



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:52 AM UTC

PDB ID : 1KD1 / pdb_00001kd1
Title : Co-crystal Structure of Spiramycin bound to the 50S Ribosomal Subunit of Haloarcula marismortui
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-11-12
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

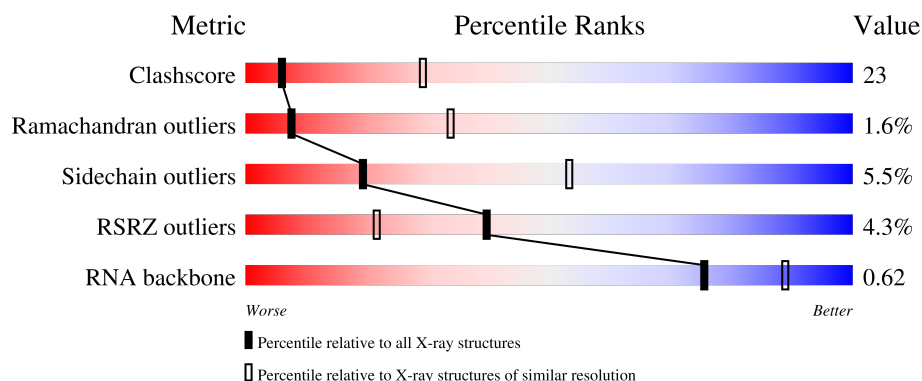
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2922	
2	B	122	
3	C	239	
4	D	337	
5	E	246	

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Mol	Chain	Length	Quality of chain
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	A	8054	-	-	X	-
34	CL	O	8507	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98587 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	conflict	? 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O		0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O		0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O		0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S	150	Total	C	N	O	S	0	0
			1149	713	209	223	4		

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	T	81	Total	C	N	O	S	0	0
			641	389	111	138	3		

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O		0	0
			949	568	180	201			

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	53	Total	C	N	O	S	0	0
			410	244	75	86	5		

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	W	65	Total	C	N	O	S	0	0
			499	304	94	100	1		

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S	0	0
			1195	737	209	243	6		

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

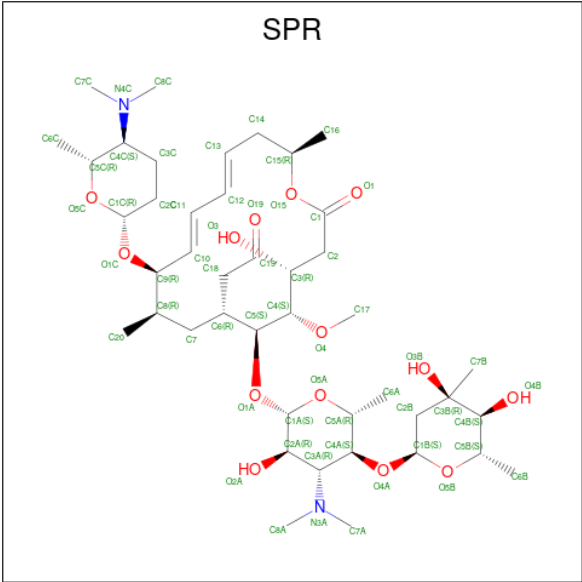
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is SPIRAMYCIN I (CCD ID: SPR) (formula: C₄₃H₇₄N₂O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			59	43	2	14		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	112	Total	Mg	0	0
			112	112		
32	B	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	1	1	Total	Mg	0	0
			1	1		
32	4	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	73	Total Na 73 73	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	J	1	Total Na 1 1	0	0
33	K	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0
33	N	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	2	Total Na 2 2	0	0
33	T	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	9	Total Cl 9 9	0	0
34	C	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	3	Total Cl 3 3	0	0
34	M	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0
34	P	1	Total Cl 1 1	0	0
34	R	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	S	1	Total 1	Cl 1	0	0
34	Z	1	Total 1	Cl 1	0	0
34	4	1	Total 1	Cl 1	0	0

- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	3	Total 3	K 3	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5910	Total 5910	O 5910	0	0
37	B	142	Total 142	O 142	0	0
37	C	126	Total 126	O 126	0	0
37	D	150	Total 150	O 150	0	0
37	E	169	Total 169	O 169	0	0
37	F	51	Total 51	O 51	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	26	Total 26	O 26	0	0
37	I	21	Total 21	O 21	0	0
37	J	78	Total 78	O 78	0	0
37	K	54	Total 54	O 54	0	0
37	L	65	Total 65	O 65	0	0
37	M	79	Total 79	O 79	0	0
37	N	132	Total 132	O 132	0	0
37	O	69	Total 69	O 69	0	0
37	P	45	Total 45	O 45	0	0
37	Q	65	Total 65	O 65	0	0
37	R	55	Total 55	O 55	0	0
37	S	83	Total 83	O 83	0	0
37	T	35	Total 35	O 35	0	0
37	U	39	Total 39	O 39	0	0
37	V	25	Total 25	O 25	0	0
37	W	15	Total 15	O 15	0	0
37	X	70	Total 70	O 70	0	0
37	Y	25	Total 25	O 25	0	0
37	Z	94	Total 94	O 94	0	0
37	1	41	Total 41	O 41	0	0

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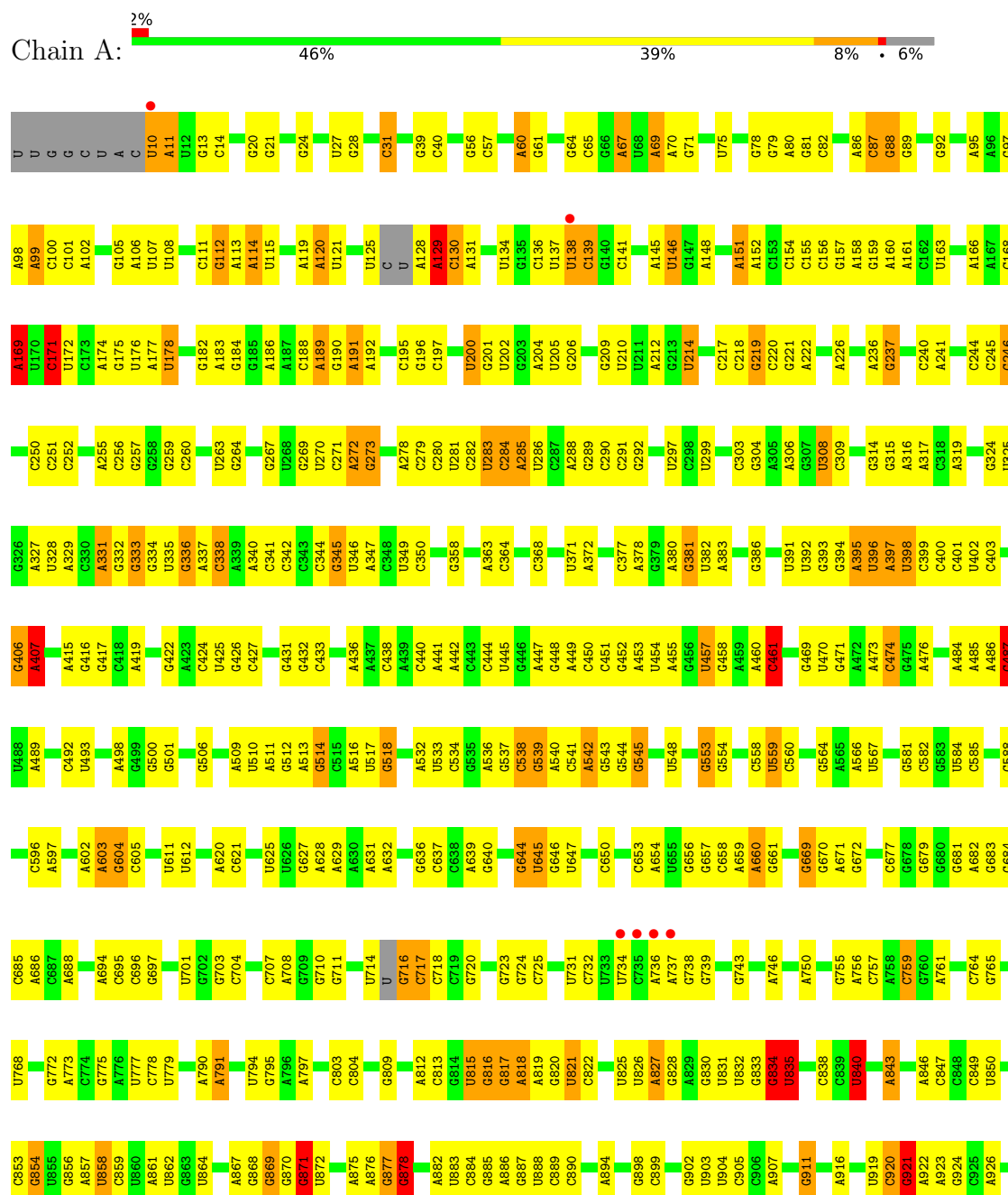
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	55	Total 55	O 55	0	0
37	3	42	Total 42	O 42	0	0
37	4	73	Total 73	O 73	0	0

3 Residue-property plots

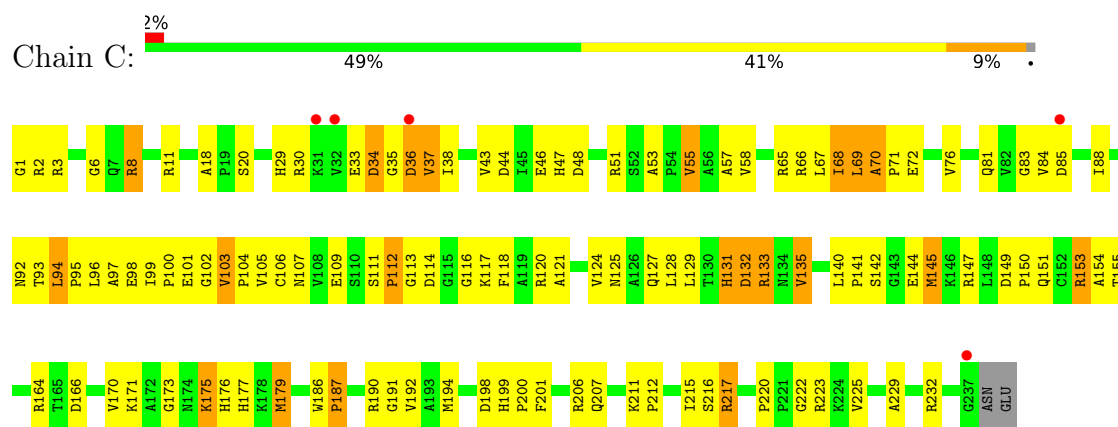
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 rRNA

