	5.88	123.32	119.20
1	A	219	G	N1-C6-O6	-5.88	116.37	119.90
1	A	1561	G	N1-C6-O6	5.88	123.43	119.90
1	A	855	G	N1-C6-O6	5.88	123.43	119.90
1	A	1408	C	C5-C4-N4	-5.88	116.09	120.20
1	A	1026	U	N3-C2-O2	-5.88	118.09	122.20
1	A	559	G	C4-N9-C1'	-5.87	118.86	126.50
1	A	1949	G	C6-C5-N7	-5.87	126.88	130.40
1	A	1429	G	C8-N9-C4	-5.87	104.05	106.40
1	A	2717	G	N3-C4-C5	-5.87	125.67	128.60
1	A	1142(A)	A	C2-N3-C4	-5.87	107.67	110.60
6	G	135	LEU	CA-CB-CG	5.87	128.80	115.30
1	A	1771	C	N3-C4-C5	5.87	124.25	121.90
1	A	1974	C	N3-C4-C5	5.86	124.25	121.90
1	A	2297	C	C5-C6-N1	5.86	123.93	121.00
1	A	1021	A	C5-C6-N1	-5.86	114.77	117.70
1	A	1256	G	C8-N9-C1'	-5.86	119.39	127.00
1	A	1395	A	N1-C6-N6	-5.86	115.09	118.60
1	A	1115	G	C8-N9-C4	5.86	108.74	106.40
1	A	1403	C	C4-C5-C6	5.86	120.33	117.40
1	A	102	G	C4-C5-N7	-5.85	108.46	110.80
1	A	1475	G	N3-C4-C5	5.85	131.53	128.60
1	A	2755	C	C6-N1-C1'	-5.85	113.78	120.80
1	A	2838	G	N1-C6-O6	5.85	123.41	119.90
1	A	1223	G	N3-C4-C5	5.85	131.53	128.60
1	A	1629	U	N1-C2-O2	-5.85	118.70	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	G	N1-C2-N2	5.85	121.46	116.20
1	A	1038	C	C5-C6-N1	5.85	123.92	121.00
1	A	1899	G	C4-C5-N7	5.85	113.14	110.80
1	A	1142(A)	A	N1-C2-N3	5.85	132.22	129.30
1	A	1526	G	N3-C4-C5	5.84	131.52	128.60
1	A	2857	G	C4-C5-N7	5.84	113.14	110.80
1	A	784	A	P-O3'-C3'	5.84	126.71	119.70
1	A	509	C	N3-C2-O2	-5.84	117.81	121.90
1	A	464	U	N3-C4-C5	-5.84	111.10	114.60
1	A	760	G	N3-C2-N2	-5.84	115.81	119.90
1	A	1497	U	C2-N1-C1'	5.84	124.71	117.70
1	A	1769	G	C6-C5-N7	-5.84	126.90	130.40
1	A	1619	G	C5-C6-N1	5.84	114.42	111.50
1	A	1355	G	C6-C5-N7	-5.83	126.90	130.40
1	A	1393	A	C5-C6-N6	-5.83	119.03	123.70
1	A	458	G	C5-C6-O6	5.83	132.10	128.60
1	A	2506	U	N3-C4-O4	-5.83	115.32	119.40
1	A	2877	G	C5-C6-N1	-5.83	108.59	111.50
1	A	1663	C	C2-N3-C4	-5.82	116.99	119.90
1	A	2259	G	N3-C2-N2	-5.82	115.83	119.90
1	A	337	C	C5-C4-N4	5.82	124.27	120.20
1	A	330	A	N9-C4-C5	-5.82	103.47	105.80
1	A	1653	G	N3-C2-N2	5.82	123.97	119.90
1	A	2007	C	N3-C2-O2	5.82	125.97	121.90
1	A	2415	G	C8-N9-C4	-5.82	104.07	106.40
1	A	1419	A	N1-C6-N6	-5.82	115.11	118.60
1	A	2590	A	C6-N1-C2	-5.82	115.11	118.60
1	A	1004	C	N1-C2-O2	-5.81	115.41	118.90
1	A	1280	G	C8-N9-C4	5.81	108.73	106.40
1	A	229	A	C3'-C2'-C1'	-5.81	96.85	101.50
1	A	733	G	C4-C5-N7	5.81	113.12	110.80
1	A	2843	G	C5-C6-O6	-5.81	125.11	128.60
1	A	986	C	N3-C2-O2	-5.81	117.83	121.90
2	B	54	G	C6-C5-N7	-5.81	126.92	130.40
1	A	135	G	N1-C6-O6	5.81	123.38	119.90
1	A	726	G	C4-C5-N7	-5.80	108.48	110.80
1	A	2191	G	C6-N1-C2	5.80	128.58	125.10
1	A	511	U	C6-N1-C2	-5.80	117.52	121.00
1	A	1569	A	C5-C6-N6	5.80	128.34	123.70
1	A	791	C	N1-C2-O2	5.79	122.38	118.90
1	A	1142(A)	A	N7-C8-N9	5.79	116.70	113.80
1	A	1026	U	N1-C2-O2	5.79	126.86	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1959	G	N3-C2-N2	-5.79	115.84	119.90
1	A	2502	G	C5-C6-O6	-5.79	125.12	128.60
1	A	2725	A	C5-C6-N1	5.79	120.60	117.70
1	A	58	G	C8-N9-C4	-5.79	104.08	106.40
1	A	1297	C	C5-C6-N1	-5.79	118.10	121.00
1	A	1631(A)	A	N1-C6-N6	5.79	122.07	118.60
1	A	2028	U	C5-C4-O4	5.79	129.37	125.90
1	A	2054	A	N1-C2-N3	5.79	132.19	129.30
1	A	102	G	C5-C6-O6	5.79	132.07	128.60
1	A	528	A	N7-C8-N9	5.79	116.69	113.80
2	B	6	C	C5-C6-N1	-5.79	118.11	121.00
1	A	844	C	C6-N1-C2	5.78	122.61	120.30
1	A	1264	G	C5-C6-N1	-5.78	108.61	111.50
1	A	2473	U	C6-N1-C2	-5.78	117.53	121.00
1	A	2565	A	C2-N3-C4	-5.78	107.71	110.60
1	A	188	G	C5-N7-C8	-5.78	101.41	104.30
1	A	787	U	C5-C4-O4	5.78	129.37	125.90
1	A	1899	G	N3-C4-N9	5.78	129.47	126.00
1	A	1964	G	C8-N9-C1'	-5.78	119.48	127.00
2	B	4	C	C6-N1-C2	5.78	122.61	120.30
1	A	2258	C	N1-C2-O2	-5.78	115.43	118.90
1	A	461	C	N3-C2-O2	5.78	125.94	121.90
1	A	583	G	C5-C6-N1	-5.78	108.61	111.50
1	A	778	G	N9-C4-C5	-5.78	103.09	105.40
1	A	1618	A	N9-C4-C5	5.77	108.11	105.80
7	H	171	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	234	C	N1-C2-O2	-5.77	115.44	118.90
1	A	566	U	C2-N1-C1'	-5.77	110.77	117.70
1	A	791	C	N3-C2-O2	-5.77	117.86	121.90
1	A	113	G	N1-C6-O6	5.77	123.36	119.90
1	A	2104	G	N3-C4-N9	5.76	129.46	126.00
1	A	687	C	N1-C2-O2	-5.76	115.44	118.90
1	A	1261	C	C6-N1-C2	5.76	122.61	120.30
1	A	2326	C	C6-N1-C1'	5.76	127.71	120.80
1	A	2535	G	C5-C6-O6	-5.76	125.14	128.60
1	A	2755	C	C5-C4-N4	-5.76	116.17	120.20
1	A	1004	C	N3-C2-O2	5.76	125.93	121.90
1	A	6	A	C5-C6-N6	-5.76	119.10	123.70
1	A	778	G	C8-N9-C4	5.75	108.70	106.40
1	A	1699	G	N9-C4-C5	5.75	107.70	105.40
1	A	2286	A	C4-N9-C1'	5.75	136.66	126.30
1	A	2027	G	N1-C6-O6	-5.75	116.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2689	U	C5-C4-O4	5.75	129.35	125.90
1	A	778	G	N1-C2-N2	-5.75	111.03	116.20
1	A	2251	G	N3-C4-N9	5.75	129.45	126.00
1	A	760	G	N9-C4-C5	5.74	107.70	105.40
1	A	22	C	N3-C4-N4	-5.74	113.98	118.00
1	A	481	G	P-O3'-C3'	5.74	126.59	119.70
1	A	1355	G	C5-C6-N1	-5.74	108.63	111.50
1	A	1774	C	C2-N1-C1'	5.74	125.11	118.80
1	A	2502	G	C5-N7-C8	-5.74	101.43	104.30
1	A	2765	A	C4-C5-C6	5.73	119.87	117.00
1	A	894	C	N1-C2-O2	5.73	122.34	118.90
1	A	1831	G	C6-C5-N7	-5.73	126.96	130.40
1	A	482	A	C5-C6-N6	-5.73	119.12	123.70
1	A	1297	C	C4-C5-C6	5.73	120.26	117.40
1	A	1616	A	N7-C8-N9	5.73	116.66	113.80
1	A	2049	G	C4-C5-N7	5.72	113.09	110.80
12	Q	64	ILE	CB-CA-C	-5.72	100.16	111.60
1	A	1223	G	C4-N9-C1'	-5.72	119.07	126.50
1	A	330	A	C5-C6-N6	-5.72	119.13	123.70
1	A	1008	C	N3-C4-C5	5.71	124.18	121.90
1	A	2425	A	C2-N3-C4	5.71	113.45	110.60
1	A	71	A	C4-C5-N7	5.71	113.55	110.70
1	A	928	G	C8-N9-C4	-5.71	104.12	106.40
1	A	1297	C	C5-C4-N4	5.71	124.19	120.20
1	A	1598	C	C2-N1-C1'	5.71	125.08	118.80
1	A	773	U	C2-N3-C4	-5.71	123.58	127.00
1	A	2200	C	C6-N1-C2	-5.71	118.02	120.30
1	A	20	C	C6-N1-C2	-5.70	118.02	120.30
26	4	42	PHE	C-N-CA	5.70	135.96	121.70
1	A	1830	C	C6-N1-C2	5.70	122.58	120.30
1	A	1027	A	N1-C6-N6	-5.70	115.18	118.60
1	A	2388	A	N9-C4-C5	5.70	108.08	105.80
1	A	2731	G	C4-C5-N7	5.70	113.08	110.80
1	A	1437	C	C2-N1-C1'	5.69	125.06	118.80
1	A	2003	G	C2-N3-C4	-5.69	109.05	111.90
1	A	314	A	N1-C6-N6	-5.69	115.19	118.60
1	A	1125	G	C8-N9-C4	5.69	108.68	106.40
1	A	533	G	N9-C4-C5	-5.69	103.12	105.40
1	A	1907	G	N3-C4-N9	-5.69	122.59	126.00
1	A	2003	G	N3-C4-N9	-5.69	122.59	126.00
1	A	2018	G	C4-N9-C1'	5.69	133.89	126.50
1	A	2771	C	N3-C2-O2	-5.69	117.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1972	A	C8-N9-C4	-5.69	103.53	105.80
1	A	74	A	C8-N9-C4	-5.68	103.53	105.80
1	A	1157	G	C8-N9-C4	-5.68	104.13	106.40
1	A	1698	A	C6-C5-N7	-5.68	128.32	132.30
1	A	2585	U	N1-C2-O2	5.68	126.78	122.80
1	A	2686	G	N7-C8-N9	5.68	115.94	113.10
1	A	371	A	N9-C4-C5	-5.68	103.53	105.80
1	A	1362	C	C6-N1-C2	-5.68	118.03	120.30
1	A	686	G	N1-C2-N3	5.68	127.31	123.90
1	A	1915	U	C2-N1-C1'	5.68	124.52	117.70
1	A	2437	U	C2-N1-C1'	-5.68	110.89	117.70
1	A	2711	A	C2-N3-C4	-5.68	107.76	110.60
1	A	803	U	N1-C2-O2	5.68	126.78	122.80
1	A	1968	G	N1-C6-O6	5.68	123.31	119.90
1	A	494	G	N1-C6-O6	5.67	123.30	119.90
1	A	2522	U	C6-N1-C2	5.67	124.40	121.00
1	A	271(O)	C	N3-C2-O2	-5.67	117.93	121.90
1	A	1470	G	N3-C4-N9	-5.67	122.60	126.00
1	A	452	G	C6-N1-C2	-5.67	121.70	125.10
1	A	679	C	N1-C2-O2	-5.67	115.50	118.90
1	A	60	G	N9-C4-C5	5.67	107.67	105.40
1	A	1210	A	C5-C6-N6	-5.67	119.17	123.70
1	A	1489	U	C5-C4-O4	5.67	129.30	125.90
1	A	1187	G	C8-N9-C4	-5.66	104.14	106.40
1	A	2598	A	C5-N7-C8	-5.66	101.07	103.90
2	B	14	U	N1-C2-O2	5.66	126.76	122.80
1	A	737	C	C2-N3-C4	-5.66	117.07	119.90
1	A	1551	C	C6-N1-C2	-5.66	118.03	120.30
1	A	805	G	C5-C6-N1	5.66	114.33	111.50
1	A	972	G	N1-C2-N3	5.66	127.30	123.90
1	A	1614	A	C2-N3-C4	-5.66	107.77	110.60
1	A	2495	G	C5-C6-O6	-5.66	125.20	128.60
1	A	1553	A	N9-C4-C5	5.66	108.06	105.80
1	A	1857	G	C6-C5-N7	-5.66	127.00	130.40
1	A	616	G	N3-C4-C5	-5.65	125.77	128.60
1	A	2392	A	N1-C6-N6	-5.65	115.21	118.60
1	A	574	C	N3-C4-N4	-5.65	114.04	118.00
1	A	216	A	N1-C2-N3	5.65	132.12	129.30
1	A	1276	A	C2-N3-C4	-5.65	107.78	110.60
1	A	1625	C	N1-C2-O2	5.65	122.29	118.90
1	A	2791	C	N3-C4-N4	5.65	121.95	118.00
1	A	1208	C	N3-C4-N4	5.64	121.95	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1314	C	N1-C2-O2	5.64	122.29	118.90
1	A	1640	C	C2-N1-C1'	5.64	125.01	118.80
1	A	1616	A	N1-C6-N6	5.64	121.99	118.60
1	A	2689	U	C4-C5-C6	5.64	123.08	119.70
1	A	2723	C	N1-C2-N3	5.64	123.15	119.20
1	A	577	G	C8-N9-C4	5.64	108.66	106.40
1	A	669	G	C4-C5-N7	-5.64	108.54	110.80
1	A	1787	A	N1-C6-N6	5.64	121.98	118.60
1	A	2607	G	N1-C2-N2	-5.64	111.12	116.20
1	A	1639	U	N3-C2-O2	-5.64	118.25	122.20
1	A	2259	G	N1-C2-N2	5.64	121.27	116.20
1	A	2778	A	C2-N3-C4	-5.64	107.78	110.60
1	A	2829	C	N3-C4-C5	5.64	124.16	121.90
1	A	2473	U	C5-C6-N1	5.64	125.52	122.70
1	A	1648	C	N1-C2-O2	-5.63	115.52	118.90
2	B	94	C	C6-N1-C2	5.63	122.55	120.30
1	A	2039	C	N3-C2-O2	-5.63	117.96	121.90
1	A	2042	A	C2-N3-C4	-5.63	107.78	110.60
1	A	85	G	C8-N9-C4	5.63	108.65	106.40
1	A	946	G	N9-C4-C5	5.63	107.65	105.40
1	A	2460	U	N3-C4-C5	-5.63	111.22	114.60
1	A	192	C	C6-N1-C2	5.63	122.55	120.30
1	A	105	C	N3-C2-O2	5.62	125.84	121.90
1	A	2222	G	C8-N9-C4	-5.62	104.15	106.40
1	A	1701	A	C8-N9-C4	-5.62	103.55	105.80
1	A	1432	C	N3-C4-N4	5.62	121.94	118.00
3	D	271	ILE	CB-CA-C	-5.62	100.36	111.60
1	A	1487	G	C8-N9-C4	-5.62	104.15	106.40
1	A	1926	U	C5-C4-O4	5.62	129.27	125.90
1	A	133	C	C6-N1-C2	5.61	122.55	120.30
1	A	889	C	C6-N1-C2	-5.61	118.05	120.30
1	A	2473	U	N1-C2-O2	5.61	126.73	122.80
1	A	1909	C	N3-C2-O2	-5.61	117.97	121.90
1	A	1992	G	C5-C6-N1	5.61	114.31	111.50
1	A	2239	G	N1-C6-O6	-5.61	116.53	119.90
1	A	2356	C	N3-C2-O2	5.61	125.83	121.90
1	A	733	G	C4-N9-C1'	5.61	133.79	126.50
1	A	1374	G	N1-C6-O6	5.61	123.27	119.90
1	A	2039	C	N1-C2-O2	5.61	122.26	118.90
1	A	2596	U	C5-C6-N1	-5.61	119.90	122.70
1	A	380	U	N3-C2-O2	5.60	126.12	122.20
1	A	407	G	C8-N9-C1'	-5.60	119.72	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1160	G	N3-C4-C5	-5.60	125.80	128.60
1	A	1427	A	C8-N9-C4	-5.60	103.56	105.80
1	A	1769	G	N7-C8-N9	5.60	115.90	113.10
1	A	962	G	C5-C6-O6	-5.60	125.24	128.60
1	A	768	G	C6-C5-N7	-5.60	127.04	130.40
1	A	1611	C	N1-C2-O2	-5.59	115.54	118.90
1	A	560	C	C2-N1-C1'	-5.59	112.65	118.80
1	A	493	G	N3-C4-C5	5.59	131.40	128.60
1	A	2788	C	C2-N1-C1'	-5.59	112.65	118.80
1	A	92	A	C5-N7-C8	-5.59	101.11	103.90
1	A	560	C	N1-C2-O2	-5.59	115.55	118.90
1	A	1160	G	N3-C4-N9	5.59	129.35	126.00
1	A	1520	G	N3-C4-N9	5.58	129.35	126.00
1	A	2482	G	C4-N9-C1'	5.58	133.76	126.50
1	A	1934	C	C5-C6-N1	-5.58	118.21	121.00
1	A	2207	G	C4-N9-C1'	5.58	133.76	126.50
1	A	2430	A	C2-N3-C4	-5.58	107.81	110.60
1	A	1983	C	N1-C2-O2	-5.58	115.55	118.90
1	A	2570	G	C8-N9-C4	5.58	108.63	106.40
1	A	1811	G	N3-C2-N2	-5.58	115.99	119.90
1	A	2455	G	C8-N9-C4	-5.58	104.17	106.40
1	A	2503	A	C5-C6-N6	-5.58	119.24	123.70
1	A	2894	G	N3-C4-N9	5.58	129.35	126.00
1	A	1281	G	C5-C6-N1	-5.58	108.71	111.50
1	A	2689	U	P-O3'-C3'	5.58	126.39	119.70
1	A	1021	A	C5-N7-C8	-5.58	101.11	103.90
1	A	2053	G	N1-C6-O6	5.58	123.25	119.90
1	A	2440	C	C5-C6-N1	-5.58	118.21	121.00
1	A	213	A	C4-C5-N7	5.57	113.49	110.70
1	A	1758	G	N9-C4-C5	5.57	107.63	105.40
2	B	56	G	N3-C4-C5	-5.57	125.81	128.60
1	A	188	G	N9-C4-C5	-5.57	103.17	105.40
1	A	1367	A	N1-C6-N6	5.57	121.94	118.60
1	A	2238	G	N3-C2-N2	-5.57	116.00	119.90
1	A	783	A	N3-C4-C5	-5.57	122.90	126.80
1	A	265	A	C4-C5-N7	5.57	113.48	110.70
1	A	583	G	C6-C5-N7	-5.57	127.06	130.40
1	A	2621	A	C2-N3-C4	-5.57	107.82	110.60
1	A	2697	G	C8-N9-C4	5.57	108.63	106.40
1	A	2056	G	C4-C5-N7	5.56	113.03	110.80
1	A	773	U	C5-C6-N1	-5.56	119.92	122.70
1	A	856	C	C3'-C2'-C1'	-5.56	97.05	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2866	U	C5-C4-O4	5.56	129.24	125.90
1	A	2283	C	N3-C2-O2	5.56	125.79	121.90
1	A	480	A	N3-C4-C5	-5.55	122.91	126.80
1	A	506	G	C4-C5-N7	5.55	113.02	110.80
1	A	1698	A	N3-C4-N9	-5.55	122.96	127.40
1	A	2708	G	C8-N9-C4	5.55	108.62	106.40
1	A	473	G	N3-C2-N2	-5.55	116.02	119.90
1	A	676	A	N1-C2-N3	5.55	132.07	129.30
1	A	197	A	C5-C6-N6	-5.54	119.26	123.70
1	A	1256	G	N1-C6-O6	5.54	123.23	119.90
1	A	1927	A	N7-C8-N9	5.54	116.57	113.80
1	A	2897	U	C6-N1-C1'	-5.54	113.44	121.20
1	A	467	G	N7-C8-N9	-5.54	110.33	113.10
1	A	1558	A	N7-C8-N9	5.54	116.57	113.80
1	A	33	U	C5-C4-O4	-5.54	122.58	125.90
1	A	975	C	C4-C5-C6	-5.54	114.63	117.40
1	A	1113	U	N3-C2-O2	-5.54	118.32	122.20
1	A	1556	C	C5-C6-N1	-5.54	118.23	121.00
1	A	30	G	N9-C4-C5	5.53	107.61	105.40
1	A	2781	A	C5-C6-N6	5.53	128.12	123.70
1	A	1983	C	C2-N3-C4	-5.53	117.14	119.90
1	A	1640	C	N3-C2-O2	-5.53	118.03	121.90
1	A	2291	U	C5-C4-O4	5.53	129.22	125.90
1	A	2318	G	C4-N9-C1'	5.53	133.68	126.50
1	A	2463	C	N1-C2-O2	-5.53	115.58	118.90
1	A	307	G	N3-C4-N9	5.52	129.31	126.00
1	A	452	G	C5-C6-N1	5.52	114.26	111.50
1	A	187	G	C6-C5-N7	-5.52	127.09	130.40
1	A	2002	G	C2-N3-C4	-5.51	109.14	111.90
1	A	25	U	N3-C2-O2	5.51	126.06	122.20
1	A	1509	C	C6-N1-C2	-5.51	118.09	120.30
1	A	2821	A	C2-N3-C4	-5.51	107.84	110.60
1	A	1293	C	N3-C4-C5	5.51	124.10	121.90
1	A	33	U	C6-N1-C2	5.51	124.30	121.00
1	A	645	C	C2-N3-C4	5.51	122.65	119.90
1	A	1235	G	C4-C5-N7	-5.51	108.60	110.80
1	A	2100	G	C5-C6-O6	5.51	131.90	128.60
1	A	2735	G	C5-C6-O6	-5.50	125.30	128.60
1	A	1233	C	C5-C6-N1	5.50	123.75	121.00
1	A	1663	C	C5-C4-N4	-5.50	116.35	120.20
1	A	62	C	C5-C6-N1	-5.50	118.25	121.00
1	A	738	G	N1-C2-N2	-5.50	111.25	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	811	U	C2-N1-C1'	-5.50	111.10	117.70
1	A	1482	G	C5-C6-N1	5.50	114.25	111.50
1	A	1647	G	N3-C4-C5	5.50	131.35	128.60
1	A	1985	G	N1-C2-N3	5.50	127.20	123.90
1	A	2023	G	N7-C8-N9	5.50	115.85	113.10
1	A	1949	G	N1-C2-N3	5.50	127.20	123.90
1	A	592	G	N3-C4-N9	5.50	129.30	126.00
1	A	678	C	N3-C4-C5	5.50	124.10	121.90
1	A	1445(A)	C	C2-N1-C1'	5.50	124.85	118.80
1	A	1754	C	C6-N1-C2	5.50	122.50	120.30
1	A	1579	A	C4-N9-C1'	5.50	136.19	126.30
1	A	1826	G	N3-C4-N9	5.50	129.30	126.00
1	A	2084	C	C6-N1-C2	5.50	122.50	120.30
1	A	1202	C	N1-C2-O2	-5.50	115.60	118.90
1	A	2205	C	C2-N3-C4	5.49	122.65	119.90
1	A	1350	C	N1-C2-O2	-5.49	115.61	118.90
1	A	1769	G	C4-C5-C6	5.49	122.09	118.80
1	A	1966	A	C5-C6-N6	5.49	128.09	123.70
1	A	2396	G	C5-C6-O6	-5.49	125.31	128.60
1	A	737	C	C5-C6-N1	-5.48	118.26	121.00
1	A	1487	G	N3-C2-N2	-5.48	116.06	119.90
1	A	509	C	C5-C6-N1	-5.48	118.26	121.00
1	A	2206	G	N7-C8-N9	-5.48	110.36	113.10
1	A	2296	U	N3-C2-O2	-5.48	118.36	122.20
1	A	2713	A	N1-C6-N6	-5.48	115.31	118.60
1	A	666	G	C2-N3-C4	-5.48	109.16	111.90
1	A	1602	U	C5-C6-N1	-5.48	119.96	122.70
1	A	2607	G	C8-N9-C1'	-5.48	119.88	127.00
2	B	113	G	C5-C6-O6	-5.48	125.31	128.60
1	A	1129	A	N1-C2-N3	-5.47	126.56	129.30
1	A	1216	G	C4-N9-C1'	5.47	133.62	126.50
1	A	1353	A	C6-N1-C2	-5.47	115.31	118.60
1	A	1661	G	N1-C6-O6	5.47	123.18	119.90
1	A	2033	A	C5-C6-N1	5.47	120.44	117.70
1	A	2828	C	C5-C6-N1	-5.47	118.26	121.00
1	A	428	A	C8-N9-C4	-5.47	103.61	105.80
1	A	443	A	C5-C6-N6	5.47	128.07	123.70
1	A	2894	G	N3-C4-C5	-5.47	125.87	128.60
1	A	676	A	O4'-C1'-N9	5.47	112.57	108.20
1	A	2876	G	N3-C4-N9	5.47	129.28	126.00
1	A	51	G	N3-C4-N9	5.46	129.28	126.00
1	A	765	G	C6-C5-N7	-5.46	127.12	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1758	G	N1-C6-O6	-5.46	116.62	119.90
1	A	1909	C	C4-C5-C6	5.46	120.13	117.40
1	A	1983	C	C4-C5-C6	5.46	120.13	117.40
1	A	1355	G	C4-C5-C6	5.46	122.08	118.80
8	I	101	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	307	G	N3-C4-C5	-5.46	125.87	128.60
1	A	1254	A	N7-C8-N9	5.46	116.53	113.80
1	A	2014	A	C6-N1-C2	-5.46	115.33	118.60
1	A	2452	C	C5-C6-N1	5.46	123.73	121.00
1	A	1655	A	C2-N3-C4	-5.45	107.87	110.60
1	A	2454	G	N1-C6-O6	-5.45	116.63	119.90
1	A	1856	G	C8-N9-C4	-5.45	104.22	106.40
5	F	170	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	1024	G	N1-C6-O6	5.45	123.17	119.90
2	B	103	G	C6-C5-N7	-5.45	127.13	130.40
1	A	590	A	N3-C4-C5	5.45	130.61	126.80
1	A	1142(A)	A	C4-C5-C6	5.45	119.72	117.00
1	A	2067	G	N3-C2-N2	-5.45	116.09	119.90
1	A	442	G	N1-C6-O6	-5.44	116.63	119.90
1	A	932	G	C4-C5-N7	-5.44	108.62	110.80
1	A	1440	G	C5-C6-O6	5.44	131.87	128.60
1	A	1656	C	C6-N1-C2	-5.44	118.12	120.30
1	A	888	C	C5-C6-N1	5.44	123.72	121.00
1	A	1192	G	C4-C5-N7	5.44	112.98	110.80
1	A	2272	U	C6-N1-C2	-5.44	117.74	121.00
1	A	2429	G	C6-C5-N7	-5.44	127.14	130.40
1	A	269	U	C2-N1-C1'	5.44	124.22	117.70
1	A	620	G	N3-C4-C5	-5.44	125.88	128.60
1	A	1240	U	C6-N1-C2	-5.44	117.74	121.00
1	A	92	A	N1-C6-N6	5.43	121.86	118.60
1	A	1678	G	N3-C4-C5	-5.43	125.88	128.60
1	A	1781	C	N1-C2-O2	5.43	122.16	118.90
1	A	659	C	N3-C4-C5	5.43	124.07	121.90
1	A	925	C	N3-C4-N4	-5.43	114.20	118.00
1	A	1681	G	N3-C4-C5	5.43	131.32	128.60
1	A	2522	U	C5-C6-N1	-5.43	119.98	122.70
1	A	2583	G	N9-C4-C5	5.43	107.57	105.40
1	A	2599	G	N3-C4-N9	-5.43	122.74	126.00
1	A	1347	G	N3-C4-N9	-5.43	122.74	126.00
1	A	479	A	C2-N3-C4	5.43	113.31	110.60
1	A	518	G	C8-N9-C4	-5.43	104.23	106.40
1	A	1666	G	N1-C6-O6	5.43	123.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	G	C6-C5-N7	-5.42	127.14	130.40
1	A	760	G	N3-C4-C5	-5.42	125.89	128.60
1	A	1319	G	N7-C8-N9	5.42	115.81	113.10
1	A	1767	C	N1-C2-N3	5.42	123.00	119.20
1	A	1143	A	C4-C5-C6	5.42	119.71	117.00
1	A	2700	C	C2-N3-C4	-5.42	117.19	119.90
1	A	489	G	C5-C6-O6	5.42	131.85	128.60
1	A	507	A	C8-N9-C4	5.42	107.97	105.80
1	A	662	G	C8-N9-C4	5.42	108.57	106.40
1	A	1681	G	N3-C4-N9	-5.42	122.75	126.00
1	A	743	G	C5-C6-O6	-5.41	125.35	128.60
1	A	797	C	N3-C4-C5	-5.41	119.73	121.90
1	A	2281	C	C6-N1-C2	-5.41	118.14	120.30
1	A	945	A	C4-C5-C6	5.41	119.70	117.00
2	B	74	U	C5-C4-O4	5.41	129.15	125.90
1	A	271	A	C8-N9-C4	5.41	107.96	105.80
1	A	1765	C	C5-C6-N1	5.41	123.70	121.00
1	A	2040	C	C6-N1-C2	5.41	122.46	120.30
1	A	533	G	N1-C2-N3	5.40	127.14	123.90
1	A	1617	C	N1-C2-O2	-5.40	115.66	118.90
1	A	142	A	N1-C6-N6	-5.40	115.36	118.60
1	A	806	C	C2-N1-C1'	5.40	124.74	118.80
1	A	1395	A	N9-C4-C5	5.40	107.96	105.80
1	A	1997	G	C6-N1-C2	-5.40	121.86	125.10
1	A	2066	C	N3-C4-N4	5.40	121.78	118.00
1	A	2831	G	C8-N9-C4	5.40	108.56	106.40
1	A	127	A	C8-N9-C4	5.40	107.96	105.80
1	A	139(A)	G	N3-C4-C5	-5.40	125.90	128.60
1	A	265	A	C4-N9-C1'	5.40	136.02	126.30
1	A	2244	U	C4-C5-C6	5.40	122.94	119.70
1	A	733	G	C8-N9-C1'	-5.40	119.98	127.00
1	A	1650	G	N1-C6-O6	5.40	123.14	119.90
1	A	1791	A	C5-C6-N6	-5.40	119.38	123.70
1	A	2191	G	N3-C4-N9	-5.40	122.76	126.00
1	A	425	G	C4-N9-C1'	5.39	133.51	126.50
1	A	702	G	C8-N9-C4	5.39	108.56	106.40
1	A	979	G	N7-C8-N9	5.39	115.80	113.10
1	A	2022	U	N1-C2-O2	-5.39	119.03	122.80
1	A	761	A	C5-N7-C8	5.39	106.59	103.90
1	A	2304	G	C8-N9-C4	-5.39	104.24	106.40
1	A	2621	A	N1-C2-N3	5.39	131.99	129.30
1	A	928	G	C4-N9-C1'	5.39	133.50	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1779	U	C2-N1-C1'	5.39	124.17	117.70
1	A	833	U	N1-C2-O2	-5.38	119.03	122.80
1	A	1569	A	C8-N9-C4	-5.38	103.65	105.80
1	A	2583	G	C8-N9-C4	-5.38	104.25	106.40
1	A	614(C)	A	N1-C6-N6	-5.38	115.37	118.60
2	B	90	A	C8-N9-C4	5.38	107.95	105.80
1	A	855	G	C6-C5-N7	-5.38	127.17	130.40
1	A	1264	G	C2-N3-C4	-5.38	109.21	111.90
1	A	1638	C	C5-C6-N1	-5.38	118.31	121.00
1	A	1558	A	C5-N7-C8	-5.38	101.21	103.90
1	A	2581	G	N3-C4-C5	-5.38	125.91	128.60
1	A	76	C	C6-N1-C2	-5.38	118.15	120.30
1	A	1587	A	C2-N3-C4	5.38	113.29	110.60
1	A	517	C	C5-C4-N4	-5.37	116.44	120.20
1	A	745	G	C5-C6-N1	-5.37	108.81	111.50
1	A	1960	A	C2-N3-C4	-5.37	107.91	110.60
2	B	25	A	N1-C6-N6	5.37	121.82	118.60
1	A	488	G	C5-N7-C8	5.37	106.99	104.30
1	A	2384	G	N1-C6-O6	5.37	123.12	119.90
1	A	893	C	C2-N1-C1'	5.37	124.71	118.80
1	A	1644	C	N3-C2-O2	-5.37	118.14	121.90
1	A	428	A	N3-C4-C5	-5.37	123.04	126.80
1	A	1265	A	C2-N3-C4	-5.37	107.92	110.60
1	A	2018	G	C8-N9-C4	-5.37	104.25	106.40
1	A	668	G	N1-C6-O6	5.37	123.12	119.90
1	A	1899	G	N9-C4-C5	-5.37	103.25	105.40
1	A	494	G	C8-N9-C4	5.36	108.55	106.40
1	A	962	G	C6-C5-N7	-5.36	127.18	130.40
1	A	1216	G	C8-N9-C1'	-5.36	120.03	127.00
1	A	1372	U	C5-C4-O4	-5.36	122.68	125.90
1	A	2099	U	C6-N1-C2	-5.36	117.78	121.00
1	A	930	U	C6-N1-C2	5.36	124.22	121.00
1	A	2771	C	N1-C2-O2	5.36	122.11	118.90
1	A	1832	C	N3-C2-O2	5.36	125.65	121.90
1	A	1839	G	C8-N9-C4	5.36	108.54	106.40
1	A	747	U	C5-C4-O4	-5.35	122.69	125.90
1	A	1273	U	C4-C5-C6	5.35	122.91	119.70
1	A	2360	A	C8-N9-C4	5.35	107.94	105.80
1	A	2503	A	C5-C6-N1	5.35	120.38	117.70
1	A	506	G	C5-C6-O6	-5.35	125.39	128.60
1	A	1519	G	C8-N9-C4	-5.35	104.26	106.40
1	A	1936	A	N1-C6-N6	5.35	121.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2235	G	C8-N9-C4	-5.35	104.26	106.40
1	A	2394	C	N3-C2-O2	-5.35	118.15	121.90
1	A	2373	G	N7-C8-N9	-5.35	110.42	113.10
1	A	188	G	N1-C6-O6	5.35	123.11	119.90
1	A	1277	G	C4-N9-C1'	-5.35	119.55	126.50
1	A	2405	G	C4-N9-C1'	5.35	133.45	126.50
1	A	895	U	C5-C6-N1	5.35	125.37	122.70
1	A	1322	A	C2-N3-C4	-5.34	107.93	110.60
1	A	1687	G	N1-C6-O6	-5.34	116.69	119.90
23	1	21	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	1831	G	C8-N9-C4	-5.34	104.26	106.40
1	A	2541	A	N1-C6-N6	5.34	121.80	118.60
1	A	2622	C	C2-N1-C1'	-5.34	112.93	118.80
1	A	1964	G	C4-N9-C1'	5.34	133.44	126.50
1	A	1330	C	N3-C2-O2	5.34	125.64	121.90
1	A	2714	G	N3-C2-N2	-5.33	116.17	119.90
1	A	482	A	C8-N9-C4	5.33	107.93	105.80
1	A	1305	C	C5-C6-N1	5.33	123.67	121.00
1	A	1999	C	C2-N3-C4	-5.33	117.23	119.90
1	A	1320	C	N1-C2-O2	-5.33	115.70	118.90
1	A	1353	A	N1-C6-N6	-5.33	115.40	118.60
1	A	2515	C	C6-N1-C2	-5.33	118.17	120.30
1	A	2766	G	C4-C5-N7	5.33	112.93	110.80
4	E	78	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	1675	C	C5-C4-N4	5.32	123.93	120.20
1	A	776	G	C8-N9-C1'	-5.32	120.08	127.00
1	A	945	A	C5-C6-N1	-5.32	115.04	117.70
1	A	789	A	C8-N9-C4	-5.32	103.67	105.80
1	A	2644	G	C4-C5-N7	-5.32	108.67	110.80
1	A	13	A	N1-C6-N6	-5.32	115.41	118.60
1	A	2191	G	N3-C4-C5	5.32	131.26	128.60
1	A	1223	G	C8-N9-C1'	5.32	133.91	127.00
1	A	1163	G	N3-C2-N2	-5.31	116.18	119.90
1	A	1894	C	N1-C2-O2	-5.31	115.71	118.90
1	A	1964	G	C6-C5-N7	-5.31	127.21	130.40
1	A	2365	G	C4-C5-N7	5.31	112.92	110.80
1	A	2829	C	C2-N1-C1'	-5.31	112.96	118.80
1	A	1626	G	C8-N9-C4	-5.31	104.28	106.40
1	A	1675	C	C6-N1-C2	-5.31	118.18	120.30
1	A	2341	G	N1-C6-O6	5.31	123.08	119.90
1	A	2459	A	C8-N9-C4	-5.31	103.68	105.80
1	A	774	A	N7-C8-N9	5.31	116.45	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1579	A	C8-N9-C1'	-5.31	118.15	127.70
1	A	946	G	C8-N9-C4	-5.30	104.28	106.40
1	A	1822	G	C5-C6-N1	-5.30	108.85	111.50
1	A	142	A	N9-C4-C5	5.30	107.92	105.80
1	A	514	A	C5-C6-N6	-5.30	119.46	123.70
1	A	2827	C	N1-C2-O2	-5.30	115.72	118.90
1	A	2877	G	C8-N9-C4	5.30	108.52	106.40
1	A	1631	C	C6-N1-C2	5.30	122.42	120.30
1	A	2519	U	C5-C6-N1	-5.30	120.05	122.70
1	A	1218	C	C6-N1-C2	-5.30	118.18	120.30
1	A	2022	U	C4-C5-C6	5.30	122.88	119.70
1	A	2791	C	N3-C4-C5	-5.30	119.78	121.90
1	A	1187	G	C4-N9-C1'	5.29	133.38	126.50
1	A	2502	G	N1-C6-O6	5.29	123.08	119.90
1	A	1984	G	N3-C2-N2	-5.29	116.20	119.90
1	A	2597	G	C8-N9-C1'	-5.29	120.12	127.00
1	A	1429	G	N9-C4-C5	5.29	107.52	105.40
1	A	512	G	N1-C6-O6	-5.29	116.73	119.90
1	A	1237	A	N1-C6-N6	-5.29	115.43	118.60
1	A	1679	U	N3-C4-C5	-5.29	111.43	114.60
1	A	1838	C	N1-C2-O2	5.29	122.07	118.90
1	A	2729	G	C4-C5-N7	5.29	112.92	110.80
1	A	1702	G	C4-N9-C1'	-5.29	119.63	126.50
1	A	838	C	C5-C6-N1	-5.28	118.36	121.00
1	A	13	A	C5-C6-N6	5.28	127.92	123.70
1	A	2447	G	N1-C2-N2	5.28	120.95	116.20
1	A	2607	G	C6-C5-N7	-5.28	127.23	130.40
1	A	2838	G	N3-C2-N2	-5.28	116.20	119.90
1	A	1788	C	C6-N1-C2	-5.28	118.19	120.30
1	A	329	G	C4-N9-C1'	5.28	133.36	126.50
1	A	1008	C	C6-N1-C2	5.28	122.41	120.30
1	A	1232	G	N3-C4-N9	-5.28	122.83	126.00
1	A	2575	C	N3-C2-O2	-5.28	118.21	121.90
1	A	1844	C	C5-C4-N4	-5.27	116.51	120.20
1	A	59	U	N1-C2-N3	5.27	118.06	114.90
1	A	534	U	N3-C4-C5	-5.27	111.44	114.60
1	A	2515	C	N1-C2-O2	-5.27	115.74	118.90
10	O	26	LYS	N-CA-C	-5.27	96.77	111.00
1	A	114	U	C2-N1-C1'	5.27	124.02	117.70
1	A	135	G	N3-C4-C5	5.27	131.23	128.60
1	A	531	C	C6-N1-C1'	5.27	127.12	120.80
1	A	294	A	N1-C6-N6	-5.27	115.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	968	G	C8-N9-C4	-5.26	104.29	106.40
1	A	1423	G	C8-N9-C4	5.26	108.51	106.40
1	A	2060	A	C5-C6-N1	5.26	120.33	117.70
1	A	2504	U	N1-C2-N3	-5.26	111.74	114.90
1	A	752	A	C8-N9-C4	-5.26	103.69	105.80
1	A	1193	G	N1-C6-O6	5.26	123.06	119.90
1	A	2049	G	C2-N3-C4	-5.26	109.27	111.90
1	A	530	G	N9-C4-C5	5.26	107.50	105.40
1	A	2049	G	N3-C4-C5	5.26	131.23	128.60
1	A	2382	G	N3-C4-C5	-5.26	125.97	128.60
1	A	2829	C	N3-C2-O2	5.26	125.58	121.90
1	A	1471	A	C8-N9-C4	-5.26	103.70	105.80
1	A	1829	A	C2-N3-C4	-5.26	107.97	110.60
2	B	19	G	N3-C4-N9	-5.26	122.85	126.00
2	B	103	G	C4-C5-N7	5.26	112.90	110.80
1	A	1619	G	C2-N3-C4	5.25	114.53	111.90
1	A	1142	U	C6-N1-C1'	-5.25	113.85	121.20
1	A	1600	C	C5-C6-N1	-5.25	118.37	121.00
1	A	2619	C	C6-N1-C2	5.25	122.40	120.30
1	A	222	A	C8-N9-C4	5.25	107.90	105.80
1	A	1970	A	N7-C8-N9	5.25	116.42	113.80
1	A	2033	A	N9-C4-C5	5.25	107.90	105.80
1	A	2566	A	N3-C4-N9	-5.25	123.20	127.40
1	A	2426	A	C4-C5-N7	5.25	113.32	110.70
1	A	2821	A	N1-C2-N3	5.25	131.92	129.30
1	A	616	G	N3-C4-N9	5.24	129.15	126.00
1	A	977	G	C4-C5-N7	5.24	112.90	110.80
1	A	1787	A	N9-C4-C5	-5.24	103.70	105.80
1	A	2583	G	C5-C6-O6	5.24	131.75	128.60
1	A	137	C	C6-N1-C2	-5.24	118.20	120.30
1	A	188	G	N3-C4-C5	5.24	131.22	128.60
1	A	893	C	C5-C6-N1	5.24	123.62	121.00
1	A	2876	G	N1-C6-O6	5.24	123.05	119.90
1	A	464	U	N3-C4-O4	5.24	123.07	119.40
1	A	473	G	C2-N3-C4	-5.24	109.28	111.90
1	A	530	G	C8-N9-C1'	5.24	133.81	127.00
1	A	1945	G	N3-C4-N9	5.24	129.14	126.00
1	A	2589	A	N7-C8-N9	-5.24	111.18	113.80
1	A	2446	G	C4-C5-N7	-5.24	108.70	110.80
1	A	1839	G	N9-C4-C5	-5.24	103.31	105.40
1	A	2775	A	C8-N9-C4	5.24	107.89	105.80
1	A	730	C	N3-C4-C5	5.23	123.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	930	U	N1-C2-N3	-5.23	111.76	114.90
1	A	1637	A	N1-C2-N3	5.23	131.92	129.30
1	A	1789	A	N1-C6-N6	-5.23	115.46	118.60
1	A	2555	U	C2-N1-C1'	-5.23	111.42	117.70
1	A	2321	G	C4-N9-C1'	5.23	133.30	126.50
1	A	1551	C	N3-C4-C5	-5.23	119.81	121.90
1	A	71	A	C4-C5-C6	5.23	119.61	117.00
1	A	132	G	C5-C6-O6	5.23	131.74	128.60
1	A	1204	A	O4'-C1'-N9	5.23	112.38	108.20
1	A	1945	G	C8-N9-C1'	-5.23	120.21	127.00
1	A	2485	G	N3-C4-N9	5.22	129.13	126.00
1	A	696	G	C5-N7-C8	5.22	106.91	104.30
1	A	1631	C	C2-N3-C4	-5.22	117.29	119.90
1	A	2571	C	C6-N1-C2	-5.22	118.21	120.30
1	A	2607	G	C8-N9-C4	5.22	108.49	106.40
1	A	1371	G	C5-C6-N1	5.22	114.11	111.50
1	A	1260	G	N7-C8-N9	-5.21	110.49	113.10
1	A	1813	G	N3-C2-N2	-5.21	116.25	119.90
1	A	1984	G	C8-N9-C4	-5.21	104.31	106.40
1	A	1441	G	C8-N9-C4	5.21	108.48	106.40
1	A	2035	G	C5-N7-C8	5.21	106.91	104.30
1	A	219	G	N3-C4-C5	-5.21	125.99	128.60
1	A	329	G	N1-C2-N2	-5.21	111.51	116.20
1	A	1683	C	C6-N1-C2	5.21	122.38	120.30
5	F	12	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	2726	U	C6-N1-C2	5.21	124.13	121.00
1	A	837	C	N3-C4-N4	5.21	121.65	118.00
1	A	298	G	C5-N7-C8	-5.21	101.70	104.30
1	A	2608	G	C5-C6-O6	5.21	131.72	128.60
1	A	1455	G	C8-N9-C4	-5.20	104.32	106.40
1	A	2089	U	N3-C2-O2	5.20	125.84	122.20
1	A	820	A	C5-C6-N6	5.20	127.86	123.70
1	A	1675	C	N3-C2-O2	-5.20	118.26	121.90
1	A	1229	G	N1-C6-O6	5.20	123.02	119.90
1	A	1394	U	N3-C2-O2	-5.20	118.56	122.20
1	A	2695	C	C5-C6-N1	-5.20	118.40	121.00
1	A	734	A	C5-N7-C8	-5.20	101.30	103.90
1	A	2443	C	N3-C2-O2	-5.20	118.26	121.90
1	A	672	C	C5-C6-N1	-5.19	118.40	121.00
1	A	574	C	C6-N1-C1'	5.19	127.03	120.80
1	A	2014	A	C4-C5-C6	5.19	119.59	117.00
1	A	2894	G	C8-N9-C1'	-5.19	120.25	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1299	G	N1-C2-N3	5.19	127.01	123.90
1	A	767	U	N3-C2-O2	-5.19	118.57	122.20
1	A	559	G	N3-C4-C5	5.18	131.19	128.60
1	A	377	C	N1-C2-O2	-5.18	115.79	118.90
1	A	552	G	N3-C4-N9	-5.18	122.89	126.00
1	A	1496	A	C8-N9-C4	-5.18	103.73	105.80
1	A	2823	A	C5-N7-C8	-5.18	101.31	103.90
1	A	1691	C	N1-C2-O2	-5.18	115.79	118.90
1	A	2288	A	C8-N9-C4	-5.18	103.73	105.80
1	A	849	A	N9-C4-C5	5.18	107.87	105.80
1	A	1992	G	C2-N3-C4	5.18	114.49	111.90
1	A	2185	C	N1-C2-O2	5.18	122.01	118.90
1	A	673	C	C2-N3-C4	-5.18	117.31	119.90
1	A	546	C	C2-N1-C1'	5.18	124.50	118.80
1	A	1645	G	N3-C4-C5	-5.18	126.01	128.60
1	A	2321	G	N3-C4-C5	-5.18	126.01	128.60
1	A	1135	C	C6-N1-C1'	-5.17	114.59	120.80
1	A	1897	G	C8-N9-C4	5.17	108.47	106.40
1	A	2054	A	C8-N9-C4	-5.17	103.73	105.80
1	A	2444	G	C4-C5-N7	-5.17	108.73	110.80
1	A	2618	G	C4-C5-N7	-5.17	108.73	110.80
1	A	1347	G	N3-C4-C5	5.17	131.19	128.60
1	A	2429	G	N1-C6-O6	5.17	123.00	119.90
1	A	196	A	C8-N9-C4	5.17	107.87	105.80
1	A	589	C	N3-C2-O2	5.17	125.52	121.90
1	A	729	G	C5-C6-O6	-5.17	125.50	128.60
1	A	1655	A	C8-N9-C4	5.17	107.87	105.80
1	A	2401	U	C2-N1-C1'	5.17	123.90	117.70
1	A	512	G	C5-C6-O6	5.17	131.70	128.60
1	A	1129	A	C4-C5-C6	-5.17	114.42	117.00
2	B	53	A	C8-N9-C4	-5.17	103.73	105.80
1	A	2775	A	C4-C5-C6	-5.17	114.42	117.00
1	A	1262	A	C5-C6-N6	-5.16	119.57	123.70
1	A	209	C	C6-N1-C2	5.16	122.36	120.30
1	A	747	U	C6-N1-C1'	-5.16	113.97	121.20
1	A	2028	U	C4-C5-C6	5.16	122.80	119.70
1	A	784	A	N9-C4-C5	5.16	107.86	105.80
1	A	1769	G	C5-C6-O6	-5.16	125.50	128.60
1	A	1792	G	C8-N9-C4	5.16	108.47	106.40
1	A	541	C	C6-N1-C2	5.16	122.36	120.30
1	A	781	A	C8-N9-C4	-5.16	103.74	105.80
1	A	135	G	N3-C4-N9	-5.15	122.91	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2365	G	C6-C5-N7	-5.15	127.31	130.40
1	A	2553	G	C8-N9-C1'	-5.15	120.30	127.00
1	A	1788	C	C2-N1-C1'	5.15	124.47	118.80
1	A	518	G	C4-N9-C1'	5.15	133.19	126.50
1	A	1470	G	N3-C2-N2	-5.15	116.30	119.90
1	A	2032	G	C5-N7-C8	5.15	106.87	104.30
1	A	2609	U	C6-N1-C2	-5.15	117.91	121.00
1	A	1214	A	C6-N1-C2	-5.15	115.51	118.60
1	A	493	G	C5-N7-C8	-5.14	101.73	104.30
1	A	467	G	N9-C4-C5	-5.14	103.34	105.40
1	A	2728	U	C5-C6-N1	-5.14	120.13	122.70
1	A	2842	G	N3-C4-C5	5.14	131.17	128.60
1	A	672	C	N1-C2-O2	-5.14	115.81	118.90
1	A	306	U	C6-N1-C2	-5.14	117.92	121.00
1	A	546	C	C6-N1-C2	-5.14	118.24	120.30
1	A	1238	G	N1-C6-O6	-5.14	116.82	119.90
1	A	2425	A	C5-C6-N1	5.14	120.27	117.70
1	A	684	G	C8-N9-C4	-5.14	104.34	106.40
1	A	2755	C	N3-C4-N4	5.14	121.60	118.00
2	B	102	A	N9-C4-C5	-5.14	103.75	105.80
1	A	1421	G	C5-C6-N1	-5.14	108.93	111.50
1	A	1678	G	C4-C5-C6	5.13	121.88	118.80
1	A	2716	U	N1-C2-N3	5.13	117.98	114.90
1	A	825	C	C4-C5-C6	5.13	119.97	117.40
1	A	1276	A	N9-C4-C5	-5.13	103.75	105.80
1	A	965	C	C6-N1-C2	-5.13	118.25	120.30
1	A	2412	A	C8-N9-C4	-5.13	103.75	105.80
1	A	451	C	N3-C4-C5	5.13	123.95	121.90
1	A	2195	C	C2-N1-C1'	-5.13	113.16	118.80
1	A	2405	G	C8-N9-C1'	-5.13	120.33	127.00
1	A	2695	C	C2-N1-C1'	-5.13	113.16	118.80
2	B	22	U	C5-C6-N1	5.13	125.26	122.70
1	A	799	G	N1-C2-N3	5.13	126.97	123.90
1	A	1256	G	C4-N9-C1'	5.12	133.16	126.50
1	A	1566	A	C2-N3-C4	-5.12	108.04	110.60
1	A	2394	C	N1-C2-O2	5.12	121.97	118.90
1	A	15	G	C8-N9-C4	5.12	108.45	106.40
1	A	34	C	N1-C2-O2	5.12	121.97	118.90
1	A	242	G	C4-N9-C1'	-5.12	119.84	126.50
1	A	2027	G	N3-C4-C5	-5.12	126.04	128.60
3	D	211	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	102	G	P-O3'-C3'	5.12	125.84	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	G	N7-C8-N9	-5.12	110.54	113.10
1	A	1128	A	C2-N3-C4	5.12	113.16	110.60
1	A	1231	G	C5-C6-N1	-5.12	108.94	111.50
1	A	1801	G	C6-N1-C2	-5.12	122.03	125.10
1	A	1961	C	C2-N1-C1'	-5.12	113.17	118.80
1	A	2007	C	C2-N1-C1'	-5.12	113.17	118.80
1	A	2751	G	C2-N3-C4	5.12	114.46	111.90
1	A	125	G	N9-C4-C5	-5.12	103.35	105.40
1	A	546	C	N1-C2-O2	5.12	121.97	118.90
1	A	2283	C	N1-C2-O2	-5.12	115.83	118.90
1	A	2831	G	N1-C6-O6	-5.12	116.83	119.90
1	A	1157	G	C4-N9-C1'	5.12	133.15	126.50
1	A	1984	G	N7-C8-N9	5.12	115.66	113.10
1	A	2006	C	C6-N1-C2	-5.11	118.25	120.30
2	B	2	C	C2-N1-C1'	5.11	124.43	118.80
1	A	624	C	N1-C2-O2	-5.11	115.83	118.90
1	A	1829	A	N1-C2-N3	5.11	131.86	129.30
1	A	1531	C	N3-C4-N4	5.11	121.58	118.00
1	A	1789	A	C8-N9-C4	5.11	107.84	105.80
1	A	1992	G	N7-C8-N9	5.11	115.65	113.10
1	A	2590	A	C5-C6-N1	5.11	120.25	117.70
1	A	1969	A	C5-N7-C8	-5.10	101.35	103.90
1	A	1115	G	C4-N9-C1'	-5.10	119.87	126.50
1	A	1670	C	N3-C2-O2	-5.10	118.33	121.90
1	A	2528	U	N3-C4-C5	-5.10	111.54	114.60
1	A	2426	A	C5-C6-N6	-5.10	119.62	123.70
1	A	1556	C	C4-C5-C6	5.10	119.95	117.40
1	A	2256	G	C2-N3-C4	5.10	114.45	111.90
1	A	265	A	N1-C2-N3	5.09	131.85	129.30
1	A	620	G	N9-C4-C5	5.09	107.44	105.40
18	W	12	ILE	N-CA-C	-5.09	97.24	111.00
1	A	2565	A	N3-C4-C5	5.09	130.37	126.80
2	B	103	G	C5-C6-O6	-5.09	125.54	128.60
1	A	187	G	N1-C2-N3	5.09	126.95	123.90
1	A	2031	A	N9-C4-C5	-5.09	103.76	105.80
1	A	2186	G	C5-C6-N1	-5.09	108.95	111.50
1	A	2302	G	N1-C6-O6	5.09	122.95	119.90
1	A	2502	G	N7-C8-N9	5.09	115.64	113.10
1	A	693	C	C5-C6-N1	-5.09	118.46	121.00
2	B	54	G	C4-N9-C1'	5.09	133.11	126.50
1	A	552	G	N3-C4-C5	5.08	131.14	128.60
1	A	1669	A	N1-C2-N3	5.08	131.84	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1814	G	N7-C8-N9	5.08	115.64	113.10
1	A	1936	A	C4-C5-N7	5.08	113.24	110.70
1	A	2012	G	C6-C5-N7	-5.08	127.35	130.40
1	A	500	G	C5-C6-N1	-5.08	108.96	111.50
1	A	2286	A	C8-N9-C1'	-5.08	118.56	127.70
1	A	1797	C	C6-N1-C2	5.08	122.33	120.30
1	A	27	G	C8-N9-C4	-5.08	104.37	106.40
1	A	930	U	C5-C4-O4	-5.08	122.85	125.90
1	A	329	G	C8-N9-C4	-5.07	104.37	106.40
1	A	1770	G	C6-C5-N7	-5.07	127.36	130.40
1	A	781	A	C5-N7-C8	-5.07	101.36	103.90
1	A	982	C	C2-N3-C4	5.07	122.44	119.90
1	A	1452	A	N1-C6-N6	5.07	121.64	118.60
1	A	2405	G	C5-C6-O6	5.07	131.64	128.60
1	A	2502	G	C4-C5-C6	5.07	121.84	118.80
1	A	1340	U	C2-N3-C4	-5.07	123.96	127.00
1	A	74	A	C5-C6-N6	5.07	127.75	123.70
1	A	341	G	N1-C2-N2	-5.07	111.64	116.20
1	A	748	G	N3-C2-N2	5.07	123.45	119.90
1	A	781	A	C5-C6-N6	-5.06	119.65	123.70
1	A	933	A	N1-C6-N6	5.06	121.64	118.60
1	A	945	A	C8-N9-C1'	-5.06	118.59	127.70
1	A	1235	G	C8-N9-C4	-5.06	104.38	106.40
1	A	1997	G	C5-C6-O6	-5.06	125.56	128.60
1	A	1694	C	C6-N1-C2	5.06	122.32	120.30
1	A	2892	A	C8-N9-C4	-5.06	103.78	105.80
1	A	1121	C	N3-C4-N4	-5.06	114.46	118.00
1	A	2857	G	C5-N7-C8	-5.06	101.77	104.30
1	A	861	A	C8-N9-C4	-5.05	103.78	105.80
1	A	1616	A	C4-C5-N7	5.05	113.22	110.70
1	A	197	A	C6-N1-C2	-5.05	115.57	118.60
1	A	510	C	C2-N1-C1'	5.05	124.36	118.80
1	A	2440	C	C4-C5-C6	5.05	119.92	117.40
1	A	253	C	C5-C4-N4	-5.05	116.67	120.20
1	A	1354	A	C5-C6-N1	5.05	120.22	117.70
1	A	1698	A	C6-N1-C2	5.05	121.63	118.60
1	A	718	A	N1-C6-N6	5.05	121.63	118.60
1	A	788	A	N9-C4-C5	-5.05	103.78	105.80
1	A	1814	G	N1-C2-N3	5.05	126.93	123.90
1	A	2608	G	C2-N3-C4	-5.05	109.38	111.90
18	W	92	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	115	C	C5-C6-N1	-5.04	118.48	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1492	G	N3-C2-N2	-5.04	116.37	119.90
1	A	116	C	C6-N1-C1'	5.04	126.85	120.80
1	A	472	A	N1-C6-N6	5.04	121.62	118.60
1	A	1774	C	C6-N1-C2	-5.04	118.28	120.30
1	A	509	C	C2-N3-C4	-5.04	117.38	119.90
1	A	1834	U	N1-C2-O2	5.04	126.33	122.80
2	B	56	G	C2-N3-C4	5.04	114.42	111.90
1	A	1187	G	N7-C8-N9	5.04	115.62	113.10
2	B	102	A	C4-C5-N7	5.04	113.22	110.70
1	A	612	C	C2-N1-C1'	-5.03	113.26	118.80
1	A	923	C	C5-C6-N1	5.03	123.52	121.00
1	A	1964	G	N3-C4-C5	-5.03	126.08	128.60
1	A	6	A	N3-C4-C5	-5.03	123.28	126.80
1	A	2104	G	N3-C2-N2	5.03	123.42	119.90
1	A	378	C	N3-C4-C5	5.03	123.91	121.90
1	A	798	G	C5-C6-N1	-5.03	108.98	111.50
1	A	2697	G	N9-C4-C5	-5.03	103.39	105.40
1	A	1354	A	N1-C6-N6	-5.03	115.58	118.60
1	A	1923	U	C5-C6-N1	5.03	125.21	122.70
1	A	1964	G	C5-C6-O6	-5.03	125.58	128.60
1	A	142	A	C8-N9-C4	-5.02	103.79	105.80
1	A	798	G	N3-C4-N9	-5.02	122.99	126.00
1	A	391	G	C5-C6-N1	-5.02	108.99	111.50
1	A	528	A	C8-N9-C4	-5.02	103.79	105.80
1	A	1219	G	N3-C4-C5	5.02	131.11	128.60
1	A	1299	G	C8-N9-C4	-5.02	104.39	106.40
1	A	2356	C	C6-N1-C2	5.02	122.31	120.30
1	A	2827	C	N3-C2-O2	5.02	125.41	121.90
1	A	760	G	N7-C8-N9	5.02	115.61	113.10
1	A	1482	G	C2-N3-C4	5.02	114.41	111.90
1	A	1377	G	C4-C5-C6	5.01	121.81	118.80
1	A	1266	G	N3-C4-N9	5.01	129.01	126.00
1	A	2246	G	C2-N3-C4	-5.01	109.39	111.90
1	A	2455	G	C4-N9-C1'	5.01	133.02	126.50
1	A	92	A	C6-C5-N7	-5.01	128.79	132.30
1	A	503	A	N9-C4-C5	5.01	107.80	105.80
1	A	755	C	N1-C2-O2	-5.01	115.89	118.90
1	A	945	A	N1-C2-N3	5.01	131.81	129.30
1	A	1667	G	C8-N9-C4	5.01	108.40	106.40
1	A	60	G	C8-N9-C1'	5.01	133.51	127.00
1	A	90	U	N3-C4-O4	5.01	122.91	119.40
1	A	574	C	C2-N3-C4	5.01	122.40	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1670	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1992	G	P-O3'-C3'	5.01	125.71	119.70
1	A	2476	A	N9-C4-C5	5.01	107.80	105.80
1	A	1670	C	N1-C2-N3	5.01	122.70	119.20
1	A	1789	A	N7-C8-N9	-5.01	111.30	113.80
1	A	2824	C	C6-N1-C2	5.01	122.30	120.30
1	A	314	A	C4-C5-C6	-5.01	114.50	117.00
1	A	1671	U	N3-C2-O2	5.01	125.70	122.20
1	A	2361	A	N1-C2-N3	5.01	131.80	129.30
1	A	603	A	C8-N9-C4	5.00	107.80	105.80
1	A	1937	A	C4-C5-C6	5.00	119.50	117.00
1	A	1990	C	C5-C4-N4	5.00	123.70	120.20
1	A	2288	A	N7-C8-N9	5.00	116.30	113.80