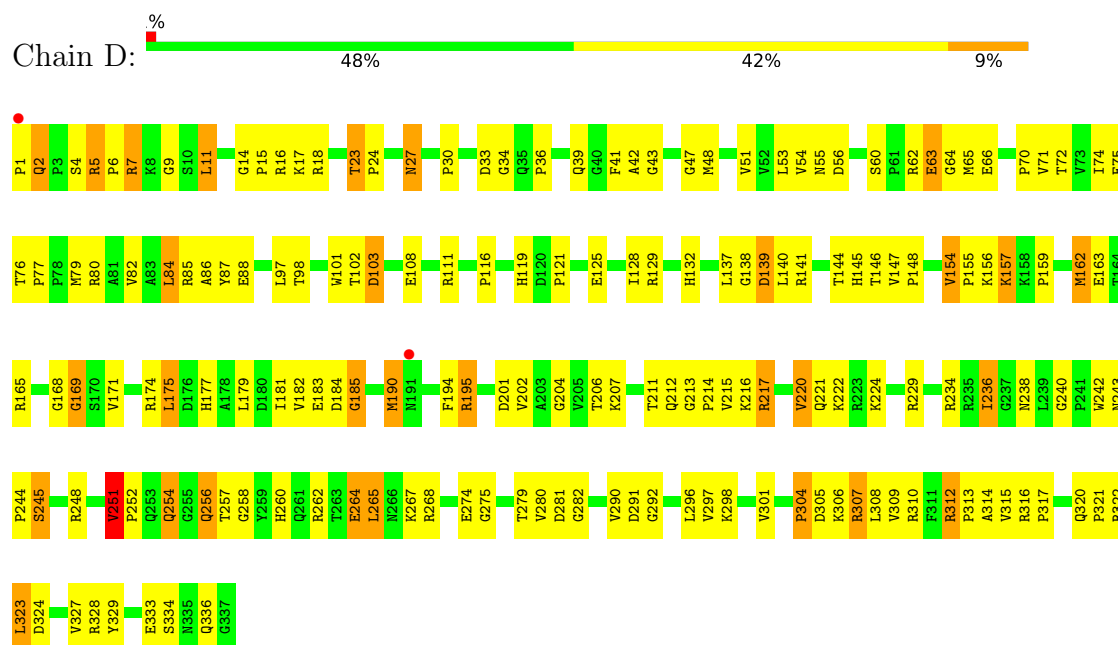


U2012	A1858	C1687	A1807	U1506	C1342	A1242	G1087	A1005	A929
G2013	A1859	G1688	G1608	C1507	U1347	C1243	A1088	A1006	U932
G2014	C1860	A1689	G1609	C1513	A1348	U1244	C1175	A1007	G940
A2015	C1861	U1770	G1610	C1514	U1435	C1245	U1095	C1008	G941
U2016	A1942	G1772	G1611	A1515	C1436	A1246	A1177	A1013	U942
A2019	C1863	G1773	A1612	C1516	G1351	U1249	U1096	A1014	A943
G2023	G1774	G1774	G1613	U1517	A1352	C1250	A1097	U1015	G946
U2030	A1778	A1778	U1440	U1441	C1353	C1251	A1180	C1019	G948
G2031	A1779	U1779	A1442	A1443	A1358	U1260	A1181	A1020	U949
U2032	C1787	U1788	A1444	G1445	U1359	G1261	C1182	G1021	G950
G2033	G1789	A1701	G1446	U1447	C1360	C1262	C1183	A1022	A951
U2034	C1790	U1702	U1448	U1449	C1361	G1263	U1184	C1023	G952
G2035	U1791	G1707	U1450	C1451	U1362	U1264	A1114	G1024	G953
C2036	C1798	C1706	U1452	C1453	G1363	U1265	U1115	C1025	U954
C2037	G1798	G1707	G1533	A1534	U1368	G1266	U1116	G1026	A955
A2038	A1804	G1707	G1534	C1535	A1369	G1267	U1117	G1027	G958
A2039	G1805	A1710	C1536	C1537	G1370	U1268	A1118	U1028	C959
G2044	G1806	A1711	U1457	A1458	U1371	U1270	G1119	G1039	A961
G2045	G1807	A1712	A1459	A1460	A1375	A1278	U1120	A1040	C962
G2046	G1808	A1713	C1462	U1463	G1376	U1279	A1123	U1041	C963
C2047	C1810	C1720	U1464	U1465	G1377	U1288	C1126	U1042	
G2050	A1815	C1721	G1468	A1469	U1380	C1289	C1127	G1043	
G2053	G1816	U1722	C1469	C1470	U1381	G1290	U1128	G1044	
A2054	U1817	G1723	A1471	A1472	C1384	U1293	U1129	G1045	
G1971	C1818	C1725	A1473	C1474	U1389	U1298	G1130		
U1972	G1819	U1730	U1474	C1475	G1390	G1299	U1131		
A1973	G1820	C1731	U1476	U1477	A1391	C1300	A1132		
G1996	U1895	A1736	G1855	C1564	C1392	C1301	G1133		
A1974	U1897	C1738	A1856	C1565	A1393	G1302	U1136		
U1978	G1902	A1737	U1857	A1559	C1394	C1303	G1137		
G1979	A1909	C1738	A1858	U	G1398	U1298	U1139		
U1980	U1903	A1742	A1859	A1580	A1399	G1299	C1140		
A1981	A1904	C1735	A1860	A1581	G1402	C1301	G1151		
C1982	C1908	A1736	G1856	C1582	A1406	G1302	C1156		
U1983	A1912	U1741	A1857	A1583	A1407	U1218	C1157		
A1984	U1915	C1834	A1858	A1584	U1408	U1219	G1158		
G1995	C1916	U1835	A1859	A1585	A1409	U1220	G1159		
U1996	G1917	A1840	U1860	A1586	G1409	G1221	A1161		
C1997	U1918	C1841	A1861	A1587	U1414	C1229	G1072		
G2000	A1919	U1748	G1670	G1588	A1415	A1328	G1075		
G2001	C1920	G1751	C1592	C1593	G1416	A1329			
G2002	A1921	G1752	C1594	C1595	G1417	A1330			
G1923	U1922	C1753	G1596	G1597	U1418	A1331	A1079		
U2003	G1923	A1848	U1596	G1497	U1419	U1332	A1080		
A2085	A1924	U1849	C1680	G1497	U1419	U1333	A1081		
G2005	G1925	U1850	A1597	U1500	C1420	C1334	G1167		
C2088	G1926	G1851	A1598	U1501	C1421	C1335	A1082		
A2089	U1761	U1761	A1603	A1502	U1422	G1339	C1083		
G2090	G1855	A1684	G1604	U1503	A1423	G1239	C1084		
A1934	C1856	A1766	A1605	A1504	A1424	G1240	A1086		
G2092	C1935	A1767	C1686	U1505		G1241			