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	1	83	GLU	Peptide
24	2	43	GLN	Peptide
26	4	42	PHE	Peptide
28	6	43	CYS	Peptide
4	E	72	VAL	Peptide
5	F	85	GLY	Peptide
6	G	13	GLU	Peptide
6	G	49	ASP	Peptide
6	G	50	ALA	Peptide
7	H	92	ILE	Peptide
10	O	48	PRO	Peptide
11	P	26	GLY	Peptide
12	Q	1	MET	Peptide
14	S	82	ILE	Peptide
15	T	126	ALA	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	58627	0	29570	1189	0
2	B	2573	0	1306	83	0
3	D	2136	0	2218	103	0
4	E	1555	0	1607	72	0
5	F	1578	0	1623	96	0
6	G	1361	0	1316	76	0
7	H	1317	0	1376	59	0
8	I	1057	0	1087	56	0
9	N	1112	0	1180	64	0
10	O	923	0	981	38	0
11	P	1131	0	1201	66	0
12	Q	1122	0	1179	66	0
13	R	968	0	1033	56	0
14	S	873	0	927	64	0
15	T	1058	0	1098	35	0
16	U	959	0	1019	49	0
17	V	770	0	838	40	0
18	W	877	0	932	32	0
19	X	732	0	777	17	0
20	Y	781	0	829	42	0
21	Z	1451	0	1421	72	0
22	0	607	0	622	39	0
23	1	745	0	804	37	0
24	2	584	0	623	26	0
25	3	453	0	501	28	0
26	4	349	0	336	19	0
27	5	451	0	461	25	0
28	6	437	0	440	16	0
29	7	402	0	434	11	0
30	8	509	0	565	26	0
31	9	292	0	313	14	0
32	0	3	0	0	0	0
32	1	1	0	0	0	0
32	6	2	0	0	0	0
32	7	1	0	0	0	0
32	A	686	0	0	0	0
32	B	16	0	0	0	0
32	D	3	0	0	0	0
32	E	4	0	0	0	0
32	F	3	0	0	0	0
32	O	1	0	0	0	0
32	P	1	0	0	0	0
32	Q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	R	1	0	0	0	0
32	T	3	0	0	0	0
32	U	1	0	0	0	0
32	V	1	0	0	0	0
32	X	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	1	2	0	0	1	0
34	3	1	0	0	0	0
34	6	2	0	0	0	0
34	7	2	0	0	0	0
34	8	4	0	0	1	0
34	A	1013	0	0	61	0
34	B	40	0	0	2	0
34	D	7	0	0	0	0
34	E	11	0	0	1	0
34	F	4	0	0	0	0
34	N	2	0	0	0	0
34	O	4	0	0	1	0
34	P	4	0	0	0	0
34	R	6	0	0	1	0
34	T	2	0	0	0	0
34	V	1	0	0	0	0
34	W	1	0	0	0	0
All	All	89631	0	58617	2284	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (2284) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:11:CYS:SG	31:9:32:HIS:HE1	1.40	1.43
1:A:885:C:N4	1:A:890:A:N6	1.81	1.27
1:A:1798:U:H5'	3:D:259:THR:HG22	1.36	1.03
1:A:31:C:OP1	34:A:3842:HOH:O	1.75	1.03
1:A:571:A:H5'	1:A:2030:A:H62	1.27	0.99
1:A:631:A:OP1	11:P:65:ARG:NH1	1.98	0.95
2:B:52:A:HO2'	2:B:53:A:H2	1.09	0.95
1:A:885:C:H42	1:A:890:A:N6	1.56	0.95

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1689:A:H62	1:A:1698:A:H2	1.14	0.94
23:1:50:ARG:HG2	23:1:59:THR:HB	1.51	0.93
1:A:271(I):G:H1	1:A:271(O):C:H42	1.13	0.90
1:A:885:C:N4	1:A:890:A:H61	1.68	0.90
28:6:16:CYS:HB3	28:6:43:CYS:SG	2.12	0.89
1:A:1038:C:H42	1:A:1117:G:H1	1.14	0.89
1:A:2407:G:OP1	34:A:4080:HOH:O	1.90	0.89
12:Q:16:ARG:HG2	12:Q:16:ARG:HH11	1.38	0.88
18:W:19:LEU:HB3	27:5:25:LEU:HD12	1.53	0.87
26:4:16:CYS:SG	26:4:36:CYS:HB3	2.16	0.86
8:I:71:ILE:HG23	8:I:72:LEU:HD23	1.58	0.86
3:D:206:LEU:HD22	3:D:211:ARG:HG2	1.56	0.86
1:A:1365:A:O2'	23:1:11:ARG:NH2	2.08	0.85
1:A:249:C:OP1	34:A:3993:HOH:O	1.94	0.85
1:A:2206:G:H5'	1:A:2207:G:N7	1.92	0.85
1:A:635:C:O2'	1:A:639:U:OP1	1.95	0.84
14:S:102:ALA:HA	14:S:105:ALA:H	1.42	0.84
1:A:2777:G:H5''	1:A:2778:A:H5'	1.59	0.84
14:S:34:HIS:HD1	14:S:53:SER:HG	1.25	0.84
1:A:2206:G:H3'	1:A:2207:G:C8	2.13	0.83
1:A:2287:A:H62	1:A:2344:U:H3	1.27	0.83
11:P:39:LYS:HB2	11:P:45:LEU:HD12	1.60	0.83
9:N:24:GLY:HA2	9:N:27:ALA:HB3	1.61	0.83
1:A:864:G:N7	12:Q:22:LYS:NZ	2.26	0.83
1:A:1210:A:H5'	1:A:1210:A:H8	1.43	0.83
1:A:1740:G:H2'	1:A:1741:A:H8	1.43	0.83
6:G:161:THR:HG22	6:G:163:ALA:H	1.43	0.82
1:A:1530:C:O2'	1:A:1531:C:O5'	1.97	0.82
15:T:54:ARG:HA	15:T:59:THR:HB	1.62	0.81
1:A:1889:A:H2'	1:A:1890:A:C8	2.15	0.81
1:A:154(A):C:H42	1:A:171:G:H1	1.28	0.81
1:A:1265:A:OP2	34:A:3900:HOH:O	1.97	0.81
1:A:1412:A:H2'	1:A:1413:G:H8	1.46	0.81
8:I:38:LEU:HB3	8:I:40:THR:HG23	1.62	0.81
1:A:826:U:H4'	11:P:55:ARG:HB2	1.63	0.80
6:G:36:LYS:HD3	6:G:95:ARG:HH12	1.45	0.80
1:A:11:G:H2'	1:A:12:U:H5'	1.64	0.80
1:A:2206:G:H3'	1:A:2207:G:H8	1.45	0.80
11:P:138:LEU:HD23	11:P:145:PRO:HG3	1.62	0.80
1:A:2276:G:H5'	12:Q:86:GLY:HA2	1.62	0.80
10:O:20:MET:HB2	10:O:44:LYS:HG2	1.64	0.80
1:A:851:U:H5'	25:3:49:LYS:HD2	1.64	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2308:G:O6	1:A:2311:A:N6	2.14	0.79
1:A:1762:A:N1	34:A:3949:HOH:O	2.14	0.79
17:V:76:LYS:HB2	17:V:81:TYR:HB3	1.63	0.79
14:S:34:HIS:ND1	14:S:53:SER:OG	2.10	0.79
1:A:299:A:H5''	20:Y:86:ARG:HH21	1.45	0.79
3:D:274:ARG:HG2	3:D:275:LYS:HB3	1.62	0.79
1:A:819:A:OP2	1:A:1187:G:N2	2.15	0.79
1:A:1365:A:OP1	23:1:41:ARG:NH1	2.17	0.78
6:G:63:ILE:HG22	6:G:64:THR:HG23	1.64	0.78
1:A:910:A:H62	12:Q:12:GLN:HA	1.49	0.78
1:A:781:A:OP1	3:D:218:ARG:NH2	2.17	0.78
1:A:784:A:OP2	34:A:3786:HOH:O	2.03	0.77
1:A:1250:G:N7	11:P:18:ARG:NH2	2.32	0.77
14:S:14:VAL:O	14:S:18:ILE:HG12	1.85	0.77
1:A:639:U:H2'	1:A:640:C:C6	2.19	0.77
1:A:317:G:N7	34:A:4589:HOH:O	2.16	0.77
1:A:271(I):G:H1	1:A:271(O):C:N4	1.81	0.77
2:B:13:A:N1	2:B:69:G:O2'	2.16	0.77
7:H:3:ARG:HD3	7:H:54:ARG:HH12	1.49	0.77
1:A:2839:G:H5'	13:R:46:GLY:HA2	1.65	0.77
1:A:1558:A:H4'	1:A:1559:G:O5'	1.85	0.77
1:A:2683:C:OP1	15:T:53:ARG:NH2	2.17	0.76
1:A:2100:G:H1	1:A:2189:U:H3	1.33	0.76
1:A:48:G:O6	34:A:4612:HOH:O	2.03	0.76
1:A:1453:U:OP1	13:R:77:ARG:NH1	2.19	0.76
1:A:2577:A:OP2	27:5:3:LYS:NZ	2.16	0.76
1:A:309:G:N3	1:A:329:G:O2'	2.18	0.76
31:9:25:VAL:HB	31:9:34:GLN:HB2	1.67	0.76
1:A:2293:C:O2	1:A:2339:G:N2	2.17	0.76
18:W:50:VAL:HG12	18:W:105:VAL:HG22	1.68	0.76
1:A:2296:U:OP2	14:S:9:ARG:NH2	2.18	0.76
10:O:35:VAL:HG11	10:O:103:ALA:HB3	1.67	0.76
1:A:2006:C:OP2	34:A:3821:HOH:O	2.02	0.76
31:9:29:ASN:HD22	31:9:32:HIS:CD2	2.03	0.75
1:A:2287:A:N6	1:A:2344:U:H3	1.82	0.75
1:A:1645:G:H5''	1:A:1646:C:H5'	1.69	0.75
1:A:676:A:H8	1:A:2069:G:H21	1.33	0.75
17:V:40:LEU:HB2	17:V:46:VAL:HG13	1.66	0.75
1:A:958:U:OP2	12:Q:14:ARG:NH1	2.17	0.75
21:Z:52:SER:OG	21:Z:53:ILE:N	2.15	0.75
21:Z:110:GLY:HA3	21:Z:174:VAL:HG11	1.68	0.75
1:A:1557:C:OP2	1:A:1558:A:O2'	2.03	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:83:ALA:HB1	8:I:87:LYS:O	1.87	0.75
1:A:1567:A:H5'	3:D:58:HIS:CD2	2.21	0.75
1:A:1740:G:H2'	1:A:1741:A:C8	2.22	0.74
1:A:300:A:P	20:Y:86:ARG:HH22	2.09	0.74
2:B:48:A:H4'	14:S:95:HIS:HD2	1.51	0.74
1:A:120:U:OP2	34:A:4223:HOH:O	2.04	0.74
23:1:21:ARG:HD3	23:1:35:THR:HG21	1.69	0.74
1:A:1316:U:H2'	1:A:1317:A:H8	1.53	0.74
1:A:500:G:N1	1:A:503:A:OP2	2.20	0.74
1:A:134:C:H42	1:A:145:G:H1	1.36	0.73
7:H:106:THR:HG22	7:H:112:PRO:HB3	1.69	0.73
3:D:182:LEU:HB3	3:D:271:ILE:HD12	1.70	0.73
3:D:177:LEU:HD12	3:D:181:GLU:HB3	1.69	0.73
5:F:185:ASP:HA	5:F:188:ARG:HD3	1.69	0.73
1:A:2712:U:O2'	1:A:2712(A):A:OP2	2.06	0.73
11:P:111:ARG:HG2	11:P:128:HIS:CG	2.23	0.73
1:A:468:G:N7	29:7:39:ARG:NH2	2.34	0.73
1:A:7:G:H2'	1:A:8:A:C8	2.23	0.73
1:A:1639:U:H2'	1:A:1640:C:H5''	1.71	0.73
8:I:72:LEU:C	8:I:74:ASN:H	1.90	0.73
1:A:1412:A:H2'	1:A:1413:G:C8	2.24	0.73
1:A:2567:G:H2'	1:A:2568:C:C6	2.23	0.73
1:A:2884:U:H1'	27:5:53:ALA:HB2	1.70	0.73
7:H:8:PRO:HB3	7:H:51:ARG:HG3	1.71	0.73
8:I:72:LEU:HA	8:I:75:LEU:HD12	1.69	0.73
7:H:80:SER:OG	7:H:81:GLU:N	2.21	0.73
6:G:47:LYS:HB3	6:G:82:LEU:HD13	1.71	0.73
1:A:587:C:OP2	11:P:21:ARG:NH2	2.21	0.73
13:R:51:LEU:HD22	13:R:66:VAL:HG13	1.69	0.72
1:A:1403:C:H5''	1:A:1471:A:H1'	1.71	0.72
12:Q:36:ALA:HB1	12:Q:127:ILE:HD11	1.71	0.72
4:E:128:SER:OG	4:E:129:HIS:N	2.20	0.72
1:A:2781:A:H5''	1:A:2782:G:H5'	1.70	0.72
23:1:23:LYS:HB3	23:1:29:GLY:HA3	1.70	0.72
9:N:58:ASP:N	9:N:58:ASP:OD1	2.14	0.72
1:A:885:C:C4	1:A:890:A:N6	2.54	0.72
20:Y:49:VAL:HG22	20:Y:61:ILE:HG22	1.70	0.72
1:A:863:A:H3'	12:Q:22:LYS:HE2	1.71	0.72
1:A:139(A):G:N2	19:X:44:GLU:OE1	2.22	0.72
1:A:33:U:O4	1:A:446:G:O2'	2.08	0.72
1:A:2692:C:HO2'	1:A:2847:U:HO2'	1.37	0.72
1:A:620:G:N3	1:A:620:G:H5''	2.05	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1009:A:OP1	9:N:37:LYS:NZ	2.20	0.71
25:3:23:LEU:HD12	25:3:28:LEU:HB2	1.72	0.71
1:A:2378:A:H4'	14:S:23:ARG:NH1	2.05	0.71
3:D:127:VAL:HA	3:D:193:VAL:HG23	1.71	0.71
1:A:479:A:N3	1:A:481:G:H5''	2.05	0.71
1:A:994:C:OP2	16:U:54:LYS:NZ	2.21	0.71
1:A:2307:G:H4'	1:A:2308:G:H5'	1.71	0.71
11:P:39:LYS:HD2	11:P:45:LEU:HD12	1.72	0.71
12:Q:34:LEU:HB2	12:Q:118:LEU:HD22	1.72	0.71
1:A:548:A:N6	17:V:19:LYS:H	1.89	0.71
1:A:991:C:H5'	1:A:991:C:H6	1.56	0.71
1:A:1266:G:O5'	18:W:15:ARG:NH2	2.23	0.71
23:1:54:ALA:HB1	23:1:83:GLU:HG3	1.73	0.70
9:N:34:LEU:O	9:N:49:GLY:HA3	1.91	0.70
1:A:384:U:H2'	1:A:385:C:H6	1.54	0.70
1:A:1721:G:H8	1:A:1741:A:H62	1.38	0.70
10:O:23:ARG:HG3	10:O:24:VAL:N	2.07	0.70
1:A:849:A:N1	25:3:25:ALA:HB2	2.05	0.70
1:A:1803:A:O2'	3:D:259:THR:HG21	1.91	0.70
11:P:120:ALA:HB1	11:P:138:LEU:HD12	1.71	0.70
1:A:1149:G:H2'	1:A:1150:C:C6	2.27	0.70
1:A:572:A:OP2	17:V:78:LYS:NZ	2.24	0.70
1:A:1332:G:N2	1:A:1609:A:O2'	2.23	0.70
1:A:2528:U:H5'	31:9:31:LYS:HD3	1.74	0.70
1:A:298:G:N7	34:A:3715:HOH:O	2.24	0.70
1:A:71:A:H5''	1:A:73:A:C8	2.27	0.70
12:Q:43:THR:HG22	12:Q:94:VAL:HG12	1.74	0.69
21:Z:156:LYS:HD2	21:Z:158:PRO:HG3	1.73	0.69
1:A:19:C:H2'	1:A:20:C:H6	1.57	0.69
1:A:2055:C:N3	34:A:3889:HOH:O	2.24	0.69
1:A:1021:A:H62	1:A:1141:U:H3	1.39	0.69
1:A:272(G):C:H42	1:A:363(C):G:H1	1.40	0.69
1:A:287:C:H42	1:A:354:G:H1	1.39	0.69
1:A:1776:G:OP2	34:A:3826:HOH:O	2.10	0.69
5:F:185:ASP:OD1	5:F:188:ARG:NH1	2.25	0.69
22:O:27:GLU:HB2	22:O:69:PHE:HD1	1.57	0.69
4:E:135:HIS:CD2	4:E:135:HIS:H	2.09	0.69
1:A:574:C:OP2	34:A:3915:HOH:O	2.10	0.69
6:G:108:ASN:HA	26:4:37:SER:HB3	1.74	0.69
1:A:71:A:OP2	1:A:71:A:H3'	1.92	0.69
6:G:96:ARG:O	6:G:99:MET:HB3	1.93	0.69
10:O:73:ASP:OD1	15:T:32:TYR:OH	2.10	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:51:VAL:HG12	3:D:54:ARG:HD3	1.75	0.68
4:E:143:ASN:HB2	4:E:147:PRO:HD2	1.75	0.68
1:A:152:G:H1	1:A:174:C:H42	1.40	0.68
1:A:2556:C:H2'	1:A:2557:G:O4'	1.92	0.68
1:A:637:A:H8	11:P:117:GLU:HG3	1.58	0.68
1:A:989:G:OP2	25:3:11:SER:OG	2.12	0.68
1:A:1980:G:O2'	1:A:1982:C:OP2	2.08	0.68
10:O:87:ILE:HG22	10:O:93:PRO:HA	1.75	0.68
1:A:495:G:H21	18:W:61:ASN:HD21	1.41	0.68
28:6:3:SER:H	28:6:6:ARG:HB3	1.57	0.68
2:B:90:A:C5	2:B:91:C:H1'	2.28	0.68
1:A:1721:G:H2'	1:A:1740:G:O6	1.94	0.68
1:A:2641:G:H5''	9:N:76:SER:HB3	1.75	0.68
1:A:9:U:H3	1:A:2629:A:H2	1.41	0.68
1:A:2570:G:N7	34:A:4170:HOH:O	2.26	0.68
1:A:1140:C:O3'	9:N:25:ARG:NH1	2.27	0.68
7:H:20:ALA:HB3	7:H:23:ARG:HB2	1.76	0.68
20:Y:61:ILE:HG13	20:Y:62:GLU:N	2.09	0.68
1:A:995:C:O2	9:N:3:THR:OG1	2.11	0.68
10:O:24:VAL:HA	10:O:39:ILE:HG22	1.74	0.68
1:A:1693:U:O2'	3:D:14:ARG:NH2	2.26	0.68
1:A:2816:C:O3'	13:R:99:LYS:NZ	2.25	0.68
1:A:1970:A:OP1	34:A:4202:HOH:O	2.12	0.68
1:A:928:G:O6	34:A:4218:HOH:O	2.09	0.68
1:A:848:G:H2'	1:A:849:A:C8	2.29	0.67
5:F:157:VAL:HB	5:F:194:MET:HG2	1.76	0.67
1:A:248:G:OP1	34:A:4615:HOH:O	2.11	0.67
13:R:21:TYR:CZ	13:R:43:GLU:HG2	2.29	0.67
1:A:2789:C:O3'	1:A:2790:A:H4'	1.93	0.67
7:H:9:ILE:HB	7:H:50:VAL:HB	1.76	0.67
1:A:1983:C:H2'	1:A:1984:G:H5''	1.76	0.67
1:A:2820:A:OP2	13:R:2:ARG:NH2	2.27	0.67
1:A:531:C:OP1	1:A:561:G:N1	2.28	0.67
1:A:827:U:OP1	34:A:4414:HOH:O	2.10	0.67
3:D:69:ARG:NH2	3:D:128:GLY:O	2.28	0.67
12:Q:57:HIS:CD2	12:Q:117:ALA:HB2	2.29	0.67
1:A:2577:A:H5''	1:A:2578:G:H5'	1.77	0.67
1:A:323:G:HO2'	1:A:1205:U:H3	1.43	0.67
25:3:10:LYS:HB3	25:3:53:LEU:HA	1.75	0.67
14:S:18:ILE:O	14:S:21:THR:HG22	1.94	0.67
1:A:1337:G:OP2	19:X:73:ARG:NH2	2.27	0.67
1:A:1405:U:H2'	1:A:1406:U:C6	2.29	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:N:104:LYS:HA	9:N:107:LEU:HD12	1.77	0.67
1:A:1721:G:N1	1:A:1739:U:OP2	2.28	0.66
1:A:660:G:H5'	5:F:99:TYR:CD2	2.30	0.66
14:S:96:GLY:HA2	14:S:100:ALA:H	1.60	0.66
12:Q:35:VAL:HG22	12:Q:36:ALA:H	1.60	0.66
1:A:15:G:OP2	34:A:4271:HOH:O	2.12	0.66
1:A:2019:A:O3'	16:U:27:LEU:HD12	1.95	0.66
3:D:5:LYS:HA	3:D:17:THR:HG22	1.76	0.66
1:A:548:A:H61	17:V:19:LYS:H	1.43	0.66
12:Q:37:LEU:HD21	12:Q:130:LYS:HB2	1.77	0.66
7:H:113:VAL:HG21	7:H:151:ILE:HG21	1.77	0.66
14:S:96:GLY:HA2	14:S:97:ARG:C	2.16	0.66
1:A:301:G:OP2	20:Y:84:ARG:NH2	2.22	0.66
22:O:65:GLY:HA3	22:O:81:VAL:HG12	1.77	0.66
20:Y:23:ARG:HG2	20:Y:42:VAL:HG22	1.77	0.66
1:A:1316:U:H2'	1:A:1317:A:C8	2.30	0.66
8:I:54:GLN:HG2	8:I:57:ARG:HH21	1.61	0.66
1:A:602:G:O2'	1:A:655:A:N6	2.29	0.66
1:A:363:G:H2'	1:A:363(A):A:H8	1.59	0.66
5:F:162:LEU:H	5:F:162:LEU:HD22	1.60	0.66
7:H:8:PRO:O	7:H:69:ARG:NH1	2.29	0.66
1:A:1599:C:H2'	1:A:1600:C:H6	1.60	0.66
1:A:1204:A:H2	1:A:1241:A:H62	1.44	0.66
1:A:2313:C:H2'	1:A:2314:C:H6	1.61	0.65
1:A:783:A:OP2	34:A:3786:HOH:O	2.12	0.65
16:U:92:ARG:HA	16:U:95:LEU:HB2	1.77	0.65
7:H:90:LYS:NZ	7:H:159:GLU:OE1	2.29	0.65
1:A:1614:A:OP1	34:A:4107:HOH:O	2.13	0.65
1:A:2316:C:H4'	6:G:128:ARG:HD2	1.79	0.65
1:A:1762:A:H2'	34:A:4674:HOH:O	1.97	0.65
26:4:33:VAL:HG12	26:4:34:GLU:H	1.61	0.65
2:B:40:U:O4	26:4:1:MET:N	2.22	0.65
1:A:997:G:OP2	16:U:58:ARG:NH1	2.30	0.65
1:A:607:U:OP1	5:F:102:PRO:HA	1.95	0.65
6:G:39:ILE:HG23	6:G:157:ILE:HG12	1.78	0.65
1:A:987:G:OP2	34:A:4245:HOH:O	2.14	0.65
24:2:65:ASN:OD1	24:2:69:ARG:NH1	2.30	0.65
4:E:116:VAL:HG13	4:E:122:PHE:HB2	1.77	0.65
8:I:29:TYR:O	8:I:33:ARG:HG3	1.97	0.65
1:A:2574:G:OP1	34:A:3846:HOH:O	2.13	0.65
23:1:26:ARG:N	34:1:201:HOH:O	2.29	0.65
1:A:1315:C:OP2	34:A:3805:HOH:O	2.13	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:V:6:LYS:HE3	17:V:9:GLY:HA2	1.78	0.65
1:A:2282:G:O2'	1:A:2283:C:OP2	2.11	0.65
1:A:2659:G:N7	34:A:4709:HOH:O	2.28	0.65
14:S:59:LYS:H	14:S:60:GLY:HA3	1.62	0.65
1:A:2689:U:OP2	1:A:2719:G:N2	2.30	0.65
7:H:9:ILE:N	7:H:50:VAL:O	2.30	0.65
5:F:34:TRP:CZ2	11:P:8:PRO:HG3	2.32	0.65
7:H:159:GLU:HG3	7:H:169:VAL:HG21	1.79	0.65
1:A:1430:C:H2'	1:A:1431:U:C6	2.32	0.65
1:A:994:C:OP1	16:U:53:ARG:NH2	2.30	0.64
1:A:1503:U:H2'	1:A:1504:C:H6	1.62	0.64
1:A:1252:G:N3	16:U:33:ARG:HD2	2.12	0.64
8:I:110:ASP:N	8:I:130:TYR:OH	2.22	0.64
3:D:176:ARG:HG3	3:D:176:ARG:O	1.96	0.64
3:D:242:ARG:N	3:D:242:ARG:HD3	2.12	0.64
1:A:1031:G:H21	31:9:36:GLN:HE22	1.44	0.64
1:A:1529:G:O6	1:A:1530:C:N4	2.31	0.64
17:V:29:PRO:HA	17:V:61:VAL:HG22	1.79	0.64
1:A:102:G:OP1	24:2:7:ARG:NH2	2.31	0.64
1:A:1614:A:OP1	34:A:4108:HOH:O	2.15	0.64
2:B:55:U:O3'	6:G:27:ASN:ND2	2.31	0.64
1:A:2712(A):A:H5''	1:A:2713:A:OP2	1.98	0.64
1:A:288:C:H2'	1:A:289:A:H8	1.63	0.64
1:A:1503:U:H2'	1:A:1504:C:C6	2.32	0.64
2:B:103:G:N7	34:B:320:HOH:O	2.30	0.64
1:A:601:C:O2'	5:F:104:LYS:NZ	2.30	0.64
10:O:19:ILE:HG22	10:O:43:VAL:HA	1.80	0.64
1:A:1876:A:H2'	1:A:1877:A:C8	2.33	0.64
24:2:50:ILE:O	24:2:51:ARG:HB3	1.97	0.64
20:Y:13:VAL:HG12	20:Y:74:PRO:HA	1.78	0.64
1:A:1654:A:H1'	1:A:2823:A:H5'	1.80	0.64
15:T:81:PRO:HG2	15:T:82:LEU:HD12	1.80	0.64
11:P:121:LYS:HG2	11:P:122:PRO:HD2	1.79	0.64
1:A:1378:A:OP1	29:7:10:ARG:NH2	2.31	0.64
8:I:72:LEU:HD21	8:I:107:VAL:HG11	1.80	0.64
1:A:804:A:H5''	1:A:805:G:OP1	1.98	0.63
1:A:993:G:C4	1:A:994:C:H5	2.16	0.63
1:A:2101:G:C2	1:A:2102:U:H1'	2.32	0.63
6:G:33:ARG:NE	6:G:162:THR:HG21	2.13	0.63
1:A:1210:A:H5''	1:A:1212:G:H5'	1.79	0.63
11:P:100:LEU:HD22	11:P:105:LEU:HB2	1.80	0.63
6:G:76:SER:HA	6:G:83:ARG:HA	1.78	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:43:C:O2	6:G:95:ARG:NH2	2.31	0.63
23:1:77:ALA:HB2	23:1:94:LEU:HD21	1.80	0.63
5:F:110:LEU:HD22	5:F:202:PHE:HE1	1.64	0.63
28:6:16:CYS:CB	28:6:43:CYS:SG	2.78	0.63
1:A:1529:G:C6	1:A:1530:C:N4	2.67	0.63
10:O:68:GLU:OE2	10:O:78:ARG:NH1	2.32	0.63
1:A:1495:A:H2'	1:A:1496:A:C8	2.32	0.63
3:D:132:PRO:HD3	3:D:190:TYR:CZ	2.34	0.63
1:A:2080:G:H5'	23:1:19:GLN:HG3	1.78	0.63
5:F:164:ARG:HD2	5:F:175:THR:HG23	1.81	0.63
4:E:120:TRP:CE3	4:E:155:LYS:HD3	2.34	0.63
9:N:62:VAL:HG21	9:N:87:LEU:HD11	1.81	0.63
1:A:1313:U:H2'	1:A:1610:A:C2	2.34	0.63
3:D:71:ASP:OD1	3:D:103:ARG:NH2	2.31	0.63
1:A:2356:C:O3'	22:O:20:ARG:HD3	1.99	0.63
1:A:674:G:O2'	5:F:74:ARG:HD3	1.99	0.63
1:A:1448:G:H4'	1:A:1542:A:OP1	1.99	0.63
5:F:197:ASP:OD2	5:F:197:ASP:N	2.32	0.63
21:Z:54:HIS:ND1	21:Z:101:PRO:HG3	2.14	0.63
1:A:2183:C:H2'	1:A:2184:G:C8	2.33	0.62
7:H:95:ARG:HB2	7:H:128:PRO:HB3	1.81	0.62
30:8:58:ILE:HA	30:8:61:LEU:HD12	1.82	0.62
1:A:89:G:H3'	1:A:90:U:H5''	1.81	0.62
21:Z:145:GLU:HG3	21:Z:146:ILE:H	1.64	0.62
1:A:1019:U:H3	1:A:1142(A):A:H62	1.47	0.62
1:A:1472:A:H2'	1:A:1473:G:O4'	1.99	0.62
1:A:1899:G:N3	1:A:1899:G:H2'	2.14	0.62
8:I:92:VAL:HG22	8:I:120:ILE:HB	1.81	0.62
1:A:2324:C:H5''	1:A:2325:G:H5'	1.80	0.62
2:B:31:C:O2'	2:B:53:A:N6	2.31	0.62
8:I:75:LEU:HD23	8:I:105:HIS:NE2	2.14	0.62
1:A:1557:C:P	1:A:1558:A:HO2'	2.22	0.62
21:Z:94:GLU:O	21:Z:130:PRO:HD3	1.99	0.62
14:S:88:ASP:OD1	14:S:90:GLY:N	2.32	0.62
1:A:2847:U:OP1	15:T:98:LYS:NZ	2.33	0.62
15:T:26:ASP:O	15:T:49:VAL:HG12	2.00	0.62
8:I:77:LEU:HG	8:I:101:LEU:HD23	1.80	0.62
1:A:2533:A:OP1	1:A:2665:A:O2'	2.16	0.62
15:T:27:THR:HB	15:T:89:VAL:HG22	1.82	0.62
1:A:1857:G:O5'	1:A:1857:G:H8	1.83	0.62
1:A:2218:U:H4'	1:A:2219:G:OP2	1.98	0.62
5:F:9:ILE:HG21	5:F:125:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:954:G:H5''	12:Q:13:GLN:HB3	1.82	0.62
1:A:833:U:O2	11:P:55:ARG:NH2	2.32	0.62
1:A:342:G:N7	34:A:4230:HOH:O	2.31	0.62
13:R:52:ILE:HD12	13:R:94:TYR:HB2	1.81	0.62
5:F:135:LYS:HB2	5:F:138:GLU:HG3	1.82	0.62
1:A:1530:C:N4	1:A:1539:G:H1	1.97	0.62
1:A:271(U):G:H2'	1:A:271(V):G:H8	1.65	0.62
1:A:2277:G:H3'	22:O:12:ASN:HD21	1.65	0.62
4:E:14:ILE:HD11	4:E:173:VAL:HG11	1.82	0.62
21:Z:126:VAL:HG13	21:Z:163:LEU:HA	1.81	0.61
1:A:2448:A:OP2	34:A:4694:HOH:O	2.16	0.61
3:D:58:HIS:ND1	3:D:59:LYS:N	2.48	0.61
1:A:1789:A:H5'	3:D:221:VAL:HG12	1.82	0.61
17:V:5:VAL:HG11	17:V:57:VAL:HG21	1.82	0.61
1:A:2439:A:H5''	1:A:2439:A:C8	2.35	0.61
1:A:994:C:O2'	1:A:996:A:OP1	2.09	0.61
1:A:2364:C:H4'	22:O:56:ASP:OD2	2.00	0.61
11:P:38:GLN:O	11:P:39:LYS:HB3	2.00	0.61
1:A:708:C:H42	1:A:723:G:H1	1.47	0.61
1:A:1449:A:O2'	1:A:1529:G:N2	2.28	0.61
1:A:826:U:C4'	11:P:55:ARG:HB2	2.30	0.61
7:H:54:ARG:NE	7:H:57:ASP:OD1	2.34	0.61
2:B:20:C:H42	2:B:63:G:H1	1.48	0.61
4:E:47:VAL:HG21	4:E:86:PRO:HD2	1.83	0.61
21:Z:157:LEU:HD21	21:Z:163:LEU:HB2	1.83	0.61
26:4:18:CYS:HB3	26:4:39:CYS:HB3	1.83	0.61
1:A:1190:G:H5''	11:P:32:THR:HA	1.83	0.61
15:T:36:GLU:OE1	15:T:41:ARG:NE	2.33	0.61
1:A:83:G:N2	1:A:103:A:OP2	2.32	0.61
1:A:89:G:H3'	1:A:90:U:C5'	2.31	0.61
21:Z:30:ASN:HB3	21:Z:90:VAL:HB	1.83	0.61
1:A:1292:U:H2'	1:A:1293:C:C6	2.36	0.61
4:E:12:THR:HG22	4:E:13:ARG:H	1.66	0.61
1:A:1028:A:N6	1:A:1125:G:H2'	2.15	0.61
30:8:6:THR:HG22	30:8:63:PRO:HD2	1.83	0.60
3:D:159:ALA:HB1	3:D:198:ASN:O	2.01	0.60
1:A:2313:C:H2'	1:A:2314:C:C6	2.35	0.60
18:W:36:LEU:HD13	18:W:48:ALA:HA	1.83	0.60
1:A:212:G:H2'	1:A:213:A:O4'	2.00	0.60
1:A:1331:A:O2'	1:A:1332:G:H8	1.85	0.60
1:A:2478:A:H5'	31:9:31:LYS:HD2	1.83	0.60
7:H:20:ALA:HB1	7:H:21:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:4:14:ILE:HG22	26:4:33:VAL:HG22	1.82	0.60
1:A:1790:C:H5''	1:A:1791:A:OP1	2.01	0.60
26:4:36:CYS:SG	26:4:37:SER:N	2.74	0.60
17:V:50:PRO:HG2	17:V:51:VAL:HG12	1.83	0.60
1:A:1358:G:O2'	1:A:1359:A:H5''	2.00	0.60
4:E:27:LEU:HD22	15:T:1:MET:HE3	1.82	0.60
1:A:581:C:H2'	1:A:582:G:H8	1.66	0.60
10:O:88:ASN:H	10:O:88:ASN:HD22	1.48	0.60
1:A:1221(A):C:H42	1:A:1228:G:H1	1.49	0.60
1:A:1427:A:H4'	1:A:1428:C:O5'	2.01	0.60
1:A:1169:G:H1	1:A:1180:C:H42	1.49	0.60
1:A:1818:U:H2'	3:D:157:ARG:HG3	1.83	0.60
1:A:370:G:OP1	1:A:403:U:N3	2.31	0.60
21:Z:53:ILE:HG22	21:Z:71:VAL:HB	1.82	0.60
1:A:976:C:H5'	1:A:1156:A:N6	2.16	0.60
1:A:2563:U:H4'	10:O:28:SER:HA	1.83	0.60
1:A:2705:A:OP2	34:A:4340:HOH:O	2.15	0.60
1:A:154(A):C:N4	1:A:171:G:H1	1.98	0.60
1:A:1496:A:N3	1:A:1577:C:O2'	2.30	0.60
5:F:11:VAL:HG22	5:F:125:LEU:HB2	1.83	0.60
1:A:1247:A:OP1	5:F:95:ARG:NH2	2.35	0.60
17:V:98:GLU:OE1	17:V:100:ARG:NH1	2.35	0.60
7:H:149:ARG:HD2	7:H:164:TYR:CE1	2.37	0.60
17:V:60:GLU:HB2	17:V:97:LYS:HE2	1.82	0.60
1:A:875:G:O6	1:A:902:C:N4	2.25	0.59
1:A:608:A:H2'	1:A:609:A:C8	2.37	0.59
5:F:53:THR:HG22	5:F:56:GLU:OE2	2.02	0.59
1:A:1607:C:H4'	1:A:1608:A:O5'	2.02	0.59
1:A:90:U:O2'	1:A:92:A:C8	2.56	0.59
6:G:109:VAL:HG11	6:G:142:PRO:HB3	1.85	0.59
1:A:918:A:H5''	2:B:98:G:O2'	2.03	0.59
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.38	0.59
29:7:12:ARG:NH2	29:7:44:PRO:HB3	2.17	0.59
6:G:106:LEU:HA	6:G:110:ALA:HB3	1.83	0.59
1:A:1803:A:H4'	3:D:259:THR:HG23	1.83	0.59
26:4:16:CYS:HB2	26:4:20:ASN:O	2.02	0.59
6:G:38:VAL:HG22	6:G:93:THR:HG23	1.85	0.59
4:E:38:THR:O	4:E:42:ASP:N	2.30	0.59
1:A:2647:U:H2'	1:A:2648:C:H6	1.68	0.59
14:S:36:TYR:HA	14:S:52:SER:HB3	1.85	0.59
1:A:1283:G:H22	1:A:1286:A:H5'	1.66	0.59
13:R:79:LEU:HA	13:R:83:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:A:C8	1:A:1408:C:O2'	2.52	0.59
1:A:1329:U:H5''	1:A:1330:C:H5	1.66	0.59
13:R:24:GLN:OE1	13:R:36:THR:HG21	2.03	0.59
1:A:1593:G:H2'	1:A:1594:G:C8	2.37	0.59
1:A:1379:A:H4'	1:A:1380:G:OP2	2.02	0.59
13:R:72:ASP:OD1	13:R:75:LEU:HB2	2.02	0.59
1:A:2014:A:H4'	18:W:92:ARG:NH2	2.17	0.59
9:N:37:LYS:HG3	9:N:42:TRP:CE2	2.37	0.59
1:A:528:A:C2	1:A:2043:C:H4'	2.38	0.59
17:V:58:VAL:HB	17:V:97:LYS:HB2	1.85	0.59
20:Y:2:ARG:O	20:Y:2:ARG:HG3	2.00	0.59
1:A:1227:G:OP2	16:U:16:LYS:NZ	2.36	0.59
2:B:44:G:OP1	6:G:98:ARG:NH2	2.35	0.59
1:A:1237:A:OP1	34:A:4013:HOH:O	2.16	0.59
2:B:12:C:H2'	22:O:73:GLY:HA3	1.83	0.59
2:B:52:A:O2'	2:B:53:A:H2	1.81	0.59
11:P:91:PHE:O	11:P:121:LYS:NZ	2.35	0.59
12:Q:31:ASP:O	12:Q:134:ARG:HG2	2.03	0.59
1:A:311:A:C6	1:A:328:U:C4	2.90	0.59
18:W:79:GLY:HA3	18:W:100:THR:HG22	1.84	0.59
31:9:10:ILE:HD12	31:9:32:HIS:HA	1.85	0.59
1:A:1210:A:C8	1:A:1210:A:H5'	2.32	0.59
21:Z:157:LEU:HD23	21:Z:161:VAL:HG13	1.83	0.59
1:A:800:A:OP1	1:A:800:A:H8	1.86	0.59
9:N:123:TYR:HH	9:N:130:HIS:CE1	2.19	0.59
1:A:644:A:H4'	1:A:645:C:C5	2.37	0.59
11:P:39:LYS:HB2	11:P:45:LEU:CD1	2.31	0.59
16:U:58:ARG:HA	16:U:61:TRP:CE3	2.37	0.59
1:A:1856:G:H2'	1:A:1857:G:H5'	1.85	0.59
1:A:2390:U:O2'	1:A:2391:G:H5'	2.02	0.59
4:E:52:LEU:HB2	4:E:76:ARG:HG2	1.84	0.59
1:A:288:C:H2'	1:A:289:A:C8	2.37	0.59
2:B:17:C:N4	2:B:109:C:N3	2.51	0.59
1:A:1593:G:H2'	1:A:1594:G:H8	1.67	0.59
2:B:113:G:H2'	2:B:114:C:C6	2.38	0.59
13:R:19:ALA:O	13:R:23:ASN:ND2	2.29	0.59
1:A:1354:A:H2'	1:A:1355:G:O4'	2.02	0.59
1:A:1545:A:H2'	1:A:1546:C:O4'	2.02	0.59
1:A:2009:G:H1'	13:R:107:ASP:O	2.03	0.59
13:R:81:ASP:O	13:R:85:PRO:HG3	2.02	0.59
8:I:75:LEU:HD23	8:I:105:HIS:CD2	2.38	0.58
1:A:784:A:H5'	1:A:785:G:OP1	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2689:U:P	1:A:2719:G:H22	2.24	0.58
6:G:106:LEU:O	6:G:111:LEU:N	2.26	0.58
21:Z:48:PHE:HE2	21:Z:71:VAL:HG11	1.68	0.58
1:A:1857:G:H2'	1:A:1858:G:O4'	2.04	0.58
13:R:29:LEU:HB3	13:R:75:LEU:HD11	1.84	0.58
8:I:5:LEU:HD11	8:I:19:VAL:HG22	1.84	0.58
1:A:1266:G:O2'	1:A:2012:G:O6	2.18	0.58
4:E:143:ASN:HD22	4:E:147:PRO:CD	2.15	0.58
1:A:2572:A:OP1	1:A:2574:G:O2'	2.17	0.58
4:E:33:VAL:HG11	4:E:36:ARG:HH21	1.68	0.58
23:1:5:CYS:SG	23:1:62:VAL:HG23	2.43	0.58
1:A:185:U:H4'	1:A:218:A:H4'	1.84	0.58
3:D:144:ALA:HB3	3:D:192:THR:HG23	1.84	0.58
1:A:2275:C:H5'	1:A:2275:C:H6	1.68	0.58
12:Q:21:THR:HG21	12:Q:101:ARG:HB2	1.85	0.58
3:D:24:ILE:HD13	3:D:84:TYR:HB2	1.85	0.58
1:A:34:C:O2'	1:A:35:G:OP1	2.18	0.58
11:P:38:GLN:HA	11:P:41:ARG:HG2	1.86	0.58
18:W:26:GLY:H	18:W:71:VAL:HG12	1.67	0.58
6:G:23:PHE:HB2	6:G:25:TYR:CZ	2.38	0.58
7:H:11:VAL:HG13	7:H:15:VAL:HG13	1.86	0.58
21:Z:9:TYR:HE2	21:Z:35:ARG:HG3	1.68	0.58
1:A:2286:A:OP1	28:6:29:ASN:ND2	2.37	0.58
1:A:2611:U:H2'	27:5:2:ALA:O	2.02	0.58
1:A:2722:G:H5'	13:R:4:LEU:HD12	1.86	0.58
16:U:27:LEU:HA	16:U:30:LYS:HB2	1.86	0.58
1:A:2033:A:P	34:A:4575:HOH:O	2.61	0.58
14:S:66:ALA:HA	14:S:69:VAL:HG12	1.85	0.58
1:A:72:U:OP1	34:A:4067:HOH:O	2.16	0.58
1:A:66:C:H2'	1:A:67:U:H6	1.69	0.58
1:A:492:A:H2'	1:A:493:G:O4'	2.02	0.58
5:F:32:LEU:HD11	5:F:105:VAL:HG13	1.85	0.58
1:A:848:G:N9	1:A:933:A:H8	2.02	0.58
1:A:2872:G:O2'	1:A:2873:A:H5'	2.03	0.58
3:D:274:ARG:CG	3:D:275:LYS:HB3	2.31	0.58
8:I:104:GLN:O	8:I:105:HIS:ND1	2.35	0.58
9:N:30:ILE:HG22	9:N:34:LEU:HD22	1.84	0.58
1:A:637:A:H5''	11:P:117:GLU:HG2	1.86	0.58
10:O:63:VAL:HG22	10:O:84:ALA:HA	1.86	0.58
1:A:1336:A:H2'	1:A:1337:G:H8	1.69	0.57
1:A:581:C:H2'	1:A:582:G:C8	2.39	0.57
1:A:2425:A:H4'	1:A:2426:A:H5''	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:14:GLU:O	6:G:18:GLU:HB3	2.03	0.57
1:A:1224:C:O2'	17:V:86:GLY:N	2.34	0.57
2:B:53:A:H2'	2:B:54:G:O4'	2.04	0.57
7:H:88:LEU:HB2	7:H:163:TYR:HB2	1.85	0.57
4:E:23:VAL:HG21	4:E:183:LEU:HG	1.86	0.57
12:Q:62:GLY:O	21:Z:178:GLU:HG2	2.03	0.57
1:A:1914:C:O2'	1:A:1915:U:OP1	2.21	0.57
1:A:1359:A:N6	1:A:1372:U:H3	2.02	0.57
15:T:53:ARG:NH1	15:T:60:THR:HG23	2.19	0.57
1:A:1149:G:H2'	1:A:1150:C:H6	1.66	0.57
9:N:104:LYS:HB2	9:N:117:PHE:CE1	2.38	0.57
2:B:113:G:H2'	2:B:114:C:H6	1.69	0.57
1:A:1040:C:H2'	1:A:1041:C:O4'	2.04	0.57
1:A:2331:G:O3'	22:O:43:THR:HG22	2.03	0.57
1:A:857:C:H2'	1:A:858:U:C6	2.39	0.57
18:W:76:VAL:HG22	18:W:103:ILE:HG23	1.86	0.57
20:Y:90:LEU:HB3	20:Y:92:ASN:H	1.69	0.57
1:A:993:G:C5	1:A:994:C:H5	2.22	0.57
21:Z:128:VAL:HG22	21:Z:129:SER:H	1.69	0.57
6:G:105:LYS:NZ	26:4:25:TYR:O	2.37	0.57
1:A:1396:U:OP2	34:A:4658:HOH:O	2.17	0.57
1:A:1359:A:C2	1:A:1372:U:O4	2.58	0.57
1:A:926:A:N7	34:A:4215:HOH:O	2.32	0.57
2:B:15:A:OP2	2:B:69:G:N2	2.38	0.57
1:A:10:G:O2'	1:A:2801(A):A:N7	2.38	0.57
1:A:2014:A:H5'	18:W:94:ASP:OD2	2.04	0.57
15:T:118:ARG:NH2	15:T:121:ILE:HG21	2.19	0.57
1:A:1973:G:H2'	1:A:1974:C:C6	2.39	0.57
3:D:72:LYS:HE3	3:D:75:ILE:HD12	1.87	0.57
1:A:1589:C:H2'	1:A:1590:U:H6	1.69	0.57
1:A:2592:G:H2'	1:A:2593:U:O4'	2.03	0.57
5:F:130:ALA:CB	5:F:142:TRP:HD1	2.18	0.57
30:8:15:LYS:HB2	34:8:101:HOH:O	2.04	0.57
1:A:2074:U:H2'	1:A:2075:U:C6	2.38	0.57
1:A:520:G:H2'	1:A:521:G:C8	2.40	0.57
1:A:657:U:H2'	1:A:658:C:C6	2.40	0.57
1:A:247:G:H4'	1:A:386:G:C5	2.40	0.57
12:Q:16:ARG:HG2	12:Q:16:ARG:NH1	2.13	0.57
1:A:1187:G:H5''	17:V:81:TYR:CE2	2.38	0.57
1:A:1019:U:H3	1:A:1142(A):A:N6	2.02	0.57
1:A:1225:G:H4'	17:V:84:LYS:HG2	1.87	0.57
1:A:619:G:H5''	1:A:620:G:OP2	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:Y:19:LYS:HE3	20:Y:20:TYR:HE1	1.70	0.57
1:A:2849:U:OP2	15:T:95:ARG:NH1	2.37	0.57
12:Q:126:PRO:HG2	12:Q:127:ILE:HG23	1.87	0.57
1:A:1336:A:H2'	1:A:1337:G:C8	2.39	0.57
20:Y:14:LEU:HG	20:Y:15:VAL:N	2.20	0.57
1:A:2394:C:OP2	30:8:30:ARG:NH1	2.38	0.57
14:S:59:LYS:HB3	14:S:60:GLY:HA2	1.87	0.56
8:I:93:THR:HG23	8:I:119:PRO:HG3	1.87	0.56
1:A:62:C:H42	1:A:93:G:H1	1.53	0.56
20:Y:99:CYS:CB	20:Y:102:CYS:SG	2.92	0.56
1:A:2364:C:H2'	1:A:2365:G:O4'	2.04	0.56
1:A:857:C:H2'	1:A:858:U:H6	1.69	0.56
1:A:652(A):A:H4'	1:A:652(B):A:OP2	2.05	0.56
1:A:1359:A:N1	1:A:1372:U:C4	2.72	0.56
13:R:2:ARG:NH1	13:R:5:LYS:O	2.37	0.56
1:A:1429:G:H2'	1:A:1430:C:C6	2.41	0.56
1:A:978:G:O6	34:A:4248:HOH:O	2.18	0.56
1:A:2300:G:H2'	1:A:2301:C:H6	1.70	0.56
19:X:57:LEU:HD13	19:X:78:LYS:HG2	1.87	0.56
7:H:70:THR:HA	7:H:73:ALA:HB3	1.86	0.56
1:A:1403:C:H5''	1:A:1471:A:C1'	2.34	0.56
1:A:71:A:H5''	1:A:73:A:N7	2.21	0.56
9:N:63:THR:HG22	9:N:66:LYS:HZ2	1.71	0.56
4:E:135:HIS:HD2	4:E:135:HIS:H	1.53	0.56
1:A:2659:G:P	7:H:158:HIS:HE2	2.28	0.56
1:A:971:C:H2'	1:A:972:G:H5'	1.88	0.56
1:A:796:C:H2'	1:A:797:C:C6	2.40	0.56
4:E:4:ILE:HG12	4:E:5:LEU:H	1.70	0.56
1:A:2833:G:O2'	1:A:2834:G:OP1	2.23	0.56
1:A:1019:U:HO2'	1:A:1021:A:H2	1.52	0.56
1:A:1486:A:O2'	1:A:1487:G:H5'	2.05	0.56
1:A:1762:A:H8	34:A:4674:HOH:O	1.87	0.56
16:U:102:GLU:HG3	17:V:2:PHE:CE1	2.41	0.56
1:A:2296:U:OP2	14:S:6:ALA:HB2	2.05	0.56
1:A:2387:U:OP1	22:O:55:ARG:NH2	2.38	0.56
1:A:1971:A:C4	3:D:241:PRO:HD3	2.41	0.56
1:A:229:A:H5''	1:A:230:U:H5'	1.88	0.56
21:Z:104:PHE:HB3	21:Z:141:VAL:HG21	1.87	0.56
21:Z:180:VAL:O	21:Z:183:LEU:HB2	2.05	0.56
22:O:27:GLU:HG3	22:O:68:GLU:HA	1.88	0.56
1:A:2641:G:P	9:N:74:ARG:HH21	2.29	0.56
1:A:528:A:C2	1:A:2042:A:H2'	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:229:A:H3'	1:A:229:A:C8	2.41	0.56
1:A:2395:C:O2'	23:1:30:VAL:O	2.24	0.56
1:A:2061:G:H5''	1:A:2503:A:C2	2.41	0.56
5:F:129:PHE:O	5:F:132:VAL:HG22	2.06	0.56
10:O:77:ILE:HG13	15:T:74:ARG:HG2	1.87	0.56
18:W:50:VAL:HG12	18:W:105:VAL:CG2	2.36	0.56
14:S:58:LEU:HD12	14:S:59:LYS:HB2	1.87	0.56
1:A:2277:G:H3'	22:0:12:ASN:ND2	2.21	0.56
1:A:2463:C:C2'	1:A:2464:C:H5'	2.35	0.56
2:B:22:U:H3	2:B:61:G:H1	1.53	0.56
1:A:2404:C:H2'	1:A:2405:G:H5'	1.88	0.56
1:A:2320:A:N3	1:A:2320:A:H2'	2.19	0.56
1:A:1209:G:H21	1:A:1210:A:H62	1.54	0.55
1:A:1167:U:O2	1:A:1183:G:N2	2.39	0.55
1:A:1939:U:OP1	1:A:2604:U:O2'	2.24	0.55
1:A:1859:A:N6	1:A:1883:G:O2'	2.37	0.55
8:I:68:LEU:HA	8:I:71:ILE:HG22	1.87	0.55
25:3:27:GLY:HA3	25:3:35:ARG:NH1	2.21	0.55
1:A:2870:C:H5''	13:R:65:LEU:HD21	1.88	0.55
1:A:1366:A:OP1	23:1:3:LYS:NZ	2.38	0.55
1:A:2329:G:N2	22:0:41:ARG:HG3	2.21	0.55
1:A:2463:C:H2'	1:A:2464:C:H5'	1.88	0.55
1:A:242:G:H5''	30:8:64:TYR:CE2	2.42	0.55
1:A:448:U:C4	1:A:583:G:H1'	2.41	0.55
1:A:639:U:H2'	1:A:640:C:H6	1.70	0.55
5:F:36:VAL:O	5:F:40:GLN:HG3	2.07	0.55
8:I:56:LYS:O	8:I:60:GLU:N	2.36	0.55
2:B:30:C:H2'	2:B:31:C:H5'	1.89	0.55
5:F:32:LEU:O	5:F:36:VAL:HG23	2.07	0.55
1:A:2371:G:O2'	28:6:46:HIS:ND1	2.33	0.55
7:H:44:VAL:HB	7:H:51:ARG:H	1.71	0.55
1:A:579:G:H2'	1:A:580:C:C6	2.41	0.55
30:8:32:LEU:O	30:8:36:LYS:HE3	2.06	0.55
1:A:1259:G:H2'	1:A:1260:G:C8	2.40	0.55
1:A:2755:C:O3'	1:A:2756:U:H6	1.90	0.55
16:U:19:LYS:O	16:U:22:LYS:HG3	2.07	0.55
1:A:2239:G:H5'	3:D:251:GLY:HA3	1.87	0.55
9:N:67:LEU:HD13	9:N:87:LEU:HD13	1.88	0.55
13:R:78:LYS:HE2	13:R:83:ILE:HD11	1.89	0.55
4:E:178:GLU:OE2	4:E:178:GLU:N	2.23	0.55
2:B:4:C:H42	2:B:117:G:H1	1.55	0.55
8:I:102:SER:OG	8:I:103:ARG:N	2.39	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:8:37:SER:OG	30:8:40:GLU:HG3	2.07	0.55
7:H:144:VAL:O	7:H:148:ILE:HG12	2.07	0.55
1:A:2028:U:H5	34:A:4576:HOH:O	1.89	0.55
1:A:2658:C:H5''	7:H:158:HIS:CD2	2.42	0.55
21:Z:126:VAL:HG11	21:Z:161:VAL:HG22	1.88	0.55
10:O:120:GLU:HG2	10:O:122:LEU:HG	1.89	0.55
3:D:95:LEU:HD11	3:D:105:ILE:HG12	1.88	0.55
1:A:442:G:H4'	5:F:46:ARG:HG3	1.89	0.55
25:3:8:LEU:HD13	25:3:31:LEU:HD23	1.87	0.55
1:A:2037:G:H2'	1:A:2038:G:C8	2.42	0.55
1:A:1034:G:H5'	31:9:18:ARG:HD2	1.88	0.54
19:X:3:THR:OG1	19:X:5:TYR:N	2.37	0.54
21:Z:3:TYR:HB2	21:Z:56:VAL:O	2.06	0.54
21:Z:100:VAL:HG13	21:Z:136:PHE:HA	1.89	0.54
14:S:53:SER:OG	14:S:54:LEU:N	2.39	0.54
25:3:22:ALA:HB2	25:3:49:LYS:HD3	1.90	0.54
1:A:829:A:H5''	1:A:831:G:N7	2.22	0.54
1:A:1688:U:O2	1:A:1700:A:H5'	2.07	0.54
17:V:56:SER:H	17:V:100:ARG:HB2	1.71	0.54
4:E:4:ILE:HD13	4:E:28:ALA:HB1	1.89	0.54
12:Q:1:MET:HG2	12:Q:1:MET:O	2.07	0.54
21:Z:111:VAL:C	21:Z:113:ALA:H	2.10	0.54
17:V:72:VAL:HG13	17:V:85:LYS:HB3	1.89	0.54
1:A:2661:G:H2'	1:A:2662:A:C8	2.43	0.54
27:5:35:GLU:HG3	27:5:51:TYR:CD2	2.41	0.54
1:A:2405:G:H4'	1:A:2406:U:OP2	2.08	0.54
1:A:7:G:H2'	1:A:8:A:H8	1.70	0.54
3:D:172:TYR:CD1	3:D:186:HIS:HA	2.42	0.54
1:A:22:C:H42	1:A:518:G:H1	1.55	0.54
10:O:15:GLY:HA2	10:O:47:ILE:HD11	1.90	0.54
2:B:55:U:C1'	6:G:29:TRP:HE1	2.21	0.54
20:Y:13:VAL:HB	20:Y:72:VAL:HG22	1.88	0.54
1:A:795:C:H2'	1:A:796:C:H6	1.73	0.54
11:P:52:GLU:O	11:P:54:GLY:N	2.41	0.54
1:A:455:C:N3	1:A:472:A:H2'	2.21	0.54
1:A:1359:A:H61	1:A:1372:U:H3	1.56	0.54
21:Z:24:LEU:HB2	21:Z:41:LEU:HD22	1.89	0.54
1:A:2632:A:O2'	1:A:2811:G:O2'	2.16	0.54
1:A:126:A:OP2	29:7:19:ARG:HB2	2.07	0.54
1:A:889:C:HO2'	1:A:890:A:H8	1.54	0.54
3:D:127:VAL:HA	3:D:193:VAL:CG2	2.38	0.54
1:A:2689:U:H5	34:A:3701:HOH:O	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:857:C:H4'	22:0:23:VAL:HG21	1.90	0.54
6:G:24:GLY:O	6:G:26:GLN:NE2	2.36	0.54
9:N:61:ARG:HH11	9:N:61:ARG:HB2	1.73	0.54
26:4:14:ILE:HG23	26:4:31:ILE:HD12	1.90	0.54
1:A:2329:G:H21	22:0:41:ARG:HG3	1.73	0.54
8:I:114:LEU:HD21	8:I:128:LEU:HD13	1.89	0.54
5:F:130:ALA:HB2	5:F:142:TRP:HD1	1.72	0.54
6:G:124:SER:HB2	6:G:131:TYR:CE1	2.43	0.54
1:A:1638:C:O2	1:A:2698:U:O2'	2.26	0.54
4:E:112:GLY:O	4:E:159:HIS:HA	2.08	0.54
1:A:576:U:H5	34:A:3913:HOH:O	1.91	0.54
1:A:631:A:H1'	11:P:66:GLY:HA2	1.89	0.54
1:A:1970:A:OP1	34:A:4200:HOH:O	2.17	0.54
1:A:531:C:OP2	34:A:4407:HOH:O	2.18	0.54
8:I:29:TYR:HD2	8:I:30:LEU:HD23	1.72	0.54
2:B:24:G:H5'	2:B:25:A:N7	2.23	0.54
1:A:2406:U:OP1	1:A:2411:A:N6	2.41	0.54
5:F:117:ARG:HD2	5:F:190:GLU:O	2.08	0.54
1:A:2444:G:OP2	5:F:68:LYS:HE2	2.07	0.54
1:A:1786:A:H1'	1:A:1938:A:N6	2.21	0.54
1:A:852:G:N2	1:A:926:A:H1'	2.23	0.54
1:A:1022:G:H22	1:A:1142(A):A:H2	1.56	0.54
18:W:40:ASN:O	18:W:41:LYS:HG2	2.08	0.54
7:H:118:PRO:HD2	7:H:121:ILE:HG13	1.90	0.54
24:2:32:LEU:HB2	24:2:53:LEU:HD13	1.90	0.54
2:B:50:G:OP1	14:S:63:THR:OG1	2.20	0.53
1:A:886:C:OP1	1:A:886:C:H4'	2.08	0.53
6:G:44:GLY:HA2	6:G:88:ILE:HG22	1.89	0.53
1:A:1470:G:H5''	1:A:1471:A:OP1	2.09	0.53
1:A:300:A:N6	34:A:3865:HOH:O	2.41	0.53
1:A:363:G:H2'	1:A:363(A):A:C8	2.41	0.53
4:E:72:VAL:HA	4:E:73:GLU:HB3	1.90	0.53
1:A:1651:G:OP1	13:R:40:LYS:HE3	2.08	0.53
12:Q:20:ALA:HA	12:Q:99:PRO:HD2	1.90	0.53
14:S:27:SER:HA	14:S:88:ASP:HB3	1.90	0.53
13:R:104:ARG:HG3	13:R:107:ASP:OD2	2.09	0.53
1:A:2300:G:H2'	1:A:2301:C:C6	2.43	0.53
21:Z:74:VAL:HG22	21:Z:86:VAL:HG13	1.88	0.53
13:R:33:ARG:NH2	27:5:57:VAL:O	2.34	0.53
9:N:48:MET:HE2	9:N:48:MET:H	1.73	0.53
1:A:2680:C:H5'	4:E:189:PRO:HA	1.90	0.53
1:A:907:U:O2'	12:Q:101:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:U:72:HIS:HE2	16:U:107:ALA:HB2	1.73	0.53
1:A:2881:C:H2'	1:A:2882:A:O4'	2.08	0.53
8:I:77:LEU:HD11	8:I:101:LEU:HB2	1.91	0.53
21:Z:128:VAL:HG23	21:Z:161:VAL:H	1.73	0.53
6:G:44:GLY:CA	6:G:88:ILE:HG22	2.38	0.53
1:A:2359:C:H2'	1:A:2360:A:O4'	2.09	0.53
14:S:95:HIS:N	14:S:99:LYS:HB3	2.23	0.53
5:F:182:ASN:HD21	5:F:185:ASP:CG	2.12	0.53
7:H:43:VAL:HG12	7:H:44:VAL:H	1.74	0.53
20:Y:76:CYS:SG	20:Y:99:CYS:HB2	2.48	0.53
8:I:94:ALA:HA	8:I:97:ILE:HB	1.90	0.53
4:E:101:ARG:CZ	4:E:171:GLU:HB2	2.39	0.53
1:A:1267:U:H2'	1:A:1268:A:H8	1.74	0.53
6:G:107:LEU:HD23	6:G:111:LEU:HD12	1.90	0.53
1:A:184:C:H2'	1:A:185:U:C6	2.43	0.53
21:Z:18:LEU:HD23	21:Z:25:PRO:HG3	1.91	0.53
1:A:263:C:H2'	1:A:264:C:O4'	2.09	0.53
8:I:72:LEU:O	8:I:74:ASN:N	2.38	0.53
15:T:53:ARG:O	15:T:53:ARG:HG3	2.09	0.53
4:E:107:THR:O	4:E:190:GLY:HA2	2.08	0.53
1:A:330:A:HO2'	1:A:331:A:H8	1.57	0.53
7:H:3:ARG:HG2	7:H:6:ARG:CZ	2.38	0.53
3:D:182:LEU:HD12	3:D:272:ALA:HB3	1.90	0.53
1:A:2527:C:C4	1:A:2528:U:C5	2.97	0.53
1:A:323:G:O2'	1:A:1205:U:N3	2.35	0.53
1:A:2345:G:OP2	28:6:38:LYS:HG3	2.09	0.53
12:Q:111:GLU:O	12:Q:115:MET:HG2	2.09	0.53
8:I:72:LEU:C	8:I:74:ASN:N	2.61	0.52
1:A:994:C:O2	1:A:994:C:H2'	2.09	0.52
1:A:1430:C:H2'	1:A:1431:U:H6	1.72	0.52
1:A:795:C:H2'	1:A:796:C:C6	2.44	0.52
5:F:129:PHE:CD2	5:F:163:VAL:HG21	2.44	0.52
1:A:2351:G:HO2'	1:A:2352:A:H8	1.54	0.52
12:Q:63:LYS:HE3	12:Q:65:PHE:CE1	2.44	0.52
1:A:1739:U:HO2'	1:A:1740:G:H8	1.57	0.52
22:O:47:PRO:HA	22:O:51:VAL:HG12	1.91	0.52
1:A:2273:A:H2'	1:A:2274:A:C8	2.43	0.52
25:3:26:LEU:HD21	25:3:46:ASN:HB2	1.91	0.52
1:A:2647:U:H2'	1:A:2648:C:C6	2.44	0.52
1:A:2275:C:O2'	12:Q:85:LYS:N	2.35	0.52
1:A:2869:G:H2'	1:A:2870:C:O4'	2.09	0.52
1:A:1506:C:H2'	1:A:1507:A:H5'	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:636:G:C2	11:P:115:LEU:HD11	2.44	0.52
1:A:41:C:H2'	1:A:42:G:H8	1.75	0.52
1:A:1477:A:H2'	1:A:1478:G:O4'	2.09	0.52
5:F:28:ILE:HA	5:F:112:MET:HG2	1.91	0.52
1:A:2019:A:H2'	1:A:2020:A:O5'	2.09	0.52
1:A:1849:G:H2'	1:A:1850:G:H8	1.74	0.52
2:B:6:C:O2'	14:S:29:PHE:HE1	1.93	0.52
1:A:9:U:O2'	1:A:10:G:OP1	2.24	0.52
1:A:747:U:O2	1:A:2014:A:H1'	2.09	0.52
2:B:114:C:H4'	14:S:46:VAL:HG13	1.91	0.52