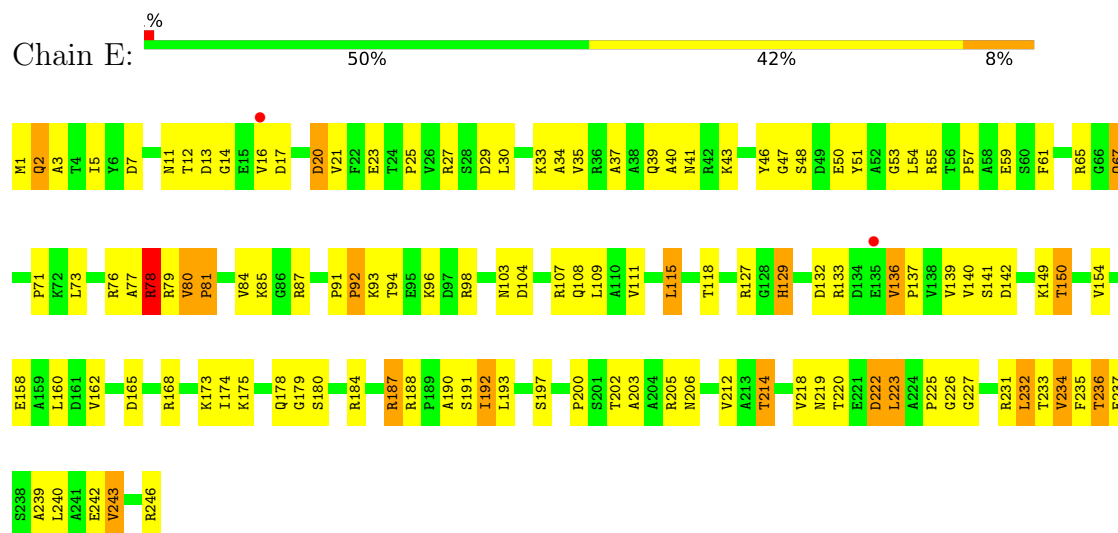




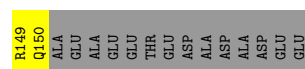
• Molecule 4: RIBOSOMAL PROTEIN L3



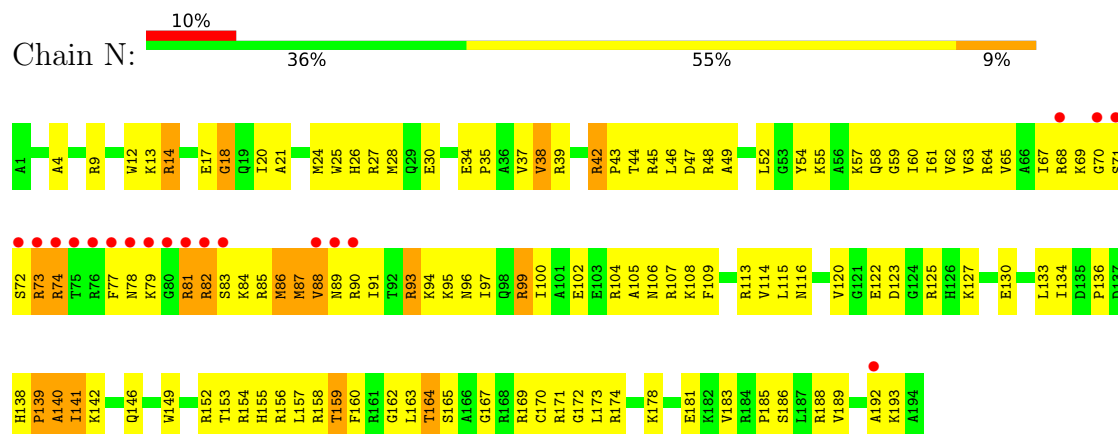
• Molecule 5: RIBOSOMAL PROTEIN L4



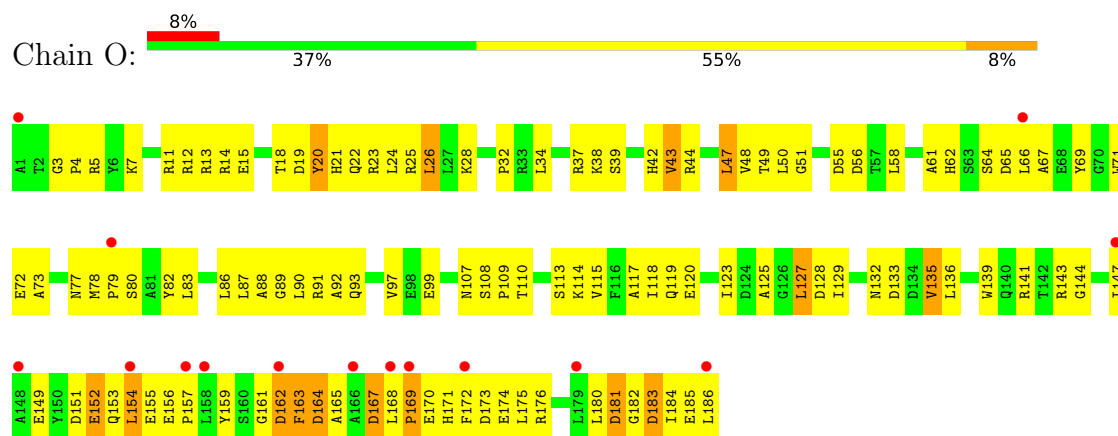
• Molecule 6: RIBOSOMAL PROTEIN L5



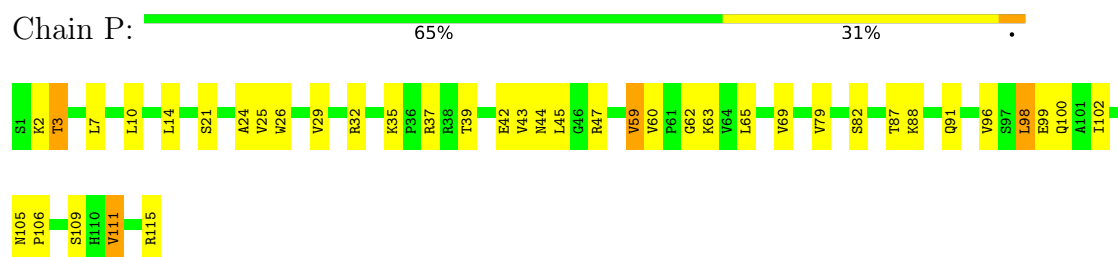
• Molecule 14: RIBOSOMAL PROTEIN L15E



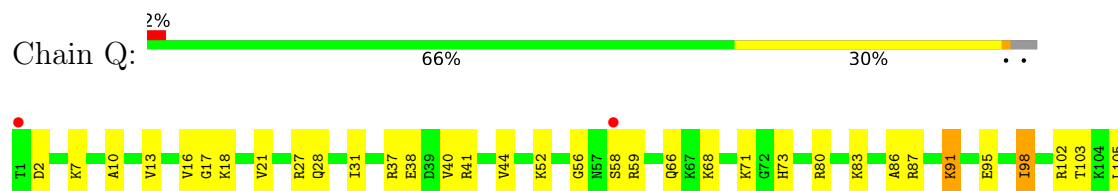
• Molecule 15: RIBOSOMAL PROTEIN L18



• Molecule 16: RIBOSOMAL PROTEIN L18E



• Molecule 17: RIBOSOMAL PROTEIN L19E

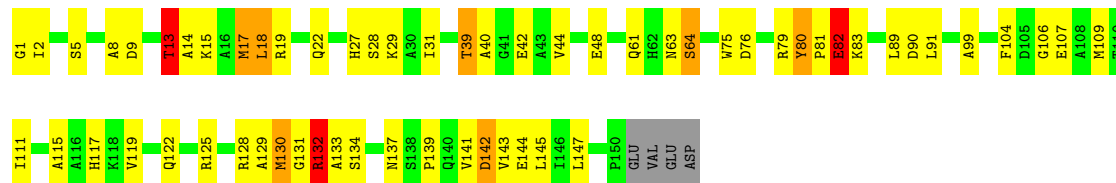




● Molecule 18: RIBOSOMAL PROTEIN L21E



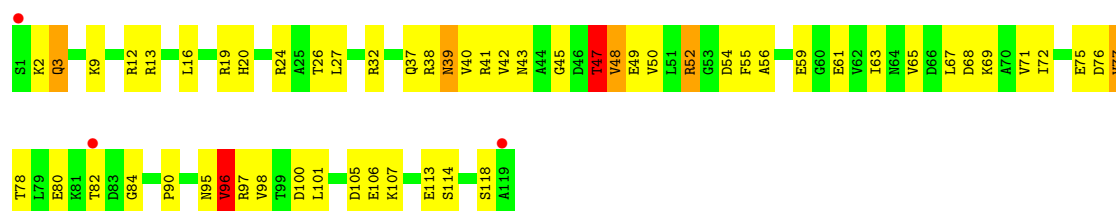
● Molecule 19: RIBOSOMAL PROTEIN L22



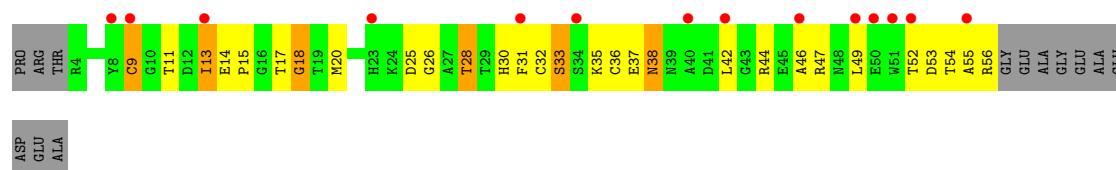
● Molecule 20: RIBOSOMAL PROTEIN L23



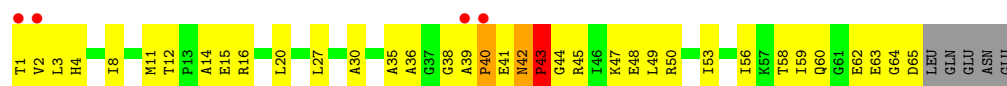
● Molecule 21: RIBOSOMAL PROTEIN L24



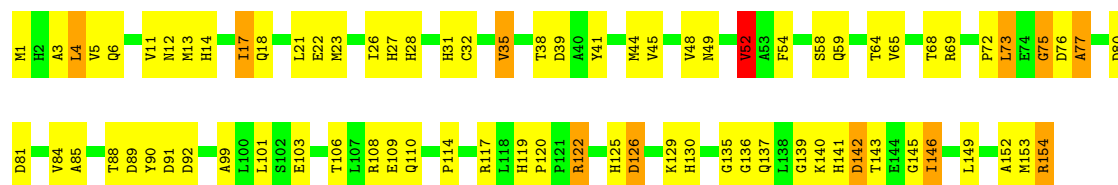
● Molecule 22: RIBOSOMAL PROTEIN L24E



- Molecule 23: RIBOSOMAL PROTEIN L29



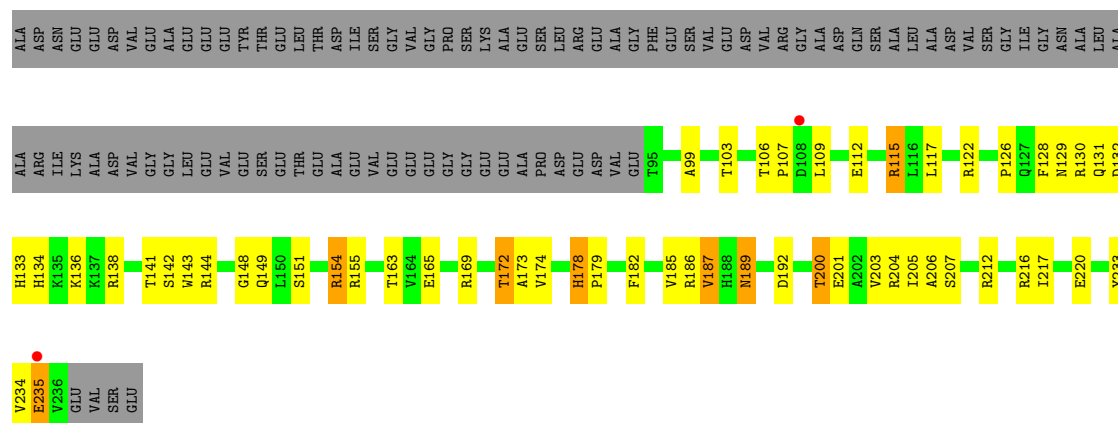
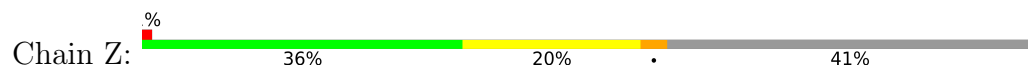
- Molecule 24: RIBOSOMAL PROTEIN L30



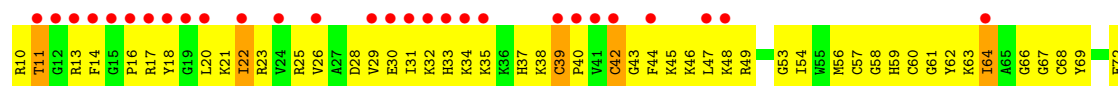
- Molecule 25: RIBOSOMAL PROTEIN L31E

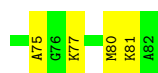


- Molecule 26: RIBOSOMAL PROTEIN L32E



- Molecule 27: RIBOSOMAL PROTEIN L37Ae





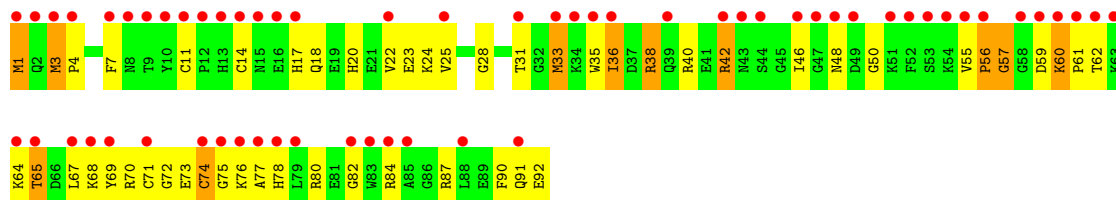
• Molecule 28: RIBOSOMAL PROTEIN L37E



• Molecule 29: RIBOSOMAL PROTEIN L39E



• Molecule 30: RIBOSOMAL PROTEIN L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.7 (19.99-3.00) 91.4 (19.99-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.269 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	98587	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CD, SPR, K, CL, MG, NA

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	0.51	3/66076 (0.0%)	0.78	70/103052 (0.1%)
2	B	0.74	7/2905 (0.2%)	0.90	17/4528 (0.4%)
3	C	0.68	1/1787 (0.1%)	1.18	12/2409 (0.5%)
4	D	0.67	0/2689	1.18	24/3652 (0.7%)
5	E	0.69	0/1883	1.16	13/2551 (0.5%)
6	F	0.50	0/1111	0.97	4/1498 (0.3%)
7	G	0.63	0/1382	0.99	3/1880 (0.2%)
8	H	0.54	0/896	0.98	3/1219 (0.2%)
9	I	0.56	0/241	0.89	0/324
10	J	0.69	0/1246	1.37	19/1686 (1.1%)
11	K	0.67	0/1135	1.01	4/1530 (0.3%)
12	L	0.65	0/1003	1.18	5/1351 (0.4%)
13	M	0.57	0/1126	1.10	6/1504 (0.4%)
14	N	0.87	2/1633 (0.1%)	1.27	13/2180 (0.6%)
15	O	0.60	0/1473	1.19	14/1999 (0.7%)
16	P	0.67	0/873	1.09	6/1181 (0.5%)
17	Q	0.62	0/1143	1.02	1/1521 (0.1%)
18	R	0.64	0/748	1.17	6/1005 (0.6%)
19	S	0.91	5/1172 (0.4%)	1.21	12/1578 (0.8%)
20	T	0.56	0/648	1.01	4/875 (0.5%)
21	U	0.58	0/957	1.12	8/1289 (0.6%)
22	V	0.99	1/417 (0.2%)	1.23	4/562 (0.7%)
23	W	0.57	0/502	1.07	2/675 (0.3%)
24	X	0.74	0/1218	1.08	6/1655 (0.4%)
25	Y	0.69	0/664	1.09	2/895 (0.2%)
26	Z	0.66	0/1146	1.08	4/1536 (0.3%)
27	1	1.09	0/575	1.26	1/763 (0.1%)
28	2	0.67	0/437	1.16	5/578 (0.9%)
29	3	0.60	0/398	0.89	0/527
30	4	1.36	4/771 (0.5%)	1.18	4/1024 (0.4%)
All	All	0.59	23/98255 (0.0%)	0.89	272/147027 (0.2%)