14:S:48:LEU:HD12	14:S:48:LEU:H	1.74	0.52
1:A:1819:A:H4'	1:A:1820:U:O5'	2.08	0.52
1:A:1652:A:C2'	1:A:1653:G:H5'	2.39	0.52
1:A:2302:G:H2'	1:A:2303:G:H8	1.75	0.52
1:A:2262:U:O2'	1:A:2263:C:H5'	2.09	0.52
7:H:149:ARG:HA	7:H:162:ILE:HG21	1.92	0.52
12:Q:42:ILE:HD13	12:Q:97:VAL:CG2	2.39	0.52
4:E:175:VAL:HG23	4:E:177:PRO:HD3	1.92	0.52
1:A:244:A:C2	1:A:255:A:C4	2.97	0.52
1:A:632:A:H2'	1:A:633:A:C8	2.45	0.52
22:O:29:GLN:O	22:O:67:VAL:HG23	2.10	0.52
6:G:16:ARG:NE	6:G:31:VAL:HG21	2.25	0.52
1:A:2206:G:C3'	1:A:2207:G:C8	2.91	0.52
9:N:24:GLY:HA2	9:N:27:ALA:CB	2.37	0.52
1:A:300:A:P	20:Y:86:ARG:NH2	2.80	0.52
1:A:142:A:HO2'	1:A:1407:C:HO2'	1.58	0.52
1:A:1607:C:N4	1:A:1622:G:OP2	2.43	0.52
1:A:608:A:H2'	1:A:609:A:H8	1.73	0.52
26:4:3:GLU:H	26:4:3:GLU:CD	2.12	0.52
1:A:195:A:H61	1:A:198:C:H3'	1.75	0.52
1:A:1537:G:H2'	1:A:1538:G:H8	1.74	0.52
6:G:7:LEU:HD22	6:G:100:TRP:CE3	2.44	0.52
1:A:2576:G:H1'	34:A:3834:HOH:O	2.10	0.52
1:A:1472:A:H61	1:A:1519:G:H1'	1.74	0.52
13:R:52:ILE:HB	13:R:94:TYR:HD1	1.73	0.52
12:Q:21:THR:HG21	12:Q:101:ARG:HH11	1.74	0.52
6:G:3:LEU:HD13	26:4:25:TYR:CZ	2.45	0.52
1:A:1653:G:C6	13:R:9:LYS:HB2	2.45	0.52
15:T:127:ALA:HA	15:T:129:ARG:N	2.25	0.52
1:A:698:C:O2'	1:A:734:A:N6	2.43	0.52
1:A:1198:U:H2'	1:A:1199:U:H6	1.75	0.52
1:A:479:A:H1'	1:A:480:A:H5''	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:155:LEU:HB3	21:Z:157:LEU:HD12	1.91	0.52
12:Q:63:LYS:O	12:Q:107:ALA:N	2.43	0.52
22:O:26:TYR:O	22:O:29:GLN:HB2	2.09	0.52
5:F:7:TYR:OH	5:F:119:ARG:HD3	2.09	0.52
27:5:41:PRO:O	27:5:44:THR:OG1	2.27	0.52
1:A:1579:A:H2'	1:A:1580:A:C8	2.44	0.52
1:A:71:A:C2	19:X:31:HIS:HE1	2.28	0.52
20:Y:20:TYR:CD2	20:Y:42:VAL:HG13	2.45	0.52
3:D:71:ASP:CG	3:D:103:ARG:HH22	2.14	0.52
19:X:35:THR:HG23	19:X:38:GLU:H	1.74	0.52
5:F:51:THR:HG23	5:F:92:PRO:HG2	1.92	0.52
11:P:29:LYS:HG2	11:P:30:THR:N	2.24	0.52
1:A:864:G:C6	1:A:865:C:N4	2.78	0.51
1:A:827:U:H4'	1:A:828:U:C5	2.45	0.51
12:Q:57:HIS:HD2	12:Q:117:ALA:HB2	1.72	0.51
1:A:2316:C:O2'	6:G:128:ARG:NH1	2.42	0.51
13:R:103:ARG:HD3	13:R:108:GLY:O	2.10	0.51
1:A:972:G:OP2	1:A:973:A:O2'	2.20	0.51
1:A:2464:C:O2'	1:A:2465:C:H5''	2.11	0.51
1:A:363(E):U:O2'	1:A:363(F):A:OP1	2.24	0.51
1:A:944:G:H5''	1:A:945:A:O5'	2.10	0.51
6:G:16:ARG:O	6:G:20:ILE:HG13	2.10	0.51
1:A:1371:G:H2'	1:A:1372:U:H5	1.74	0.51
1:A:1434:A:H61	1:A:1558:A:H62	1.58	0.51
3:D:221:VAL:HG23	3:D:226:MET:CE	2.40	0.51
1:A:2238:G:H2'	1:A:2238:G:N3	2.26	0.51
1:A:610:G:H2'	1:A:611:C:C6	2.45	0.51
1:A:84:A:H5''	20:Y:8:LYS:HG2	1.92	0.51
18:W:54:ALA:HB1	18:W:107:LEU:HD22	1.92	0.51
1:A:2022:U:O2'	1:A:2617:C:H5'	2.10	0.51
1:A:1267:U:H2'	1:A:1268:A:C8	2.46	0.51
9:N:19:GLU:HG3	9:N:20:GLY:H	1.75	0.51
14:S:4:LEU:HD11	14:S:12:PHE:HE1	1.75	0.51
1:A:1480:G:C6	1:A:1481:U:N3	2.78	0.51
2:B:55:U:H1'	6:G:29:TRP:HE1	1.75	0.51
1:A:2505:G:O6	1:A:2576:G:H2'	2.10	0.51
9:N:38:HIS:ND1	9:N:39:ARG:HG3	2.25	0.51
12:Q:48:GLU:O	12:Q:52:VAL:HG23	2.11	0.51
4:E:108:SER:HB3	4:E:165:VAL:HG21	1.91	0.51
1:A:1529:G:O6	1:A:1541:G:N2	2.42	0.51
1:A:272(G):C:N4	1:A:363(C):G:H1	2.08	0.51
1:A:1514:U:H2'	1:A:1515:G:C8	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:1:67:ILE:N	23:1:68:PRO:HD2	2.25	0.51
2:B:94:C:H2'	2:B:95:C:H6	1.75	0.51
1:A:1257:C:H4'	5:F:83:PHE:CE2	2.46	0.51
18:W:72:LYS:N	18:W:106:ILE:O	2.35	0.51
1:A:57:C:H2'	1:A:58:G:O4'	2.10	0.51
1:A:1754:C:OP1	15:T:96:ARG:NH1	2.41	0.51
1:A:1945:G:H2'	1:A:1946:U:H6	1.75	0.51
1:A:2820:A:C5	13:R:4:LEU:HD11	2.46	0.51
17:V:57:VAL:HG12	17:V:99:ILE:HG23	1.93	0.51
6:G:101:ILE:HG21	26:4:25:TYR:HB2	1.91	0.51
25:3:44:ARG:O	25:3:48:GLU:HG2	2.10	0.51
14:S:26:LEU:HD22	14:S:87:PHE:CD1	2.45	0.51
1:A:2777:G:C5'	1:A:2778:A:H5'	2.37	0.51
1:A:192:C:O2'	1:A:802:A:N3	2.42	0.51
12:Q:43:THR:N	12:Q:46:GLN:OE1	2.31	0.51
1:A:1384:A:O2'	1:A:1404:C:O2	2.25	0.51
15:T:127:ALA:HA	15:T:129:ARG:H	1.75	0.51
1:A:307:G:N2	1:A:310:A:O5'	2.43	0.51
9:N:97:ARG:O	9:N:100:GLU:N	2.43	0.51
6:G:167:GLU:HA	6:G:170:ARG:HB2	1.92	0.51
1:A:267:C:H42	1:A:425:G:H1	1.58	0.51
1:A:954:G:O2'	1:A:2274:A:N1	2.41	0.51
6:G:64:THR:HG22	6:G:94:LEU:HD11	1.91	0.51
1:A:1558:A:C4'	1:A:1559:G:O5'	2.56	0.51
6:G:125:PHE:HB3	6:G:166:ASP:OD2	2.11	0.51
4:E:9:VAL:HG13	4:E:25:VAL:O	2.10	0.51
25:3:6:VAL:HG12	25:3:56:VAL:HG22	1.93	0.51
14:S:41:ASP:OD2	14:S:44:LYS:HD3	2.11	0.51
9:N:47:ALA:HB2	9:N:112:LEU:HD11	1.92	0.51
1:A:2055:C:H5'	1:A:2056:G:H5''	1.92	0.51
1:A:1788:C:OP1	3:D:222:ARG:NH2	2.44	0.51
1:A:1169:G:H2'	1:A:1170:G:O4'	2.11	0.51
1:A:328:U:H4'	20:Y:68:HIS:CD2	2.46	0.51
1:A:1589:C:H2'	1:A:1590:U:C6	2.46	0.51
1:A:2833:G:N3	1:A:2833:G:O2'	2.43	0.51
2:B:116:G:H8	2:B:116:G:OP2	1.93	0.51
1:A:1668:A:H4'	1:A:1669:A:O5'	2.10	0.51
1:A:271(J):C:O2'	1:A:271(K):U:OP2	2.21	0.51
2:B:79:C:H6	2:B:79:C:O5'	1.94	0.51
12:Q:114:ALA:O	12:Q:118:LEU:HB2	2.11	0.51
3:D:68:LYS:O	3:D:69:ARG:HB2	2.10	0.51
10:O:15:GLY:O	10:O:47:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:271(L):U:H4'	1:A:271(M):G:H5'	1.92	0.51
1:A:1694:C:H4'	1:A:1695:G:O5'	2.11	0.51
1:A:662:G:H5''	11:P:16:ARG:HG2	1.93	0.51
12:Q:10:ARG:HH11	12:Q:10:ARG:HG3	1.75	0.51
1:A:2432:A:N1	23:1:35:THR:HG22	2.25	0.50
1:A:2357:U:OP1	22:0:20:ARG:NH1	2.43	0.50
11:P:48:PRO:O	30:8:57:ARG:NH2	2.45	0.50
2:B:64:C:H2'	2:B:65:C:C6	2.46	0.50
21:Z:29:TYR:HA	21:Z:33:LEU:O	2.12	0.50
1:A:1257:C:H4'	5:F:83:PHE:CD2	2.45	0.50
1:A:2821:A:OP2	1:A:2822:G:OP2	2.29	0.50
2:B:32:C:O2	2:B:50:G:N2	2.33	0.50
1:A:2692:C:O2'	1:A:2847:U:O2'	2.19	0.50
1:A:2562:U:H1'	10:O:23:ARG:HH11	1.76	0.50
1:A:1514:U:H2'	1:A:1515:G:H8	1.76	0.50
21:Z:124:ILE:HD11	21:Z:165:VAL:HG21	1.93	0.50
5:F:8:GLN:OE1	5:F:21:ALA:N	2.44	0.50
1:A:718:A:H3'	1:A:719:C:H6	1.76	0.50
6:G:15:VAL:HG12	6:G:19:LEU:HG	1.92	0.50
1:A:1446:C:H2'	1:A:1447:G:H8	1.76	0.50
1:A:575:A:OP2	1:A:2055:C:N4	2.31	0.50
1:A:2789:C:H4'	1:A:2790:A:OP1	2.12	0.50
1:A:2302:G:N1	1:A:2315:G:C6	2.80	0.50
6:G:33:ARG:H	6:G:162:THR:HG23	1.74	0.50
9:N:38:HIS:CE1	9:N:39:ARG:HG3	2.46	0.50
1:A:197:A:N6	1:A:2430:A:H2'	2.25	0.50
5:F:13:SER:HB2	5:F:18:ARG:HE	1.76	0.50
1:A:189:G:OP2	23:1:39:LYS:NZ	2.45	0.50
21:Z:153:SER:HB3	21:Z:167:PRO:O	2.11	0.50
1:A:27:G:N2	1:A:512:G:H1'	2.26	0.50
1:A:2399:G:H2'	1:A:2400:G:O4'	2.11	0.50
2:B:89:G:H2'	2:B:90:A:C8	2.46	0.50
3:D:177:LEU:HD11	3:D:183:ARG:HB2	1.93	0.50
4:E:135:HIS:CD2	4:E:135:HIS:N	2.79	0.50
1:A:2285:C:OP2	28:6:6:ARG:NH1	2.42	0.50
17:V:5:VAL:HG11	17:V:57:VAL:CG2	2.41	0.50
1:A:1025:G:C5	1:A:1135:C:H1'	2.47	0.50
12:Q:32:TYR:HE2	12:Q:133:ARG:HG3	1.76	0.50
1:A:2673:G:O3'	10:O:26:LYS:NZ	2.44	0.50
1:A:1747:G:H2'	1:A:1747(A):G:H8	1.76	0.50
21:Z:43:GLU:O	21:Z:47:VAL:HG23	2.11	0.50
1:A:1803:A:H4'	3:D:259:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1406:U:H2'	1:A:1407:C:C6	2.46	0.50
1:A:1003:G:N2	1:A:1153:C:C2	2.80	0.50
18:W:40:ASN:C	18:W:41:LYS:HG2	2.31	0.50
18:W:14:PRO:HG2	18:W:78:GLU:HG2	1.93	0.50
4:E:115:GLY:O	4:E:119:ARG:HB2	2.12	0.50
1:A:271(I):G:N2	1:A:271(O):C:N3	2.46	0.50
14:S:105:ALA:O	14:S:110:LEU:HB2	2.12	0.50
5:F:184:TYR:HE1	11:P:3:LEU:HD21	1.77	0.50
1:A:271(M):G:H4'	1:A:271(N):U:OP1	2.10	0.50
1:A:718:A:O5'	1:A:718:A:H8	1.94	0.50
23:1:86:SER:HB3	23:1:89:GLU:HG2	1.94	0.50
1:A:2262:U:H4'	1:A:2328:A:H2	1.76	0.50
1:A:1313:U:H2'	1:A:1610:A:N1	2.27	0.50
13:R:84:ALA:N	13:R:85:PRO:HD2	2.27	0.50
1:A:973:A:H5'	1:A:1188:U:H1'	1.93	0.50
1:A:2879:C:OP2	34:A:4332:HOH:O	2.18	0.50
14:S:41:ASP:OD1	14:S:43:GLU:HB2	2.11	0.50
1:A:1878:G:C6	1:A:1879:C:C4	3.00	0.50
21:Z:21:ALA:O	21:Z:23:LYS:N	2.45	0.50
5:F:6:VAL:O	5:F:22:ALA:HB3	2.12	0.50
4:E:75:VAL:HG13	4:E:77:ILE:H	1.76	0.50
3:D:147:LEU:HD12	3:D:155:LEU:HD21	1.93	0.50
1:A:571:A:OP2	1:A:2030:A:N6	2.44	0.50
1:A:910:A:N7	12:Q:12:GLN:HB2	2.27	0.50
28:6:6:ARG:O	28:6:6:ARG:HG3	2.12	0.50
25:3:12:PRO:O	25:3:15:TYR:HB2	2.11	0.50
3:D:148:GLU:HB2	3:D:151:LYS:HD3	1.93	0.50
2:B:49:C:OP1	14:S:97:ARG:N	2.45	0.50
1:A:2103:C:O2	1:A:2187:G:N1	2.45	0.50
20:Y:98:VAL:HG23	20:Y:99:CYS:O	2.12	0.50
1:A:2473:U:H2'	1:A:2473:U:O2	2.11	0.50
2:B:9:G:OP1	14:S:15:ARG:NH1	2.42	0.50
17:V:74:LYS:HB2	17:V:83:ARG:HB2	1.94	0.50
1:A:1006:C:C2	1:A:1138:G:N2	2.80	0.50
14:S:96:GLY:H	14:S:99:LYS:H	1.60	0.49
1:A:2712:U:H1'	1:A:2712(A):A:C8	2.47	0.49
1:A:848:G:C4	1:A:933:A:H8	2.30	0.49
1:A:173:G:H2'	1:A:174:C:C6	2.48	0.49
13:R:21:TYR:OH	13:R:43:GLU:HG2	2.11	0.49
4:E:35:GLN:HB3	4:E:48:GLN:HB3	1.93	0.49
16:U:72:HIS:N	16:U:72:HIS:ND1	2.60	0.49
1:A:1006:C:H1'	9:N:106:MET:HB3	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:58:LEU:HD13	8:I:59:ALA:HB2	1.94	0.49
1:A:1341:U:H1'	19:X:55:ASN:HD22	1.76	0.49
1:A:1709:U:H2'	1:A:1710:C:C6	2.46	0.49
9:N:26:LEU:HD23	9:N:60:ILE:HD11	1.92	0.49
3:D:145:VAL:HG11	3:D:175:LEU:HD11	1.94	0.49
1:A:631:A:OP2	30:8:47:LYS:NZ	2.34	0.49
1:A:1540:U:H2'	1:A:1541:G:O4'	2.12	0.49
1:A:579:G:H2'	1:A:580:C:H6	1.77	0.49
16:U:76:TYR:O	16:U:80:ILE:HG12	2.12	0.49
1:A:2331:G:N3	1:A:2336:A:H2	2.10	0.49
5:F:158:THR:HG21	5:F:163:VAL:HG11	1.94	0.49
1:A:1300:U:H4'	1:A:1301:A:H5''	1.94	0.49
16:U:49:HIS:HA	16:U:52:ARG:HB3	1.94	0.49
1:A:294:A:H2'	1:A:295:G:O4'	2.12	0.49
1:A:1239:G:H2'	1:A:1240:U:O4'	2.12	0.49
4:E:54:GLN:HB2	4:E:76:ARG:HB3	1.94	0.49
17:V:52:VAL:CG2	17:V:55:ALA:HB3	2.42	0.49
3:D:52:ARG:HB2	3:D:53:PHE:CD2	2.47	0.49
12:Q:55:VAL:HG12	12:Q:64:ILE:HD12	1.95	0.49
1:A:539:G:H2'	1:A:540:C:C6	2.47	0.49
17:V:20:LEU:O	17:V:93:GLU:HG2	2.12	0.49
8:I:4:ILE:HG12	8:I:18:VAL:HG22	1.95	0.49
28:6:16:CYS:HB2	28:6:18:ARG:HH11	1.78	0.49
7:H:9:ILE:HD12	7:H:72:ILE:HG22	1.94	0.49
1:A:900:A:H2'	1:A:901:A:O4'	2.13	0.49
17:V:5:VAL:HG12	17:V:37:VAL:HG22	1.94	0.49
1:A:2439:A:H1'	1:A:2587:A:OP1	2.13	0.49
2:B:20:C:H2'	2:B:21:G:H5'	1.94	0.49
4:E:47:VAL:HG12	4:E:49:LEU:HD13	1.94	0.49
1:A:588:U:H2'	1:A:589:C:C6	2.48	0.49
10:O:115:VAL:HG12	10:O:121:VAL:HG21	1.94	0.49
24:2:44:LEU:HD23	24:2:45:SER:O	2.13	0.49
25:3:5:LYS:HE2	25:3:57:GLU:HG3	1.95	0.49
22:0:52:GLY:O	22:0:59:LEU:HA	2.11	0.49
1:A:667:U:H2'	1:A:668:G:O4'	2.13	0.49
1:A:2307:G:H4'	1:A:2308:G:C5'	2.40	0.49
5:F:188:ARG:HA	11:P:3:LEU:HD11	1.95	0.49
7:H:7:LEU:HB3	7:H:69:ARG:NH1	2.26	0.49
1:A:1252:G:O4'	16:U:33:ARG:HD3	2.12	0.49
4:E:4:ILE:HG12	4:E:5:LEU:N	2.27	0.49
12:Q:55:VAL:HG12	12:Q:64:ILE:CD1	2.42	0.49
3:D:239:ARG:O	3:D:239:ARG:HG3	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:S:7:TYR:HA	14:S:10:ARG:HH12	1.76	0.49
1:A:2716:U:O2'	1:A:2717:G:H5'	2.13	0.49
31:9:30:PRO:O	31:9:33:LYS:HB2	2.13	0.49
1:A:1319:G:H5''	1:A:1319:G:H8	1.78	0.49
1:A:19:C:H2'	1:A:20:C:C6	2.43	0.49
1:A:1019:U:O2'	1:A:1021:A:H2	1.94	0.49
1:A:1022:G:C6	1:A:1140:C:C4	3.00	0.49
1:A:2465:C:O2	1:A:2486:G:C2	2.65	0.49
19:X:5:TYR:CE2	24:2:30:ARG:HB2	2.48	0.49
24:2:46:GLN:O	24:2:49:LYS:HG3	2.13	0.49
3:D:120:GLY:O	3:D:131:LEU:HG	2.13	0.49
20:Y:43:ASN:OD1	20:Y:65:ALA:HB3	2.12	0.49
5:F:39:TRP:CH2	5:F:106:ARG:HD3	2.47	0.49
2:B:105:A:OP1	21:Z:72:ARG:NH1	2.46	0.49
14:S:35:ILE:HD11	14:S:101:LEU:HD12	1.93	0.49
7:H:69:ARG:HG3	7:H:70:THR:N	2.27	0.49
1:A:2550:G:C5	1:A:2551:C:C5	3.01	0.49
24:2:45:SER:O	24:2:46:GLN:HB2	2.13	0.49
10:O:114:ILE:O	10:O:117:LEU:N	2.45	0.49
5:F:178:PRO:HB2	5:F:201:VAL:HG22	1.94	0.49
6:G:28:VAL:O	6:G:31:VAL:HG13	2.11	0.49
1:A:1357:U:H2'	1:A:1358:G:C8	2.48	0.49
3:D:218:ARG:HB3	3:D:219:PRO:HD2	1.95	0.49
1:A:637:A:C8	11:P:117:GLU:HG3	2.45	0.49
1:A:998:C:P	16:U:92:ARG:HH22	2.36	0.49
1:A:1789:A:H5''	3:D:220:HIS:O	2.13	0.49
12:Q:108:GLY:HA3	21:Z:116:VAL:HG11	1.95	0.49
5:F:167:ALA:HB1	5:F:173:VAL:HG11	1.95	0.49
3:D:78:LYS:HE2	3:D:114:GLY:HA2	1.93	0.49
4:E:132:HIS:CD2	34:E:410:HOH:O	2.65	0.49
1:A:12:U:H2'	1:A:12:U:O2	2.12	0.49
1:A:321:G:C5	1:A:341:G:H4'	2.47	0.49
1:A:2801(A):A:H5''	1:A:2802:G:H5'	1.93	0.49
27:5:29:THR:O	27:5:30:LEU:HD23	2.13	0.49
5:F:17:ARG:HG3	5:F:18:ARG:H	1.78	0.49
4:E:200:GLU:HG3	4:E:201:THR:H	1.78	0.49
1:A:38:A:H2'	1:A:39:C:C6	2.48	0.49
8:I:14:ASP:N	8:I:17:GLN:OE1	2.44	0.49
2:B:2:C:O2'	2:B:3:C:H5'	2.12	0.49
8:I:38:LEU:O	8:I:43:ASN:ND2	2.46	0.49
13:R:94:TYR:N	13:R:94:TYR:CD2	2.79	0.49
1:A:1154:G:H8	1:A:1154:G:O5'	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1339:G:N2	1:A:1603:A:H1'	2.27	0.49
1:A:1450(A):C:N4	1:A:1451:C:H41	2.11	0.49
1:A:2319:G:O4'	1:A:2319:G:N3	2.45	0.49
11:P:143:GLY:O	11:P:145:PRO:HD3	2.13	0.48
15:T:53:ARG:HH11	15:T:60:THR:HG23	1.77	0.48
1:A:1019:U:H2'	1:A:1020:A:H8	1.78	0.48
3:D:68:LYS:C	3:D:70:TRP:H	2.15	0.48
1:A:1001:A:H2'	1:A:1002:G:O4'	2.13	0.48
16:U:76:TYR:OH	16:U:92:ARG:NH1	2.40	0.48
1:A:2261:C:C5	22:O:16:SER:HB3	2.48	0.48
4:E:67:PHE:HB3	4:E:72:VAL:O	2.12	0.48
1:A:1005:C:C2	1:A:1143:A:C5	3.01	0.48
7:H:153:LYS:HG3	7:H:154:PRO:HD2	1.94	0.48
8:I:123:LEU:HA	8:I:144:VAL:HG13	1.95	0.48
1:A:776:G:H4'	1:A:777:A:O5'	2.12	0.48
1:A:1141:U:P	9:N:25:ARG:HH11	2.36	0.48
6:G:33:ARG:HB2	6:G:33:ARG:HE	1.46	0.48
1:A:1494:A:H2'	1:A:1495:A:C8	2.48	0.48
21:Z:30:ASN:N	21:Z:33:LEU:O	2.38	0.48
1:A:1859:A:C2	1:A:1884:A:H1'	2.48	0.48
1:A:1936:A:H2'	1:A:1945:G:O6	2.14	0.48
1:A:1963:U:H4'	1:A:1964:G:OP1	2.13	0.48
7:H:26:VAL:HG12	7:H:79:VAL:HG21	1.95	0.48
20:Y:79:CYS:HB2	20:Y:81:LYS:H	1.77	0.48
2:B:66:A:H61	2:B:109:C:H5''	1.77	0.48
24:2:9:GLN:HE22	24:2:56:GLN:HB3	1.78	0.48
1:A:673:C:H5''	5:F:81:PRO:HD2	1.94	0.48
14:S:101:LEU:HD22	14:S:102:ALA:HB2	1.94	0.48
1:A:2575:C:H2'	1:A:2578:G:O6	2.12	0.48
1:A:2884:U:O2	27:5:53:ALA:HB2	2.13	0.48
1:A:660:G:H5'	5:F:99:TYR:CE2	2.48	0.48
1:A:2102:U:O2	1:A:2187:G:O6	2.31	0.48
15:T:91:ARG:HD2	15:T:120:ARG:NH1	2.29	0.48
21:Z:34:ASN:O	21:Z:35:ARG:HD2	2.13	0.48
14:S:26:LEU:HA	14:S:39:ILE:HD13	1.95	0.48
21:Z:151:HIS:C	21:Z:153:SER:H	2.17	0.48
9:N:18:ALA:HB1	9:N:60:ILE:HD13	1.94	0.48
16:U:104:GLN:OE1	16:U:105:VAL:HG23	2.13	0.48
4:E:24:THR:HG22	4:E:186:GLY:O	2.13	0.48
1:A:898:C:H2'	1:A:899:A:O4'	2.13	0.48
1:A:2805:G:H2'	1:A:2807:G:O4'	2.13	0.48
1:A:659:C:H4'	5:F:100:THR:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2887:U:H2'	1:A:2888:C:H6	1.79	0.48
1:A:1689:A:N6	1:A:1698:A:H2	1.97	0.48
1:A:1448:G:O2'	1:A:1528:A:N6	2.38	0.48
1:A:2295:C:C2	1:A:2296:U:H5	2.31	0.48
7:H:30:LYS:HG3	7:H:80:SER:O	2.13	0.48
1:A:287:C:N4	1:A:354:G:H1	2.10	0.48
1:A:988:A:P	25:3:11:SER:HB2	2.54	0.48
1:A:533:G:H21	16:U:45:TYR:HE2	1.61	0.48
1:A:770:G:N3	1:A:1354:A:H2	2.12	0.48
12:Q:97:VAL:HG13	12:Q:101:ARG:HB3	1.95	0.48
25:3:43:ILE:O	25:3:47:VAL:HG23	2.13	0.48
28:6:9:LEU:CD2	28:6:25:LYS:HB3	2.43	0.48
1:A:537:C:O2'	9:N:5:VAL:HG21	2.13	0.48
15:T:109:GLU:O	15:T:113:LYS:N	2.45	0.48
3:D:273:ARG:HG2	3:D:274:ARG:N	2.28	0.48
1:A:102:G:O2'	1:A:103:A:P	2.71	0.48
1:A:1008:C:N4	1:A:1136:G:C6	2.82	0.48
9:N:42:TRP:HA	9:N:48:MET:SD	2.53	0.48
1:A:2054:A:H5''	1:A:2055:C:O5'	2.12	0.48
1:A:520:G:H2'	1:A:521:G:H8	1.76	0.48
12:Q:32:TYR:HB2	12:Q:106:VAL:HG23	1.95	0.48
1:A:2376:A:H8	1:A:2376:A:OP1	1.97	0.48
16:U:17:ILE:HA	16:U:20:LEU:HD12	1.95	0.48
19:X:84:ALA:O	19:X:87:GLN:HG3	2.13	0.48
21:Z:108:PRO:HA	21:Z:142:SER:HA	1.96	0.48
1:A:2326:C:H5''	1:A:2327:A:OP2	2.13	0.48
1:A:2751:G:C8	7:H:2:SER:N	2.81	0.48
2:B:37:C:C5	2:B:38:C:C5	3.02	0.48
1:A:2529:G:H5''	1:A:2530:A:H5''	1.95	0.48
1:A:531:C:H4'	1:A:532:A:H5''	1.94	0.48
1:A:1292:U:H2'	1:A:1293:C:H6	1.79	0.48
15:T:6:LEU:HD13	15:T:6:LEU:HA	1.47	0.48
1:A:2469:A:H5''	1:A:2470:G:OP2	2.14	0.48
19:X:36:LYS:HE3	19:X:56:THR:OG1	2.14	0.48
1:A:2780:G:H4'	1:A:2781:A:OP2	2.14	0.48
9:N:62:VAL:CG1	9:N:66:LYS:HB2	2.44	0.48
13:R:25:ALA:O	13:R:29:LEU:HB2	2.14	0.48
1:A:1638:C:H4'	1:A:2710:C:O2	2.14	0.48
24:2:32:LEU:HD12	24:2:53:LEU:HB3	1.96	0.48
1:A:2534:A:C2	1:A:2535:G:H1'	2.49	0.48
1:A:614(C):A:N3	1:A:615:G:H1'	2.29	0.48
1:A:1802:A:N1	1:A:1822:G:H1'	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1200:C:H1'	16:U:2:PRO:HG3	1.95	0.48
1:A:1839:G:C8	1:A:1927:A:H1'	2.49	0.48
1:A:2228:G:OP1	3:D:261:LYS:HE2	2.14	0.48
1:A:2783:G:H2'	1:A:2784:C:C6	2.49	0.48
1:A:109:G:H2'	1:A:110:G:O4'	2.13	0.48
1:A:854:G:H2'	1:A:855:G:H8	1.79	0.48
1:A:1356:G:C6	1:A:1357:U:N3	2.81	0.48
1:A:875:G:N2	1:A:903:C:C2	2.81	0.48
9:N:53:VAL:HG11	9:N:128:HIS:HB2	1.96	0.48
1:A:2009:G:OP1	18:W:41:LYS:HE3	2.14	0.48
1:A:2833:G:O2'	1:A:2834:G:P	2.71	0.48
12:Q:63:LYS:HE3	12:Q:65:PHE:CZ	2.49	0.48
1:A:2361:A:OP1	30:8:27:THR:HG23	2.13	0.48
1:A:705:A:H1'	3:D:9:TYR:CE1	2.49	0.48
6:G:32:PRO:HB2	6:G:172:LEU:HD22	1.96	0.48
1:A:1810:A:H2'	1:A:1811:G:O4'	2.13	0.48
23:1:76:ARG:HE	23:1:97:LEU:HD22	1.79	0.48
1:A:754:C:H2'	1:A:755:C:C6	2.49	0.48
29:7:24:THR:O	29:7:28:ARG:HG3	2.13	0.48
1:A:2052:G:O4'	4:E:142:GLY:HA3	2.14	0.48
1:A:483:A:O2'	20:Y:49:VAL:O	2.21	0.48
1:A:2657:A:C2	1:A:2665:A:C4	3.02	0.48
21:Z:128:VAL:HG23	21:Z:161:VAL:N	2.29	0.48
5:F:53:THR:O	5:F:55:GLY:N	2.47	0.48
9:N:128:HIS:O	9:N:130:HIS:N	2.47	0.48
5:F:89:VAL:HG12	5:F:90:PHE:N	2.28	0.48
1:A:1339:G:H21	1:A:1603:A:H1'	1.79	0.48
18:W:59:VAL:HG12	18:W:60:ASN:OD1	2.13	0.48
1:A:2461:C:H2'	1:A:2462:U:C6	2.49	0.48
1:A:296:C:O3'	20:Y:95:LYS:NZ	2.47	0.48
1:A:297:C:OP1	20:Y:87:LYS:HD2	2.14	0.47
5:F:184:TYR:CE2	5:F:188:ARG:HD2	2.49	0.47
1:A:2779:U:H4'	1:A:2780:G:H5''	1.95	0.47
1:A:2528:U:O2'	1:A:2529:G:H3'	2.13	0.47
1:A:1788:C:C2	1:A:1789:A:C8	3.01	0.47
1:A:1183:G:O3'	25:3:29:ARG:NH1	2.47	0.47
4:E:51:PHE:HB3	4:E:77:ILE:HG22	1.95	0.47
1:A:872:A:C6	1:A:873:G:C6	3.01	0.47
10:O:64:ARG:HB3	10:O:79:PHE:CG	2.49	0.47
17:V:64:HIS:ND1	17:V:92:THR:OG1	2.38	0.47
1:A:2334:G:H8	1:A:2334:G:OP1	1.96	0.47
2:B:55:U:HO2'	6:G:29:TRP:HD1	1.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:45:A:OP1	6:G:95:ARG:HD2	2.14	0.47
1:A:2712:U:OP1	1:A:2714:G:H4'	2.15	0.47
12:Q:35:VAL:HG22	12:Q:36:ALA:N	2.28	0.47
1:A:1021:A:H3'	1:A:1021:A:C8	2.50	0.47
1:A:533:G:H5'	16:U:24:TYR:CD2	2.49	0.47
1:A:1497:U:H5''	1:A:1498:C:H5	1.79	0.47
20:Y:92:ASN:N	20:Y:93:GLY:HA2	2.28	0.47
1:A:886:C:H2'	1:A:887:A:H5'	1.96	0.47
16:U:8:VAL:HG13	16:U:12:ARG:HE	1.79	0.47
1:A:646:A:H2'	1:A:647:G:O4'	2.13	0.47
27:5:45:VAL:HG22	27:5:52:TYR:HB2	1.94	0.47
1:A:2653:U:H3	1:A:2667:C:H42	1.61	0.47
1:A:565:C:H2'	1:A:566:U:O4'	2.14	0.47
1:A:321:G:OP2	5:F:136:THR:OG1	2.32	0.47
1:A:152:G:H2'	1:A:153:C:O4'	2.14	0.47
1:A:2572:A:N7	4:E:145:LYS:HB2	2.29	0.47
1:A:1302:A:H5'	1:A:1608:A:OP1	2.15	0.47
1:A:1283:G:H2'	1:A:1285:G:OP2	2.14	0.47
1:A:1283:G:N2	1:A:1286:A:H5'	2.29	0.47
29:7:8:ASN:OD1	29:7:8:ASN:C	2.53	0.47
23:1:73:LEU:HD22	23:1:73:LEU:HA	1.80	0.47
1:A:960:A:H5''	1:A:961:C:OP2	2.14	0.47
8:I:88:ILE:HD12	8:I:121:LYS:C	2.34	0.47
1:A:2262:U:OP1	22:0:19:LYS:HD3	2.13	0.47
4:E:18:ASP:HB3	15:T:82:LEU:HD21	1.95	0.47
1:A:1686:C:O2'	1:A:1687:G:H5'	2.14	0.47
6:G:106:LEU:HG	6:G:111:LEU:HG	1.97	0.47
18:W:71:VAL:HA	18:W:107:LEU:HD12	1.95	0.47
1:A:1915:U:H3'	1:A:1916:A:H8	1.78	0.47
1:A:2050:C:H1'	4:E:156:MET:CE	2.44	0.47
1:A:1515:G:H2'	1:A:1516:C:H6	1.79	0.47
1:A:2808:U:H5''	1:A:2891:G:O6	2.14	0.47
1:A:2634:G:O6	1:A:2784:C:N4	2.34	0.47
21:Z:19:ARG:HB2	21:Z:19:ARG:HE	1.42	0.47
17:V:42:GLY:O	17:V:43:GLU:HG2	2.14	0.47
1:A:1796:U:H2'	1:A:1797:C:C6	2.50	0.47
1:A:1438:U:O2'	1:A:1439:A:H5'	2.14	0.47
3:D:16:MET:HB2	3:D:207:GLY:HA3	1.96	0.47
1:A:480:A:OP2	20:Y:47:LYS:HD3	2.14	0.47
1:A:2256:G:H2'	1:A:2257:U:H6	1.79	0.47
1:A:1927:A:H2'	1:A:1928:A:C8	2.50	0.47
1:A:832:G:H21	11:P:53:GLY:HA3	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1242:A:N1	11:P:4:SER:HB2	2.29	0.47
1:A:251:A:C5	1:A:252:G:H1'	2.50	0.47
1:A:29:U:H6	1:A:29:U:O5'	1.98	0.47
1:A:2787:C:O2'	4:E:61:ARG:HD3	2.14	0.47
1:A:2467:C:H4'	12:Q:123:HIS:ND1	2.30	0.47
29:7:35:ARG:HG3	29:7:42:LEU:HD11	1.95	0.47
6:G:16:ARG:CZ	6:G:31:VAL:HG21	2.44	0.47
1:A:953:A:H2'	1:A:954:G:H8	1.80	0.47
8:I:65:ALA:O	8:I:68:LEU:HB2	2.14	0.47
1:A:71:A:C2	19:X:31:HIS:CE1	3.02	0.47
11:P:86:LYS:HB3	11:P:118:GLY:HA2	1.97	0.47
1:A:830:G:H4'	1:A:831:G:OP2	2.15	0.47
22:0:56:ASP:O	22:0:57:PHE:HB2	2.14	0.47
12:Q:60:ARG:NH2	21:Z:177:PRO:HG3	2.30	0.47
1:A:729:G:O5'	3:D:208:LYS:NZ	2.48	0.47
1:A:1529:G:C6	1:A:1530:C:C4	3.02	0.47
2:B:45:A:C6	2:B:46:A:C5	3.02	0.47
1:A:2070:G:C2	1:A:2442:C:C2	3.02	0.47
14:S:95:HIS:C	14:S:99:LYS:HB3	2.35	0.47
1:A:144:C:H2'	1:A:145:G:H8	1.80	0.47
5:F:28:ILE:HG13	5:F:112:MET:HG2	1.97	0.47
25:3:46:ASN:O	25:3:50:VAL:HG22	2.14	0.47
1:A:475:U:C4	1:A:481:G:O6	2.68	0.47
1:A:9:U:HO2'	1:A:10:G:P	2.36	0.47
16:U:41:ALA:O	16:U:45:TYR:HD1	1.97	0.47
1:A:323:G:H2'	5:F:169:ASN:ND2	2.30	0.47
20:Y:19:LYS:HE3	20:Y:20:TYR:CE1	2.50	0.47
1:A:987:G:O2'	1:A:1000:A:N3	2.37	0.47
1:A:2261:C:C6	22:0:16:SER:HB3	2.50	0.47
6:G:33:ARG:HE	6:G:162:THR:HG21	1.78	0.47
7:H:88:LEU:N	7:H:163:TYR:O	2.47	0.47
1:A:2464:C:C2	1:A:2487:G:C2	3.02	0.47
4:E:98:PRO:HD3	4:E:175:VAL:HG13	1.95	0.47
1:A:614:U:H5'	1:A:614(C):A:N6	2.30	0.47
12:Q:2:LEU:HA	12:Q:2:LEU:HD12	1.61	0.47
1:A:176:G:O2'	1:A:177:G:H5'	2.15	0.47
16:U:88:ILE:HG23	17:V:48:GLY:O	2.14	0.47
12:Q:110:THR:HG23	12:Q:113:GLN:OE1	2.14	0.47
2:B:66:A:H61	2:B:109:C:C5'	2.27	0.47
1:A:1820:U:C2	3:D:202:LYS:HG2	2.50	0.47
6:G:19:LEU:HA	6:G:22:ARG:HB2	1.96	0.47
23:1:85:LEU:HB3	23:1:89:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:U:18:LEU:HA	16:U:18:LEU:HD23	1.64	0.47
28:6:8:LYS:HD3	30:8:34:TRP:CD2	2.49	0.47
1:A:1782:C:H1'	1:A:2609:U:H5''	1.97	0.47
1:A:686:G:N2	1:A:788:A:H61	2.12	0.47
3:D:109:ASP:HB2	3:D:197:GLY:HA2	1.96	0.47
1:A:2524:G:N2	1:A:2539:C:O2	2.42	0.47
11:P:60:MET:HA	30:8:13:ARG:NH1	2.29	0.47
7:H:137:ASP:HB3	7:H:140:LYS:HB2	1.97	0.47
20:Y:9:LYS:HB2	20:Y:27:VAL:O	2.14	0.47
1:A:572:A:H2'	1:A:573:G:O4'	2.15	0.47
1:A:533:G:H5'	16:U:24:TYR:CE2	2.50	0.47
30:8:57:ARG:HG3	30:8:57:ARG:H	1.44	0.47
1:A:1914:C:HO2'	1:A:1915:U:P	2.35	0.47
1:A:198:C:H5'	1:A:2244:U:OP1	2.14	0.47
1:A:2537:U:H2'	1:A:2538:C:C6	2.50	0.47
1:A:257:A:H2'	1:A:258:G:O4'	2.15	0.47
1:A:1441:G:H2'	1:A:1442:G:H8	1.79	0.47
11:P:38:GLN:C	11:P:40:SER:H	2.18	0.47
1:A:93:G:H2'	1:A:94:C:C6	2.50	0.47
1:A:2410:G:N2	1:A:2411:A:H1'	2.30	0.47
5:F:178:PRO:HB2	5:F:201:VAL:CG2	2.45	0.47
1:A:1420:U:HO2'	1:A:1421:G:P	2.36	0.47
11:P:112:LEU:HD22	11:P:113:LYS:N	2.30	0.47
6:G:11:TYR:CZ	6:G:16:ARG:HD3	2.51	0.46
2:B:48:A:H4'	14:S:95:HIS:CD2	2.41	0.46
1:A:991:C:C6	1:A:991:C:H5'	2.44	0.46
1:A:1331:A:O2'	1:A:1332:G:C8	2.66	0.46
1:A:2275:C:C6	1:A:2275:C:H5'	2.47	0.46
1:A:1849:G:H2'	1:A:1850:G:C8	2.50	0.46
1:A:1815:A:C5	1:A:1817:G:C6	3.03	0.46
1:A:1655:A:C8	1:A:1656:C:C5	3.02	0.46
1:A:1364:G:N7	23:1:3:LYS:HE2	2.31	0.46
14:S:94:TYR:CE2	14:S:99:LYS:HD2	2.50	0.46
1:A:2680:C:OP2	4:E:111:ARG:NH2	2.44	0.46
3:D:68:LYS:HD2	3:D:70:TRP:CZ2	2.50	0.46
1:A:320:A:H4'	1:A:322:A:N7	2.30	0.46
6:G:25:TYR:HB3	6:G:30:GLU:HB2	1.97	0.46
1:A:970:C:H2'	1:A:971:C:C6	2.50	0.46
1:A:1676:A:OP2	1:A:1676:A:H8	1.99	0.46
18:W:31:GLU:O	18:W:34:ASN:HB2	2.16	0.46
1:A:236:C:H2'	1:A:237:C:C6	2.50	0.46
1:A:947:G:N3	1:A:984:A:H2	2.13	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2016:U:O2	27:5:7:PRO:HG2	2.14	0.46
1:A:681:G:H2'	1:A:682:G:O4'	2.16	0.46
1:A:736:C:H42	1:A:760:G:H1	1.63	0.46
7:H:52:VAL:HG12	7:H:65:HIS:CD2	2.50	0.46
11:P:26:GLY:HA3	11:P:27:HIS:CB	2.45	0.46
4:E:150:VAL:HG13	4:E:154:LYS:HG3	1.96	0.46
1:A:2567:G:H2'	1:A:2568:C:H6	1.78	0.46
1:A:847:U:H5'	1:A:848:G:OP2	2.15	0.46
24:2:50:ILE:C	24:2:52:ASP:H	2.19	0.46
7:H:149:ARG:HD2	7:H:164:TYR:HE1	1.79	0.46
2:B:7:G:H4'	14:S:29:PHE:CD1	2.51	0.46
9:N:33:LEU:HD12	9:N:38:HIS:CD2	2.51	0.46
6:G:145:THR:OG1	6:G:146:TYR:N	2.44	0.46
1:A:817:C:H2'	1:A:818:G:H8	1.80	0.46
3:D:179:SER:O	3:D:275:LYS:HB2	2.15	0.46
1:A:826:U:OP1	1:A:2428:G:H3'	2.15	0.46
12:Q:38:GLU:HB2	12:Q:127:ILE:HB	1.97	0.46
1:A:14:A:H5''	1:A:15:G:OP2	2.16	0.46
20:Y:28:LYS:HG2	20:Y:40:GLU:HG3	1.97	0.46
8:I:29:TYR:CD2	8:I:30:LEU:HD23	2.49	0.46
5:F:53:THR:O	5:F:56:GLU:N	2.42	0.46
1:A:1420:U:O2'	1:A:1421:G:OP1	2.28	0.46
22:0:34:GLY:N	22:0:61:ALA:O	2.28	0.46
5:F:70:THR:C	5:F:72:ARG:H	2.18	0.46
21:Z:24:LEU:HD23	21:Z:44:PHE:CD1	2.51	0.46
1:A:2302:G:H2'	1:A:2303:G:C8	2.50	0.46
22:0:41:ARG:HD3	22:0:41:ARG:HA	1.63	0.46
1:A:2611:U:OP2	1:A:2611:U:H3'	2.16	0.46
14:S:66:ALA:O	14:S:69:VAL:HG12	2.16	0.46
1:A:1515:G:H2'	1:A:1516:C:C6	2.49	0.46
28:6:17:LYS:HA	28:6:17:LYS:HD3	1.73	0.46
24:2:21:LEU:HD23	24:2:21:LEU:HA	1.60	0.46
1:A:2278:A:OP1	12:Q:11:LYS:HE2	2.16	0.46
11:P:95:VAL:CG2	11:P:125:VAL:HG12	2.45	0.46
1:A:2766:G:H5''	1:A:2767:C:OP2	2.14	0.46
13:R:67:LEU:HD13	13:R:76:VAL:HG21	1.96	0.46
1:A:841:A:H2'	1:A:842:G:C8	2.50	0.46
14:S:78:LEU:HD22	14:S:82:ILE:O	2.15	0.46
17:V:87:HIS:NE2	17:V:89:GLN:HG2	2.31	0.46
1:A:1495:A:H2'	1:A:1496:A:H8	1.74	0.46
5:F:164:ARG:O	5:F:168:ARG:HB2	2.16	0.46
1:A:590:A:OP1	5:F:95:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:9:TYR:CE2	21:Z:35:ARG:HG3	2.50	0.46
27:5:51:TYR:CE1	27:5:56:LYS:HG3	2.50	0.46
5:F:51:THR:HB	5:F:88:VAL:HG11	1.96	0.46
8:I:140:LEU:HA	8:I:140:LEU:HD23	1.73	0.46
6:G:121:ASN:HA	6:G:122:PRO:HD3	1.68	0.46
30:8:16:ILE:HD12	30:8:59:LYS:HD2	1.97	0.46
3:D:36:PRO:HA	3:D:61:LEU:CD1	2.46	0.46
1:A:671:C:H2'	1:A:672:C:C6	2.51	0.46
1:A:774:A:H2'	1:A:774:A:N3	2.31	0.46
1:A:2295:C:H5	14:S:13:ARG:NH2	2.13	0.46
1:A:2295:C:H5	14:S:13:ARG:HH22	1.63	0.46
23:1:94:LEU:HA	23:1:94:LEU:HD23	1.70	0.46
1:A:854:G:H2'	1:A:855:G:C8	2.50	0.46
1:A:2461:C:H2'	1:A:2462:U:H6	1.81	0.46
10:O:89:ASN:OD1	10:O:89:ASN:N	2.48	0.46
1:A:137:C:N4	1:A:139:G:O6	2.48	0.46
3:D:65:ILE:HG21	3:D:106:ILE:HG22	1.98	0.46
16:U:79:PHE:CZ	16:U:83:LEU:HD21	2.51	0.46
1:A:2418:A:C2	1:A:2419:U:C2	3.03	0.46
5:F:149:ASP:N	5:F:149:ASP:OD2	2.47	0.46
2:B:90:A:C6	2:B:91:C:H1'	2.50	0.46
1:A:330:A:O2'	1:A:331:A:H2'	2.15	0.46
1:A:1007:C:H2'	1:A:1008:C:H5	1.80	0.46
1:A:1021:A:H3'	1:A:1021:A:H8	1.80	0.46
3:D:51:VAL:CG1	3:D:54:ARG:HD3	2.46	0.46
25:3:52:HIS:CD2	25:3:53:LEU:HG	2.51	0.46
15:T:11:GLU:O	15:T:15:VAL:HG23	2.16	0.46
1:A:41:C:H2'	1:A:42:G:C8	2.51	0.46
4:E:117:MET:HG3	4:E:117:MET:H	1.62	0.46
5:F:181:LEU:O	5:F:205:ARG:NH2	2.44	0.46
1:A:850:C:O3'	25:3:49:LYS:HE2	2.16	0.46
5:F:187:VAL:HG12	11:P:3:LEU:HD12	1.96	0.46
1:A:1332:G:H4'	1:A:1333:C:OP2	2.16	0.46
1:A:528:A:C8	1:A:528:A:H3'	2.50	0.46
17:V:37:VAL:HG12	17:V:39:LEU:H	1.81	0.46
1:A:370:G:H4'	1:A:371:A:OP2	2.16	0.46
1:A:1827:C:C2'	1:A:1828:G:H5'	2.46	0.46
10:O:113:LYS:O	10:O:117:LEU:HD12	2.15	0.46
1:A:517:C:OP1	27:5:16:ARG:NH2	2.45	0.46
1:A:704:G:H1'	1:A:726:G:N2	2.30	0.46
7:H:13:LYS:HA	7:H:14:GLY:HA2	1.57	0.46
1:A:1464:C:C2	1:A:1465:G:C8	3.04	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1925:C:O2'	1:A:1926:U:H5'	2.15	0.46
18:W:51:LEU:O	18:W:54:ALA:HB3	2.16	0.46
24:2:32:LEU:O	24:2:35:LEU:N	2.49	0.46
13:R:118:GLU:H	13:R:118:GLU:HG3	1.26	0.46
8:I:41:GLU:HA	8:I:44:LEU:HB3	1.97	0.46
1:A:699:A:H2'	1:A:700:G:O4'	2.16	0.46
5:F:184:TYR:CE1	11:P:3:LEU:HD21	2.51	0.45
1:A:848:G:C4	1:A:933:A:C8	3.04	0.45
8:I:126:TYR:HB2	8:I:142:VAL:O	2.15	0.45
2:B:6:C:C2	2:B:116:G:N2	2.84	0.45
1:A:271(K):U:O2'	1:A:271(M):G:N2	2.49	0.45
1:A:2335:A:O2'	1:A:2337:G:N7	2.41	0.45
1:A:1164:G:H2'	1:A:1165:U:C6	2.52	0.45
1:A:2032:G:H4'	34:A:4573:HOH:O	2.15	0.45
13:R:97:VAL:HG23	13:R:114:VAL:HG23	1.98	0.45
1:A:271(Q):G:O2'	1:A:271(R):G:OP2	2.30	0.45
8:I:26:ALA:HA	8:I:30:LEU:HB2	1.98	0.45
1:A:1124:C:H1'	31:9:36:GLN:NE2	2.31	0.45
13:R:107:ASP:OD2	13:R:108:GLY:N	2.50	0.45
7:H:87:LEU:HA	7:H:163:TYR:O	2.16	0.45
2:B:83:G:H1	2:B:94:C:H42	1.64	0.45
1:A:1006:C:N3	1:A:1138:G:C2	2.84	0.45
1:A:1341:U:OP1	1:A:1397:U:N3	2.37	0.45
16:U:104:GLN:OE1	16:U:105:VAL:N	2.49	0.45
1:A:2419:U:H2'	1:A:2420:C:C6	2.52	0.45
1:A:1115:G:OP2	1:A:1115:G:H8	1.99	0.45
3:D:264:LYS:O	3:D:267:SER:HB2	2.16	0.45
1:A:506:G:O3'	1:A:507:A:H8	1.98	0.45
1:A:600:G:N2	1:A:605:C:O3'	2.49	0.45
5:F:59:TYR:CD1	5:F:78:ILE:HD12	2.50	0.45
22:O:27:GLU:HB2	22:O:69:PHE:CD1	2.45	0.45
20:Y:39:VAL:HG12	20:Y:42:VAL:HG21	1.98	0.45
7:H:95:ARG:CB	7:H:128:PRO:HB3	2.45	0.45
4:E:12:THR:HG22	4:E:13:ARG:N	2.31	0.45
1:A:1017:G:O6	34:A:4524:HOH:O	2.20	0.45
1:A:1952:A:C6	1:A:1953:A:N1	2.85	0.45
1:A:1468:C:H2'	1:A:1469:A:C8	2.52	0.45
1:A:2571:C:H5''	1:A:2572:A:H5''	1.98	0.45
10:O:43:VAL:HG23	10:O:56:ASP:O	2.16	0.45
1:A:990:A:N6	1:A:1186:G:H1'	2.31	0.45
1:A:141:A:H8	1:A:1408:C:HO2'	1.53	0.45
1:A:1375:C:H2'	1:A:1376:C:H6	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:22:GLY:O	21:Z:23:LYS:HD3	2.16	0.45
6:G:120:LEU:HB2	6:G:180:PHE:HD2	1.82	0.45
7:H:92:ILE:O	7:H:94:TYR:HB2	2.16	0.45
1:A:280:C:N3	1:A:361:G:N2	2.64	0.45
1:A:571:A:H1'	1:A:573:G:H5''	1.98	0.45
1:A:563:G:H5'	1:A:572:A:H4'	1.98	0.45
1:A:573:G:O2'	1:A:574:C:H3'	2.15	0.45
1:A:874:G:H2'	1:A:875:G:O4'	2.17	0.45
1:A:2023:G:H5'	1:A:2617:C:H4'	1.98	0.45
23:1:66:HIS:C	23:1:68:PRO:HD2	2.37	0.45
10:O:107:ARG:HB2	10:O:115:VAL:HG11	1.98	0.45
1:A:507:A:H5''	1:A:508:G:H3'	1.98	0.45
21:Z:14:LYS:HA	21:Z:15:PRO:HD3	1.75	0.45
12:Q:69:PHE:CD1	12:Q:70:PRO:HD2	2.52	0.45
1:A:1942:C:OP2	1:A:1943:U:O2'	2.28	0.45
1:A:953:A:C4	1:A:954:G:C8	3.04	0.45
23:1:41:ARG:HD3	23:1:43:TYR:CE2	2.52	0.45
2:B:28:C:H2'	2:B:29:A:O4'	2.17	0.45
1:A:2557:G:H2'	1:A:2558:C:C6	2.51	0.45
1:A:997:G:H5''	16:U:92:ARG:HH21	1.81	0.45
1:A:2262:U:H2'	1:A:2263:C:C6	2.52	0.45
1:A:184:C:H2'	1:A:185:U:H6	1.81	0.45
1:A:2331:G:H4'	22:0:43:THR:H	1.81	0.45
1:A:970:C:H2'	1:A:971:C:H6	1.81	0.45
1:A:95:G:O2'	24:2:46:GLN:HA	2.16	0.45
1:A:2462:U:H1'	1:A:2491:U:O4	2.17	0.45
7:H:71:LEU:O	7:H:74:ASN:N	2.49	0.45
18:W:12:ILE:HD13	18:W:17:VAL:HG22	1.97	0.45
5:F:24:LEU:HD21	5:F:199:TRP:HH2	1.81	0.45
12:Q:132:VAL:HG11	21:Z:81:ARG:NH2	2.31	0.45
23:1:41:ARG:HD3	23:1:43:TYR:HE2	1.82	0.45
1:A:1359:A:H2	1:A:1372:U:O4	2.00	0.45
1:A:103:A:H8	1:A:103:A:OP2	2.00	0.45
1:A:579:G:C8	1:A:2017:U:C4	3.05	0.45
5:F:9:ILE:HA	5:F:10:PRO:HD2	1.65	0.45
2:B:108:U:H2'	2:B:109:C:H5''	1.98	0.45
1:A:1198:U:H2'	1:A:1199:U:C6	2.50	0.45
1:A:1936:A:C8	1:A:1940:U:O2	2.70	0.45
25:3:4:LEU:O	25:3:36:VAL:HA	2.17	0.45
5:F:13:SER:O	5:F:16:GLY:N	2.50	0.45
3:D:145:VAL:HG13	3:D:191:ALA:HB2	1.99	0.45
4:E:61:ARG:HB3	4:E:62:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:31:ARG:H	21:Z:31:ARG:HG3	1.24	0.45
3:D:2:ALA:HB3	3:D:20:ASP:HB3	1.99	0.45
5:F:19:GLU:O	5:F:20:LEU:HD23	2.16	0.45
1:A:1309:G:HO2'	1:A:1611:C:HO2'	1.59	0.45
13:R:56:LYS:NZ	13:R:90:ARG:O	2.50	0.45
1:A:1274:A:N3	1:A:1297:C:H1'	2.32	0.45
1:A:139(A):G:O2'	1:A:140:G:H5'	2.17	0.45
17:V:87:HIS:CE1	17:V:89:GLN:HG2	2.52	0.45
1:A:2019:A:C2'	1:A:2020:A:O5'	2.65	0.45
10:O:68:GLU:CD	10:O:68:GLU:H	2.19	0.45
8:I:92:VAL:CG2	8:I:120:ILE:HB	2.46	0.45
2:B:19:G:H2'	2:B:20:C:O4'	2.17	0.45
1:A:1221(A):C:C2	1:A:1229:G:C2	3.05	0.45
18:W:80:PRO:O	18:W:100:THR:HB	2.17	0.45
14:S:66:ALA:O	14:S:69:VAL:N	2.50	0.45
1:A:2393:A:C2'	1:A:2394:C:H5'	2.47	0.45
13:R:65:LEU:HA	13:R:65:LEU:HD12	1.72	0.45
1:A:1669:A:H5''	1:A:2550:G:OP1	2.17	0.45
3:D:35:LYS:HG3	3:D:64:ILE:HD11	1.98	0.45
2:B:77:U:H4'	21:Z:84:GLU:CD	2.37	0.45
1:A:792:G:N3	1:A:2072:G:O2'	2.41	0.45
3:D:76:PRO:HA	3:D:118:VAL:HB	1.99	0.45
24:2:22:GLU:HG3	24:2:64:LEU:HD11	1.98	0.45
9:N:11:PRO:O	9:N:13:TRP:HD1	2.00	0.45
1:A:1298:C:H5''	1:A:1299:G:OP2	2.17	0.45
1:A:362:U:O2'	1:A:363:G:H5''	2.17	0.45
4:E:12:THR:HG21	15:T:11:GLU:HG2	1.99	0.45
1:A:1354:A:C8	1:A:1355:G:C8	3.04	0.45
2:B:6:C:HO2'	14:S:29:PHE:HE1	1.64	0.45
8:I:124:GLY:H	8:I:144:VAL:HG13	1.82	0.45
27:5:16:ARG:HG3	27:5:17:ASP:H	1.82	0.45
19:X:25:LYS:HA	19:X:81:VAL:O	2.16	0.45
5:F:132:VAL:HG23	5:F:132:VAL:O	2.17	0.45
1:A:363(E):U:HO2'	1:A:363(F):A:P	2.37	0.45
26:4:8:LYS:HE3	26:4:8:LYS:HB3	1.66	0.45
1:A:389:G:O5'	1:A:389:G:H8	1.99	0.45
1:A:527:C:H5	34:A:4174:HOH:O	1.99	0.45
18:W:75:TYR:HE2	18:W:104:THR:HG1	1.63	0.45
1:A:720:C:H2'	1:A:721:C:H6	1.82	0.45
1:A:36:G:N3	1:A:450:G:O2'	2.49	0.45
18:W:86:LEU:HD12	18:W:87:PRO:HD2	1.99	0.45
3:D:96:HIS:NE2	3:D:102:LYS:HE2	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1288:U:C2	1:A:1327:C:O2	2.70	0.45
16:U:5:LYS:HG2	16:U:7:GLY:H	1.81	0.45
2:B:46:A:H2'	2:B:47:C:C6	2.52	0.44
1:A:1020:A:H4'	1:A:1021:A:O5'	2.17	0.44
1:A:2555:U:C5	1:A:2556:C:C2	3.05	0.44
5:F:34:TRP:CE2	11:P:8:PRO:HG3	2.51	0.44
1:A:247:G:H4'	1:A:386:G:C6	2.53	0.44
20:Y:76:CYS:HA	20:Y:77:PRO:HD3	1.77	0.44
14:S:7:TYR:CZ	14:S:91:PRO:HG3	2.52	0.44
23:1:46:LEU:HD22	23:1:46:LEU:HA	1.80	0.44
14:S:8:GLU:H	14:S:8:GLU:HG3	1.47	0.44
1:A:308:G:O2'	34:A:3720:HOH:O	2.21	0.44
12:Q:19:GLY:O	12:Q:98:LYS:HB3	2.17	0.44
1:A:2850:A:OP2	1:A:2866:U:H5	2.00	0.44
1:A:628:G:H2'	1:A:629:G:C8	2.53	0.44
1:A:300:A:OP2	20:Y:86:ARG:NH2	2.50	0.44
7:H:3:ARG:HG3	7:H:3:ARG:NH1	2.30	0.44
1:A:192:C:C2'	1:A:193:U:H5'	2.47	0.44
9:N:63:THR:HG22	9:N:66:LYS:NZ	2.30	0.44
20:Y:84:ARG:O	20:Y:100:ALA:HB2	2.17	0.44
30:8:4:MET:HE3	30:8:63:PRO:HG3	1.99	0.44
1:A:857:C:O2'	1:A:858:U:H5'	2.17	0.44
12:Q:108:GLY:HA3	21:Z:116:VAL:CG1	2.48	0.44
3:D:36:PRO:HA	3:D:61:LEU:HD12	1.99	0.44
11:P:2:LYS:O	11:P:5:ASP:HB2	2.17	0.44
20:Y:24:VAL:HG12	20:Y:25:GLY:N	2.32	0.44
5:F:140:LEU:HD11	5:F:170:LEU:HD11	1.98	0.44
13:R:111:LEU:HD12	13:R:111:LEU:HA	1.73	0.44
1:A:921:G:H2'	1:A:922:U:C6	2.53	0.44