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
1	A	1	198
2	B	0	6
28	2	0	1
All	All	1	205

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3023	U	O5'-C5'	9.65	1.56	1.42
30	4	33	MET	SD-CE	9.59	2.03	1.79
2	B	3026	C	P-OP2	-9.26	1.30	1.49
2	B	3025	G	O3'-P	9.25	1.75	1.61
19	S	129	ALA	C-O	-7.71	1.14	1.23
19	S	130	MET	CB-CG	-7.50	1.29	1.52
2	B	3023	U	C2'-O2'	7.26	1.53	1.42
1	A	2104	C	O5'-C5'	-7.17	1.31	1.42
2	B	3025	G	P-OP2	-7.14	1.34	1.49
19	S	132	ARG	N-CA	7.11	1.54	1.45
2	B	3025	G	C4'-O4'	6.80	1.55	1.45
2	B	3026	C	P-O5'	-6.54	1.50	1.59
3	C	145	MET	SD-CE	6.42	1.95	1.79
30	4	1	MET	SD-CE	6.40	1.95	1.79
30	4	36	ILE	CA-CB	6.38	1.63	1.54
14	N	86	MET	SD-CE	6.22	1.95	1.79
1	A	2103	A	C5-C6	5.99	1.53	1.41
19	S	132	ARG	CA-CB	-5.90	1.44	1.53
19	S	17	MET	SD-CE	-5.68	1.65	1.79
22	V	13	ILE	CA-CB	5.55	1.60	1.54
1	A	2106	C	O3'-P	-5.43	1.53	1.61
14	N	82	ARG	CA-C	5.28	1.59	1.52
30	4	3	MET	SD-CE	5.05	1.92	1.79

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP2-P-O3'	-14.70	63.89	108.00
1	A	1164	U	OP1-P-O3'	-14.38	64.85	108.00
1	A	1563	G	C2'-C3'-O3'	13.12	129.18	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	74	ASN	N-CA-C	-13.02	95.51	114.39
14	N	141	ILE	N-CA-C	-12.80	101.53	111.90
15	O	135	VAL	N-CA-C	-12.43	100.92	113.47
10	J	141	ASN	N-CA-C	-12.41	98.24	113.50
1	A	1979	G	C2'-C3'-O3'	10.14	124.71	109.50
1	A	1563	G	C4'-C3'-O3'	9.64	123.86	109.40
1	A	1942	A	C5'-C4'-C3'	9.61	130.41	116.00
10	J	1	LYS	CA-C-N	9.44	129.38	119.85
10	J	1	LYS	C-N-CA	9.44	129.38	119.85
21	U	52	ARG	N-CA-C	9.33	125.59	113.18
4	D	213	GLY	CA-C-N	9.22	128.56	118.97
4	D	213	GLY	C-N-CA	9.22	128.56	118.97
1	A	2103	A	C5'-C4'-O4'	8.91	122.46	109.10
4	D	23	THR	CA-C-N	8.77	128.81	119.78
4	D	23	THR	C-N-CA	8.77	128.81	119.78
5	E	80	VAL	CA-C-N	8.54	129.05	119.32
5	E	80	VAL	C-N-CA	8.54	129.05	119.32
14	N	139	PRO	N-CA-C	-8.35	99.39	111.33
18	R	17	LYS	N-CA-C	-8.27	99.33	109.83
4	D	157	LYS	N-CA-C	-8.24	103.82	114.04
1	A	2103	A	C4'-C3'-O3'	-8.21	97.08	109.40
15	O	169	PRO	N-CA-C	-8.15	104.01	114.03
7	G	11	VAL	N-CA-C	8.13	121.81	109.20
5	E	175	LYS	N-CA-C	8.07	120.73	110.24
10	J	113	ALA	CA-C-N	8.06	128.75	120.04
10	J	113	ALA	C-N-CA	8.06	128.75	120.04
10	J	156	THR	N-CA-C	-7.99	98.65	110.48
10	J	147	ARG	N-CA-C	-7.98	102.57	111.82
2	B	3025	G	C1'-C2'-O2'	-7.87	96.59	108.40
2	B	3026	C	C3'-C2'-O2'	7.82	122.43	110.70
5	E	78	ARG	N-CA-C	7.73	119.89	108.60
6	F	136	ARG	CA-C-N	7.70	129.46	119.84
6	F	136	ARG	C-N-CA	7.70	129.46	119.84
4	D	323	LEU	N-CA-C	7.70	120.24	110.24
13	M	57	VAL	N-CA-C	-7.62	105.42	112.43
28	2	21	ARG	N-CA-C	7.58	121.02	111.69
30	4	55	VAL	CA-C-N	7.50	129.21	119.84
30	4	55	VAL	C-N-CA	7.50	129.21	119.84
15	O	153	GLN	N-CA-C	-7.41	103.12	113.20
14	N	42	ARG	CA-C-N	7.35	127.77	119.83
14	N	42	ARG	C-N-CA	7.35	127.77	119.83
13	M	145	LEU	N-CA-C	-7.35	103.35	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	74	ARG	N-CA-C	7.34	120.48	108.52
19	S	137	ASN	N-CA-C	7.31	121.28	110.46
15	O	13	ARG	N-CA-C	-7.30	104.00	113.12
4	D	265	LEU	N-CA-C	7.21	121.16	110.48
16	P	79	VAL	N-CA-C	-7.21	103.43	110.72
23	W	42	ASN	CA-C-N	7.21	128.85	119.84
23	W	42	ASN	C-N-CA	7.21	128.85	119.84
3	C	198	ASP	N-CA-C	7.05	121.88	113.28
15	O	117	ALA	N-CA-C	-7.01	103.72	111.36
18	R	86	VAL	N-CA-C	6.98	117.56	108.35
19	S	18	LEU	N-CA-C	-6.96	98.58	109.72
22	V	38	ASN	N-CA-C	6.91	118.81	111.28
3	C	222	GLY	N-CA-C	-6.83	105.76	114.37
20	T	57	THR	N-CA-C	6.82	120.57	110.48
2	B	3002	U	C4'-C3'-O3'	6.76	119.54	109.40
1	A	1942	A	C5'-C4'-O4'	6.74	119.91	109.80
10	J	137	ASN	N-CA-C	-6.70	101.39	110.36
10	J	155	PRO	N-CA-C	6.68	121.42	111.41
2	B	3039	U	C4'-C3'-O3'	-6.66	103.00	113.00
2	B	3025	G	O3'-P-O5'	6.66	113.99	104.00
13	M	47	GLY	N-CA-C	6.65	118.90	111.85
5	E	192	ILE	N-CA-C	6.64	118.24	109.21
1	A	335	U	C4'-C3'-O3'	-6.63	103.05	113.00
2	B	3024	U	C4'-C3'-O3'	6.59	122.89	113.00
1	A	835	U	C4'-C3'-O3'	-6.55	103.17	113.00
24	X	126	ASP	N-CA-C	6.55	120.87	113.01
6	F	100	ASP	N-CA-C	-6.55	105.29	113.28
16	P	82	SER	N-CA-C	-6.54	101.89	110.53
14	N	73	ARG	N-CA-C	-6.54	95.69	107.98
3	C	70	ALA	N-CA-C	6.50	119.04	109.42
2	B	3023	U	P-O5'-C5'	6.48	130.62	120.90
16	P	69	VAL	N-CA-C	6.47	117.17	108.11
2	B	3025	G	C3'-C2'-O2'	6.46	120.39	110.70
10	J	162	SER	CA-C-N	-6.46	111.76	119.84
10	J	162	SER	C-N-CA	-6.46	111.76	119.84
12	L	8	VAL	N-CA-C	6.46	117.78	108.48
24	X	75	GLY	N-CA-C	6.46	120.14	112.33
4	D	220	VAL	N-CA-C	-6.43	103.04	110.05
4	D	154	VAL	N-CA-C	6.43	113.91	107.55
4	D	282	GLY	N-CA-C	-6.39	107.48	115.08
15	O	3	GLY	CA-C-N	6.38	126.30	119.28
15	O	3	GLY	C-N-CA	6.38	126.30	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	20	TYR	N-CA-C	6.34	119.00	111.71
19	S	142	ASP	N-CA-C	-6.33	99.84	109.85
8	H	62	HIS	N-CA-C	6.33	119.17	111.82
22	V	18	GLY	N-CA-C	6.29	122.12	112.81
4	D	217	ARG	N-CA-C	6.27	118.20	111.36
1	A	1738	C	C5'-C4'-C3'	6.25	125.38	116.00
1	A	2103	A	OP2-P-O3'	6.24	126.73	108.00
3	C	118	PHE	N-CA-C	6.24	120.24	110.32
2	B	3039	U	N1-C1'-C2'	6.22	121.33	112.00
12	L	111	GLY	CA-C-N	6.20	126.17	120.21
12	L	111	GLY	C-N-CA	6.20	126.17	120.21
1	A	2419	U	N1-C1'-C2'	6.18	121.27	112.00
2	B	3026	C	O3'-P-O5'	6.14	113.21	104.00
19	S	130	MET	CB-CG-SD	6.12	131.06	112.70
1	A	171	C	C4'-C3'-O3'	-6.12	103.82	113.00
4	D	251	VAL	CA-C-N	6.12	127.75	120.23
4	D	251	VAL	C-N-CA	6.12	127.75	120.23
11	K	68	GLY	N-CA-C	6.10	120.36	112.18
1	A	834	G	C2'-C3'-O3'	-6.09	104.57	113.70
21	U	78	THR	N-CA-C	6.06	117.79	109.18
4	D	147	VAL	CA-C-N	6.04	126.48	119.47
4	D	147	VAL	C-N-CA	6.04	126.48	119.47
1	A	129	A	C2'-C3'-O3'	6.03	122.74	113.70
3	C	48	ASP	CA-C-N	5.98	126.41	119.47
3	C	48	ASP	C-N-CA	5.98	126.41	119.47
16	P	59	VAL	N-CA-C	5.98	116.22	107.37
1	A	2792	A	C3'-C2'-O2'	5.97	119.65	110.70
1	A	1504	A	N9-C1'-C2'	5.96	120.93	112.00
27	1	39	CYS	N-CA-C	5.95	117.20	109.64
17	Q	56	GLY	N-CA-C	-5.92	101.85	110.90
12	L	46	LYS	N-CA-C	5.91	119.69	110.17
21	U	3	GLN	CA-C-N	5.91	126.06	119.32
21	U	3	GLN	C-N-CA	5.91	126.06	119.32
11	K	89	HIS	N-CA-C	5.91	119.96	112.87
14	N	100	ILE	N-CA-C	-5.91	104.98	110.53
1	A	2106	C	N1-C1'-C2'	-5.91	103.14	112.00
10	J	129	ASN	CA-C-N	-5.90	114.58	122.72
10	J	129	ASN	C-N-CA	-5.90	114.58	122.72
1	A	2432	C	N1-C1'-C2'	5.88	120.82	112.00
8	H	8	VAL	N-CA-C	5.86	113.35	107.55
30	4	60	LYS	N-CA-C	-5.85	102.70	110.07
18	R	68	GLY	N-CA-C	-5.81	99.41	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1693	A	C3'-C2'-O2'	-5.80	105.90	114.60
1	A	171	C	C3'-C2'-O2'	5.79	119.39	110.70
1	A	1723	G	C4'-C3'-O3'	-5.79	104.32	113.00
4	D	47	GLY	N-CA-C	5.79	117.97	110.45
4	D	175	LEU	N-CA-C	-5.79	104.88	111.07
4	D	80	ARG	N-CA-C	5.75	117.76	107.80
7	G	7	ILE	CA-C-N	5.75	125.68	119.76
7	G	7	ILE	C-N-CA	5.75	125.68	119.76
19	S	80	TYR	CA-C-N	5.75	127.02	119.84
19	S	80	TYR	C-N-CA	5.75	127.02	119.84
10	J	7	ARG	N-CA-C	5.74	119.90	113.01
1	A	2106	C	C4'-C3'-O3'	-5.74	104.40	113.00
1	A	920	C	C2'-C3'-O3'	-5.73	105.11	113.70
26	Z	187	VAL	N-CA-C	5.71	116.11	108.11
3	C	220	PRO	CA-C-N	-5.71	113.88	119.76
3	C	220	PRO	C-N-CA	-5.71	113.88	119.76
15	O	51	GLY	CA-C-N	5.69	125.37	119.05
15	O	51	GLY	C-N-CA	5.69	125.37	119.05
1	A	2465	A	N9-C1'-C2'	-5.67	105.50	114.00
28	2	11	LYS	N-CA-C	5.65	118.39	108.56
4	D	154	VAL	CA-C-N	5.63	125.74	119.32
4	D	154	VAL	C-N-CA	5.63	125.74	119.32
5	E	20	ASP	N-CA-C	5.62	118.13	111.33
4	D	48	MET	N-CA-C	5.62	118.38	109.50
25	Y	79	GLU	N-CA-C	5.62	119.98	113.18
1	A	1358	A	C4'-C3'-O3'	-5.61	104.58	113.00
1	A	1721	C	N1-C1'-C2'	5.61	120.41	112.00
28	2	3	ALA	N-CA-C	-5.58	106.48	113.28
19	S	131	GLY	CA-C-O	-5.57	110.88	120.57
5	E	179	GLY	N-CA-C	-5.56	105.87	113.27
1	A	1592	G	N9-C1'-C2'	5.56	120.34	112.00
1	A	2835	C	C4'-C3'-O3'	-5.55	104.68	113.00
14	N	4	ALA	N-CA-C	-5.54	105.33	111.36
26	Z	115	ARG	N-CA-C	-5.53	105.17	111.14
1	A	2864	U	C4'-C3'-O3'	-5.53	104.71	113.00
1	A	2466	G	N9-C1'-C2'	5.53	120.29	112.00
1	A	1916	C	C3'-C2'-O2'	5.52	118.98	110.70
19	S	90	ASP	N-CA-C	-5.52	105.35	111.36
10	J	73	GLN	N-CA-C	-5.52	103.70	110.65
4	D	242	TRP	N-CA-C	-5.51	104.96	110.97
2	B	3024	U	O5'-P-OP2	5.51	124.53	108.00
16	P	2	LYS	N-CA-C	-5.50	102.33	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	38	SER	N-CA-C	-5.50	99.71	109.06
1	A	2096	A	C4'-C3'-O3'	-5.50	104.76	113.00
14	N	70	GLY	N-CA-C	5.48	122.18	112.53
19	S	13	THR	N-CA-C	5.48	118.37	109.06
1	A	2104	C	C3'-C2'-O2'	-5.47	102.49	110.70
5	E	91	PRO	CA-C-N	5.47	125.23	119.76
5	E	91	PRO	C-N-CA	5.47	125.23	119.76
10	J	91	HIS	N-CA-C	5.46	117.01	109.15
3	C	8	ARG	N-CA-C	-5.46	105.33	111.28
21	U	96	VAL	N-CA-C	5.46	117.25	108.85
1	A	2431	C	C1'-C2'-O2'	5.44	116.56	108.40
1	A	2103	A	O3'-P-O5'	5.44	112.16	104.00
14	N	90	ARG	N-CA-C	5.44	119.91	113.28
13	M	96	VAL	CB-CA-C	-5.43	105.40	111.80
25	Y	12	ILE	N-CA-C	5.42	113.23	107.76
5	E	197	SER	N-CA-C	5.40	120.23	113.43