2:B:35:U:H2'	2:B:36:C:O4'	2.17	0.44
22:0:37:LEU:HG	22:0:60:PHE:HA	1.99	0.44
1:A:888:C:H2'	1:A:889:C:C4	2.52	0.44
1:A:861:A:C2	1:A:917:A:C4	3.05	0.44
1:A:1721:G:N3	1:A:1721:G:H5''	2.31	0.44
1:A:2884:U:H1'	27:5:53:ALA:CB	2.45	0.44
21:Z:137:ILE:HG23	21:Z:156:LYS:HE3	1.99	0.44
7:H:151:ILE:HD12	7:H:151:ILE:H	1.82	0.44
2:B:42:C:O2	6:G:92:VAL:HA	2.17	0.44
1:A:2648:C:H2'	1:A:2649:U:C6	2.53	0.44
4:E:98:PRO:HG3	4:E:174:ASP:HA	2.00	0.44
1:A:236:C:H2'	1:A:237:C:H6	1.82	0.44
1:A:1142:U:OP2	34:A:3736:HOH:O	2.21	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:P:50:ARG:HH11	30:8:7:HIS:CD2	2.35	0.44
10:O:99:PHE:HB2	34:O:301:HOH:O	2.17	0.44
1:A:652(D):C:H2'	1:A:652(E):G:O4'	2.18	0.44
1:A:1774:C:H6	1:A:1774:C:O5'	2.00	0.44
3:D:258:LYS:HE2	3:D:273:ARG:NH2	2.32	0.44
1:A:1448:G:H2'	1:A:1449:A:C8	2.52	0.44
7:H:3:ARG:NE	7:H:3:ARG:HA	2.32	0.44
1:A:1007:C:H2'	1:A:1008:C:C5	2.52	0.44
1:A:1331:A:HO2'	1:A:1332:G:H8	1.65	0.44
1:A:1221(A):C:N4	1:A:1228:G:H1	2.15	0.44
1:A:734:A:O2'	1:A:1635:G:H5'	2.17	0.44
14:S:15:ARG:O	14:S:19:LYS:HG2	2.18	0.44
1:A:2854:G:H2'	1:A:2855:C:C6	2.51	0.44
17:V:24:LYS:HA	17:V:92:THR:OG1	2.18	0.44
16:U:5:LYS:HG2	16:U:6:THR:N	2.32	0.44
12:Q:24:GLY:O	12:Q:102:VAL:HG23	2.17	0.44
6:G:135:LEU:HG	6:G:155:MET:HE3	2.00	0.44
1:A:866:A:C6	1:A:914:C:C5	3.05	0.44
1:A:1142(A):A:N7	1:A:1144:G:C5	2.86	0.44
3:D:242:ARG:H	3:D:242:ARG:HD3	1.83	0.44
1:A:1498:C:O4'	1:A:1577:C:H4'	2.18	0.44
1:A:1608:A:H1'	1:A:1610:A:OP2	2.18	0.44
1:A:2356:C:H2'	1:A:2357:U:O4'	2.17	0.44
1:A:1028:A:H61	1:A:1125:G:H2'	1.83	0.44
23:1:82:LEU:HA	23:1:85:LEU:HD23	1.99	0.44
29:7:1:MET:O	29:7:3:ARG:HG2	2.18	0.44
1:A:85:G:H1	1:A:97:C:H42	1.66	0.44
1:A:1813:G:H1'	3:D:50:THR:OG1	2.18	0.44
1:A:597:U:H2'	1:A:598:G:C8	2.52	0.44
1:A:1665:A:H4'	10:O:67:LYS:HB2	2.00	0.44
1:A:1366:A:H2'	1:A:1367:A:O4'	2.18	0.44
1:A:861:A:N3	2:B:79:C:O2'	2.50	0.44
4:E:111:ARG:HA	13:R:1:MET:SD	2.58	0.44
1:A:1344:G:H4'	1:A:1384:A:C5	2.53	0.44
16:U:76:TYR:CZ	16:U:80:ILE:HG13	2.52	0.44
11:P:47:ASP:HA	11:P:48:PRO:HD3	1.72	0.44
1:A:1857:G:H1'	1:A:1885:A:N6	2.33	0.44
1:A:2405:G:H8	1:A:2405:G:O5'	2.00	0.44
1:A:2870:C:H2'	1:A:2871:C:O4'	2.17	0.44
17:V:52:VAL:HG21	17:V:55:ALA:HB3	1.98	0.44
1:A:2318:G:H2'	1:A:2319:G:OP1	2.17	0.44
28:6:9:LEU:HD21	28:6:25:LYS:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2525:G:N2	1:A:2539:C:C2	2.86	0.44
1:A:1665:A:C4'	10:O:67:LYS:HB2	2.47	0.44
1:A:2456:C:N4	34:A:3923:HOH:O	2.51	0.44
6:G:35:GLU:HB3	6:G:160:VAL:O	2.18	0.44
8:I:11:ASN:O	8:I:12:LEU:HG	2.18	0.44
1:A:299:A:H5''	20:Y:86:ARG:NH2	2.25	0.44
14:S:96:GLY:CA	14:S:100:ALA:H	2.30	0.44
1:A:2017:U:H4'	27:5:8:LYS:O	2.17	0.44
1:A:1654:A:OP1	13:R:1:MET:HA	2.18	0.44
1:A:1344:G:H4'	1:A:1384:A:N7	2.33	0.44
1:A:234:C:H2'	1:A:235:U:C6	2.53	0.44
1:A:218:A:C2	1:A:235:U:H4'	2.53	0.44
1:A:228:A:H2'	1:A:230:U:O4'	2.18	0.44
1:A:588:U:H1'	5:F:90:PHE:CG	2.53	0.44
1:A:2667:C:H1'	7:H:109:PHE:CD2	2.53	0.44
10:O:69:ILE:H	10:O:69:ILE:HG13	1.58	0.44
3:D:171:ASP:O	3:D:187:GLY:N	2.49	0.44
4:E:181:LEU:HA	4:E:181:LEU:HD13	1.60	0.44
1:A:2774:C:H2'	1:A:2775:A:O4'	2.18	0.44
1:A:2079:U:OP1	23:1:21:ARG:NH2	2.51	0.44
1:A:1022:G:N2	1:A:1142(A):A:H2	2.16	0.44
1:A:2313:C:OP1	6:G:71:THR:HG21	2.18	0.44
26:4:14:ILE:HG22	26:4:33:VAL:CG2	2.48	0.44
21:Z:160:GLY:HA2	21:Z:161:VAL:HB	2.00	0.44
1:A:519:U:O2'	1:A:520:G:H5'	2.17	0.44
1:A:971:C:C2'	1:A:972:G:H5'	2.48	0.44
4:E:119:ARG:HG2	4:E:160:TYR:HB2	2.00	0.44
11:P:46:LYS:HZ2	11:P:46:LYS:HG2	1.73	0.44
21:Z:119:GLU:OE2	21:Z:122:ARG:NH1	2.51	0.44
1:A:870:A:OP1	12:Q:6:ARG:NE	2.50	0.44
1:A:2623:G:H4'	1:A:2825:C:O2	2.18	0.44
3:D:119:ALA:HB2	3:D:130:ALA:HB3	2.00	0.44
1:A:459:U:H5''	29:7:40:TRP:CD2	2.53	0.44
2:B:8:U:H6	2:B:8:U:H5''	1.83	0.44
1:A:925:C:C2	1:A:926:A:C8	3.06	0.44
1:A:1632:A:N6	34:A:3949:HOH:O	2.50	0.44
1:A:144:C:H2'	1:A:145:G:C8	2.53	0.44
1:A:627:A:C6	1:A:637:A:C8	3.06	0.44
1:A:828:U:H4'	1:A:831:G:N1	2.33	0.44
9:N:104:LYS:HB2	9:N:117:PHE:HE1	1.78	0.44
22:O:14:ARG:HG2	22:O:14:ARG:HH11	1.83	0.44
1:A:977:G:N2	1:A:986:C:O2	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:647:G:O5'	1:A:647:G:H8	2.01	0.44
12:Q:11:LYS:HD2	12:Q:87:LYS:HD3	1.99	0.44
7:H:160:LYS:HE3	7:H:160:LYS:HB2	1.84	0.44
16:U:69:CYS:HB3	16:U:74:LEU:HD13	1.99	0.44
9:N:136:GLU:HG2	9:N:137:LYS:O	2.17	0.44
2:B:37:C:H2'	2:B:38:C:H5'	2.00	0.43
14:S:30:ARG:HG3	14:S:97:ARG:CZ	2.48	0.43
1:A:2078:C:H2'	1:A:2079:U:O4'	2.17	0.43
1:A:499:U:H2'	1:A:500:G:O4'	2.18	0.43
1:A:2713:A:N3	1:A:2713:A:H2'	2.33	0.43
2:B:42:C:O2	6:G:93:THR:N	2.38	0.43
1:A:729:G:H2'	1:A:1775:U:O2	2.17	0.43
1:A:729:G:C6	3:D:208:LYS:HB2	2.53	0.43
1:A:2536:G:C5	1:A:2537:U:C5	3.06	0.43
12:Q:24:GLY:HA2	12:Q:67:ARG:NH2	2.33	0.43
1:A:272(A):U:H6	1:A:272(A):U:H5'	1.82	0.43
1:A:225:A:N6	1:A:226:G:C2	2.86	0.43
1:A:76:C:O3'	24:2:59:ARG:HD3	2.18	0.43
4:E:21:VAL:HA	4:E:22:PRO:HD2	1.84	0.43
9:N:96:GLU:N	9:N:96:GLU:OE2	2.35	0.43
1:A:892:G:H2'	1:A:893:C:O4'	2.18	0.43
1:A:13:A:N1	1:A:525:U:H2'	2.33	0.43
1:A:1264:G:OP1	27:5:19:ARG:NH1	2.47	0.43
3:D:228:PRO:HD3	3:D:235:GLY:HA3	1.99	0.43
1:A:372:G:O2'	1:A:373:U:P	2.75	0.43
1:A:1155:A:OP1	16:U:55:ARG:HD3	2.18	0.43
5:F:183:VAL:O	5:F:187:VAL:HG23	2.17	0.43
1:A:1140:C:OP2	9:N:66:LYS:NZ	2.49	0.43
1:A:2815:C:H5'	27:5:29:THR:HG21	1.99	0.43
1:A:2820:A:C8	4:E:109:LYS:HE2	2.53	0.43
13:R:52:ILE:HD12	13:R:94:TYR:CB	2.47	0.43
1:A:2290:G:O2'	1:A:2381:C:H1'	2.18	0.43
16:U:39:LEU:HA	16:U:39:LEU:HD23	1.68	0.43
1:A:2745:C:H4'	7:H:142:GLY:O	2.19	0.43
26:4:42:PHE:CA	26:4:43:TYR:HB2	2.49	0.43
1:A:910:A:C5	12:Q:13:GLN:HG3	2.53	0.43
2:B:91:C:OP1	12:Q:16:ARG:HG2	2.17	0.43
1:A:924:C:H2'	1:A:925:C:H6	1.82	0.43
1:A:341:G:H2'	1:A:342:G:O4'	2.18	0.43
1:A:2562:U:H4'	10:O:25:LEU:HD21	1.99	0.43
1:A:9:U:N3	1:A:2629:A:H2	2.13	0.43
20:Y:39:VAL:O	20:Y:42:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2304:G:O6	34:A:4690:HOH:O	2.21	0.43
1:A:2262:U:H4'	1:A:2328:A:C2	2.53	0.43
3:D:221:VAL:HG23	3:D:226:MET:HE2	1.98	0.43
1:A:2617:C:C2	1:A:2618:G:C8	3.07	0.43
27:5:41:PRO:HG2	27:5:44:THR:OG1	2.18	0.43
1:A:539:G:H2'	1:A:540:C:H6	1.84	0.43
1:A:2807:G:C6	1:A:2808:U:C4	3.06	0.43
1:A:2228:G:C6	1:A:2229:C:C4	3.06	0.43
1:A:1815:A:C6	1:A:1817:G:O6	2.71	0.43
1:A:616:G:H5'	5:F:205:ARG:HH11	1.82	0.43
15:T:123:GLN:HG3	15:T:123:GLN:H	1.59	0.43
15:T:22:PHE:CD2	15:T:22:PHE:N	2.86	0.43
23:1:58:ILE:HD11	23:1:60:PHE:CZ	2.53	0.43
1:A:2193:G:H2'	1:A:2194:G:O4'	2.19	0.43
9:N:111:PRO:HA	9:N:114:ARG:NH1	2.33	0.43
12:Q:77:LYS:HE3	12:Q:84:GLY:O	2.18	0.43
24:2:10:LEU:HD23	24:2:10:LEU:HA	1.82	0.43
5:F:61:GLY:HA2	5:F:77:ASP:HB3	2.00	0.43
1:A:1971:A:OP2	3:D:242:ARG:NH2	2.51	0.43
24:2:51:ARG:H	24:2:54:LYS:HB2	1.83	0.43
1:A:1668:A:N3	1:A:1670:C:C4	2.86	0.43
1:A:27:G:C2	1:A:512:G:N3	2.86	0.43
12:Q:32:TYR:CE2	12:Q:133:ARG:HG3	2.53	0.43
24:2:44:LEU:HD22	24:2:47:ASN:HA	2.00	0.43
1:A:2805:G:C6	1:A:2807:G:C5	3.06	0.43
1:A:280:C:C4	1:A:361:G:N2	2.87	0.43
30:8:50:LEU:HB2	30:8:55:ALA:HB2	2.00	0.43
21:Z:150:LEU:HG	21:Z:172:ALA:HB3	2.00	0.43
1:A:651:G:H4'	30:8:18:ALA:HB3	1.99	0.43
2:B:54:G:H21	6:G:29:TRP:HZ2	1.66	0.43
1:A:953:A:OP2	12:Q:16:ARG:NE	2.50	0.43
1:A:1356:G:N1	1:A:1357:U:C2	2.86	0.43
1:A:1265:A:H8	1:A:1265:A:OP1	2.02	0.43
1:A:2307:G:H8	1:A:2307:G:OP1	2.01	0.43
1:A:637:A:H4'	1:A:638:G:O5'	2.19	0.43
2:B:110:G:H2'	2:B:111:G:H8	1.84	0.43
1:A:243:U:OP1	30:8:6:THR:OG1	2.17	0.43
1:A:34:C:H2'	1:A:35:G:H5'	2.01	0.43
6:G:23:PHE:HB2	6:G:25:TYR:HH	1.83	0.43
1:A:530:G:N1	1:A:2022:U:OP1	2.51	0.43
21:Z:99:TYR:HB3	21:Z:123:ASP:OD1	2.18	0.43
14:S:10:ARG:NE	14:S:91:PRO:O	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2791:C:H1'	1:A:2807:G:N2	2.33	0.43
1:A:612:C:H2'	1:A:613:G:O4'	2.17	0.43
5:F:78:ILE:HG13	5:F:78:ILE:H	1.57	0.43
11:P:75:ILE:HG12	11:P:75:ILE:H	1.39	0.43
1:A:691:C:H2'	1:A:692:C:H6	1.83	0.43
1:A:1778:U:P	34:A:4148:HOH:O	2.76	0.43
1:A:2013:A:H4'	18:W:96:ILE:HD13	2.00	0.43
1:A:64:A:H2'	1:A:65:C:C6	2.53	0.43
2:B:50:G:OP2	14:S:62:LYS:HD3	2.18	0.43
2:B:38:C:O4'	14:S:95:HIS:NE2	2.51	0.43
1:A:1331:A:H2'	1:A:1333:C:C5	2.53	0.43
9:N:62:VAL:HG13	9:N:66:LYS:HB2	2.01	0.43
1:A:2315:G:C6	1:A:2316:C:C4	3.07	0.43
13:R:29:LEU:HD23	13:R:70:LEU:HD11	2.00	0.43
13:R:70:LEU:HD23	13:R:70:LEU:HA	1.80	0.43
1:A:2300:G:N7	34:A:3761:HOH:O	2.36	0.43
10:O:13:ASN:C	10:O:15:GLY:N	2.71	0.43
24:2:17:SER:O	24:2:21:LEU:HB2	2.18	0.43
8:I:79:ILE:HA	8:I:80:PRO:HD3	1.69	0.43
1:A:992:C:H42	1:A:1162:G:H1	1.67	0.43
21:Z:182:LYS:O	21:Z:186:GLU:HG3	2.18	0.43
8:I:72:LEU:O	8:I:73:GLU:HB3	2.19	0.43
1:A:1007:C:OP1	9:N:37:LYS:HE2	2.19	0.43
3:D:142:VAL:HG23	3:D:193:VAL:HA	1.99	0.43
1:A:1142(A):A:C8	1:A:1144:G:N7	2.87	0.43
11:P:84:ASN:HB3	11:P:86:LYS:HG2	2.01	0.43
24:2:35:LEU:HD12	24:2:53:LEU:HD12	1.99	0.43
1:A:1945:G:H2'	1:A:1946:U:C6	2.52	0.43
6:G:139:LEU:HG	6:G:139:LEU:H	1.55	0.43
3:D:94:LEU:HD23	3:D:94:LEU:HA	1.84	0.43
1:A:2051:A:H8	1:A:2051:A:OP2	2.00	0.43
24:2:37:PHE:O	24:2:40:SER:OG	2.34	0.43
1:A:1321:A:H2'	1:A:1322:A:O4'	2.18	0.43
21:Z:93:ASP:O	21:Z:131:ARG:NH2	2.51	0.43
24:2:29:LYS:HD3	24:2:57:ILE:HD12	1.99	0.43
1:A:950:G:H2'	1:A:951:C:O4'	2.19	0.43
27:5:36:CYS:SG	27:5:48:GLU:HB2	2.59	0.43
1:A:1657:C:H2'	1:A:1658:C:H6	1.84	0.43
1:A:2286:A:H4'	1:A:2287:A:O4'	2.18	0.43
1:A:1530:C:H1'	1:A:1531:C:OP1	2.19	0.43
21:Z:44:PHE:CE2	21:Z:48:PHE:HB2	2.53	0.43
14:S:96:GLY:N	14:S:99:LYS:H	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:183:ARG:HH11	3:D:183:ARG:HG2	1.84	0.43
1:A:995:C:OP2	16:U:54:LYS:HE3	2.18	0.43
3:D:70:TRP:CZ2	3:D:150:LYS:HG3	2.53	0.43
1:A:1394:U:C4	1:A:1395:A:C5	3.06	0.43
16:U:105:VAL:O	16:U:108:GLU:HB2	2.19	0.43
30:8:34:TRP:O	30:8:35:GLN:HG2	2.19	0.43
5:F:155:LEU:HD23	5:F:186:ILE:HG13	2.00	0.43
1:A:372:G:H8	23:1:65:SER:O	2.02	0.43
7:H:32:GLU:HG2	7:H:32:GLU:H	1.70	0.43
1:A:1517:G:C6	1:A:1518:U:C4	3.06	0.43
5:F:64:ILE:HG13	5:F:65:TRP:N	2.32	0.43
1:A:740:U:H2'	1:A:741:G:C8	2.53	0.43
1:A:838:C:H2'	1:A:839:U:O4'	2.19	0.43
1:A:1889:A:H2'	1:A:1890:A:H8	1.76	0.43
1:A:993:G:O2'	17:V:89:GLN:HG3	2.19	0.43
1:A:848:G:H2'	1:A:849:A:H8	1.82	0.43
1:A:1278:A:H2'	1:A:1279:G:C8	2.53	0.43
13:R:81:ASP:N	13:R:81:ASP:OD1	2.49	0.43
1:A:2660:A:C6	1:A:2661:G:C6	3.07	0.43
19:X:35:THR:HG22	19:X:38:GLU:OE1	2.18	0.43
9:N:38:HIS:O	16:U:67:ALA:HB1	2.18	0.43
14:S:39:ILE:HA	14:S:39:ILE:HD13	1.80	0.43
1:A:2666:C:H6	1:A:2666:C:O5'	2.01	0.43
22:0:24:LYS:O	22:0:25:ARG:HD3	2.18	0.43
5:F:33:LEU:O	5:F:37:VAL:HG23	2.19	0.43
1:A:1122:G:H2'	1:A:1122:G:N3	2.34	0.43
1:A:715:G:H2'	1:A:716:A:O4'	2.18	0.43
1:A:1462:C:H4'	1:A:2703:C:H5'	2.00	0.43
3:D:97:TYR:HB2	3:D:101:GLU:O	2.19	0.43
1:A:2684:U:H2'	1:A:2685:G:O4'	2.19	0.43
8:I:6:LEU:HG	8:I:36:ALA:HA	2.01	0.43
2:B:33:G:C2	2:B:50:G:C2	3.07	0.43
1:A:2206:G:O2'	1:A:2207:G:OP1	2.34	0.43
11:P:3:LEU:HD12	11:P:3:LEU:N	2.33	0.43
1:A:1169:G:N2	1:A:1181:C:C2	2.87	0.43
1:A:234:C:H2'	1:A:235:U:H6	1.84	0.43
5:F:158:THR:HG21	5:F:163:VAL:CG1	2.49	0.43
22:0:48:GLY:H	22:0:51:VAL:HB	1.83	0.43
1:A:614(C):A:C4	5:F:180:GLY:HA2	2.54	0.43
20:Y:9:LYS:HA	20:Y:10:GLY:HA2	1.76	0.43
1:A:1815:A:C6	1:A:1817:G:C6	3.06	0.43
11:P:25:SER:OG	11:P:26:GLY:N	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1165:U:H2'	1:A:1166:C:C6	2.54	0.43
8:I:9:LEU:HB3	8:I:12:LEU:HB2	2.01	0.43
13:R:28:LEU:O	13:R:28:LEU:HD22	2.19	0.43
23:1:72:GLU:O	23:1:72:GLU:HG2	2.19	0.43
4:E:103:ASP:OD1	4:E:168:MET:HG3	2.19	0.43
31:9:9:ARG:HB3	31:9:14:CYS:HB2	2.01	0.43
1:A:1889:A:N1	1:A:2234:G:H1'	2.33	0.42
5:F:32:LEU:HD22	5:F:112:MET:HE1	2.00	0.42
1:A:1223:G:OP2	17:V:66:ARG:NH1	2.52	0.42
1:A:2872:G:C2'	1:A:2873:A:H5'	2.49	0.42
19:X:29:TRP:CE3	19:X:78:LYS:HB3	2.54	0.42
1:A:2502:G:H5''	1:A:2503:A:H5''	2.01	0.42
9:N:94:HIS:O	9:N:97:ARG:HB2	2.19	0.42
9:N:46:VAL:O	9:N:47:ALA:HB3	2.19	0.42
4:E:6:GLY:HA2	4:E:51:PHE:CZ	2.54	0.42
1:A:2016:U:H1'	27:5:6:VAL:HG13	2.00	0.42
11:P:50:ARG:HG2	11:P:51:PHE:N	2.33	0.42
13:R:38:VAL:HB	13:R:39:PRO:HD3	2.00	0.42
6:G:173:LEU:HD13	6:G:178:PHE:CD2	2.54	0.42
5:F:123:LEU:HD12	5:F:124:LEU:H	1.84	0.42
25:3:7:LYS:HG3	25:3:34:GLU:HG2	2.01	0.42
1:A:271(O):C:C4	1:A:271(P):C:C4	3.08	0.42
1:A:2207:G:O2'	1:A:2208:A:OP1	2.33	0.42
14:S:102:ALA:HA	14:S:105:ALA:N	2.22	0.42
1:A:1530:C:HO2'	1:A:1531:C:P	2.35	0.42
9:N:67:LEU:O	9:N:88:GLU:HG3	2.19	0.42
1:A:322:A:H3'	5:F:169:ASN:OD1	2.19	0.42
1:A:2183:C:H2'	1:A:2184:G:H8	1.79	0.42
1:A:722:A:H2'	1:A:723:G:C8	2.54	0.42
2:B:20:C:N4	2:B:63:G:H1	2.16	0.42
4:E:35:GLN:HG3	4:E:36:ARG:N	2.34	0.42
12:Q:21:THR:CG2	12:Q:101:ARG:HB2	2.47	0.42
1:A:977:G:C2	1:A:978:G:C8	3.07	0.42
1:A:1138:G:O2'	9:N:105:GLY:HA3	2.19	0.42
5:F:123:LEU:HD12	5:F:124:LEU:N	2.34	0.42
22:0:21:LEU:HD23	22:0:21:LEU:HA	1.87	0.42
16:U:65:ILE:HG13	16:U:96:ALA:HB2	2.01	0.42
9:N:82:LEU:HD23	9:N:84:LYS:HZ2	1.84	0.42
1:A:1388:G:H2'	1:A:1389:G:H8	1.84	0.42
1:A:31:C:N4	34:A:4010:HOH:O	2.52	0.42
1:A:1371:G:O6	34:A:4128:HOH:O	2.21	0.42
1:A:298:G:H5''	1:A:299:A:OP1	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:57:ASP:O	7:H:62:LYS:HE2	2.19	0.42
5:F:36:VAL:HG11	5:F:183:VAL:HG11	2.01	0.42
1:A:561:G:H1'	16:U:45:TYR:CE2	2.54	0.42
20:Y:20:TYR:N	20:Y:20:TYR:CD1	2.86	0.42
14:S:88:ASP:OD1	14:S:88:ASP:C	2.58	0.42
15:T:23:ARG:HG3	15:T:120:ARG:CZ	2.49	0.42
5:F:53:THR:HG23	5:F:55:GLY:H	1.83	0.42
1:A:195:A:H5''	1:A:196:A:O5'	2.18	0.42
11:P:26:GLY:HA3	11:P:27:HIS:HB2	2.02	0.42
23:1:58:ILE:HD11	23:1:60:PHE:CE2	2.54	0.42
9:N:59:LYS:HD3	9:N:59:LYS:HA	1.85	0.42
1:A:2292:C:H4'	1:A:2375:G:H4'	2.01	0.42
1:A:543:C:C2	1:A:551:G:N2	2.87	0.42
1:A:1359:A:N1	1:A:1372:U:O4	2.52	0.42
1:A:1952:A:OP1	10:O:44:LYS:HE2	2.19	0.42
1:A:926:A:C8	34:A:4215:HOH:O	2.71	0.42
1:A:2311:A:H3'	1:A:2312:U:C6	2.54	0.42
1:A:1654:A:C1'	1:A:2823:A:H5'	2.48	0.42
8:I:128:LEU:HD12	8:I:142:VAL:HG21	2.02	0.42
1:A:2324:C:H5''	1:A:2325:G:C5'	2.49	0.42
1:A:902:C:H2'	1:A:903:C:C6	2.54	0.42
1:A:902:C:H2'	1:A:903:C:H6	1.84	0.42
2:B:11:C:OP2	2:B:12:C:H5	2.03	0.42
7:H:12:PRO:O	7:H:15:VAL:HG12	2.20	0.42
28:6:25:LYS:HE3	28:6:30:THR:O	2.18	0.42
1:A:204:A:OP1	1:A:204:A:H8	2.01	0.42
1:A:2340:G:H2'	1:A:2341:G:H8	1.84	0.42
17:V:8:GLY:O	17:V:10:LYS:HE2	2.20	0.42
25:3:21:ALA:O	25:3:24:LYS:N	2.50	0.42
9:N:14:VAL:HG13	9:N:138:LEU:HB2	2.00	0.42
1:A:2546:U:H4'	1:A:2566:A:H2	1.84	0.42
5:F:150:GLY:HA2	5:F:172:TRP:CE3	2.54	0.42
1:A:438:G:H2'	1:A:440:G:H8	1.85	0.42
2:B:31:C:O2'	2:B:32:C:H5'	2.19	0.42
2:B:32:C:C2	2:B:51:G:N2	2.87	0.42
11:P:45:LEU:HA	11:P:45:LEU:HD23	1.56	0.42
9:N:37:LYS:HA	9:N:42:TRP:CD1	2.55	0.42
2:B:110:G:H2'	2:B:111:G:C8	2.54	0.42
1:A:1404:C:N3	1:A:1405:U:C5	2.88	0.42
15:T:80:SER:HA	15:T:81:PRO:HD2	1.81	0.42
15:T:117:ASP:OD2	15:T:120:ARG:NE	2.52	0.42
1:A:221:A:C4	1:A:266:G:N7	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:560:C:O2	16:U:49:HIS:NE2	2.52	0.42
7:H:52:VAL:O	7:H:65:HIS:NE2	2.48	0.42
1:A:2543:G:C1'	1:A:2766:G:H5'	2.50	0.42
1:A:524:U:H2'	1:A:525:U:C6	2.55	0.42
1:A:1023:U:O2'	1:A:1122:G:H5'	2.20	0.42
11:P:68:GLN:OE1	11:P:68:GLN:HA	2.19	0.42
8:I:7:GLU:HB3	8:I:8:PRO:HD2	2.01	0.42
1:A:2749:A:H1'	7:H:63:SER:HB3	2.02	0.42
1:A:1678:G:H2'	1:A:1679:U:H5'	2.01	0.42
3:D:179:SER:O	3:D:275:LYS:HD3	2.19	0.42
1:A:271(Q):G:O2'	1:A:271(R):G:P	2.78	0.42
3:D:206:LEU:HD23	3:D:206:LEU:HA	1.43	0.42
1:A:862:G:H2'	1:A:863:A:O4'	2.19	0.42
1:A:925:C:H2'	1:A:926:A:O4'	2.20	0.42
12:Q:41:TRP:HB3	12:Q:94:VAL:HB	2.00	0.42
1:A:1900:A:N1	1:A:1970:A:C6	2.87	0.42
1:A:2303:G:H2'	1:A:2304:G:H8	1.84	0.42
1:A:2303:G:O2'	1:A:2304:G:H5'	2.19	0.42
1:A:2328:A:H2'	1:A:2329:G:C8	2.54	0.42
11:P:100:LEU:HA	11:P:100:LEU:HD23	1.70	0.42
1:A:1688:U:H1'	1:A:1701:A:C6	2.55	0.42
1:A:271(U):G:H2'	1:A:271(V):G:C8	2.50	0.42
25:3:8:LEU:HD13	25:3:31:LEU:CD2	2.50	0.42
16:U:72:HIS:HE2	16:U:107:ALA:CB	2.32	0.42
4:E:179:GLU:HB3	4:E:181:LEU:CD2	2.50	0.42
6:G:178:PHE:HA	6:G:179:PRO:HD3	1.73	0.42
10:O:29:ASN:OD1	10:O:29:ASN:N	2.52	0.42
1:A:104:U:O5'	1:A:104:U:H6	2.02	0.42
14:S:76:LYS:O	14:S:80:LEU:HD13	2.19	0.42
6:G:86:MET:HA	6:G:87:PRO:HD3	1.78	0.42
1:A:757:U:H2'	1:A:758:C:O4'	2.20	0.42
1:A:1195:G:N7	11:P:15:ARG:NH1	2.68	0.42
7:H:3:ARG:HH11	7:H:3:ARG:HG3	1.84	0.42
14:S:96:GLY:N	14:S:99:LYS:HB3	2.34	0.42
5:F:184:TYR:O	5:F:187:VAL:N	2.53	0.42
1:A:2815:C:H2'	1:A:2816:C:C6	2.55	0.42
1:A:1204:A:H61	1:A:1240:U:H2'	1.84	0.42
11:P:83:VAL:HG21	11:P:100:LEU:HD11	2.01	0.42
1:A:90:U:HO2'	1:A:92:A:H8	1.59	0.42
1:A:990:A:H1'	1:A:1156:A:N3	2.35	0.42
1:A:2464:C:C2	1:A:2487:G:N2	2.87	0.42
6:G:73:ALA:HA	6:G:88:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1827:C:H2'	1:A:1828:G:O4'	2.18	0.42
4:E:200:GLU:HG3	4:E:201:THR:N	2.34	0.42
1:A:29:U:H2'	1:A:30:G:C8	2.54	0.42
9:N:96:GLU:HB2	9:N:122:VAL:HG12	2.02	0.42
3:D:44:ASN:OD1	3:D:46:GLN:HG3	2.20	0.42
2:B:104:U:OP2	34:B:317:HOH:O	2.21	0.42
11:P:101:VAL:HA	11:P:106:LEU:O	2.20	0.42
1:A:2342:C:O2'	1:A:2374:C:H5''	2.19	0.42
1:A:2057:A:H2'	1:A:2058:A:O4'	2.19	0.42
1:A:764:A:O4'	3:D:213:ARG:HG3	2.20	0.42
1:A:885:C:N4	1:A:890:A:C6	2.47	0.42
3:D:274:ARG:CB	3:D:275:LYS:HB3	2.49	0.42
24:2:48:HIS:O	24:2:52:ASP:HB2	2.19	0.42
1:A:990:A:C6	1:A:1186:G:H1'	2.55	0.42
3:D:108:PRO:HB3	3:D:143:HIS:HE1	1.82	0.42
1:A:66:C:H2'	1:A:67:U:C6	2.52	0.42
1:A:2320:A:H1'	1:A:2321:G:C6	2.55	0.42
1:A:1011:G:C4	1:A:1151:G:N2	2.88	0.42
28:6:33:LYS:HE3	28:6:51:GLU:HG2	2.01	0.42
1:A:2742:C:OP1	31:9:35:ARG:HD3	2.20	0.42
1:A:469:G:H2'	1:A:470:A:H5''	2.00	0.42
9:N:55:VAL:CG2	9:N:126:PRO:HA	2.50	0.42
6:G:129:GLY:O	6:G:161:THR:HB	2.19	0.42
1:A:1528:A:C6	1:A:1528(A):A:C6	3.08	0.42
1:A:2577:A:H5''	1:A:2578:G:C5'	2.48	0.42
1:A:2816:C:O2	1:A:2883:A:O2'	2.38	0.42
1:A:1614:A:C2	18:W:93:ALA:HB2	2.55	0.42
1:A:2279:G:O6	22:0:14:ARG:HG3	2.20	0.42
21:Z:129:SER:O	21:Z:133:ILE:HG23	2.19	0.42
21:Z:159:PRO:HA	21:Z:160:GLY:HA2	1.82	0.42
4:E:13:ARG:O	15:T:57:PHE:HE1	2.03	0.42
7:H:149:ARG:HA	7:H:162:ILE:CG2	2.50	0.42
6:G:107:LEU:HD13	6:G:177:GLY:O	2.20	0.42
1:A:2522:U:O2'	1:A:2647:U:OP1	2.20	0.42
21:Z:28:MET:O	21:Z:35:ARG:N	2.45	0.42
21:Z:166:SER:HA	21:Z:167:PRO:HD3	1.80	0.42
1:A:2400:G:C5	1:A:2401:U:C5	3.08	0.42
1:A:2401:U:H3'	1:A:2402:C:H6	1.85	0.42
24:2:45:SER:O	24:2:46:GLN:CB	2.68	0.42
5:F:107:LYS:HE2	5:F:205:ARG:O	2.19	0.42
13:R:37:THR:HA	13:R:111:LEU:HD12	2.02	0.42
1:A:2355:C:O3'	22:0:24:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:1:61:ARG:HE	23:1:61:ARG:HB3	1.65	0.42
1:A:545:G:OP1	1:A:545:G:H4'	2.20	0.42
18:W:43:GLY:O	18:W:47:VAL:HG23	2.20	0.42
1:A:2010:G:H5''	18:W:42:ARG:HB2	2.02	0.42
21:Z:10:ARG:NE	21:Z:37:VAL:O	2.50	0.42
27:5:46:CYS:CB	27:5:49:CYS:SG	3.02	0.42
4:E:134:ILE:O	4:E:137:HIS:HB2	2.20	0.42
14:S:21:THR:HG23	14:S:23:ARG:HB2	2.02	0.42
1:A:1639:U:H4'	1:A:2699:C:H4'	2.02	0.42
1:A:1469:A:H2'	1:A:1470:G:O4'	2.19	0.42
1:A:2557:G:H2'	1:A:2558:C:H6	1.84	0.42
1:A:2262:U:H2'	1:A:2263:C:H6	1.85	0.42
1:A:2080:G:C2'	1:A:2081:C:H5'	2.50	0.42
1:A:1788:C:H2'	1:A:1789:A:O4'	2.19	0.42
1:A:52:A:OP2	1:A:117:G:N1	2.41	0.42
1:A:1579:A:H5'	1:A:1579:A:H8	1.84	0.42
3:D:52:ARG:HB2	3:D:53:PHE:CE2	2.55	0.42
6:G:120:LEU:HB2	6:G:180:PHE:CD2	2.55	0.42
8:I:79:ILE:HG22	8:I:81:VAL:HG13	2.00	0.42
1:A:1033:U:OP1	31:9:9:ARG:NH2	2.52	0.42
9:N:133:GLN:HG2	9:N:133:GLN:H	1.59	0.42
4:E:94:GLU:HA	4:E:94:GLU:OE1	2.20	0.42
13:R:11:ASN:ND2	34:R:304:HOH:O	2.42	0.42
22:0:39:ARG:HD3	22:0:58:THR:OG1	2.20	0.42
22:0:84:LEU:HG	22:0:85:ALA:H	1.85	0.42
18:W:1:MET:HG3	18:W:2:GLU:N	2.35	0.42
1:A:2288:A:H4'	1:A:2289:G:OP2	2.20	0.42
19:X:40:LYS:HG3	19:X:51:VAL:HB	2.02	0.42
1:A:676:A:H2	1:A:802:A:H61	1.68	0.41
1:A:134:C:N4	1:A:145:G:H1	2.12	0.41
5:F:40:GLN:OE1	5:F:183:VAL:HG13	2.20	0.41
13:R:48:VAL:O	13:R:51:LEU:HB2	2.19	0.41
1:A:2820:A:P	13:R:2:ARG:HH21	2.43	0.41
20:Y:40:GLU:O	20:Y:42:VAL:HG23	2.20	0.41
15:T:26:ASP:CG	15:T:120:ARG:HH22	2.23	0.41
1:A:1223:G:C6	1:A:1227:G:C6	3.07	0.41
1:A:977:G:C4	1:A:978:G:C8	3.07	0.41
1:A:2463:C:O2'	1:A:2464:C:H5'	2.20	0.41
10:O:122:LEU:HD23	10:O:122:LEU:HA	1.54	0.41
1:A:1296:G:O2'	1:A:1297:C:H5'	2.20	0.41
8:I:25:TYR:HD2	8:I:25:TYR:HA	1.68	0.41
16:U:112:ARG:O	16:U:115:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1525:G:C2	1:A:1526:G:C4	3.08	0.41
1:A:2236:C:H2'	1:A:2237:G:H5'	2.01	0.41
1:A:1798:U:OP2	3:D:274:ARG:NH2	2.53	0.41
1:A:910:A:N3	1:A:2264:C:O2'	2.47	0.41
1:A:805:G:H4'	11:P:38:GLN:HB3	2.02	0.41
1:A:192:C:H2'	1:A:193:U:H5'	2.01	0.41
25:3:28:LEU:HD21	25:3:35:ARG:HB2	2.02	0.41
19:X:31:HIS:O	19:X:34:ALA:HB3	2.20	0.41
1:A:320:A:H4'	1:A:322:A:C8	2.55	0.41
3:D:240:ALA:HB1	3:D:241:PRO:HD2	2.02	0.41
15:T:33:LYS:HE3	15:T:82:LEU:HA	2.03	0.41
1:A:977:G:N3	1:A:978:G:C8	2.88	0.41
23:1:64:ALA:HA	23:1:67:ILE:HD12	2.02	0.41
21:Z:99:TYR:HA	21:Z:124:ILE:O	2.20	0.41
1:A:1025:G:C4	1:A:1135:C:H1'	2.55	0.41
23:1:86:SER:O	23:1:89:GLU:HG2	2.20	0.41
1:A:686:G:N7	29:7:5:TRP:CH2	2.88	0.41
3:D:77:ALA:O	3:D:116:GLN:HG3	2.21	0.41
1:A:2730:C:H4'	4:E:168:MET:O	2.20	0.41
5:F:124:LEU:HB3	5:F:193:VAL:HG22	2.02	0.41
13:R:12:ARG:HD3	13:R:16:HIS:CD2	2.55	0.41
13:R:42:LYS:HG2	13:R:45:ARG:NH2	2.34	0.41
1:A:1168:G:C2	1:A:1182:A:C2	3.08	0.41
1:A:1643:G:H2'	1:A:1644:C:H6	1.85	0.41
23:1:40:ARG:HB2	23:1:40:ARG:HE	1.59	0.41
14:S:110:LEU:HD12	14:S:110:LEU:HA	1.71	0.41
2:B:46:A:C5	2:B:47:C:C4	3.08	0.41
25:3:23:LEU:HD22	25:3:50:VAL:HG11	2.02	0.41
22:0:65:GLY:CA	22:0:81:VAL:HG12	2.47	0.41
16:U:62:ILE:HG12	16:U:76:TYR:CE1	2.56	0.41
8:I:120:ILE:HG21	8:I:126:TYR:CE1	2.56	0.41
1:A:1328:G:H2'	1:A:1330:C:C5	2.55	0.41
1:A:1915:U:H5'	1:A:1916:A:OP2	2.20	0.41
1:A:873:G:N2	1:A:905:U:C2	2.89	0.41
1:A:1416:G:O2'	1:A:1417:C:H5	2.02	0.41
18:W:4:LYS:NZ	18:W:6:ILE:HD11	2.35	0.41
4:E:78:LEU:O	4:E:79:ARG:HG2	2.20	0.41
21:Z:8:TYR:HB2	21:Z:38:TYR:CE2	2.55	0.41
6:G:11:TYR:OH	6:G:16:ARG:HD3	2.21	0.41
2:B:55:U:H4'	6:G:28:VAL:HG13	2.02	0.41
1:A:548:A:N7	17:V:19:LYS:HD2	2.36	0.41
1:A:2445:G:OP1	5:F:74:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:28:ALA:HB3	4:E:93:VAL:HG13	2.02	0.41
1:A:2405:G:HO2'	1:A:2406:U:P	2.44	0.41
1:A:1580:A:H8	1:A:1580:A:OP2	2.04	0.41
12:Q:32:TYR:CE2	12:Q:133:ARG:CG	3.03	0.41
1:A:2470:G:C2	1:A:2471:C:C6	3.08	0.41
11:P:125:VAL:O	11:P:125:VAL:HG23	2.19	0.41
8:I:41:GLU:H	8:I:41:GLU:CD	2.24	0.41
1:A:839:U:H3	1:A:939:G:H1	1.68	0.41
15:T:61:PHE:CE2	15:T:76:PHE:HB2	2.55	0.41
11:P:93:GLY:O	11:P:123:LEU:HD22	2.20	0.41
1:A:836:G:C5	1:A:837:C:C4	3.08	0.41
21:Z:70:LEU:HA	21:Z:70:LEU:HD23	1.75	0.41
6:G:16:ARG:HA	6:G:16:ARG:HD2	1.75	0.41
8:I:104:GLN:HG2	8:I:105:HIS:CE1	2.55	0.41
1:A:249:C:O2	30:8:12:LYS:NZ	2.43	0.41
9:N:27:ALA:HA	9:N:30:ILE:HD12	2.02	0.41
1:A:863:A:O2'	1:A:864:G:H5'	2.20	0.41
7:H:44:VAL:HB	7:H:51:ARG:O	2.21	0.41
21:Z:156:LYS:HE3	21:Z:156:LYS:HB3	1.88	0.41
5:F:34:TRP:CE3	5:F:35:GLU:HG2	2.56	0.41
1:A:1431:U:H2'	1:A:1432:C:C6	2.56	0.41
1:A:1224:C:H6	1:A:1224:C:O5'	2.03	0.41
9:N:93:THR:HB	9:N:94:HIS:ND1	2.35	0.41
10:O:97:ARG:HA	10:O:117:LEU:HD22	2.02	0.41
1:A:686:G:H21	1:A:788:A:H61	1.67	0.41
26:4:40:HIS:HB3	26:4:43:TYR:CD1	2.55	0.41
1:A:1778:U:H2'	1:A:1784:A:N6	2.36	0.41
1:A:1462:C:H2'	1:A:1463:C:O4'	2.21	0.41
1:A:271(E):U:H3	1:A:271(S):G:H1	1.69	0.41
1:A:1210:A:H5''	1:A:1212:G:C5'	2.49	0.41
9:N:58:ASP:OD1	9:N:124:ALA:HA	2.20	0.41
1:A:2041:U:H2'	1:A:2042:A:C8	2.55	0.41
4:E:36:ARG:HG2	4:E:47:VAL:HG22	2.02	0.41
1:A:2505:G:O2'	1:A:2506:U:H5''	2.21	0.41
1:A:57:C:O5'	1:A:57:C:H6	2.04	0.41
1:A:1796:U:H4'	3:D:256:GLY:N	2.34	0.41
2:B:76:G:H2'	2:B:77:U:O4'	2.20	0.41
26:4:42:PHE:HB3	26:4:43:TYR:HB2	2.02	0.41
1:A:2236:C:C2'	1:A:2237:G:H5'	2.51	0.41
3:D:37:LEU:HD12	3:D:37:LEU:HA	1.71	0.41
2:B:80:U:H2'	2:B:81:G:C8	2.56	0.41
17:V:62:LEU:HD11	17:V:95:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:629:G:H1'	1:A:639:U:O2'	2.20	0.41
17:V:89:GLN:HA	17:V:90:PRO:HD2	1.79	0.41
9:N:128:HIS:O	9:N:128:HIS:CG	2.73	0.41
30:8:33:ASN:HA	30:8:36:LYS:HG3	2.02	0.41
25:3:4:LEU:HD22	25:3:56:VAL:HG11	2.02	0.41
17:V:21:ARG:HD2	17:V:93:GLU:HG3	2.03	0.41
1:A:1296:G:H2'	1:A:1297:C:H6	1.86	0.41
1:A:2363:C:O2	22:0:39:ARG:NH2	2.46	0.41
12:Q:58:PHE:CD2	12:Q:58:PHE:N	2.88	0.41
1:A:315:G:H2'	1:A:316:C:O4'	2.20	0.41
8:I:98:ALA:CB	8:I:111:PRO:HG3	2.51	0.41
20:Y:30:VAL:HG22	20:Y:37:VAL:HG12	2.03	0.41
1:A:1452:A:O2'	1:A:2702:U:O4	2.28	0.41
1:A:847:U:C3'	1:A:848:G:H5'	2.51	0.41
1:A:528:A:H8	1:A:528:A:H3'	1.84	0.41
1:A:2689:U:H4'	1:A:2690:C:H5'	2.02	0.41
21:Z:128:VAL:HG22	21:Z:132:ASN:O	2.21	0.41
1:A:2834:G:C5	1:A:2879:C:C4	3.09	0.41
1:A:2345:G:N3	1:A:2381:C:H2'	2.36	0.41
1:A:1341:U:OP2	1:A:1394:U:O2'	2.23	0.41
1:A:1163:G:C2	1:A:1164:G:C8	3.09	0.41
1:A:870:A:C2	1:A:908:C:C2	3.09	0.41
3:D:44:ASN:ND2	3:D:46:GLN:HG3	2.36	0.41
27:5:46:CYS:HB3	27:5:49:CYS:SG	2.61	0.41
1:A:2619:C:H4'	4:E:151:TYR:O	2.20	0.41
14:S:32:LEU:HA	14:S:32:LEU:HD23	1.83	0.41
13:R:60:LEU:HD23	13:R:60:LEU:HA	1.67	0.41
6:G:41:GLN:NE2	6:G:153:ARG:HG2	2.36	0.41
1:A:1991:U:H2'	1:A:1992:G:H5''	2.02	0.41
10:O:45:GLU:HG2	10:O:46:ALA:N	2.36	0.41
13:R:55:ALA:HA	13:R:80:PHE:CE1	2.56	0.41
1:A:746:A:H2'	1:A:2612:C:H5''	2.02	0.41
6:G:60:LEU:HD12	6:G:68:PRO:HG3	2.01	0.41
9:N:34:LEU:HD12	9:N:34:LEU:HA	1.66	0.41
1:A:862:G:H4'	2:B:79:C:H5'	2.03	0.41
10:O:44:LYS:HA	10:O:44:LYS:HD2	1.92	0.41
1:A:781:A:C2	1:A:1776:G:H2'	2.56	0.41
1:A:856:C:O4'	22:0:27:GLU:HB3	2.21	0.41
26:4:15:ILE:O	26:4:33:VAL:HG23	2.20	0.41
22:0:19:LYS:HG2	22:0:41:ARG:HH21	1.86	0.41
1:A:2261:C:O2'	1:A:2262:U:H5'	2.21	0.41
1:A:2705:A:H2	13:R:64:ARG:HH11	1.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1278:A:H5''	13:R:36:THR:HG22	2.03	0.41
1:A:1183:G:H4'	25:3:29:ARG:HH12	1.86	0.41
1:A:1506:C:C2'	1:A:1507:A:H5'	2.51	0.41
10:O:79:PHE:CD2	15:T:72:VAL:HG22	2.56	0.41
3:D:77:ALA:HA	3:D:97:TYR:HA	2.03	0.41
11:P:101:VAL:O	11:P:104:GLY:N	2.38	0.41
9:N:55:VAL:CG1	9:N:126:PRO:HA	2.50	0.41
1:A:254:G:N7	30:8:5:LYS:HE2	2.35	0.41
1:A:1629:U:H2'	1:A:1630:G:O4'	2.20	0.41
12:Q:72:LYS:HA	12:Q:73:PRO:HD3	1.90	0.41
6:G:114:ILE:HB	6:G:117:PHE:HB2	2.02	0.41
30:8:39:LYS:O	30:8:43:GLN:HG3	2.21	0.41
8:I:61:ARG:C	8:I:63:ALA:N	2.74	0.41
1:A:2552:U:H2'	1:A:2554:U:OP2	2.21	0.41
5:F:116:ASP:OD2	11:P:1:MET:HB2	2.21	0.41
1:A:1751:C:O4'	1:A:2860:A:C2	2.74	0.41
7:H:20:ALA:HB1	7:H:21:PRO:CD	2.51	0.41
1:A:1344:G:O2'	1:A:1385:G:H2'	2.21	0.41
1:A:1252:G:C4	16:U:33:ARG:HD2	2.56	0.41
1:A:1355:G:N2	1:A:1376:C:O2	2.48	0.41
1:A:2398:U:O2'	1:A:2399:G:H5'	2.22	0.41
1:A:28:A:C2'	1:A:29:U:H5'	2.51	0.41
5:F:181:LEU:CD1	5:F:186:ILE:HD11	2.51	0.41
24:2:10:LEU:HD22	24:2:14:ARG:NH1	2.36	0.41
21:Z:38:TYR:HD1	21:Z:39:VAL:O	2.04	0.41
1:A:2531:A:H5'	7:H:157:TYR:CE1	2.56	0.41
1:A:2817:G:C4	1:A:2830:G:N2	2.89	0.41
21:Z:16:SER:O	21:Z:20:ARG:HB2	2.21	0.41
3:D:10:THR:HG23	3:D:13:ARG:HB2	2.03	0.41
1:A:1365:A:N6	1:A:1366:A:C6	2.89	0.40
1:A:864:G:H1'	1:A:914:C:N4	2.36	0.40
1:A:1528(A):A:C8	1:A:1529:G:C8	3.09	0.40
11:P:143:GLY:C	11:P:145:PRO:HD3	2.42	0.40
1:A:297:C:H2'	1:A:298:G:O4'	2.21	0.40
1:A:2577:A:O4'	27:5:3:LYS:HB2	2.21	0.40
21:Z:48:PHE:CE2	21:Z:71:VAL:HG11	2.52	0.40
1:A:2699:C:H2'	1:A:2700:C:O4'	2.21	0.40
1:A:1149:G:C2	1:A:1150:C:C4	3.09	0.40
1:A:2056:G:O2'	27:5:8:LYS:HD2	2.20	0.40
11:P:84:ASN:HB3	11:P:117:GLU:O	2.20	0.40
1:A:2329:G:H2'	1:A:2330:G:C8	2.55	0.40
1:A:1031:G:O2'	31:9:7:VAL:N	2.45	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:769:G:C2'	1:A:770:G:H5'	2.51	0.40
1:A:1945:G:C4	1:A:1946:U:C5	3.09	0.40
1:A:1792:G:H2'	1:A:1793:C:C6	2.56	0.40
1:A:872:A:OP1	12:Q:5:ARG:NH1	2.54	0.40
1:A:237:C:N3	1:A:261:G:C2	2.89	0.40
5:F:181:LEU:HD11	5:F:186:ILE:HD11	2.03	0.40
11:P:101:VAL:HG12	11:P:102:ARG:N	2.36	0.40
1:A:2510:C:H2'	1:A:2511:U:C6	2.56	0.40
19:X:2:LYS:HD2	19:X:2:LYS:HA	1.85	0.40
1:A:2740:A:C6	1:A:2764:A:C8	3.09	0.40
1:A:2296:U:H4'	1:A:2297:C:OP1	2.20	0.40
1:A:1002:G:H2'	1:A:1003:G:O4'	2.21	0.40
1:A:1153:C:OP1	16:U:92:ARG:NH1	2.55	0.40
30:8:54:GLU:HA	30:8:57:ARG:HD2	2.03	0.40
1:A:2448:A:N6	34:A:3944:HOH:O	2.54	0.40
21:Z:29:TYR:CE2	21:Z:87:ASP:HB3	2.57	0.40
4:E:4:ILE:C	4:E:5:LEU:HD23	2.42	0.40
2:B:6:C:H2'	2:B:7:G:O4'	2.21	0.40
1:A:196:A:H2'	1:A:196:A:N3	2.37	0.40
9:N:19:GLU:CG	9:N:20:GLY:H	2.34	0.40
1:A:307:G:H22	1:A:310:A:P	2.44	0.40
1:A:817:C:H2'	1:A:818:G:O4'	2.20	0.40
1:A:1131:G:H4'	9:N:82:LEU:HB2	2.03	0.40
1:A:1416:G:O2'	1:A:1417:C:C5	2.74	0.40
1:A:1418:G:O5'	1:A:1418:G:H8	2.05	0.40
1:A:346:A:N3	1:A:346:A:H2'	2.36	0.40
6:G:103:LEU:HD23	6:G:103:LEU:HA	1.82	0.40
3:D:25:THR:OG1	3:D:81:ALA:HB1	2.21	0.40
1:A:1511:C:H2'	1:A:1512:U:H6	1.85	0.40
1:A:2731:G:C6	1:A:2732:G:O6	2.74	0.40
29:7:36:GLN:O	29:7:36:GLN:HG2	2.21	0.40
3:D:274:ARG:CA	3:D:275:LYS:HB3	2.52	0.40
30:8:57:ARG:O	30:8:58:ILE:C	2.60	0.40
4:E:49:LEU:HA	4:E:49:LEU:HD12	1.72	0.40
15:T:121:ILE:HG22	15:T:122:ASP:N	2.36	0.40
3:D:75:ILE:HG21	3:D:99:ASP:HB2	2.03	0.40
1:A:2697:G:H2'	1:A:2698:U:O4'	2.21	0.40
2:B:95:C:H2'	2:B:96:U:C6	2.56	0.40
1:A:108:U:H2'	1:A:109:G:C8	2.56	0.40
6:G:122:PRO:HG3	6:G:180:PHE:HB3	2.04	0.40
16:U:55:ARG:HE	16:U:55:ARG:HB3	1.51	0.40
1:A:969:U:OP1	25:3:17:LYS:HB3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2652:C:H42	1:A:2668:G:H1	1.70	0.40
1:A:2291:U:H5''	1:A:2380:C:O2'	2.20	0.40
1:A:724:U:H2'	1:A:725:G:O4'	2.22	0.40
13:R:54:LEU:O	13:R:57:ARG:HB2	2.22	0.40
1:A:2769:C:H2'	1:A:2770:G:O4'	2.22	0.40
1:A:2687:U:H2'	1:A:2688:U:O4'	2.21	0.40
1:A:387:U:P	34:A:4616:HOH:O	2.79	0.40
1:A:2518:A:N3	1:A:2518:A:H2'	2.36	0.40
1:A:330:A:H2	1:A:1210:A:H2'	1.86	0.40
21:Z:57:ILE:HD13	21:Z:71:VAL:HG23	2.02	0.40
1:A:1319:G:O2'	1:A:1320:C:H5'	2.22	0.40
28:6:3:SER:N	28:6:6:ARG:HB3	2.31	0.40
2:B:19:G:N2	2:B:64:C:N3	2.63	0.40
18:W:100:THR:HG22	18:W:100:THR:O	2.22	0.40
1:A:2881:C:C4	1:A:2882:A:N7	2.90	0.40
9:N:39:ARG:NH2	9:N:41:ASP:OD2	2.54	0.40
3:D:148:GLU:OE1	3:D:151:LYS:NZ	2.53	0.40
1:A:1658:C:H2'	1:A:1659:U:C6	2.57	0.40
3:D:125:ILE:O	3:D:125:ILE:HG22	2.21	0.40
20:Y:67:LEU:HA	20:Y:67:LEU:HD22	1.88	0.40
8:I:132:PRO:HD3	8:I:138:ILE:HG13	2.04	0.40
1:A:2065:C:H2'	1:A:2066:C:C6	2.57	0.40
1:A:2298:A:H3'	1:A:2299:G:H8	1.85	0.40
1:A:1854:A:H2'	1:A:1855:G:O4'	2.21	0.40
1:A:271(P):C:C2'	1:A:271(Q):G:H5'	2.52	0.40
1:A:1721:G:O6	1:A:1739:U:H5''	2.21	0.40
1:A:2295:C:O2	1:A:2338:G:C2	2.74	0.40
7:H:9:ILE:HD11	7:H:69:ARG:HD2	2.03	0.40
23:1:83:GLU:HA	23:1:84:GLY:HA2	1.86	0.40
1:A:848:G:N9	1:A:933:A:C8	2.88	0.40
13:R:1:MET:HB3	13:R:2:ARG:H	1.54	0.40
1:A:288:C:O2	1:A:353:G:N2	2.29	0.40
8:I:116:LEU:HD11	8:I:120:ILE:HG13	2.02	0.40
2:B:14:U:H1'	2:B:108:U:O2'	2.21	0.40
21:Z:30:ASN:HB2	21:Z:89:PHE:CE2	2.56	0.40
1:A:1328:G:H2'	1:A:1330:C:C4	2.56	0.40
1:A:328:U:H4'	20:Y:68:HIS:NE2	2.36	0.40
1:A:2709:G:H2'	1:A:2710:C:C6	2.57	0.40
14:S:26:LEU:HD12	14:S:39:ILE:HD11	2.04	0.40
6:G:15:VAL:HG13	6:G:175:LEU:HB3	2.04	0.40
17:V:20:LEU:HA	17:V:20:LEU:HD12	1.84	0.40
1:A:872:A:C5	1:A:906:G:N2	2.90	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:60:ASN:OD1	4:E:62:PRO:HD2	2.22	0.40
1:A:704:G:N3	1:A:726:G:C2	2.90	0.40
3:D:228:PRO:HD3	3:D:235:GLY:CA	2.51	0.40
8:I:62:LYS:O	8:I:66:GLU:HB2	2.20	0.40
1:A:513:A:C2	1:A:514:A:C5	3.09	0.40
1:A:2091:U:O2'	23:1:47:GLN:HG3	2.22	0.40
1:A:2489:G:C6	1:A:2490:G:N1	2.90	0.40
1:A:68:G:H2'	1:A:69:C:O4'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	273/276 (99%)	255 (93%)	16 (6%)	2 (1%)	30	80
4	E	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	15	64
5	F	198/210 (94%)	175 (88%)	23 (12%)	0	100	100
6	G	178/182 (98%)	150 (84%)	28 (16%)	0	100	100
7	H	172/180 (96%)	153 (89%)	17 (10%)	2 (1%)	19	70
8	I	144/148 (97%)	119 (83%)	23 (16%)	2 (1%)	16	66
9	N	138/140 (99%)	117 (85%)	19 (14%)	2 (1%)	16	66
10	O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	P	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	16	66
12	Q	139/141 (99%)	121 (87%)	18 (13%)	0	100	100
13	R	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
14	S	108/112 (96%)	88 (82%)	18 (17%)	2 (2%)	12	59
15	T	128/146 (88%)	119 (93%)	9 (7%)	0	100	100
16	U	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
17	V	98/101 (97%)	89 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	W	109/113 (96%)	97 (89%)	12 (11%)	0	100	100
19	X	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
20	Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	22	74
21	Z	187/206 (91%)	163 (87%)	21 (11%)	3 (2%)	14	63
22	0	75/85 (88%)	67 (89%)	8 (11%)	0	100	100
23	1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	2	69/72 (96%)	60 (87%)	9 (13%)	0	100	100
25	3	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
26	4	44/71 (62%)	34 (77%)	9 (20%)	1 (2%)	10	52
27	5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	6	51/54 (94%)	45 (88%)	6 (12%)	0	100	100
29	7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	10	53
30	8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
31	9	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
All	All	3357/3526 (95%)	2996 (89%)	340 (10%)	21 (1%)	33	83