1	A	854	G	C4'-C3'-O3'	-5.38	104.93	113.00
8	H	111	ILE	N-CA-C	-5.38	105.28	110.72
10	J	86	ARG	N-CA-C	5.38	119.69	113.18
24	X	52	VAL	N-CA-CB	-5.38	106.14	112.32
1	A	2526	C	N1-C1'-C2'	5.37	120.06	112.00
21	U	47	THR	N-CA-C	-5.36	101.43	109.95
1	A	2433	A	C1'-C2'-O2'	5.36	116.44	108.40
22	V	33	SER	N-CA-C	5.35	116.93	108.96
1	A	2291	A	C4'-C3'-O3'	-5.35	104.98	113.00
1	A	921	G	N9-C1'-C2'	5.34	120.01	112.00
28	2	29	THR	N-CA-C	5.33	118.89	112.38
1	A	1095	U	C3'-C2'-O2'	5.33	118.69	110.70
22	V	36	CYS	CA-CB-SG	-5.32	102.16	114.40
10	J	114	PRO	N-CA-C	5.32	121.45	114.27
2	B	3003	A	C4'-C3'-C2'	-5.32	97.28	102.60
2	B	3022	G	N9-C1'-C2'	5.32	119.97	112.00
1	A	146	U	N1-C1'-C2'	5.31	119.97	112.00
15	O	165	ALA	N-CA-C	-5.30	106.87	113.55
14	N	14	ARG	CA-C-N	5.29	125.01	119.82
14	N	14	ARG	C-N-CA	5.29	125.01	119.82
24	X	143	THR	N-CA-C	-5.29	105.63	111.71
1	A	1120	U	C5'-C4'-C3'	-5.29	108.07	116.00
18	R	49	ASN	N-CA-C	5.29	117.35	110.53
20	T	10	VAL	N-CA-C	5.28	115.38	107.51
18	R	47	VAL	CA-C-N	5.28	126.44	119.84
18	R	47	VAL	C-N-CA	5.28	126.44	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	137	PRO	N-CA-C	5.28	123.34	112.47
24	X	49	ASN	N-CA-C	5.28	122.04	110.80
1	A	1189	A	N9-C1'-C2'	5.26	119.89	112.00
1	A	843	A	C4'-C3'-O3'	-5.25	105.12	113.00
13	M	37	LYS	N-CA-C	5.25	116.46	108.12
3	C	133	ARG	N-CA-C	-5.24	106.73	113.23
19	S	63	ASN	N-CA-C	5.23	119.63	112.88
15	O	39	SER	N-CA-C	-5.22	101.17	108.96
19	S	122	GLN	N-CA-C	-5.22	100.57	108.67
1	A	2315	C	C5'-C4'-C3'	-5.22	108.17	116.00
1	A	1819	G	C5'-C4'-C3'	5.22	123.83	116.00
20	T	59	ASP	N-CA-C	-5.21	106.98	113.38
4	D	236	ILE	CB-CA-C	-5.20	105.62	111.45
1	A	1205	U	C3'-C2'-O2'	5.20	118.50	110.70
26	Z	143	TRP	N-CA-C	5.19	117.74	109.96
24	X	17	ILE	N-CA-C	-5.18	106.09	111.58
15	O	168	LEU	N-CA-C	5.17	119.91	108.64
3	C	103	VAL	N-CA-C	5.17	114.14	108.05
1	A	2432	C	C1'-C2'-O2'	5.16	116.13	108.40
1	A	1409	G	C3'-C2'-O2'	5.15	118.43	110.70
1	A	1651	C	N1-C1'-C2'	5.15	119.73	112.00
14	N	88	VAL	CB-CA-C	-5.15	102.84	111.29
3	C	135	VAL	N-CA-C	5.15	116.13	108.46
1	A	407	A	O4'-C4'-C3'	-5.13	98.87	104.00
1	A	386	G	C3'-C2'-O2'	5.13	118.40	110.70
1	A	189	A	C4'-C3'-O3'	-5.13	105.31	113.00
5	E	92	PRO	N-CA-C	-5.13	103.14	111.19
1	A	2667	G	O5'-C5'-C4'	5.13	119.19	111.50
2	B	3024	U	P-O5'-C5'	5.12	128.59	120.90
21	U	101	LEU	N-CA-C	5.12	117.84	109.59
1	A	2099	G	C3'-C2'-O2'	5.12	118.38	110.70
1	A	267	G	C3'-C2'-O2'	5.12	118.38	110.70
1	A	2296	C	C3'-C2'-O2'	5.12	118.37	110.70
2	B	3023	U	C3'-C2'-O2'	5.11	118.37	110.70
16	P	43	VAL	N-CA-C	5.11	116.32	108.71
1	A	2106	C	C1'-C2'-O2'	5.11	116.06	108.40
15	O	133	ASP	N-CA-C	5.10	121.67	110.80
1	A	1917	G	C3'-C2'-O2'	5.10	118.35	110.70
28	2	43	ALA	N-CA-C	-5.10	105.80	111.36
1	A	2433	A	N9-C1'-C2'	5.08	119.63	112.00
2	B	3003	A	C5'-C4'-C3'	5.08	122.82	115.20
26	Z	178	HIS	N-CA-C	-5.08	103.06	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	42	ASN	N-CA-C	5.07	118.73	112.24
1	A	2136	G	C2'-C3'-O3'	5.07	121.30	113.70
4	D	222	LYS	N-CA-C	-5.07	102.56	110.42
1	A	911	G	C3'-C2'-O2'	5.06	118.29	110.70
21	U	77	VAL	CB-CA-C	-5.06	107.55	113.22
1	A	959	C	C4'-C3'-O3'	-5.05	105.42	113.00
5	E	129	HIS	N-CA-C	5.04	117.54	110.23
1	A	2103	A	C2'-C3'-O3'	5.03	117.05	109.50
2	B	3026	C	C5'-C4'-O4'	5.03	117.35	109.80
20	T	14	ALA	N-CA-C	-5.03	105.88	111.36
5	E	150	THR	N-CA-C	-5.02	105.69	111.07
11	K	71	TYR	CA-C-N	5.02	124.78	119.76
11	K	71	TYR	C-N-CA	5.02	124.78	119.76
19	S	82	GLU	N-CA-C	5.01	116.44	111.07
30	4	59	ASP	N-CA-C	5.01	116.99	109.23
1	A	1504	A	C4'-C3'-O3'	-5.00	105.49	113.00
1	A	2104	C	O5'-P-OP1	-5.00	92.99	108.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (205) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	2	48	TYR	Sidechain
1	A	1005	A	Sidechain
1	A	1023	C	Sidechain
1	A	1027	G	Sidechain
1	A	1039	G	Sidechain
1	A	1042	U	Sidechain
1	A	1055	G	Sidechain
1	A	112	G	Sidechain
1	A	1127	C	Sidechain
1	A	1134	G	Sidechain
1	A	1136	U	Sidechain
1	A	1156	C	Sidechain
1	A	1206	U	Sidechain
1	A	1237	U	Sidechain
1	A	1260	G	Sidechain
1	A	1264	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1288	U	Sidechain
1	A	1298	U	Sidechain
1	A	1300	G	Sidechain
1	A	1309	U	Sidechain
1	A	1339	G	Sidechain
1	A	1347	U	Sidechain
1	A	1368	U	Sidechain
1	A	1376	G	Sidechain
1	A	1377	C	Sidechain
1	A	138	U	Sidechain
1	A	1389	G	Sidechain
1	A	1402	G	Sidechain
1	A	1408	U	Sidechain
1	A	1417	G	Sidechain
1	A	1418	U	Sidechain
1	A	1421	C	Sidechain
1	A	1430	G	Sidechain
1	A	1433	G	Sidechain
1	A	1447	U	Sidechain
1	A	1458	A	Sidechain
1	A	146	U	Sidechain
1	A	1468	G	Sidechain
1	A	1487	A	Sidechain
1	A	1501	A	Sidechain
1	A	1503	U	Sidechain
1	A	1614	G	Sidechain
1	A	1621	G	Sidechain
1	A	1628	G	Sidechain
1	A	163	U	Sidechain
1	A	1647	G	Sidechain
1	A	1677	U	Sidechain
1	A	1683	G	Sidechain
1	A	1684	A	Sidechain
1	A	1688	G	Sidechain
1	A	1689	A	Sidechain
1	A	169	A	Sidechain
1	A	171	C	Sidechain
1	A	1720	C	Sidechain
1	A	1736	A	Sidechain
1	A	174	A	Sidechain
1	A	1747	A	Sidechain
1	A	1748	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	176	U	Sidechain
1	A	1761	U	Sidechain
1	A	1771	U	Sidechain
1	A	178	U	Sidechain
1	A	1809	G	Sidechain
1	A	1816	C	Sidechain
1	A	1819	G	Sidechain
1	A	1823	G	Sidechain
1	A	1826	C	Sidechain
1	A	1833	U	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1848	G	Sidechain
1	A	1860	U	Sidechain
1	A	1861	C	Sidechain
1	A	1867	G	Sidechain
1	A	1878	G	Sidechain
1	A	1882	C	Sidechain
1	A	1908	G	Sidechain
1	A	191	A	Sidechain
1	A	1933	G	Sidechain
1	A	197	C	Sidechain
1	A	1972	U	Sidechain
1	A	2000	G	Sidechain
1	A	2001	G	Sidechain
1	A	2002	C	Sidechain
1	A	2035	C	Sidechain
1	A	2045	G	Sidechain
1	A	2053	G	Sidechain
1	A	2063	U	Sidechain
1	A	2068	G	Sidechain
1	A	2070	G	Sidechain
1	A	2076	U	Sidechain
1	A	2092	G	Sidechain
1	A	2101	A	Sidechain
1	A	2106	C	Sidechain
1	A	2120	U	Sidechain
1	A	2123	A	Sidechain
1	A	2128	G	Sidechain
1	A	2133	U	Sidechain
1	A	214	U	Sidechain
1	A	2244	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2273	C	Sidechain
1	A	2294	C	Sidechain
1	A	2304	G	Sidechain
1	A	2308	U	Sidechain
1	A	2310	G	Sidechain
1	A	2312	G	Sidechain
1	A	2313	C	Sidechain
1	A	2325	C	Sidechain
1	A	2337	G	Sidechain
1	A	2359	G	Sidechain
1	A	2363	G	Sidechain
1	A	2364	A	Sidechain
1	A	2378	U	Sidechain
1	A	2412	G	Sidechain
1	A	2422	U	Sidechain
1	A	2423	C	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	2453	G	Sidechain
1	A	2458	U	Sidechain
1	A	2459	G	Sidechain
1	A	246	G	Sidechain
1	A	2462	G	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2526	C	Sidechain
1	A	2575	C	Sidechain
1	A	2630	G	Sidechain
1	A	2631	U	Sidechain
1	A	264	G	Sidechain
1	A	2640	U	Sidechain
1	A	2643	G	Sidechain
1	A	2663	U	Sidechain
1	A	2673	U	Sidechain
1	A	2720	C	Sidechain
1	A	2721	U	Sidechain
1	A	2727	A	Sidechain
1	A	2730	G	Sidechain
1	A	2759	C	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	2800	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2811	A	Sidechain
1	A	2833	C	Sidechain
1	A	2840	A	Sidechain
1	A	2864	U	Sidechain
1	A	2891	A	Sidechain
1	A	331	A	Sidechain
1	A	333	G	Sidechain
1	A	395	A	Sidechain
1	A	396	U	Sidechain
1	A	398	U	Sidechain
1	A	406	G	Sidechain
1	A	407	A	Sidechain
1	A	436	A	Sidechain
1	A	458	G	Sidechain
1	A	461	C	Sidechain
1	A	474	C	Sidechain
1	A	476	A	Sidechain
1	A	486	A	Sidechain
1	A	487	G	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	554	G	Sidechain
1	A	650	C	Sidechain
1	A	669	G	Sidechain
1	A	720	G	Sidechain
1	A	723	G	Sidechain
1	A	743	G	Sidechain
1	A	75	U	Sidechain
1	A	750	A	Sidechain
1	A	755	G	Sidechain
1	A	756	A	Sidechain
1	A	757	C	Sidechain
1	A	759	C	Sidechain
1	A	761	A	Sidechain
1	A	768	U	Sidechain
1	A	791	A	Sidechain
1	A	815	U	Sidechain
1	A	816	G	Sidechain
1	A	817	G	Sidechain
1	A	818	A	Sidechain
1	A	827	A	Sidechain
1	A	838	C	Sidechain

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Mol	Chain	Res	Type	Group
1	A	840	U	Sidechain
1	A	864	U	Sidechain
1	A	867	A	Sidechain
1	A	871	G	Sidechain
1	A	878	G	Sidechain
1	A	882	A	Sidechain
1	A	887	G	Sidechain
1	A	888	U	Sidechain
1	A	889	C	Sidechain
1	A	904	U	Sidechain
1	A	916	A	Sidechain
1	A	919	U	Sidechain
1	A	946	C	Sidechain
1	A	954	U	Sidechain
1	A	99	A	Sidechain
2	B	3023	U	Sidechain
2	B	3025	G	Sidechain
2	B	3065	A	Sidechain
2	B	3069	U	Sidechain
2	B	3087	U	Sidechain
2	B	3094	G	Sidechain

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29802	1302	0
2	B	2600	0	1326	82	0
3	C	1754	0	1763	141	0
4	D	2624	0	2533	197	0
5	E	1858	0	1816	153	0
6	F	1094	0	1085	142	0
7	G	1357	0	1266	92	0
8	H	885	0	854	70	0
9	I	240	0	231	22	0
10	J	1215	0	1215	184	0
11	K	1119	0	1098	72	0
12	L	993	0	1027	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1114	0	1072	76	0
14	N	1605	0	1676	200	0
15	O	1444	0	1401	148	0
16	P	864	0	873	38	0
17	Q	1133	0	1127	53	0
18	R	734	0	727	31	0
19	S	1149	0	1122	65	0
20	T	641	0	605	24	0
21	U	949	0	923	60	0
22	V	410	0	368	44	0
23	W	499	0	511	35	0
24	X	1195	0	1137	105	0
25	Y	654	0	653	53	0
26	Z	1130	0	1133	75	0
27	1	563	0	601	82	0
28	2	430	0	426	27	0
29	3	393	0	406	28	0
30	4	755	0	732	58	0
31	A	59	0	73	9	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	112	0	0	5	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	73	0	0	1	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	1	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
34	4	1	0	0	0	0
34	A	9	0	0	2	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	K	3	0	0	2	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	3	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	41	0	0	13	0
37	2	55	0	0	5	0
37	3	42	0	0	5	0
37	4	73	0	0	6	0
37	A	5910	0	0	302	0
37	B	142	0	0	16	0
37	C	126	0	0	22	0
37	D	150	0	0	28	0
37	E	169	0	0	40	0
37	F	51	0	0	23	0
37	G	42	0	0	14	0
37	H	26	0	0	9	0
37	I	21	0	0	5	0
37	J	78	0	0	26	0
37	K	54	0	0	7	0
37	L	65	0	0	10	0
37	M	79	0	0	18	0
37	N	132	0	0	37	0
37	O	69	0	0	23	0
37	P	45	0	0	10	0
37	Q	65	0	0	4	0
37	R	55	0	0	6	0
37	S	83	0	0	10	0
37	T	35	0	0	3	0
37	U	39	0	0	4	0
37	V	25	0	0	8	0
37	W	15	0	0	2	0
37	X	70	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	Y	25	0	0	11	0
37	Z	94	0	0	18	0
All	All	98587	0	59582	3425	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (3425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:33:MET:CE	30:4:33:MET:SD	2.03	1.47
5:E:236:THR:HG22	5:E:239:ALA:H	1.09	1.15
1:A:2121:G:OP2	37:A:3494:HOH:O	1.64	1.15
1:A:2122:C:OP2	37:A:6549:HOH:O	1.64	1.15
6:F:25:MET:HE2	6:F:41:LEU:HG	1.29	1.14
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.28	1.12
1:A:1134:G:H4'	10:J:151:MET:HE1	1.28	1.11
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.23	1.10
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.64	1.09
4:D:162:MET:HE1	4:D:308:LEU:HD21	1.35	1.09
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.37	1.07
10:J:165:GLY:HA3	37:J:8386:HOH:O	1.54	1.07
1:A:871:G:H5'	1:A:871:G:H8	1.15	1.06
1:A:1160:G:H5'	1:A:1161:A:H5'	1.31	1.06
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.32	1.06
14:N:164:THR:HG22	14:N:167:GLY:H	1.14	1.06
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.35	1.05
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.38	1.04
31:A:9001:SPR:H6A3	31:A:9001:SPR:H2B1	1.32	1.03
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.89	1.02
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.38	1.02
12:L:10:GLN:NE2	12:L:10:GLN:H	1.58	1.01
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.41	1.01
1:A:871:G:H5'	1:A:871:G:C8	1.95	1.00
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.42	1.00
1:A:856:G:H2'	37:A:5401:HOH:O	1.62	1.00
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.77	0.99
1:A:2432:C:O4'	37:A:9718:HOH:O	1.80	0.99
14:N:87:MET:CG	30:4:46:ILE:HG21	1.92	0.99
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.39	0.99
1:A:2717:C:H2'	1:A:2718:C:H5''	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:115:SER:H	17:Q:118:GLN:HE21	1.00	0.98
24:X:88:THR:HB	37:X:6679:HOH:O	1.63	0.98
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.41	0.98
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.41	0.98
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.46	0.98
1:A:156:C:H5''	14:N:171:ARG:HD3	1.43	0.97
1:A:2123:A:OP2	37:A:5266:HOH:O	1.81	0.97
1:A:962:C:H1'	15:O:5:ARG:NH1	1.79	0.97
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.46	0.97
2:B:3023:U:H5''	2:B:3024:U:OP2	1.62	0.97
4:D:86:ALA:HA	37:D:8581:HOH:O	1.63	0.97
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.43	0.97
1:A:542:A:H5'	1:A:542:A:H8	1.29	0.97
2:B:3056:A:H2'	2:B:3057:A:H5''	1.47	0.96
1:A:1474:C:H6	1:A:1474:C:H5'	1.31	0.95
14:N:52:LEU:HD11	37:N:8616:HOH:O	1.65	0.94
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.33	0.94
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.78	0.94
11:K:76:ASP:HA	37:K:8565:HOH:O	1.66	0.94
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.28	0.94
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.06	0.94
27:1:39:CYS:SG	27:1:47:LEU:HD21	2.08	0.94
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.49	0.93
1:A:870:G:H2'	1:A:871:G:H5''	1.46	0.93
4:D:140:LEU:HA	37:D:8581:HOH:O	1.67	0.93
13:M:68:GLU:HA	37:M:8546:HOH:O	1.67	0.93
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.50	0.93
1:A:1667:A:H5'	1:A:1667:A:H8	1.34	0.92
4:D:62:ARG:HA	4:D:65:MET:HE3	1.49	0.92
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.15	0.92
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.83	0.92
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.03	0.92
1:A:1751:G:H2'	1:A:1752:G:H5''	1.52	0.92
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.51	0.92
14:N:87:MET:HG2	30:4:46:ILE:CG2	2.00	0.92
6:F:105:SER:HB2	6:F:131:THR:HG23	1.50	0.92
1:A:1835:U:H5	1:A:1840:A:N7	1.66	0.91
5:E:140:VAL:HB	37:E:8450:HOH:O	1.69	0.91
10:J:2:PRO:HB2	37:J:8354:HOH:O	1.69	0.91
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.36	0.91
12:L:10:GLN:H	12:L:10:GLN:HE21	1.08	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:67:ARG:O	13:M:71:GLU:HG3	1.71	0.91
20:T:57:THR:HG22	20:T:59:ASP:H	1.36	0.91
37:A:3764:HOH:O	14:N:189:VAL:HG21	1.72	0.90
4:D:238:ASN:HD22	4:D:240:GLY:H	1.19	0.90
1:A:871:G:H8	1:A:871:G:C5'	1.83	0.90
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.36	0.90
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.50	0.90
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.51	0.90
26:Z:216:ARG:HD3	37:Z:8569:HOH:O	1.70	0.90
1:A:541:C:H2'	1:A:542:A:H5''	1.52	0.90
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.72	0.90
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.53	0.89
22:V:9:CYS:SG	22:V:11:THR:HG23	2.13	0.89
5:E:2:GLN:HB3	37:E:8337:HOH:O	1.71	0.89
10:J:27:LYS:H	10:J:58:HIS:HD2	1.19	0.88
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.54	0.88
1:A:1205:U:H2'	1:A:1206:U:H5'	1.54	0.88
1:A:2426:G:H1'	37:A:6061:HOH:O	1.73	0.88
2:B:3076:G:H3'	2:B:3077:A:H5''	1.56	0.88
14:N:24:MET:HE3	14:N:28:MET:HE3	1.55	0.88
19:S:9:ASP:O	19:S:13:THR:HB	1.74	0.88
1:A:2466:G:OP1	37:A:3625:HOH:O	1.90	0.88
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.74	0.88
1:A:962:C:H1'	15:O:5:ARG:HH12	1.38	0.87
1:A:2533:C:H6	1:A:2533:C:H5'	1.39	0.87
15:O:144:GLY:O	15:O:147:ILE:HG22	1.75	0.87
1:A:1120:U:H6	1:A:1120:U:H5''	1.39	0.87
1:A:2506:A:HO2'	1:A:2507:G:H8	0.91	0.87
1:A:2812:A:H2	1:A:2814:A:H62	1.22	0.87
37:A:6265:HOH:O	6:F:99:ASP:HA	1.73	0.87
13:M:79:ASP:HB3	37:M:8559:HOH:O	1.75	0.87
5:E:236:THR:HG21	37:E:8372:HOH:O	1.74	0.87
1:A:1184:C:H1'	37:A:7445:HOH:O	1.74	0.87
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.56	0.87
1:A:541:C:C2'	1:A:542:A:H5''	2.05	0.86
6:F:154:LYS:H	6:F:154:LYS:HD2	1.39	0.86
37:A:3703:HOH:O	14:N:157:LEU:HD11	1.74	0.86
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.05	0.86
1:A:1886:A:N3	37:A:4796:HOH:O	2.07	0.86
1:A:1242:A:H5'	11:K:82:THR:HG23	1.55	0.86
2:B:3069:U:OP1	15:O:4:PRO:HG3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:162:MET:HE2	4:D:310:ARG:HD3	1.57	0.86
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.74	0.85
1:A:960:G:H4'	37:A:7406:HOH:O	1.77	0.85
10:J:150:LYS:HE2	37:J:8372:HOH:O	1.75	0.85
15:O:7:LYS:HE3	18:R:21:ARG:O	1.75	0.85
1:A:1116:U:HO2'	1:A:1118:A:H2	0.88	0.85
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.06	0.85
13:M:133:VAL:HA	37:M:8572:HOH:O	1.74	0.85
24:X:88:THR:HG22	24:X:89:ASP:H	1.41	0.85
14:N:69:LYS:O	14:N:73:ARG:NH2	2.10	0.85
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.56	0.85
23:W:1:THR:HG23	23:W:2:VAL:H	1.41	0.85
37:A:4928:HOH:O	2:B:3103:A:H4'	1.75	0.85
10:J:162:SER:HB2	10:J:163:PRO:CD	2.06	0.85
8:H:91:VAL:HG12	8:H:92:GLY:H	1.42	0.84
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.76	0.84
1:A:1134:G:C4'	10:J:151:MET:HE1	2.08	0.84
24:X:122:ARG:NH2	24:X:154:ARG:HD2	1.91	0.84
1:A:1166:A:H1'	1:A:1192:A:C2	2.12	0.84
16:P:7:LEU:HD22	37:P:5650:HOH:O	1.76	0.84
1:A:2468:A:H61	30:4:48:ASN:HD21	1.26	0.84
37:A:3661:HOH:O	14:N:79:LYS:HD3	1.77	0.84
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.76	0.84
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.58	0.83
1:A:2274:A:N3	14:N:86:MET:HE1	1.93	0.83
6:F:20:LYS:HA	6:F:75:LEU:O	1.78	0.83
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.13	0.83
8:H:96:ALA:HA	37:H:3111:HOH:O	1.76	0.83
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.08	0.83
1:A:2586:U:H3	1:A:2592:G:H22	1.26	0.83
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.59	0.83
26:Z:141:THR:HG23	37:Z:8589:HOH:O	1.78	0.83
4:D:321:PRO:HA	37:D:8659:HOH:O	1.79	0.83
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.60	0.83
1:A:544:G:H2'	1:A:545:G:H5''	1.60	0.83
2:B:3023:U:C5'	2:B:3024:U:OP2	2.26	0.83
12:L:10:GLN:HE21	12:L:10:GLN:N	1.77	0.83
22:V:20:MET:HE2	22:V:30:HIS:NE2	1.92	0.82
24:X:88:THR:HG23	24:X:110:GLN:NE2	1.95	0.82
19:S:17:MET:SD	37:S:8548:HOH:O	2.37	0.82
15:O:37:ARG:HD3	34:O:8507:CL:CL	2.17	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2717:C:C2'	1:A:2718:C:H5''	2.10	0.82
10:J:142:VAL:HG13	37:J:8370:HOH:O	1.80	0.82
26:Z:133:HIS:HD2	37:Z:8583:HOH:O	1.63	0.82
10:J:26:LYS:HG2	10:J:28:ILE:H	1.44	0.81