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	47	ALA
7	H	71	LEU
14	S	62	LYS
8	I	10	GLU
20	Y	2	ARG
3	D	3	VAL
3	D	275	LYS
7	H	92	ILE
8	I	107	VAL
9	N	129	PRO
11	P	53	GLY
14	S	63	THR
29	7	46	VAL
4	E	52	LEU
21	Z	128	VAL
21	Z	161	VAL
26	4	33	VAL
4	E	72	VAL

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Mol	Chain	Res	Type
21	Z	47	VAL
4	E	30	PRO
11	P	72	PRO

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%)	167 (78%)	48 (22%)	1	6
4	E	163/166 (98%)	128 (78%)	35 (22%)	1	7
5	F	159/166 (96%)	128 (80%)	31 (20%)	2	10
6	G	127/156 (81%)	95 (75%)	32 (25%)	1	3
7	H	141/148 (95%)	111 (79%)	30 (21%)	1	7
8	I	104/124 (84%)	76 (73%)	28 (27%)	1	2
9	N	117/119 (98%)	90 (77%)	27 (23%)	1	5
10	O	98/100 (98%)	70 (71%)	28 (29%)	0	1
11	P	114/116 (98%)	90 (79%)	24 (21%)	1	8
12	Q	111/111 (100%)	93 (84%)	18 (16%)	3	15
13	R	101/101 (100%)	79 (78%)	22 (22%)	1	7
14	S	86/88 (98%)	68 (79%)	18 (21%)	1	8
15	T	110/127 (87%)	82 (74%)	28 (26%)	1	3
16	U	93/94 (99%)	77 (83%)	16 (17%)	3	14
17	V	81/82 (99%)	56 (69%)	25 (31%)	0	1
18	W	89/92 (97%)	74 (83%)	15 (17%)	3	14
19	X	73/78 (94%)	61 (84%)	12 (16%)	3	15
20	Y	79/91 (87%)	59 (75%)	20 (25%)	1	3
21	Z	152/179 (85%)	119 (78%)	33 (22%)	1	7
22	0	61/67 (91%)	47 (77%)	14 (23%)	1	5
23	1	78/83 (94%)	58 (74%)	20 (26%)	1	2
24	2	63/67 (94%)	50 (79%)	13 (21%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	3	49/52 (94%)	40 (82%)	9 (18%)	2	11
26	4	39/63 (62%)	25 (64%)	14 (36%)	0	0
27	5	49/52 (94%)	39 (80%)	10 (20%)	2	8
28	6	48/52 (92%)	38 (79%)	10 (21%)	2	8
29	7	38/42 (90%)	30 (79%)	8 (21%)	1	8
30	8	52/55 (94%)	43 (83%)	9 (17%)	3	13
31	9	32/34 (94%)	25 (78%)	7 (22%)	1	7
All	All	2722/2923 (93%)	2118 (78%)	604 (22%)	1	6

All (604) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	3	VAL
3	D	4	LYS
3	D	10	THR
3	D	12	SER
3	D	27	THR
3	D	30	GLU
3	D	32	SER
3	D	46	GLN
3	D	58	HIS
3	D	61	LEU
3	D	64	ILE
3	D	71	ASP
3	D	72	LYS
3	D	73	VAL
3	D	94	LEU
3	D	103	ARG
3	D	105	ILE
3	D	106	ILE
3	D	111	LEU
3	D	112	GLN
3	D	113	VAL
3	D	126	GLN
3	D	127	VAL
3	D	131	LEU
3	D	136	ILE
3	D	138	VAL
3	D	147	LEU
3	D	150	LYS

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Mol	Chain	Res	Type
3	D	155	LEU
3	D	165	ILE
3	D	171	ASP
3	D	176	ARG
3	D	192	THR
3	D	200	ASP
3	D	202	LYS
3	D	211	ARG
3	D	215	LEU
3	D	218	ARG
3	D	229	VAL
3	D	239	ARG
3	D	242	ARG
3	D	257	LEU
3	D	259	THR
3	D	260	ARG
3	D	264	LYS
3	D	270	ILE
3	D	275	LYS
3	D	276	LYS
4	E	1	MET
4	E	5	LEU
4	E	9	VAL
4	E	11	MET
4	E	12	THR
4	E	21	VAL
4	E	24	THR
4	E	34	VAL
4	E	40	GLU
4	E	45	THR
4	E	49	LEU
4	E	52	LEU
4	E	63	LEU
4	E	72	VAL
4	E	75	VAL
4	E	77	ILE
4	E	79	ARG
4	E	82	ARG
4	E	84	PHE
4	E	89	ASP
4	E	92	THR
4	E	93	VAL

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Mol	Chain	Res	Type
4	E	113	PHE
4	E	116	VAL
4	E	119	ARG
4	E	121	ASN
4	E	144	ARG
4	E	149	ARG
4	E	154	LYS
4	E	168	MET
4	E	170	LEU
4	E	179	GLU
4	E	181	LEU
4	E	182	LEU
4	E	188	VAL
5	F	6	VAL
5	F	13	SER
5	F	18	ARG
5	F	23	ASP
5	F	24	LEU
5	F	33	LEU
5	F	43	LYS
5	F	68	LYS
5	F	74	ARG
5	F	78	ILE
5	F	82	ILE
5	F	98	SER
5	F	99	TYR
5	F	110	LEU
5	F	112	MET
5	F	126	VAL
5	F	140	LEU
5	F	149	ASP
5	F	158	THR
5	F	161	GLU
5	F	162	LEU
5	F	169	ASN
5	F	170	LEU
5	F	174	VAL
5	F	179	GLU
5	F	183	VAL
5	F	186	ILE
5	F	195	ASP
5	F	197	ASP

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Mol	Chain	Res	Type
5	F	200	GLU
5	F	201	VAL
6	G	9	ARG
6	G	12	TYR
6	G	13	GLU
6	G	14	GLU
6	G	18	GLU
6	G	21	ARG
6	G	33	ARG
6	G	34	LEU
6	G	39	ILE
6	G	60	LEU
6	G	63	ILE
6	G	80	PHE
6	G	88	ILE
6	G	91	ARG
6	G	101	ILE
6	G	116	ASP
6	G	128	ARG
6	G	130	ASN
6	G	133	LEU
6	G	135	LEU
6	G	138	GLN
6	G	139	LEU
6	G	140	ILE
6	G	148	MET
6	G	149	VAL
6	G	150	ASP
6	G	155	MET
6	G	162	THR
6	G	165	THR
6	G	167	GLU
6	G	170	ARG
6	G	173	LEU
7	H	3	ARG
7	H	7	LEU
7	H	15	VAL
7	H	17	VAL
7	H	32	GLU
7	H	41	MET
7	H	43	VAL
7	H	47	GLU

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Mol	Chain	Res	Type
7	H	59	ARG
7	H	63	SER
7	H	64	LEU
7	H	69	ARG
7	H	70	THR
7	H	97	ARG
7	H	104	GLU
7	H	105	LEU
7	H	121	ILE
7	H	124	GLU
7	H	127	GLU
7	H	129	THR
7	H	130	ARG
7	H	134	SER
7	H	136	ILE
7	H	140	LYS
7	H	148	ILE
7	H	153	LYS
7	H	158	HIS
7	H	167	GLU
7	H	169	VAL
7	H	171	LEU
8	I	1	MET
8	I	2	LYS
8	I	22	LYS
8	I	25	TYR
8	I	35	LEU
8	I	37	VAL
8	I	38	LEU
8	I	41	GLU
8	I	43	ASN
8	I	57	ARG
8	I	58	LEU
8	I	61	ARG
8	I	72	LEU
8	I	74	ASN
8	I	75	LEU
8	I	77	LEU
8	I	78	THR
8	I	85	GLU
8	I	86	THR
8	I	93	THR

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Mol	Chain	Res	Type
8	I	97	ILE
8	I	116	LEU
8	I	123	LEU
8	I	127	VAL
8	I	129	THR
8	I	138	ILE
8	I	140	LEU
8	I	142	VAL
9	N	1	MET
9	N	9	VAL
9	N	12	ARG
9	N	32	THR
9	N	33	LEU
9	N	34	LEU
9	N	37	LYS
9	N	38	HIS
9	N	43	THR
9	N	48	MET
9	N	55	VAL
9	N	58	ASP
9	N	60	ILE
9	N	61	ARG
9	N	62	VAL
9	N	83	LYS
9	N	87	LEU
9	N	93	THR
9	N	99	LEU
9	N	106	MET
9	N	119	ARG
9	N	120	LEU
9	N	127	ASP
9	N	133	GLN
9	N	137	LYS
9	N	138	LEU
9	N	140	VAL
10	O	7	TYR
10	O	8	LEU
10	O	10	VAL
10	O	17	ARG
10	O	23	ARG
10	O	24	VAL
10	O	28	SER

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Mol	Chain	Res	Type
10	O	32	TYR
10	O	39	ILE
10	O	44	LYS
10	O	47	ILE
10	O	58	VAL
10	O	59	LYS
10	O	62	VAL
10	O	66	LYS
10	O	69	ILE
10	O	73	ASP
10	O	75	SER
10	O	78	ARG
10	O	82	ASN
10	O	85	VAL
10	O	86	ILE
10	O	88	ASN
10	O	89	ASN
10	O	94	ARG
10	O	99	PHE
10	O	115	VAL
10	O	117	LEU
11	P	21	ARG
11	P	30	THR
11	P	39	LYS
11	P	42	SER
11	P	46	LYS
11	P	50	ARG
11	P	55	ARG
11	P	56	SER
11	P	58	THR
11	P	59	LEU
11	P	64	LYS
11	P	75	ILE
11	P	92	GLU
11	P	96	THR
11	P	100	LEU
11	P	106	LEU
11	P	111	ARG
11	P	112	LEU
11	P	119	GLU
11	P	133	SER
11	P	135	LEU

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Mol	Chain	Res	Type
11	P	139	LYS
11	P	144	GLU
11	P	146	VAL
12	Q	1	MET
12	Q	5	ARG
12	Q	6	ARG
12	Q	11	LYS
12	Q	16	ARG
12	Q	21	THR
12	Q	45	GLN
12	Q	54	MET
12	Q	55	VAL
12	Q	56	ARG
12	Q	60	ARG
12	Q	63	LYS
12	Q	79	LEU
12	Q	81	VAL
12	Q	90	VAL
12	Q	106	VAL
12	Q	110	THR
12	Q	112	GLU
13	R	6	SER
13	R	9	LYS
13	R	18	LEU
13	R	28	LEU
13	R	29	LEU
13	R	37	THR
13	R	44	LEU
13	R	45	ARG
13	R	54	LEU
13	R	60	LEU
13	R	65	LEU
13	R	73	VAL
13	R	75	LEU
13	R	79	LEU
13	R	81	ASP
13	R	86	ARG
13	R	97	VAL
13	R	100	LEU
13	R	102	GLU
13	R	104	ARG
13	R	111	LEU

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Mol	Chain	Res	Type
13	R	118	GLU
14	S	4	LEU
14	S	10	ARG
14	S	14	VAL
14	S	19	LYS
14	S	20	ARG
14	S	29	PHE
14	S	30	ARG
14	S	36	TYR
14	S	40	ILE
14	S	43	GLU
14	S	48	LEU
14	S	52	SER
14	S	64	GLU
14	S	78	LEU
14	S	83	LYS
14	S	98	VAL
14	S	101	LEU
14	S	110	LEU
15	T	6	LEU
15	T	21	GLU
15	T	23	ARG
15	T	27	THR
15	T	34	VAL
15	T	36	GLU
15	T	39	ARG
15	T	40	THR
15	T	51	ARG
15	T	54	ARG
15	T	58	ASN
15	T	59	THR
15	T	64	ARG
15	T	67	SER
15	T	73	GLU
15	T	74	ARG
15	T	85	LYS
15	T	89	VAL
15	T	90	GLN
15	T	93	ARG
15	T	95	ARG
15	T	96	ARG
15	T	105	LEU

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Mol	Chain	Res	Type
15	T	109	GLU
15	T	111	ARG
15	T	118	ARG
15	T	121	ILE
15	T	123	GLN
16	U	20	LEU
16	U	31	SER
16	U	36	ARG
16	U	51	LYS
16	U	55	ARG
16	U	58	ARG
16	U	59	ARG
16	U	63	VAL
16	U	72	HIS
16	U	74	LEU
16	U	83	LEU
16	U	88	ILE
16	U	90	VAL
16	U	100	VAL
16	U	104	GLN
16	U	108	GLU
17	V	6	LYS
17	V	10	LYS
17	V	12	TYR
17	V	13	ARG
17	V	14	VAL
17	V	18	LEU
17	V	21	ARG
17	V	28	GLU
17	V	32	THR
17	V	33	VAL
17	V	35	LEU
17	V	39	LEU
17	V	43	GLU
17	V	46	VAL
17	V	51	VAL
17	V	53	GLU
17	V	61	VAL
17	V	62	LEU
17	V	72	VAL
17	V	73	SER
17	V	79	VAL

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Mol	Chain	Res	Type
17	V	85	LYS
17	V	93	GLU
17	V	95	LEU
17	V	98	GLU
18	W	11	ARG
18	W	17	VAL
18	W	18	ARG
18	W	23	LEU
18	W	39	THR
18	W	51	LEU
18	W	52	GLU
18	W	65	LEU
18	W	66	GLU
18	W	92	ARG
18	W	94	ASP
18	W	95	ILE
18	W	100	THR
18	W	105	VAL
18	W	107	LEU
19	X	8	ILE
19	X	23	GLU
19	X	27	THR
19	X	38	GLU
19	X	53	LYS
19	X	56	THR
19	X	57	LEU
19	X	70	LEU
19	X	76	ARG
19	X	80	ILE
19	X	81	VAL
19	X	92	LEU
20	Y	1	MET
20	Y	2	ARG
20	Y	9	LYS
20	Y	28	LYS
20	Y	30	VAL
20	Y	34	LYS
20	Y	38	ILE
20	Y	44	ILE
20	Y	45	VAL
20	Y	49	VAL
20	Y	52	SER

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Mol	Chain	Res	Type
20	Y	61	ILE
20	Y	67	LEU
20	Y	72	VAL
20	Y	83	THR
20	Y	85	VAL
20	Y	86	ARG
20	Y	90	LEU
20	Y	97	ARG
20	Y	107	ASP
21	Z	1	MET
21	Z	11	GLU
21	Z	19	ARG
21	Z	24	LEU
21	Z	29	TYR
21	Z	30	ASN
21	Z	31	ARG
21	Z	40	ASP
21	Z	41	LEU
21	Z	56	VAL
21	Z	58	VAL
21	Z	66	SER
21	Z	72	ARG
21	Z	73	GLN
21	Z	74	VAL
21	Z	82	ARG
21	Z	86	VAL
21	Z	87	ASP
21	Z	93	ASP
21	Z	94	GLU
21	Z	100	VAL
21	Z	119	GLU
21	Z	129	SER
21	Z	131	ARG
21	Z	133	ILE
21	Z	135	GLU
21	Z	140	ASP
21	Z	157	LEU
21	Z	161	VAL
21	Z	170	THR
21	Z	175	VAL
21	Z	179	ASP
21	Z	185	GLU

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Mol	Chain	Res	Type
22	0	10	THR
22	0	14	ARG
22	0	16	SER
22	0	19	LYS
22	0	20	ARG
22	0	41	ARG
22	0	43	THR
22	0	53	MET
22	0	55	ARG
22	0	56	ASP
22	0	72	ARG
22	0	74	ARG
22	0	81	VAL
22	0	84	LEU
23	1	3	LYS
23	1	4	VAL
23	1	11	ARG
23	1	21	ARG
23	1	38	SER
23	1	40	ARG
23	1	41	ARG
23	1	46	LEU
23	1	51	VAL
23	1	53	VAL
23	1	58	ILE
23	1	59	THR
23	1	61	ARG
23	1	62	VAL
23	1	73	LEU
23	1	80	LEU
23	1	90	ILE
23	1	95	LEU
23	1	97	LEU
23	1	98	LEU
24	2	1	MET
24	2	3	LEU
24	2	17	SER
24	2	21	LEU
24	2	26	ARG
24	2	30	ARG
24	2	43	GLN
24	2	45	SER

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Mol	Chain	Res	Type
24	2	51	ARG
24	2	53	LEU
24	2	62	THR
24	2	64	LEU
24	2	65	ASN
25	3	8	LEU
25	3	11	SER
25	3	23	LEU
25	3	28	LEU
25	3	31	LEU
25	3	36	VAL
25	3	37	LEU
25	3	56	VAL
25	3	57	GLU
26	4	1	MET
26	4	5	ILE
26	4	8	LYS
26	4	10	VAL
26	4	13	ARG
26	4	14	ILE
26	4	16	CYS
26	4	18	CYS
26	4	31	ILE
26	4	36	CYS
26	4	39	CYS
26	4	43	TYR
26	4	44	THR
26	4	46	GLN
27	5	6	VAL
27	5	9	LYS
27	5	15	ARG
27	5	16	ARG
27	5	25	LEU
27	5	26	THR
27	5	33	CYS
27	5	40	LYS
27	5	55	ARG
27	5	57	VAL
28	6	4	GLU
28	6	5	VAL
28	6	8	LYS
28	6	13	CYS

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Mol	Chain	Res	Type
28	6	18	ARG
28	6	34	LEU
28	6	38	LYS
28	6	40	CYS
28	6	43	CYS
28	6	44	ARG
29	7	1	MET
29	7	8	ASN
29	7	12	ARG
29	7	14	LYS
29	7	19	ARG
29	7	24	THR
29	7	32	LYS
29	7	43	THR
30	8	4	MET
30	8	13	ARG
30	8	14	VAL
30	8	23	VAL
30	8	25	MET
30	8	26	LYS
30	8	32	LEU
30	8	34	TRP
30	8	41	ILE
31	9	2	LYS
31	9	4	ARG
31	9	7	VAL
31	9	12	ASP
31	9	22	ARG
31	9	26	ILE
31	9	33	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	135	HIS
5	F	75	HIS
9	N	133	GLN
10	O	88	ASN
16	U	81	HIS
19	X	31	HIS
19	X	55	ASN
22	0	12	ASN

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Mol	Chain	Res	Type
27	5	4	HIS
31	9	29	ASN
31	9	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2711/2915 (93%)	632 (23%)	55 (2%)
2	B	119/122 (97%)	26 (21%)	2 (1%)
All	All	2830/3037 (93%)	658 (23%)	57 (2%)

All (658) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	10	G
1	A	14	A
1	A	15	G
1	A	30	G
1	A	34	C
1	A	35	G
1	A	36	G
1	A	45	C
1	A	55	G
1	A	61	G
1	A	64	A
1	A	70	G
1	A	71	A
1	A	72	U
1	A	74	A
1	A	75	G
1	A	84	A
1	A	90	U
1	A	92	A
1	A	100	G
1	A	102	G
1	A	103	A
1	A	118	A
1	A	120	U
1	A	133	C
1	A	141	A

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Mol	Chain	Res	Type
1	A	153	C
1	A	154	G
1	A	154(A)	C
1	A	157	U
1	A	172	C
1	A	173	G
1	A	181	A
1	A	182	A
1	A	183	C
1	A	196	A
1	A	197	A
1	A	199	A
1	A	200	U
1	A	204	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	224	G
1	A	228	A
1	A	229	A
1	A	232	G
1	A	233	A
1	A	245	G
1	A	248	G
1	A	250	G
1	A	252	G
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(O)	C
1	A	271(R)	G
1	A	272(A)	U
1	A	272(B)	G
1	A	281	G
1	A	287	C
1	A	308	G
1	A	311	A
1	A	324	A

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Mol	Chain	Res	Type
1	A	329	G
1	A	330	A
1	A	342	G
1	A	352	G
1	A	353	G
1	A	363	G
1	A	363(B)	G
1	A	363(C)	G
1	A	363(F)	A
1	A	386	G
1	A	387	U
1	A	389	G
1	A	396	G
1	A	406	G
1	A	407	G
1	A	411	G
1	A	412	A
1	A	427	U
1	A	428	A
1	A	444	C
1	A	447	A
1	A	455	C
1	A	456	C
1	A	457	A
1	A	464	U
1	A	470	A
1	A	471	A
1	A	472	A
1	A	474	G
1	A	475	U
1	A	481	G
1	A	482	A
1	A	501	A
1	A	504	U
1	A	505	A
1	A	508	G
1	A	509	C
1	A	510	C
1	A	521	G
1	A	530	G
1	A	531	C
1	A	532	A

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Mol	Chain	Res	Type
1	A	533	G
1	A	545	G
1	A	546	C
1	A	549	G
1	A	563	G
1	A	571	A
1	A	573	G
1	A	574	C
1	A	575	A
1	A	587	C
1	A	588	U
1	A	603	A
1	A	604	G
1	A	607	U
1	A	615	G
1	A	616	G
1	A	620	G
1	A	627	A
1	A	637	A
1	A	645	C
1	A	646	A
1	A	652(B)	A
1	A	652(C)	G
1	A	652(E)	G
1	A	652(U)	G
1	A	653	A
1	A	668	G
1	A	669	G
1	A	670	A
1	A	684	G
1	A	686	G
1	A	701	G
1	A	708	C
1	A	709	U
1	A	717	G
1	A	718	A
1	A	726	G
1	A	730	C
1	A	731	C
1	A	738	G
1	A	740	U
1	A	746	A

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Mol	Chain	Res	Type
1	A	747	U
1	A	748	G
1	A	749	C
1	A	753	C
1	A	762	U
1	A	765	G
1	A	775	G
1	A	776	G
1	A	779	U
1	A	782	A
1	A	783	A
1	A	784	A
1	A	785	G
1	A	790	C
1	A	792	G
1	A	805	G
1	A	812	C
1	A	819	A
1	A	822	U
1	A	827	U
1	A	828	U
1	A	829	A
1	A	830	G
1	A	839	U
1	A	840	C
1	A	846	C
1	A	848	G
1	A	855	G
1	A	857	C
1	A	859	G
1	A	869	G
1	A	874	G
1	A	875	G
1	A	880	G
1	A	884	C
1	A	885	C
1	A	886	C
1	A	887	A
1	A	888	C
1	A	889	C
1	A	890	A
1	A	893	C

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Mol	Chain	Res	Type
1	A	894	C
1	A	896	A
1	A	900	A
1	A	901	A
1	A	905	U
1	A	910	A
1	A	911	A
1	A	917	A
1	A	931	G
1	A	932	G
1	A	933	A
1	A	934	G
1	A	938	G
1	A	941	A
1	A	944	G
1	A	945	A
1	A	946	G
1	A	947	G
1	A	957	A
1	A	958	U
1	A	959	A
1	A	961	C
1	A	968	G
1	A	974	G
1	A	975	C
1	A	975(A)	G
1	A	983	A
1	A	991	C
1	A	996	A
1	A	999	U
1	A	1004	C
1	A	1005	C
1	A	1009	A
1	A	1010	A
1	A	1012	U
1	A	1013	C
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1026	U
1	A	1027	A

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Mol	Chain	Res	Type
1	A	1033	U
1	A	1035	U
1	A	1041	C
1	A	1042	G
1	A	1113	U
1	A	1114	G
1	A	1115	G
1	A	1118	C
1	A	1126	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1137	G
1	A	1139	G
1	A	1142(A)	A
1	A	1143	A
1	A	1150	C
1	A	1155	A
1	A	1170	G
1	A	1171	G
1	A	1204	A
1	A	1205	U
1	A	1210	A
1	A	1211	U
1	A	1212	G
1	A	1213	A
1	A	1219	G
1	A	1220	A
1	A	1236	G
1	A	1237	A
1	A	1240	U
1	A	1241	A
1	A	1244	G
1	A	1253	A
1	A	1256	G
1	A	1262	A
1	A	1264	G
1	A	1268	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1278	A

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Mol	Chain	Res	Type
1	A	1287	A
1	A	1298	C
1	A	1300	U
1	A	1301	A
1	A	1308	A
1	A	1314	C
1	A	1319	G
1	A	1329	U
1	A	1332	G
1	A	1333	C
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	1379	A
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1416	G
1	A	1419	A
1	A	1420	U
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1437	C
1	A	1445	A
1	A	1448	G
1	A	1449	A
1	A	1450	G
1	A	1452	A
1	A	1455	G
1	A	1465	G
1	A	1467	C
1	A	1471	A
1	A	1478	G
1	A	1482	G
1	A	1489	U
1	A	1493	C

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Mol	Chain	Res	Type
1	A	1496	A
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	1525	G
1	A	1531	C
1	A	1537	G
1	A	1541	G
1	A	1542	A
1	A	1543	C
1	A	1547	C
1	A	1558	A
1	A	1559	G
1	A	1569	A
1	A	1578	U
1	A	1579	A
1	A	1581	G
1	A	1584	C
1	A	1586	A
1	A	1598	C
1	A	1603	A
1	A	1608	A
1	A	1609	A
1	A	1616	A
1	A	1617	C
1	A	1619	G
1	A	1621	U
1	A	1625	C
1	A	1640	C
1	A	1648	C
1	A	1654	A
1	A	1655	A
1	A	1665	A
1	A	1674	G
1	A	1676	A
1	A	1695	G
1	A	1696	G
1	A	1700	A
1	A	1701	A

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Mol	Chain	Res	Type
1	A	1703	G
1	A	1721	G
1	A	1722	A
1	A	1740	G
1	A	1742	G
1	A	1746	G
1	A	1752	C
1	A	1756	G
1	A	1758	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1769	G
1	A	1773	A
1	A	1779	U
1	A	1780	A
1	A	1781	C
1	A	1782	C
1	A	1786	A
1	A	1791	A
1	A	1799	G
1	A	1800	C
1	A	1801	G
1	A	1811	G
1	A	1812	A
1	A	1816	G
1	A	1819	A
1	A	1820	U
1	A	1827	C
1	A	1828	G
1	A	1829	A
1	A	1834	U
1	A	1835	G
1	A	1842	G
1	A	1847	A
1	A	1859	A
1	A	1860	G
1	A	1861	G
1	A	1877	A
1	A	1878	G
1	A	1896	G
1	A	1900	A

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Mol	Chain	Res	Type
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1915	U
1	A	1920	C
1	A	1929	G
1	A	1930	G
1	A	1934	C
1	A	1936	A
1	A	1938	A
1	A	1950	G
1	A	1955	U
1	A	1963	U
1	A	1964	G
1	A	1967	C
1	A	1968	G
1	A	1969	A
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1979	C
1	A	1980	G
1	A	1982	C
1	A	1984	G
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1996	C
1	A	1997	G
1	A	2018	G
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	2039	C
1	A	2043	C
1	A	2049	G
1	A	2052	G
1	A	2055	C
1	A	2056	G

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Mol	Chain	Res	Type
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2070	G
1	A	2082	A
1	A	2097	C
1	A	2099	U
1	A	2103	C
1	A	2104	G
1	A	2105	C
1	A	2185	C
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	2201	C
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2219	G
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2240	C
1	A	2257	U
1	A	2275	C
1	A	2279	G
1	A	2283	C
1	A	2287	A
1	A	2288	A
1	A	2289	G
1	A	2298	A
1	A	2304	G
1	A	2305	A
1	A	2311	A
1	A	2319	G
1	A	2320	A

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Mol	Chain	Res	Type
1	A	2321	G
1	A	2322	A
1	A	2324	C
1	A	2325	G
1	A	2327	A
1	A	2328	A
1	A	2334	G
1	A	2336	A
1	A	2343	C
1	A	2347	C
1	A	2349	G
1	A	2350	C
1	A	2352	A
1	A	2359	C
1	A	2366	A
1	A	2375	G
1	A	2383	G
1	A	2384	G
1	A	2385	C
1	A	2388	A
1	A	2391	G
1	A	2392	A
1	A	2400	G
1	A	2406	U
1	A	2410	G
1	A	2414	G
1	A	2416	C
1	A	2421	G
1	A	2422	A
1	A	2423	U
1	A	2425	A
1	A	2426	A
1	A	2427	C
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2432	A
1	A	2435	A
1	A	2436	G
1	A	2439	A
1	A	2440	C
1	A	2441	C

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Mol	Chain	Res	Type
1	A	2445	G
1	A	2448	A
1	A	2459	A
1	A	2469	A
1	A	2470	G
1	A	2474	C
1	A	2476	A
1	A	2479	G
1	A	2480	C
1	A	2481	G
1	A	2486	G
1	A	2497	A
1	A	2502	G
1	A	2504	U
1	A	2505	G
1	A	2506	U
1	A	2509	G
1	A	2517	C
1	A	2518	A
1	A	2520	C
1	A	2525	G
1	A	2529	G
1	A	2535	G
1	A	2553	G
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2569	G
1	A	2572	A
1	A	2573	C
1	A	2582	G
1	A	2585	U
1	A	2586	C
1	A	2601	C
1	A	2602	A
1	A	2608	G
1	A	2609	U
1	A	2611	U
1	A	2612	C
1	A	2615	U
1	A	2623	G
1	A	2629	A

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Mol	Chain	Res	Type
1	A	2630	G
1	A	2632	A
1	A	2636	U
1	A	2646	C
1	A	2663	G
1	A	2669	G
1	A	2673	G
1	A	2675	A
1	A	2679	A
1	A	2686	G
1	A	2689	U
1	A	2690	C
1	A	2691	C
1	A	2702	U
1	A	2711	A
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2722	G
1	A	2726	U
1	A	2727	G
1	A	2733	A
1	A	2735	G
1	A	2744	G
1	A	2752	C
1	A	2756	U
1	A	2758	A
1	A	2761	G
1	A	2764	A
1	A	2765	A
1	A	2766	G
1	A	2769	C
1	A	2778	A
1	A	2780	G
1	A	2787	C
1	A	2789	C
1	A	2790	A
1	A	2791	C
1	A	2802	G
1	A	2803	C
1	A	2807	G
1	A	2808	U

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Mol	Chain	Res	Type
1	A	2812	G
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2825	C
1	A	2833	G
1	A	2834	G
1	A	2835	A
1	A	2836	U
1	A	2850	A
1	A	2851	A
1	A	2872	G
1	A	2873	A
1	A	2879	C
1	A	2880	C
1	A	2892	A
1	A	2895	U
2	B	2	C
2	B	7	G
2	B	9	G
2	B	12	C
2	B	13	A
2	B	23	G
2	B	24	G
2	B	30	C
2	B	31	C
2	B	40	U
2	B	44	G
2	B	45	A
2	B	52	A
2	B	53	A
2	B	54	G
2	B	56	G
2	B	67	G
2	B	73	A
2	B	84	C
2	B	96	U
2	B	97	G
2	B	106	G
2	B	110	G
2	B	116	G
2	B	117	G

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Mol	Chain	Res	Type
2	B	120	A

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	34	C
1	A	71	A
1	A	102	G
1	A	196	A
1	A	249	C
1	A	271(M)	G
1	A	310	A
1	A	363(E)	U
1	A	474	G
1	A	481	G
1	A	503	A
1	A	587	C
1	A	669	G
1	A	685	A
1	A	746	A
1	A	752	A
1	A	774	A
1	A	827	U
1	A	856	C
1	A	888	C
1	A	900	A
1	A	974	G
1	A	1026	U
1	A	1210	A
1	A	1332	G
1	A	1378	A
1	A	1379	A
1	A	1420	U
1	A	1427	A
1	A	1507	A
1	A	1530	C
1	A	1558	A
1	A	1559	G
1	A	1608	A
1	A	1653	G
1	A	1819	A

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Mol	Chain	Res	Type
1	A	1914	C
1	A	1963	U
1	A	1992	G
1	A	2019	A
1	A	2238	G
1	A	2282	G
1	A	2288	A
1	A	2318	G
1	A	2319	G
1	A	2326	C
1	A	2335	A
1	A	2405	G
1	A	2439	A
1	A	2689	U
1	A	2726	U
1	A	2778	A
1	A	2789	C
1	A	2802	G
2	B	44	G
2	B	52	A

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 735 ligands modelled in this entry, 735 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2722/2915 (93%)	0.09	57 (2%) 60 15	44, 74, 127, 170	0
2	B	120/122 (98%)	0.49	5 (4%) 35 7	73, 114, 129, 146	0
3	D	275/276 (99%)	0.10	3 (1%) 77 27	41, 62, 82, 100	0
4	E	204/206 (99%)	0.08	2 (0%) 79 29	43, 74, 100, 113	0
5	F	203/210 (96%)	0.20	2 (0%) 79 29	47, 88, 114, 127	0
6	G	180/182 (98%)	0.54	14 (7%) 13 3	101, 117, 127, 136	0
7	H	174/180 (96%)	0.75	23 (13%) 4 1	96, 116, 130, 140	0
8	I	146/148 (98%)	0.17	1 (0%) 84 38	68, 108, 126, 131	0
9	N	140/140 (100%)	0.30	4 (2%) 49 10	64, 86, 107, 117	0
10	O	122/122 (100%)	0.01	1 (0%) 83 35	57, 73, 88, 96	0
11	P	149/150 (99%)	0.40	7 (4%) 30 6	52, 91, 116, 127	0
12	Q	141/141 (100%)	0.28	4 (2%) 50 11	67, 90, 106, 114	0
13	R	118/118 (100%)	0.23	1 (0%) 83 35	49, 65, 86, 95	0
14	S	110/112 (98%)	0.45	4 (3%) 41 8	90, 109, 119, 127	0
15	T	130/146 (89%)	0.07	3 (2%) 57 13	62, 77, 108, 123	0
16	U	116/118 (98%)	0.22	1 (0%) 81 32	54, 82, 103, 108	0
17	V	100/101 (99%)	0.34	3 (3%) 48 10	56, 98, 119, 123	0
18	W	111/113 (98%)	-0.04	1 (0%) 81 32	49, 63, 89, 114	0
19	X	95/96 (98%)	0.14	1 (1%) 77 27	61, 77, 100, 107	0
20	Y	107/110 (97%)	0.72	18 (16%) 2 1	77, 96, 112, 124	0
21	Z	189/206 (91%)	0.53	12 (6%) 19 4	98, 114, 131, 139	0
22	0	77/85 (90%)	0.26	4 (5%) 26 5	73, 85, 101, 124	0
23	1	97/98 (98%)	0.26	4 (4%) 35 7	50, 72, 105, 115	0
24	2	71/72 (98%)	0.32	5 (7%) 16 4	78, 94, 106, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	3	58/60 (96%)	0.29	1 (1%) 67 19	71, 84, 114, 128	0
26	4	46/71 (64%)	0.25	3 (6%) 18 4	118, 126, 136, 138	0
27	5	59/60 (98%)	0.04	2 (3%) 43 9	47, 66, 85, 106	0
28	6	53/54 (98%)	0.16	2 (3%) 38 7	67, 81, 93, 101	0
29	7	48/49 (97%)	0.48	3 (6%) 19 4	41, 53, 82, 105	0
30	8	64/65 (98%)	0.22	1 (1%) 68 20	60, 71, 83, 94	0
31	9	35/37 (94%)	0.95	7 (20%) 2 1	73, 88, 103, 115	0
All	All	6260/6563 (95%)	0.21	199 (3%) 43 9	41, 81, 124, 170	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	171	LEU	7.9
1	A	2191	G	5.8
1	A	652(B)	A	5.7
1	A	361	G	5.7
1	A	1533	G	5.4
3	D	276	LYS	5.1
7	H	172	LYS	4.9
1	A	362	U	4.7
1	A	652(A)	A	4.6
20	Y	94	LYS	4.6
1	A	2790	A	4.5
20	Y	29	GLU	4.2
1	A	1113	U	4.2
12	Q	1	MET	4.1
1	A	280	C	4.0
7	H	173	PRO	3.9
1	A	271(K)	U	3.8
11	P	109	GLY	3.7
7	H	58	GLU	3.6
20	Y	1	MET	3.6
7	H	43	VAL	3.5
31	9	17	ILE	3.5
31	9	21	GLY	3.5
2	B	6	C	3.5
7	H	156	ALA	3.4
24	2	46	GLN	3.4
1	A	655	A	3.4
1	A	889	C	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	2190	G	3.4
1	A	2189	U	3.3
1	A	352	G	3.3
5	F	131	GLY	3.3
7	H	157	TYR	3.3
1	A	1032	A	3.2
20	Y	91	GLU	3.2
21	Z	2	GLU	3.2
6	G	35	GLU	3.1
31	9	22	ARG	3.1
16	U	89	GLU	3.1
20	Y	22	GLY	3.1
7	H	97	ARG	3.1
1	A	2188	C	3.1
7	H	42	ARG	3.0
21	Z	9	TYR	3.0
1	A	2789	C	3.0
7	H	159	GLU	3.0
7	H	98	LEU	3.0
17	V	72	VAL	3.0
20	Y	55	TYR	3.0
1	A	1041	C	3.0
21	Z	141	VAL	2.9
3	D	262	ARG	2.9
7	H	101	ARG	2.9
20	Y	93	GLY	2.9
6	G	162	THR	2.9
1	A	2273	A	2.9
20	Y	3	VAL	2.9
1	A	2792	G	2.9
6	G	182	LYS	2.9
1	A	1919	A	2.9
1	A	2068	U	2.9
23	1	38	SER	2.9
6	G	61	ALA	2.8
21	Z	3	TYR	2.8
1	A	1207	C	2.8
17	V	71	LEU	2.8
1	A	360	G	2.8
29	7	48	LYS	2.8
1	A	2833	G	2.8
20	Y	89	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
17	V	68	LYS	2.7
1	A	12	U	2.7
3	D	261	LYS	2.7
23	1	37	ILE	2.7
1	A	2062	A	2.7
26	4	34	GLU	2.7
4	E	204	ALA	2.7
1	A	1034	G	2.7
23	1	15	ALA	2.7
1	A	2894	G	2.7
20	Y	95	LYS	2.7
1	A	6	A	2.7
7	H	40	GLU	2.7
14	S	84	GLN	2.7
22	0	74	ARG	2.6
14	S	54	LEU	2.6
24	2	1	MET	2.6
7	H	20	ALA	2.6
9	N	71	ILE	2.6
7	H	41	MET	2.6
1	A	154	G	2.6
21	Z	1	MET	2.6
1	A	1461	G	2.6
12	Q	59	ARG	2.6
31	9	18	ARG	2.6
20	Y	90	LEU	2.6
1	A	2602	A	2.6
1	A	1415	U	2.5
1	A	32	C	2.5
1	A	1450(A)	C	2.5
1	A	932	G	2.5
15	T	78	LEU	2.5
7	H	111	HIS	2.5
29	7	32	LYS	2.5
6	G	137	GLU	2.5
21	Z	4	ARG	2.5
9	N	10	GLU	2.5
24	2	9	GLN	2.5
6	G	3	LEU	2.5
31	9	36	GLN	2.5
15	T	113	LYS	2.5
1	A	1536	C	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1886	C	2.4
2	B	27	C	2.4
6	G	62	LEU	2.4
7	H	82	GLY	2.4
4	E	58	ARG	2.4
27	5	58	LEU	2.4
22	0	17	GLN	2.4
1	A	701	G	2.4
11	P	110	TYR	2.4
10	O	48	PRO	2.4
1	A	150	C	2.4
20	Y	2	ARG	2.3
11	P	79	ARG	2.3
20	Y	56	PRO	2.3
21	Z	38	TYR	2.3
1	A	896	A	2.3
1	A	11	G	2.3
6	G	66	GLN	2.3
25	3	20	LYS	2.3
24	2	7	ARG	2.3
7	H	81	GLU	2.3
1	A	1509	C	2.3
6	G	97	ASP	2.3
7	H	155	SER	2.3
2	B	59	A	2.3
2	B	104	U	2.3
9	N	70	LYS	2.2
1	A	1641	A	2.2
23	1	16	ASN	2.2
1	A	2281	C	2.2
1	A	2442	C	2.2
12	Q	141	GLN	2.2
22	0	42	GLY	2.2
28	6	11	LEU	2.2
20	Y	82	PRO	2.2
11	P	62	LEU	2.2
28	6	50	ARG	2.2
20	Y	57	GLN	2.2
27	5	25	LEU	2.2
1	A	1532	C	2.2
20	Y	41	GLY	2.2
11	P	73	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1183	G	2.2
21	Z	142	SER	2.1
6	G	145	THR	2.1
19	X	1	MET	2.1
7	H	22	GLY	2.1
20	Y	4	LYS	2.1
21	Z	175	VAL	2.1
7	H	13	LYS	2.1
14	S	3	ARG	2.1
22	O	71	ASP	2.1
18	W	86	LEU	2.1
30	8	2	PRO	2.1
21	Z	140	ASP	2.1
6	G	139	LEU	2.1
13	R	111	LEU	2.1
9	N	118	LYS	2.1
1	A	864	G	2.1
6	G	30	GLU	2.1
15	T	14	TYR	2.1
31	9	20	HIS	2.1
1	A	863	A	2.1
24	2	49	LYS	2.1
31	9	24	TYR	2.1
1	A	892	G	2.1
1	A	1921	G	2.1
20	Y	40	GLU	2.1
8	I	1	MET	2.1
11	P	75	ILE	2.1
6	G	138	GLN	2.1
21	Z	51	ALA	2.1
26	4	2	LYS	2.1
12	Q	6	ARG	2.1
11	P	28	GLY	2.1
1	A	2646	C	2.1
5	F	96	ASP	2.1
21	Z	50	GLN	2.0
1	A	1112	G	2.0
26	4	23	GLU	2.0
7	H	12	PRO	2.0
29	7	38	GLY	2.0
14	S	20	ARG	2.0
1	A	1033	U	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	4	C	2.0
6	G	64	THR	2.0
7	H	19	VAL	2.0

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

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

6.3 Carbohydrates i

There are no carbohydrates in this entry.

6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	3080	1/1	2.05	-	92,92,92,92	0
32	MG	A	3115	1/1	0.45	-	69,69,69,69	0
32	MG	A	3411	1/1	0.07	-	52,52,52,52	0
32	MG	A	3206	1/1	0.26	-	68,68,68,68	0
32	MG	A	3398	1/1	0.24	-	71,71,71,71	0
32	MG	A	3497	1/1	1.16	-	109,109,109,109	0
32	MG	A	3513	1/1	0.13	-	86,86,86,86	0
32	MG	A	3028	1/1	0.23	-	78,78,78,78	0
32	MG	A	3373	1/1	0.37	-	76,76,76,76	0
32	MG	A	3641	1/1	0.81	-	61,61,61,61	0
32	MG	A	3037	1/1	0.78	-	76,76,76,76	0
32	MG	A	3659	1/1	0.15	-	93,93,93,93	0
32	MG	A	3612	1/1	0.68	-	74,74,74,74	0
32	MG	A	3033	1/1	0.27	-	62,62,62,62	0
32	MG	A	3190	1/1	0.88	-	80,80,80,80	0
32	MG	A	3562	1/1	0.24	-	45,45,45,45	0
32	MG	A	3019	1/1	0.14	-	49,49,49,49	0
32	MG	A	3516	1/1	0.32	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3626	1/1	0.74	-	78,78,78,78	0
32	MG	A	3157	1/1	0.24	-	53,53,53,53	0
32	MG	A	3166	1/1	0.50	-	75,75,75,75	0
32	MG	A	3025	1/1	0.27	-	83,83,83,83	0
32	MG	A	3266	1/1	0.40	-	67,67,67,67	0
32	MG	A	3453	1/1	0.14	-	68,68,68,68	0
32	MG	A	3172	1/1	0.20	-	106,106,106,106	0
32	MG	A	3046	1/1	0.36	-	83,83,83,83	0
32	MG	A	3600	1/1	0.55	-	97,97,97,97	0
32	MG	A	3225	1/1	0.56	-	68,68,68,68	0
32	MG	A	3160	1/1	0.80	-	66,66,66,66	0
32	MG	A	3350	1/1	0.21	-	61,61,61,61	0
32	MG	A	3257	1/1	0.45	-	64,64,64,64	0
32	MG	A	3452	1/1	0.11	-	50,50,50,50	0
32	MG	A	3211	1/1	0.78	-	73,73,73,73	0
32	MG	A	3322	1/1	0.83	-	50,50,50,50	0
32	MG	A	3557	1/1	0.31	-	77,77,77,77	0
32	MG	A	3365	1/1	0.47	-	84,84,84,84	0
32	MG	A	3133	1/1	0.53	-	71,71,71,71	0
32	MG	B	209	1/1	0.68	-	86,86,86,86	0
32	MG	A	3481	1/1	0.78	-	101,101,101,101	0
32	MG	E	301	1/1	0.37	-	64,64,64,64	0
32	MG	A	3173	1/1	1.03	-	57,57,57,57	0
32	MG	A	3492	1/1	0.51	-	68,68,68,68	0
32	MG	A	3067	1/1	0.22	-	57,57,57,57	0
32	MG	A	3551	1/1	0.18	-	70,70,70,70	0
32	MG	A	3036	1/1	0.39	-	74,74,74,74	0
32	MG	A	3315	1/1	0.69	-	62,62,62,62	0
32	MG	A	3569	1/1	0.15	-	104,104,104,104	0
32	MG	A	3610	1/1	0.50	-	95,95,95,95	0
32	MG	P	201	1/1	0.18	-	67,67,67,67	0
32	MG	A	3382	1/1	0.08	-	42,42,42,42	0
32	MG	A	3342	1/1	1.33	-	68,68,68,68	0
32	MG	A	3213	1/1	0.90	-	75,75,75,75	0
32	MG	A	3113	1/1	0.42	-	62,62,62,62	0
32	MG	A	3011	1/1	0.31	-	56,56,56,56	0
32	MG	O	103	1/1	0.53	-	86,86,86,86	0
32	MG	A	3145	1/1	0.23	-	57,57,57,57	0
32	MG	A	3468	1/1	0.33	-	90,90,90,90	0
32	MG	A	3096	1/1	0.36	-	45,45,45,45	0
32	MG	A	3268	1/1	0.15	-	74,74,74,74	0
32	MG	A	3085	1/1	0.13	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3469	1/1	0.16	-	68,68,68,68	0
32	MG	A	3391	1/1	0.34	-	36,36,36,36	0
32	MG	A	3597	1/1	0.23	-	90,90,90,90	0
32	MG	A	3410	1/1	0.09	-	38,38,38,38	0
32	MG	A	3531	1/1	0.28	-	106,106,106,106	0
32	MG	A	3101	1/1	0.46	-	59,59,59,59	0
32	MG	A	3617	1/1	0.18	-	81,81,81,81	0
32	MG	A	3669	1/1	0.16	-	76,76,76,76	0
32	MG	A	3134	1/1	0.52	-	41,41,41,41	0
32	MG	A	3097	1/1	0.43	-	74,74,74,74	0
32	MG	A	3429	1/1	0.15	-	42,42,42,42	0
32	MG	A	3074	1/1	0.19	-	32,32,32,32	0
32	MG	A	3397	1/1	0.07	-	44,44,44,44	0
32	MG	7	101	1/1	0.50	-	63,63,63,63	0
32	MG	A	3366	1/1	0.42	-	69,69,69,69	0
32	MG	A	3288	1/1	0.40	-	57,57,57,57	0
32	MG	A	3233	1/1	0.43	-	64,64,64,64	0
32	MG	A	3055	1/1	0.28	-	45,45,45,45	0
32	MG	A	3665	1/1	0.21	-	75,75,75,75	0
32	MG	A	3675	1/1	0.29	-	96,96,96,96	0
32	MG	A	3449	1/1	0.13	-	46,46,46,46	0
32	MG	A	3633	1/1	0.23	-	89,89,89,89	0
32	MG	A	3107	1/1	0.36	-	39,39,39,39	0
32	MG	A	3130	1/1	0.21	-	60,60,60,60	0
32	MG	A	3180	1/1	0.19	-	77,77,77,77	0
32	MG	A	3149	1/1	0.66	-	69,69,69,69	0
32	MG	A	3605	1/1	0.28	-	77,77,77,77	0
32	MG	A	3006	1/1	0.61	-	51,51,51,51	0
32	MG	B	204	1/1	0.39	-	107,107,107,107	0
32	MG	A	3142	1/1	1.11	-	66,66,66,66	0
32	MG	A	3105	1/1	0.32	-	70,70,70,70	0
32	MG	A	3267	1/1	0.31	-	66,66,66,66	0
32	MG	A	3451	1/1	0.14	-	50,50,50,50	0
32	MG	A	3440	1/1	0.20	-	59,59,59,59	0
32	MG	A	3571	1/1	0.06	-	46,46,46,46	0
32	MG	A	3230	1/1	0.34	-	76,76,76,76	0
32	MG	A	3324	1/1	0.41	-	74,74,74,74	0
32	MG	A	3169	1/1	0.25	-	75,75,75,75	0
32	MG	A	3283	1/1	0.16	-	82,82,82,82	0
32	MG	A	3305	1/1	1.18	-	80,80,80,80	0
32	MG	A	3368	1/1	0.33	-	64,64,64,64	0
32	MG	A	3250	1/1	0.95	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3235	1/1	0.23	-	48,48,48,48	0
32	MG	A	3247	1/1	0.65	-	91,91,91,91	0
32	MG	A	3392	1/1	0.10	-	38,38,38,38	0
32	MG	A	3680	1/1	0.26	-	107,107,107,107	0
32	MG	A	3333	1/1	0.57	-	70,70,70,70	0
32	MG	A	3509	1/1	0.18	-	93,93,93,93	0
32	MG	A	3684	1/1	0.20	-	95,95,95,95	0
32	MG	A	3389	1/1	0.28	-	47,47,47,47	0
32	MG	A	3044	1/1	0.49	-	59,59,59,59	0
32	MG	A	3188	1/1	0.68	-	81,81,81,81	0
32	MG	A	3443	1/1	0.20	-	77,77,77,77	0
32	MG	A	3403	1/1	0.46	-	40,40,40,40	0
32	MG	A	3444	1/1	0.71	-	91,91,91,91	0
32	MG	A	3547	1/1	0.23	-	93,93,93,93	0
32	MG	A	3255	1/1	0.31	-	62,62,62,62	0
32	MG	A	3639	1/1	0.20	-	73,73,73,73	0
32	MG	A	3152	1/1	0.62	-	68,68,68,68	0
32	MG	A	3201	1/1	0.27	-	66,66,66,66	0
32	MG	A	3654	1/1	0.44	-	97,97,97,97	0
32	MG	A	3238	1/1	0.34	-	55,55,55,55	0
32	MG	A	3644	1/1	0.75	-	118,118,118,118	0
32	MG	A	3603	1/1	0.22	-	60,60,60,60	0
32	MG	A	3660	1/1	0.86	-	83,83,83,83	0
32	MG	A	3161	1/1	0.46	-	51,51,51,51	0
32	MG	A	3094	1/1	0.24	-	48,48,48,48	0
32	MG	A	3493	1/1	0.33	-	80,80,80,80	0
32	MG	A	3378	1/1	0.20	-	74,74,74,74	0
32	MG	A	3360	1/1	0.63	-	67,67,67,67	0
32	MG	A	3185	1/1	0.48	-	77,77,77,77	0
32	MG	A	3264	1/1	0.29	-	42,42,42,42	0
32	MG	A	3167	1/1	0.76	-	77,77,77,77	0
32	MG	A	3532	1/1	0.11	-	84,84,84,84	0
32	MG	A	3388	1/1	0.24	-	58,58,58,58	0
32	MG	A	3611	1/1	0.20	-	73,73,73,73	0
32	MG	A	3362	1/1	0.32	-	78,78,78,78	0
32	MG	R	201	1/1	0.41	-	44,44,44,44	0
33	ZN	5	101	1/1	0.03	-	88,88,88,88	0
32	MG	A	3123	1/1	0.23	-	61,61,61,61	0
32	MG	A	3564	1/1	0.27	-	53,53,53,53	0
32	MG	A	3062	1/1	0.33	-	69,69,69,69	0
32	MG	A	3272	1/1	0.28	-	76,76,76,76	0
32	MG	A	3269	1/1	1.09	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3681	1/1	0.15	-	91,91,91,91	0
32	MG	A	3064	1/1	0.90	-	51,51,51,51	0
32	MG	A	3390	1/1	0.26	-	53,53,53,53	0
32	MG	A	3490	1/1	0.16	-	68,68,68,68	0
32	MG	A	3108	1/1	0.22	-	42,42,42,42	0
32	MG	A	3575	1/1	1.10	-	104,104,104,104	0
32	MG	A	3114	1/1	0.18	-	65,65,65,65	0
32	MG	A	3319	1/1	0.80	-	78,78,78,78	0
32	MG	A	3222	1/1	0.78	-	80,80,80,80	0
32	MG	A	3402	1/1	0.20	-	52,52,52,52	0
32	MG	A	3303	1/1	1.44	-	52,52,52,52	0
32	MG	A	3623	1/1	0.19	-	62,62,62,62	0
32	MG	A	3581	1/1	0.15	-	86,86,86,86	0
32	MG	A	3223	1/1	0.58	-	62,62,62,62	0
32	MG	A	3394	1/1	0.15	-	56,56,56,56	0
32	MG	A	3422	1/1	0.31	-	85,85,85,85	0
32	MG	B	207	1/1	0.24	-	79,79,79,79	0
32	MG	A	3579	1/1	0.62	-	81,81,81,81	0
32	MG	Q	202	1/1	0.37	-	77,77,77,77	0
32	MG	A	3192	1/1	0.37	-	91,91,91,91	0
32	MG	A	3465	1/1	0.28	-	78,78,78,78	0
32	MG	A	3131	1/1	0.14	-	50,50,50,50	0
32	MG	A	3542	1/1	0.30	-	39,39,39,39	0
32	MG	A	3148	1/1	0.79	-	66,66,66,66	0
32	MG	A	3252	1/1	0.41	-	67,67,67,67	0
32	MG	A	3132	1/1	0.29	-	50,50,50,50	0
32	MG	F	302	1/1	0.60	-	75,75,75,75	0
32	MG	A	3038	1/1	0.46	-	67,67,67,67	0
32	MG	A	3666	1/1	0.14	-	94,94,94,94	0
32	MG	A	3445	1/1	0.40	-	61,61,61,61	0
32	MG	A	3434	1/1	0.10	-	54,54,54,54	0
32	MG	A	3278	1/1	0.41	-	86,86,86,86	0
32	MG	B	201	1/1	0.20	-	61,61,61,61	0
32	MG	A	3437	1/1	0.39	-	62,62,62,62	0
32	MG	A	3174	1/1	0.39	-	58,58,58,58	0
32	MG	A	3344	1/1	0.25	-	43,43,43,43	0
32	MG	A	3474	1/1	0.12	-	45,45,45,45	0
32	MG	A	3471	1/1	0.34	-	85,85,85,85	0
32	MG	A	3554	1/1	0.31	-	88,88,88,88	0
32	MG	A	3380	1/1	0.13	-	55,55,55,55	0
32	MG	A	3031	1/1	0.37	-	61,61,61,61	0
32	MG	A	3313	1/1	0.46	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3587	1/1	0.17	-	57,57,57,57	0
32	MG	B	208	1/1	0.33	-	98,98,98,98	0
32	MG	A	3298	1/1	0.59	-	88,88,88,88	0
32	MG	A	3171	1/1	0.43	-	68,68,68,68	0
32	MG	A	3139	1/1	0.36	-	65,65,65,65	0
32	MG	A	3068	1/1	0.28	-	36,36,36,36	0
32	MG	A	3596	1/1	0.26	-	76,76,76,76	0
32	MG	A	3176	1/1	0.29	-	109,109,109,109	0
32	MG	A	3003	1/1	0.15	-	66,66,66,66	0
32	MG	A	3087	1/1	0.23	-	42,42,42,42	0
32	MG	A	3561	1/1	0.43	-	57,57,57,57	0
32	MG	1	101	1/1	0.34	-	61,61,61,61	0
32	MG	A	3526	1/1	0.12	-	54,54,54,54	0
32	MG	A	3325	1/1	0.36	-	71,71,71,71	0
32	MG	A	3408	1/1	0.12	-	52,52,52,52	0
32	MG	A	3558	1/1	0.39	-	82,82,82,82	0
32	MG	A	3150	1/1	0.12	-	45,45,45,45	0
32	MG	A	3291	1/1	0.85	-	76,76,76,76	0
32	MG	A	3245	1/1	0.36	-	73,73,73,73	0
32	MG	A	3072	1/1	0.32	-	76,76,76,76	0
32	MG	A	3242	1/1	0.26	-	67,67,67,67	0
32	MG	A	3537	1/1	0.56	-	83,83,83,83	0
32	MG	T	203	1/1	0.29	-	73,73,73,73	0
32	MG	A	3358	1/1	0.18	-	80,80,80,80	0
32	MG	A	3489	1/1	0.18	-	68,68,68,68	0
32	MG	A	3619	1/1	0.65	-	104,104,104,104	0
32	MG	A	3463	1/1	0.16	-	81,81,81,81	0
32	MG	A	3589	1/1	0.32	-	50,50,50,50	0
32	MG	A	3191	1/1	0.11	-	73,73,73,73	0
32	MG	A	3423	1/1	0.17	-	46,46,46,46	0
32	MG	A	3565	1/1	0.16	-	65,65,65,65	0
32	MG	A	3254	1/1	0.36	-	68,68,68,68	0
32	MG	A	3367	1/1	0.39	-	89,89,89,89	0
32	MG	A	3393	1/1	0.19	-	60,60,60,60	0
32	MG	A	3582	1/1	0.09	-	69,69,69,69	0
32	MG	A	3655	1/1	0.25	-	87,87,87,87	0
32	MG	A	3275	1/1	0.64	-	69,69,69,69	0
32	MG	A	3124	1/1	0.30	-	66,66,66,66	0
32	MG	A	3457	1/1	0.22	-	91,91,91,91	0
32	MG	A	3335	1/1	1.10	-	67,67,67,67	0
32	MG	A	3385	1/1	0.15	-	58,58,58,58	0
32	MG	A	3505	1/1	0.15	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3604	1/1	0.27	-	98,98,98,98	0
32	MG	A	3277	1/1	0.33	-	83,83,83,83	0
32	MG	A	3092	1/1	1.19	-	60,60,60,60	0
32	MG	A	3672	1/1	0.39	-	90,90,90,90	0
32	MG	A	3091	1/1	0.32	-	45,45,45,45	0
32	MG	A	3528	1/1	0.27	-	96,96,96,96	0
32	MG	A	3189	1/1	0.30	-	53,53,53,53	0
32	MG	A	3147	1/1	0.66	-	82,82,82,82	0
32	MG	B	216	1/1	0.14	-	109,109,109,109	0
32	MG	A	3638	1/1	0.13	-	53,53,53,53	0
32	MG	A	3051	1/1	0.51	-	50,50,50,50	0
32	MG	A	3648	1/1	0.24	-	79,79,79,79	0
32	MG	A	3649	1/1	0.33	-	77,77,77,77	0
32	MG	A	3455	1/1	0.53	-	104,104,104,104	0
32	MG	B	212	1/1	0.25	-	111,111,111,111	0
32	MG	A	3073	1/1	0.30	-	64,64,64,64	0
32	MG	D	302	1/1	0.35	-	59,59,59,59	0
32	MG	A	3081	1/1	0.15	-	77,77,77,77	0
32	MG	A	3228	1/1	0.77	-	62,62,62,62	0
32	MG	A	3079	1/1	0.20	-	47,47,47,47	0
32	MG	A	3614	1/1	0.23	-	82,82,82,82	0
32	MG	A	3013	1/1	1.29	-	76,76,76,76	0
32	MG	A	3204	1/1	0.61	-	46,46,46,46	0
32	MG	A	3496	1/1	0.15	-	66,66,66,66	0
32	MG	A	3347	1/1	0.33	-	51,51,51,51	0
32	MG	A	3164	1/1	0.43	-	75,75,75,75	0
32	MG	A	3332	1/1	0.95	-	79,79,79,79	0
32	MG	A	3486	1/1	0.14	-	47,47,47,47	0
32	MG	6	103	1/1	0.53	-	93,93,93,93	0
32	MG	A	3439	1/1	0.24	-	45,45,45,45	0
32	MG	A	3301	1/1	0.30	-	52,52,52,52	0
32	MG	A	3034	1/1	0.22	-	79,79,79,79	0
32	MG	A	3396	1/1	0.12	-	48,48,48,48	0
32	MG	A	3478	1/1	0.43	-	73,73,73,73	0
32	MG	A	3341	1/1	0.47	-	57,57,57,57	0
32	MG	A	3063	1/1	0.18	-	84,84,84,84	0
32	MG	A	3336	1/1	1.10	-	70,70,70,70	0
32	MG	A	3572	1/1	0.37	-	85,85,85,85	0
32	MG	B	215	1/1	1.01	-	94,94,94,94	0
32	MG	A	3307	1/1	0.67	-	83,83,83,83	0
32	MG	F	301	1/1	0.33	-	71,71,71,71	0
32	MG	A	3021	1/1	0.21	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3232	1/1	0.28	-	78,78,78,78	0
32	MG	A	3109	1/1	0.31	-	37,37,37,37	0
32	MG	A	3584	1/1	0.18	-	44,44,44,44	0
32	MG	A	3343	1/1	0.26	-	80,80,80,80	0
32	MG	A	3686	1/1	0.46	-	96,96,96,96	0
32	MG	A	3472	1/1	0.16	-	63,63,63,63	0
32	MG	A	3010	1/1	0.31	-	46,46,46,46	0
32	MG	A	3563	1/1	0.10	-	42,42,42,42	0
32	MG	A	3568	1/1	0.22	-	50,50,50,50	0
32	MG	A	3640	1/1	0.29	-	43,43,43,43	0
32	MG	A	3210	1/1	0.17	-	82,82,82,82	0
32	MG	A	3177	1/1	0.76	-	77,77,77,77	0
32	MG	A	3374	1/1	0.15	-	51,51,51,51	0
32	MG	A	3299	1/1	0.71	-	72,72,72,72	0
32	MG	A	3370	1/1	0.19	-	84,84,84,84	0
32	MG	A	3071	1/1	0.64	-	82,82,82,82	0
32	MG	A	3286	1/1	0.28	-	81,81,81,81	0
32	MG	O	201	1/1	0.17	-	79,79,79,79	0
32	MG	A	3609	1/1	0.19	-	39,39,39,39	0
32	MG	A	3095	1/1	0.34	-	58,58,58,58	0
32	MG	A	3685	1/1	0.30	-	107,107,107,107	0
32	MG	A	3039	1/1	0.67	-	60,60,60,60	0
32	MG	A	3137	1/1	1.21	-	80,80,80,80	0
32	MG	A	3682	1/1	0.15	-	46,46,46,46	0
32	MG	A	3146	1/1	0.80	-	82,82,82,82	0
32	MG	A	3428	1/1	0.30	-	66,66,66,66	0
33	ZN	Y	201	1/1	0.04	-	123,123,123,123	0
32	MG	A	3318	1/1	0.50	-	63,63,63,63	0
32	MG	A	3351	1/1	0.76	-	60,60,60,60	0
32	MG	A	3328	1/1	0.68	-	74,74,74,74	0
32	MG	A	3432	1/1	0.10	-	56,56,56,56	0
32	MG	A	3009	1/1	0.36	-	58,58,58,58	0
32	MG	A	3338	1/1	0.30	-	77,77,77,77	0
32	MG	A	3620	1/1	0.20	-	47,47,47,47	0
32	MG	A	3012	1/1	0.53	-	60,60,60,60	0
32	MG	A	3200	1/1	0.54	-	83,83,83,83	0
32	MG	A	3218	1/1	0.54	-	52,52,52,52	0
32	MG	A	3418	1/1	0.17	-	53,53,53,53	0
32	MG	A	3121	1/1	0.20	-	66,66,66,66	0
32	MG	A	3320	1/1	0.44	-	77,77,77,77	0
32	MG	A	3514	1/1	0.67	-	99,99,99,99	0
32	MG	A	3314	1/1	0.90	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3076	1/1	0.57	-	73,73,73,73	0
32	MG	A	3220	1/1	0.56	-	74,74,74,74	0
32	MG	A	3578	1/1	0.11	-	109,109,109,109	0
32	MG	A	3548	1/1	0.32	-	59,59,59,59	0
32	MG	A	3197	1/1	0.33	-	91,91,91,91	0
32	MG	A	3088	1/1	0.25	-	45,45,45,45	0
32	MG	A	3128	1/1	0.46	-	64,64,64,64	0
32	MG	A	3631	1/1	0.10	-	50,50,50,50	0
32	MG	A	3041	1/1	0.48	-	55,55,55,55	0
32	MG	A	3194	1/1	0.41	-	68,68,68,68	0
32	MG	A	3375	1/1	0.16	-	48,48,48,48	0
32	MG	A	3165	1/1	0.96	-	67,67,67,67	0
32	MG	A	3637	1/1	0.28	-	70,70,70,70	0
32	MG	A	3352	1/1	0.82	-	75,75,75,75	0
32	MG	B	202	1/1	0.28	-	73,73,73,73	0
32	MG	A	3016	1/1	0.39	-	56,56,56,56	0
32	MG	A	3261	1/1	0.37	-	68,68,68,68	0
32	MG	A	3534	1/1	0.48	-	79,79,79,79	0
32	MG	A	3424	1/1	0.22	-	48,48,48,48	0
32	MG	A	3621	1/1	0.31	-	94,94,94,94	0
32	MG	A	3507	1/1	0.19	-	64,64,64,64	0
32	MG	A	3136	1/1	0.71	-	70,70,70,70	0
32	MG	A	3381	1/1	0.10	-	48,48,48,48	0
32	MG	A	3664	1/1	0.09	-	105,105,105,105	0
32	MG	A	3425	1/1	0.19	-	70,70,70,70	0
32	MG	A	3263	1/1	0.57	-	70,70,70,70	0
32	MG	A	3116	1/1	0.17	-	37,37,37,37	0
32	MG	A	3022	1/1	0.51	-	77,77,77,77	0
32	MG	A	3656	1/1	0.23	-	100,100,100,100	0
32	MG	A	3625	1/1	0.15	-	88,88,88,88	0
32	MG	A	3527	1/1	0.48	-	68,68,68,68	0
32	MG	A	3337	1/1	0.43	-	77,77,77,77	0
32	MG	A	3642	1/1	0.19	-	85,85,85,85	0
32	MG	A	3306	1/1	1.44	-	84,84,84,84	0
32	MG	A	3334	1/1	0.69	-	88,88,88,88	0
32	MG	A	3540	1/1	0.13	-	42,42,42,42	0
32	MG	A	3387	1/1	0.11	-	35,35,35,35	0
32	MG	A	3627	1/1	0.28	-	57,57,57,57	0
32	MG	A	3480	1/1	0.16	-	45,45,45,45	0
32	MG	A	3683	1/1	0.46	-	103,103,103,103	0
32	MG	A	3543	1/1	0.14	-	46,46,46,46	0
32	MG	A	3100	1/1	0.61	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3024	1/1	0.38	-	57,57,57,57	0
32	MG	A	3140	1/1	0.20	-	45,45,45,45	0
32	MG	A	3075	1/1	0.39	-	40,40,40,40	0
32	MG	A	3103	1/1	0.73	-	75,75,75,75	0
32	MG	A	3399	1/1	0.13	-	64,64,64,64	0
32	MG	A	3415	1/1	0.08	-	50,50,50,50	0
32	MG	A	3506	1/1	0.10	-	50,50,50,50	0
32	MG	A	3061	1/1	0.32	-	63,63,63,63	0
32	MG	A	3508	1/1	0.19	-	46,46,46,46	0
32	MG	A	3574	1/1	0.05	-	76,76,76,76	0
32	MG	A	3058	1/1	1.37	-	74,74,74,74	0
32	MG	A	3662	1/1	0.13	-	87,87,87,87	0
32	MG	A	3417	1/1	0.25	-	45,45,45,45	0
32	MG	A	3181	1/1	0.45	-	71,71,71,71	0
32	MG	A	3384	1/1	0.06	-	36,36,36,36	0
32	MG	A	3078	1/1	1.05	-	76,76,76,76	0
32	MG	A	3234	1/1	0.65	-	39,39,39,39	0
32	MG	A	3227	1/1	0.68	-	65,65,65,65	0
32	MG	A	3327	1/1	0.62	-	69,69,69,69	0
32	MG	A	3615	1/1	0.19	-	80,80,80,80	0
32	MG	A	3049	1/1	0.88	-	78,78,78,78	0
32	MG	A	3364	1/1	0.96	-	75,75,75,75	0
32	MG	A	3484	1/1	0.28	-	70,70,70,70	0
32	MG	A	3473	1/1	0.18	-	84,84,84,84	0
32	MG	A	3441	1/1	0.23	-	39,39,39,39	0
32	MG	A	3240	1/1	0.23	-	62,62,62,62	0
32	MG	A	3244	1/1	0.82	-	72,72,72,72	0
32	MG	U	201	1/1	0.47	-	72,72,72,72	0
32	MG	A	3646	1/1	0.17	-	90,90,90,90	0
32	MG	A	3483	1/1	0.39	-	80,80,80,80	0
32	MG	A	3202	1/1	1.06	-	89,89,89,89	0
32	MG	A	3464	1/1	0.22	-	76,76,76,76	0
32	MG	A	3636	1/1	0.20	-	62,62,62,62	0
32	MG	A	3361	1/1	1.17	-	65,65,65,65	0
32	MG	A	3670	1/1	0.23	-	79,79,79,79	0
32	MG	A	3354	1/1	0.27	-	94,94,94,94	0
32	MG	A	3265	1/1	0.29	-	63,63,63,63	0
32	MG	A	3529	1/1	0.23	-	102,102,102,102	0
32	MG	A	3294	1/1	0.24	-	76,76,76,76	0
32	MG	A	3577	1/1	0.71	-	86,86,86,86	0
32	MG	A	3154	1/1	0.50	-	65,65,65,65	0
32	MG	A	3650	1/1	0.21	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3284	1/1	0.21	-	75,75,75,75	0
32	MG	A	3419	1/1	0.23	-	73,73,73,73	0
32	MG	A	3117	1/1	0.30	-	59,59,59,59	0
32	MG	A	3098	1/1	0.40	-	60,60,60,60	0
32	MG	A	3292	1/1	0.23	-	54,54,54,54	0
32	MG	A	3005	1/1	0.35	-	69,69,69,69	0
32	MG	A	3667	1/1	0.18	-	51,51,51,51	0
32	MG	A	3125	1/1	0.70	-	67,67,67,67	0
32	MG	A	3089	1/1	0.29	-	53,53,53,53	0
32	MG	A	3329	1/1	0.39	-	55,55,55,55	0
32	MG	A	3586	1/1	0.38	-	67,67,67,67	0
32	MG	V	201	1/1	0.70	-	62,62,62,62	0
32	MG	A	3053	1/1	0.91	-	59,59,59,59	0
32	MG	A	3599	1/1	0.81	-	75,75,75,75	0
32	MG	A	3414	1/1	0.11	-	72,72,72,72	0
32	MG	A	3512	1/1	0.39	-	76,76,76,76	0
32	MG	A	3285	1/1	1.63	-	80,80,80,80	0
32	MG	A	3635	1/1	0.23	-	93,93,93,93	0
32	MG	A	3216	1/1	0.37	-	79,79,79,79	0
32	MG	A	3535	1/1	0.14	-	83,83,83,83	0
33	ZN	9	101	1/1	0.10	-	117,117,117,117	0
32	MG	A	3056	1/1	0.23	-	44,44,44,44	0
32	MG	A	3241	1/1	0.13	-	58,58,58,58	0
32	MG	A	3309	1/1	0.46	-	56,56,56,56	0
32	MG	A	3657	1/1	0.17	-	74,74,74,74	0
32	MG	A	3458	1/1	0.06	-	80,80,80,80	0
32	MG	A	3195	1/1	0.51	-	92,92,92,92	0
32	MG	A	3179	1/1	0.77	-	70,70,70,70	0
32	MG	A	3182	1/1	0.30	-	67,67,67,67	0
32	MG	A	3590	1/1	0.40	-	57,57,57,57	0
32	MG	A	3430	1/1	0.24	-	47,47,47,47	0
32	MG	A	3221	1/1	0.49	-	91,91,91,91	0
32	MG	A	3503	1/1	0.23	-	59,59,59,59	0
32	MG	A	3273	1/1	0.43	-	75,75,75,75	0
32	MG	A	3015	1/1	1.12	-	72,72,72,72	0
32	MG	A	3549	1/1	0.33	-	76,76,76,76	0
32	MG	A	3014	1/1	0.23	-	64,64,64,64	0
32	MG	A	3467	1/1	0.20	-	78,78,78,78	0
32	MG	0	101	1/1	1.41	-	99,99,99,99	0
33	ZN	6	101	1/1	0.09	-	106,106,106,106	0
32	MG	A	3326	1/1	0.46	-	65,65,65,65	0
32	MG	A	3608	1/1	0.22	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3522	1/1	0.24	-	90,90,90,90	0
32	MG	A	3461	1/1	0.23	-	87,87,87,87	0
32	MG	A	3539	1/1	0.37	-	87,87,87,87	0
32	MG	A	3163	1/1	1.38	-	68,68,68,68	0
32	MG	A	3077	1/1	0.55	-	82,82,82,82	0
32	MG	A	3676	1/1	0.14	-	74,74,74,74	0
32	MG	A	3520	1/1	0.14	-	72,72,72,72	0
32	MG	A	3279	1/1	0.52	-	79,79,79,79	0
32	MG	X	101	1/1	0.43	-	55,55,55,55	0
32	MG	6	102	1/1	0.19	-	82,82,82,82	0
32	MG	B	206	1/1	0.93	-	77,77,77,77	0
32	MG	A	3239	1/1	0.23	-	62,62,62,62	0
32	MG	B	205	1/1	1.41	-	79,79,79,79	0
32	MG	A	3634	1/1	0.40	-	80,80,80,80	0
32	MG	A	3438	1/1	0.17	-	73,73,73,73	0
32	MG	A	3274	1/1	0.30	-	62,62,62,62	0
32	MG	A	3661	1/1	0.20	-	92,92,92,92	0
32	MG	A	3155	1/1	0.46	-	66,66,66,66	0
32	MG	A	3588	1/1	0.14	-	69,69,69,69	0
32	MG	A	3372	1/1	0.49	-	72,72,72,72	0
32	MG	A	3004	1/1	0.57	-	42,42,42,42	0
32	MG	A	3495	1/1	0.62	-	81,81,81,81	0
32	MG	A	3412	1/1	0.50	-	47,47,47,47	0
32	MG	A	3409	1/1	0.14	-	35,35,35,35	0
32	MG	A	3175	1/1	0.37	-	76,76,76,76	0
32	MG	A	3456	1/1	0.13	-	75,75,75,75	0
32	MG	A	3122	1/1	0.28	-	51,51,51,51	0
32	MG	A	3030	1/1	1.30	-	47,47,47,47	0
32	MG	A	3093	1/1	0.27	-	52,52,52,52	0
32	MG	A	3401	1/1	0.17	-	55,55,55,55	0
32	MG	A	3208	1/1	0.78	-	67,67,67,67	0
32	MG	A	3356	1/1	0.40	-	81,81,81,81	0
32	MG	A	3371	1/1	0.32	-	88,88,88,88	0
32	MG	A	3207	1/1	0.20	-	71,71,71,71	0
32	MG	A	3331	1/1	0.25	-	70,70,70,70	0
32	MG	A	3376	1/1	0.15	-	47,47,47,47	0
32	MG	A	3308	1/1	0.51	-	69,69,69,69	0
32	MG	A	3127	1/1	0.39	-	58,58,58,58	0
32	MG	A	3260	1/1	0.56	-	68,68,68,68	0
32	MG	A	3249	1/1	1.30	-	71,71,71,71	0
32	MG	A	3106	1/1	0.25	-	50,50,50,50	0
32	MG	A	3259	1/1	0.48	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3293	1/1	0.71	-	67,67,67,67	0
32	MG	E	304	1/1	0.91	-	70,70,70,70	0
32	MG	A	3517	1/1	0.45	-	81,81,81,81	0
32	MG	A	3652	1/1	0.13	-	53,53,53,53	0
32	MG	A	3156	1/1	0.46	-	67,67,67,67	0
32	MG	A	3295	1/1	0.19	-	106,106,106,106	0
32	MG	A	3060	1/1	0.35	-	65,65,65,65	0
32	MG	A	3511	1/1	0.31	-	60,60,60,60	0
32	MG	A	3183	1/1	0.44	-	65,65,65,65	0
32	MG	A	3515	1/1	0.36	-	77,77,77,77	0
32	MG	A	3086	1/1	0.20	-	39,39,39,39	0
32	MG	A	3258	1/1	0.15	-	85,85,85,85	0
32	MG	A	3007	1/1	0.17	-	65,65,65,65	0
32	MG	A	3607	1/1	0.19	-	86,86,86,86	0
32	MG	A	3251	1/1	0.41	-	67,67,67,67	0
32	MG	A	3349	1/1	0.16	-	59,59,59,59	0
32	MG	A	3426	1/1	0.20	-	50,50,50,50	0
32	MG	A	3645	1/1	0.20	-	75,75,75,75	0
32	MG	A	3530	1/1	0.13	-	57,57,57,57	0
32	MG	A	3678	1/1	0.88	-	80,80,80,80	0
32	MG	A	3144	1/1	0.17	-	56,56,56,56	0
32	MG	A	3679	1/1	0.27	-	104,104,104,104	0
32	MG	A	3212	1/1	0.60	-	70,70,70,70	0
32	MG	A	3536	1/1	0.17	-	73,73,73,73	0
32	MG	A	3052	1/1	0.35	-	66,66,66,66	0
32	MG	A	3466	1/1	0.12	-	71,71,71,71	0
32	MG	A	3316	1/1	0.78	-	64,64,64,64	0
32	MG	A	3236	1/1	0.33	-	58,58,58,58	0
32	MG	A	3027	1/1	0.34	-	50,50,50,50	0
32	MG	A	3624	1/1	0.13	-	70,70,70,70	0
32	MG	A	3518	1/1	0.49	-	88,88,88,88	0
32	MG	A	3226	1/1	0.35	-	61,61,61,61	0
32	MG	A	3110	1/1	0.44	-	65,65,65,65	0
32	MG	A	3193	1/1	0.55	-	76,76,76,76	0
32	MG	A	3330	1/1	0.52	-	60,60,60,60	0
32	MG	B	211	1/1	0.24	-	83,83,83,83	0
32	MG	B	210	1/1	0.37	-	91,91,91,91	0
32	MG	A	3111	1/1	0.32	-	61,61,61,61	0
32	MG	A	3544	1/1	0.22	-	49,49,49,49	0
32	MG	A	3462	1/1	0.34	-	78,78,78,78	0
32	MG	A	3168	1/1	0.28	-	67,67,67,67	0
32	MG	A	3248	1/1	0.89	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3618	1/1	0.30	-	80,80,80,80	0
32	MG	A	3043	1/1	1.11	-	57,57,57,57	0
32	MG	A	3499	1/1	0.14	-	122,122,122,122	0
32	MG	A	3482	1/1	0.17	-	63,63,63,63	0
32	MG	A	3018	1/1	0.52	-	66,66,66,66	0
32	MG	A	3119	1/1	0.41	-	52,52,52,52	0
32	MG	A	3120	1/1	0.23	-	46,46,46,46	0
32	MG	T	202	1/1	0.34	-	38,38,38,38	0
32	MG	A	3158	1/1	0.29	-	51,51,51,51	0
32	MG	A	3521	1/1	0.42	-	66,66,66,66	0
32	MG	A	3566	1/1	0.23	-	75,75,75,75	0
32	MG	A	3377	1/1	0.10	-	40,40,40,40	0
32	MG	A	3346	1/1	0.21	-	85,85,85,85	0
32	MG	A	3674	1/1	0.34	-	98,98,98,98	0
32	MG	A	3345	1/1	0.26	-	55,55,55,55	0
32	MG	A	3282	1/1	0.23	-	94,94,94,94	0
32	MG	A	3436	1/1	0.12	-	40,40,40,40	0
32	MG	A	3386	1/1	0.10	-	37,37,37,37	0
32	MG	A	3383	1/1	0.16	-	63,63,63,63	0
32	MG	B	203	1/1	0.28	-	105,105,105,105	0
32	MG	A	3129	1/1	0.26	-	44,44,44,44	0
32	MG	A	3246	1/1	0.29	-	51,51,51,51	0
32	MG	A	3632	1/1	0.39	-	71,71,71,71	0
32	MG	A	3598	1/1	0.15	-	82,82,82,82	0
32	MG	A	3491	1/1	0.15	-	81,81,81,81	0
32	MG	A	3001	1/1	0.24	-	97,97,97,97	0
32	MG	A	3287	1/1	0.65	-	55,55,55,55	0
32	MG	A	3421	1/1	0.09	-	33,33,33,33	0
32	MG	A	3510	1/1	0.20	-	67,67,67,67	0
32	MG	A	3280	1/1	0.28	-	50,50,50,50	0
32	MG	A	3553	1/1	0.22	-	73,73,73,73	0
32	MG	A	3002	1/1	0.18	-	38,38,38,38	0
32	MG	A	3196	1/1	0.29	-	74,74,74,74	0
32	MG	A	3070	1/1	0.25	-	89,89,89,89	0
32	MG	A	3413	1/1	0.16	-	45,45,45,45	0
32	MG	A	3591	1/1	0.20	-	53,53,53,53	0
32	MG	D	301	1/1	0.36	-	48,48,48,48	0
32	MG	A	3498	1/1	0.22	-	87,87,87,87	0
32	MG	A	3262	1/1	0.41	-	62,62,62,62	0
32	MG	A	3008	1/1	0.34	-	75,75,75,75	0
32	MG	A	3570	1/1	0.31	-	76,76,76,76	0
32	MG	A	3602	1/1	0.25	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3032	1/1	0.21	-	62,62,62,62	0
32	MG	A	3448	1/1	0.29	-	49,49,49,49	0
32	MG	A	3524	1/1	0.15	-	73,73,73,73	0
32	MG	A	3035	1/1	0.27	-	65,65,65,65	0
32	MG	A	3065	1/1	0.49	-	74,74,74,74	0
32	MG	A	3219	1/1	0.43	-	68,68,68,68	0
32	MG	A	3304	1/1	0.21	-	47,47,47,47	0
32	MG	A	3485	1/1	0.17	-	62,62,62,62	0
32	MG	O	102	1/1	0.14	-	55,55,55,55	0
32	MG	A	3083	1/1	0.29	-	41,41,41,41	0
32	MG	A	3205	1/1	0.43	-	46,46,46,46	0
32	MG	A	3045	1/1	0.66	-	66,66,66,66	0
32	MG	A	3215	1/1	0.66	-	62,62,62,62	0
32	MG	A	3487	1/1	0.25	-	70,70,70,70	0
32	MG	A	3653	1/1	0.38	-	81,81,81,81	0
32	MG	A	3395	1/1	0.24	-	43,43,43,43	0
32	MG	A	3126	1/1	0.20	-	39,39,39,39	0
32	MG	A	3673	1/1	0.16	-	94,94,94,94	0
32	MG	A	3459	1/1	0.24	-	84,84,84,84	0
32	MG	A	3663	1/1	0.19	-	111,111,111,111	0
32	MG	A	3143	1/1	0.40	-	65,65,65,65	0
32	MG	A	3559	1/1	0.12	-	76,76,76,76	0
32	MG	A	3256	1/1	0.29	-	66,66,66,66	0
32	MG	A	3214	1/1	0.25	-	43,43,43,43	0
32	MG	A	3369	1/1	0.62	-	80,80,80,80	0
32	MG	A	3407	1/1	0.19	-	46,46,46,46	0
32	MG	A	3477	1/1	0.17	-	70,70,70,70	0
32	MG	A	3040	1/1	0.92	-	79,79,79,79	0
32	MG	A	3141	1/1	0.61	-	69,69,69,69	0
32	MG	A	3450	1/1	0.19	-	67,67,67,67	0
32	MG	A	3271	1/1	0.49	-	75,75,75,75	0
32	MG	A	3545	1/1	0.21	-	94,94,94,94	0
32	MG	A	3042	1/1	0.51	-	78,78,78,78	0
32	MG	A	3593	1/1	0.43	-	100,100,100,100	0
32	MG	A	3541	1/1	0.17	-	42,42,42,42	0
32	MG	A	3613	1/1	0.20	-	85,85,85,85	0
32	MG	A	3104	1/1	0.43	-	79,79,79,79	0
32	MG	A	3668	1/1	0.82	-	89,89,89,89	0
32	MG	A	3427	1/1	0.20	-	70,70,70,70	0
32	MG	A	3317	1/1	0.39	-	59,59,59,59	0
32	MG	A	3355	1/1	0.25	-	71,71,71,71	0
32	MG	E	303	1/1	0.58	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3310	1/1	0.28	-	50,50,50,50	0
32	MG	A	3560	1/1	0.55	-	79,79,79,79	0
32	MG	A	3525	1/1	0.37	-	96,96,96,96	0
32	MG	A	3017	1/1	0.41	-	68,68,68,68	0
32	MG	A	3628	1/1	0.27	-	48,48,48,48	0
32	MG	E	302	1/1	0.61	-	55,55,55,55	0
33	ZN	4	101	1/1	0.13	-	178,178,178,178	0
32	MG	A	3501	1/1	0.23	-	77,77,77,77	0
32	MG	A	3616	1/1	0.31	-	103,103,103,103	0
32	MG	A	3435	1/1	0.10	-	43,43,43,43	0
32	MG	A	3296	1/1	0.39	-	65,65,65,65	0
32	MG	A	3594	1/1	0.38	-	97,97,97,97	0
32	MG	A	3400	1/1	0.23	-	55,55,55,55	0
32	MG	A	3184	1/1	0.37	-	58,58,58,58	0
32	MG	A	3546	1/1	0.14	-	58,58,58,58	0
32	MG	A	3302	1/1	0.63	-	74,74,74,74	0
32	MG	A	3580	1/1	0.38	-	89,89,89,89	0
32	MG	A	3186	1/1	0.63	-	82,82,82,82	0
32	MG	A	3203	1/1	0.29	-	64,64,64,64	0
32	MG	A	3359	1/1	0.58	-	94,94,94,94	0
32	MG	D	303	1/1	0.77	-	65,65,65,65	0
32	MG	A	3243	1/1	0.25	-	71,71,71,71	0
32	MG	A	3460	1/1	0.49	-	73,73,73,73	0
32	MG	A	3023	1/1	1.26	-	76,76,76,76	0
32	MG	A	3433	1/1	0.19	-	70,70,70,70	0
32	MG	A	3519	1/1	0.23	-	82,82,82,82	0
32	MG	A	3404	1/1	0.71	-	50,50,50,50	0
32	MG	A	3601	1/1	0.64	-	80,80,80,80	0
32	MG	A	3020	1/1	0.28	-	51,51,51,51	0
32	MG	B	213	1/1	0.56	-	115,115,115,115	0
32	MG	A	3138	1/1	0.25	-	51,51,51,51	0
32	MG	A	3573	1/1	0.48	-	96,96,96,96	0
32	MG	A	3237	1/1	0.40	-	53,53,53,53	0
32	MG	A	3431	1/1	0.19	-	72,72,72,72	0
32	MG	A	3217	1/1	0.64	-	90,90,90,90	0
32	MG	A	3054	1/1	0.39	-	68,68,68,68	0
32	MG	A	3348	1/1	0.13	-	60,60,60,60	0
32	MG	A	3658	1/1	0.17	-	100,100,100,100	0
32	MG	A	3029	1/1	0.55	-	54,54,54,54	0
32	MG	A	3647	1/1	0.31	-	89,89,89,89	0
32	MG	A	3502	1/1	0.33	-	49,49,49,49	0
32	MG	A	3630	1/1	0.21	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3671	1/1	0.23	-	71,71,71,71	0
32	MG	B	214	1/1	0.25	-	83,83,83,83	0
32	MG	A	3470	1/1	0.17	-	70,70,70,70	0
32	MG	A	3281	1/1	0.31	-	69,69,69,69	0
32	MG	A	3446	1/1	0.34	-	56,56,56,56	0
32	MG	A	3135	1/1	0.33	-	66,66,66,66	0
32	MG	A	3442	1/1	0.22	-	60,60,60,60	0
32	MG	A	3170	1/1	0.22	-	59,59,59,59	0
32	MG	A	3595	1/1	0.36	-	101,101,101,101	0
32	MG	A	3651	1/1	0.17	-	61,61,61,61	0
32	MG	A	3488	1/1	0.18	-	51,51,51,51	0
32	MG	A	3209	1/1	0.47	-	83,83,83,83	0
32	MG	A	3567	1/1	0.51	-	95,95,95,95	0
32	MG	A	3270	1/1	0.37	-	70,70,70,70	0
32	MG	A	3069	1/1	0.66	-	65,65,65,65	0
32	MG	A	3622	1/1	0.24	-	69,69,69,69	0
32	MG	A	3084	1/1	0.26	-	41,41,41,41	0
32	MG	A	3379	1/1	0.15	-	66,66,66,66	0
32	MG	Q	201	1/1	0.40	-	43,43,43,43	0
32	MG	A	3340	1/1	0.54	-	72,72,72,72	0
32	MG	A	3059	1/1	0.34	-	44,44,44,44	0
32	MG	A	3290	1/1	0.34	-	62,62,62,62	0
32	MG	A	3585	1/1	0.10	-	43,43,43,43	0
32	MG	A	3229	1/1	0.62	-	74,74,74,74	0
32	MG	A	3500	1/1	0.33	-	77,77,77,77	0
32	MG	A	3047	1/1	0.58	-	67,67,67,67	0
32	MG	A	3253	1/1	0.39	-	74,74,74,74	0
32	MG	A	3416	1/1	0.41	-	42,42,42,42	0
32	MG	A	3363	1/1	0.67	-	75,75,75,75	0
32	MG	A	3494	1/1	0.22	-	94,94,94,94	0
32	MG	A	3592	1/1	0.29	-	47,47,47,47	0
32	MG	A	3552	1/1	0.35	-	69,69,69,69	0
32	MG	F	303	1/1	0.31	-	77,77,77,77	0
32	MG	A	3289	1/1	0.28	-	55,55,55,55	0
32	MG	A	3231	1/1	0.89	-	77,77,77,77	0
32	MG	A	3112	1/1	0.31	-	50,50,50,50	0
32	MG	A	3339	1/1	0.36	-	72,72,72,72	0
32	MG	A	3199	1/1	1.23	-	74,74,74,74	0
32	MG	A	3555	1/1	0.25	-	50,50,50,50	0
32	MG	A	3454	1/1	0.18	-	82,82,82,82	0
32	MG	A	3311	1/1	0.15	-	52,52,52,52	0
32	MG	A	3447	1/1	0.36	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3297	1/1	0.15	-	60,60,60,60	0
32	MG	A	3090	1/1	0.34	-	60,60,60,60	0
32	MG	A	3353	1/1	0.56	-	64,64,64,64	0
32	MG	T	201	1/1	0.20	-	73,73,73,73	0
32	MG	A	3550	1/1	0.29	-	64,64,64,64	0
32	MG	A	3504	1/1	0.14	-	76,76,76,76	0
32	MG	A	3050	1/1	0.37	-	65,65,65,65	0
32	MG	A	3420	1/1	0.59	-	83,83,83,83	0
32	MG	A	3153	1/1	0.26	-	87,87,87,87	0
32	MG	A	3066	1/1	0.62	-	75,75,75,75	0
32	MG	A	3556	1/1	0.25	-	84,84,84,84	0
32	MG	A	3057	1/1	0.35	-	83,83,83,83	0
32	MG	A	3677	1/1	0.09	-	64,64,64,64	0
32	MG	A	3099	1/1	0.38	-	51,51,51,51	0
32	MG	A	3151	1/1	0.66	-	54,54,54,54	0
32	MG	A	3082	1/1	0.58	-	34,34,34,34	0
32	MG	A	3224	1/1	0.64	-	53,53,53,53	0
32	MG	A	3479	1/1	0.20	-	68,68,68,68	0
32	MG	A	3178	1/1	0.31	-	63,63,63,63	0
32	MG	A	3048	1/1	0.31	-	90,90,90,90	0
32	MG	A	3405	1/1	0.30	-	33,33,33,33	0
32	MG	A	3187	1/1	0.46	-	80,80,80,80	0
32	MG	A	3406	1/1	0.20	-	53,53,53,53	0
32	MG	A	3475	1/1	0.12	-	42,42,42,42	0
32	MG	A	3312	1/1	0.59	-	57,57,57,57	0
32	MG	A	3629	1/1	0.20	-	82,82,82,82	0
32	MG	A	3606	1/1	0.72	-	115,115,115,115	0
32	MG	A	3583	1/1	0.11	-	75,75,75,75	0
32	MG	A	3118	1/1	0.35	-	53,53,53,53	0
32	MG	A	3300	1/1	0.95	-	68,68,68,68	0
32	MG	A	3576	1/1	0.17	-	50,50,50,50	0
32	MG	A	3276	1/1	0.32	-	62,62,62,62	0
32	MG	A	3523	1/1	0.46	-	95,95,95,95	0
32	MG	A	3538	1/1	0.16	-	72,72,72,72	0
32	MG	A	3323	1/1	0.91	-	83,83,83,83	0
32	MG	A	3102	1/1	0.45	-	70,70,70,70	0
32	MG	A	3533	1/1	0.16	-	74,74,74,74	0
32	MG	A	3198	1/1	0.27	-	89,89,89,89	0
32	MG	A	3026	1/1	0.16	-	50,50,50,50	0
32	MG	A	3159	1/1	0.26	-	96,96,96,96	0
32	MG	A	3321	1/1	0.48	-	63,63,63,63	0
32	MG	A	3643	1/1	0.33	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3357	1/1	0.23	-	75,75,75,75	0
32	MG	A	3476	1/1	0.14	-	42,42,42,42	0
32	MG	A	3162	1/1	0.44	-	62,62,62,62	0

6.5 Other polymers

There are no such residues in this entry.