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.61	0.81
3:C:199:HIS:HD2	3:C:201:PHE:H	1.28	0.81
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.45	0.81
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.61	0.81
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.44	0.81
1:A:338:C:H4'	5:E:174:ILE:CD1	2.09	0.81
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.14	0.81
10:J:139:ASP:HA	37:J:8360:HOH:O	1.79	0.81
1:A:1474:C:H5'	1:A:1474:C:C6	2.16	0.81
1:A:1701:A:H5'	37:A:6253:HOH:O	1.81	0.81
24:X:149:LEU:HG	24:X:153:MET:HE2	1.62	0.81
22:V:9:CYS:HA	22:V:52:THR:HG23	1.59	0.81
1:A:2716:G:H5''	4:D:206:THR:HG21	1.63	0.81
37:A:6840:HOH:O	14:N:178:LYS:HB2	1.81	0.81
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.61	0.81
30:4:74:CYS:SG	30:4:76:LYS:HB2	2.21	0.81
1:A:1120:U:H5''	1:A:1120:U:C6	2.16	0.80
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.11	0.80
1:A:2467:A:OP1	37:A:9038:HOH:O	1.98	0.80
1:A:1735:C:O2'	1:A:1736:A:H5'	1.81	0.80
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.61	0.80
1:A:1372:A:H3'	37:A:7165:HOH:O	1.81	0.80
10:J:139:ASP:N	10:J:140:PRO:HD3	1.97	0.80
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.64	0.80
5:E:236:THR:HG22	5:E:239:ALA:N	1.93	0.80
14:N:164:THR:HG23	14:N:165:SER:N	1.94	0.80
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.47	0.80
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.63	0.80
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.80	0.80
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.81	0.80
1:A:288:A:H61	1:A:364:C:H42	1.29	0.80
14:N:164:THR:HG22	14:N:167:GLY:N	1.96	0.80
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.80	0.80
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.65	0.79
1:A:1603:A:H5'	1:A:1605:G:O4'	1.81	0.79
1:A:1209:C:H4'	37:A:5257:HOH:O	1.83	0.79
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:4:PRO:HD2	37:O:8558:HOH:O	1.80	0.79
1:A:1118:A:H8	1:A:1118:A:H3'	1.47	0.79
1:A:2064:U:H4'	1:A:2653:A:OP1	1.83	0.79
1:A:1835:U:C5	1:A:1840:A:N7	2.51	0.79
10:J:163:PRO:HG2	37:J:8325:HOH:O	1.81	0.79
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.64	0.79
1:A:1116:U:H3	1:A:1246:A:H62	1.31	0.79
1:A:2420:G:O2'	1:A:2421:G:H5'	1.81	0.79
1:A:272:A:H3'	37:A:7510:HOH:O	1.82	0.79
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.18	0.79
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.63	0.79
1:A:1119:G:H2'	11:K:52:GLN:NE2	1.97	0.78
1:A:282:C:H1'	1:A:368:C:N4	1.98	0.78
2:B:3014:G:H5'	2:B:3014:G:H8	1.49	0.78
34:K:8501:CL:CL	37:K:8548:HOH:O	2.38	0.78
1:A:1116:U:O2'	1:A:1118:A:H2	1.67	0.78
1:A:1118:A:H3'	1:A:1118:A:C8	2.18	0.78
13:M:53:ARG:NH2	13:M:57:VAL:HG12	1.98	0.78
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.66	0.78
37:A:7536:HOH:O	30:4:60:LYS:HG3	1.83	0.78
27:1:23:ARG:NH1	37:1:8404:HOH:O	2.17	0.78
3:C:223:ARG:HG3	37:C:8606:HOH:O	1.84	0.78
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.48	0.78
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.82	0.78
1:A:545:G:H5'	1:A:545:G:H8	1.49	0.77
1:A:711:G:H1'	37:A:7067:HOH:O	1.82	0.77
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.67	0.77
1:A:111:C:O2'	28:2:20:ARG:HG2	1.84	0.77
1:A:1165:G:H4'	1:A:1174:A:O2'	1.84	0.77
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.67	0.77
1:A:2004:U:H4'	37:A:5284:HOH:O	1.82	0.77
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.66	0.77
10:J:136:VAL:HG23	37:J:8330:HOH:O	1.84	0.77
1:A:559:U:H6	1:A:559:U:H5'	1.49	0.77
37:A:4837:HOH:O	14:N:14:ARG:HG2	1.83	0.77
1:A:645:U:OP2	13:M:4:LYS:HE2	1.85	0.77
1:A:2508:C:H2'	37:A:6723:HOH:O	1.85	0.77
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.67	0.77
11:K:74:ARG:HB3	11:K:74:ARG:HH11	1.49	0.77
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.14	0.77
3:C:199:HIS:CD2	3:C:201:PHE:H	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.14	0.77
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.49	0.76
1:A:542:A:H5'	1:A:542:A:C8	2.19	0.76
1:A:1187:U:H2'	37:A:6864:HOH:O	1.85	0.76
14:N:64:ARG:HD2	37:N:8586:HOH:O	1.84	0.76
1:A:870:G:C2'	1:A:871:G:H5''	2.15	0.76
1:A:1450:C:H4'	1:A:1451:C:OP2	1.86	0.76
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.66	0.76
1:A:797:A:C4'	27:1:10:ARG:N	2.48	0.76
1:A:289:G:H22	1:A:363:A:H2	1.33	0.76
2:B:3039:U:H1'	2:B:3044:A:H61	1.51	0.76
2:B:3056:A:C2'	2:B:3057:A:H5''	2.15	0.76
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.24	0.76
8:H:91:VAL:HG12	8:H:92:GLY:N	1.99	0.76
14:N:84:LYS:HE2	37:N:8577:HOH:O	1.85	0.76
29:3:41:HIS:H	29:3:45:ASN:HD22	1.30	0.76
1:A:1160:G:C5'	1:A:1161:A:H5'	2.11	0.76
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.67	0.76
1:A:797:A:H4'	27:1:10:ARG:N	2.01	0.76
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.84	0.76
25:Y:30:MET:HE1	25:Y:58:ALA:HB3	1.68	0.76
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.26	0.76
1:A:1666:C:O2'	1:A:1667:A:H5''	1.86	0.76
10:J:137:ASN:O	10:J:139:ASP:N	2.19	0.76
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.85	0.76
26:Z:220:GLU:HG2	37:Z:8550:HOH:O	1.85	0.76
9:I:12:ILE:N	9:I:13:PRO:HD3	2.01	0.76
25:Y:25:ARG:NH1	37:Y:3861:HOH:O	2.19	0.76
1:A:541:C:H2'	1:A:542:A:C5'	2.15	0.75
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.49	0.75
10:J:14:TYR:H	10:J:91:HIS:CE1	2.04	0.75
14:N:61:ILE:HG13	37:N:8623:HOH:O	1.85	0.75
14:N:87:MET:CB	30:4:46:ILE:HG21	2.16	0.75
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.50	0.75
1:A:236:A:H4'	1:A:237:G:H5'	1.69	0.75
1:A:450:C:OP1	5:E:184:ARG:NH2	2.16	0.75
1:A:506:G:H22	1:A:509:A:C5'	1.98	0.75
6:F:27:ILE:HG22	6:F:28:GLY:H	1.51	0.75
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.19	0.75
17:Q:143:ALA:HA	37:Q:2178:HOH:O	1.87	0.75
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2506:A:O2'	1:A:2507:G:H8	1.68	0.75
37:A:4432:HOH:O	14:N:146:GLN:HG2	1.86	0.75
4:D:62:ARG:CA	4:D:65:MET:HE3	2.17	0.75
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.68	0.75
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.85	0.74
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.70	0.74
6:F:135:VAL:HG22	6:F:136:ARG:H	1.51	0.74
3:C:35:GLY:O	3:C:36:ASP:HB3	1.86	0.74
16:P:32:ARG:O	16:P:32:ARG:HD3	1.85	0.74
21:U:32:ARG:NH1	21:U:38:ARG:HH12	1.85	0.74
1:A:346:U:H4'	37:A:6811:HOH:O	1.87	0.74
5:E:76:ARG:HD2	37:E:8432:HOH:O	1.87	0.74
10:J:41:THR:HA	37:J:8384:HOH:O	1.87	0.74
27:I:49:ARG:HD2	37:I:8431:HOH:O	1.87	0.74
1:A:1160:G:H5'	1:A:1161:A:C5'	2.15	0.74
1:A:1701:A:H4'	1:A:1702:U:H5''	1.68	0.74
1:A:2466:G:H5''	37:A:3625:HOH:O	1.87	0.74
5:E:178:GLN:OE1	37:E:8465:HOH:O	2.04	0.74
26:Z:185:VAL:HA	37:Z:8564:HOH:O	1.86	0.74
1:A:21:G:H5'	19:S:2:ILE:HA	1.70	0.74
37:A:9110:HOH:O	14:N:82:ARG:HD2	1.88	0.74
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.23	0.74
1:A:1329:A:H2	37:A:4655:HOH:O	1.69	0.74
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.15	0.74
13:M:143:THR:HG22	13:M:144:ASP:N	2.02	0.74
24:X:154:ARG:C	37:X:4276:HOH:O	2.30	0.74
1:A:1058:A:H2'	1:A:1060:C:H5''	1.68	0.74
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.36	0.74
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.88	0.74
14:N:48:ARG:NH2	37:N:8563:HOH:O	2.21	0.74
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.17	0.73
10:J:71:TYR:C	10:J:73:GLN:H	1.96	0.73
5:E:78:ARG:HG3	5:E:78:ARG:NH1	2.03	0.73
14:N:172:GLY:O	14:N:183:VAL:HG11	1.89	0.73
1:A:2100:A:N1	31:A:9001:SPR:H2A	2.03	0.73
11:K:99:GLU:HA	37:K:8573:HOH:O	1.88	0.73
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.35	0.73
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.83	0.73
1:A:1130:U:H2'	1:A:1131:G:O4'	1.89	0.73
2:B:3029:C:H2'	2:B:3030:C:H5'	1.70	0.73
4:D:162:MET:HE2	4:D:310:ARG:CD	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:59:ASN:HD22	10:J:59:ASN:N	1.87	0.73
14:N:60:ILE:C	14:N:61:ILE:HD12	2.14	0.73
19:S:39:THR:HG22	19:S:42:GLU:H	1.54	0.73
25:Y:15:ARG:HB3	25:Y:15:ARG:HH11	1.54	0.73
5:E:132:ASP:HB3	37:E:8361:HOH:O	1.88	0.73
9:I:12:ILE:HA	37:I:4499:HOH:O	1.89	0.73
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.19	0.73
24:X:130:HIS:O	24:X:136:GLY:HA3	1.89	0.73
1:A:2271:G:OP2	37:A:9415:HOH:O	2.07	0.73
4:D:62:ARG:HA	4:D:65:MET:CE	2.17	0.72
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.34	0.72
1:A:172:U:OP2	37:A:6180:HOH:O	2.06	0.72
1:A:1667:A:H5'	1:A:1667:A:C8	2.21	0.72
1:A:1743:G:N7	37:A:9244:HOH:O	2.21	0.72
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.71	0.72
11:K:19:MET:HE3	11:K:132:LEU:CD1	2.17	0.72
19:S:99:ALA:HB1	19:S:109:MET:CE	2.16	0.72
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.19	0.72
1:A:31:C:H4'	37:A:7400:HOH:O	1.89	0.72
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.71	0.72
5:E:214:THR:HG21	37:E:8399:HOH:O	1.87	0.72
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.24	0.72
11:K:133:GLY:O	11:K:137:GLU:HG3	1.90	0.72
14:N:35:PRO:O	37:N:8539:HOH:O	2.06	0.72
19:S:132:ARG:NH2	37:S:8582:HOH:O	2.22	0.72
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.71	0.72
1:A:1170:U:O2'	1:A:1172:G:N7	2.23	0.72
1:A:1834:C:H2'	1:A:1840:A:N6	2.04	0.72
13:M:136:ALA:HB3	37:M:8572:HOH:O	1.89	0.72
25:Y:31:ILE:O	25:Y:35:GLU:HG3	1.90	0.72
1:A:1118:A:H62	1:A:1244:U:H3	1.37	0.72
12:L:39:GLY:HA2	37:L:4183:HOH:O	1.89	0.72
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.71	0.72
20:T:57:THR:HG22	20:T:59:ASP:N	2.05	0.72
1:A:1353:C:P	37:A:4650:HOH:O	2.48	0.72
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.72	0.72
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.90	0.72
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.71	0.72
26:Z:212:ARG:HD2	37:Z:8600:HOH:O	1.89	0.72
1:A:1164:U:H3	1:A:1192:A:H2	1.35	0.72
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:31:THR:HB	30:4:33:MET:HE3	1.71	0.72
1:A:506:G:H22	1:A:509:A:H5'	1.53	0.71
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.72	0.71
1:A:560:C:H42	1:A:597:A:H61	1.38	0.71
1:A:284:C:H4'	1:A:285:A:O5'	1.89	0.71
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.53	0.71
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.13	0.71
1:A:2301:A:H5''	1:A:2302:A:H5'	1.71	0.71
1:A:2467:A:H2'	37:A:5431:HOH:O	1.90	0.71
15:O:113:SER:HB2	37:O:8560:HOH:O	1.89	0.71
2:B:3013:A:O2'	2:B:3014:G:H5''	1.90	0.71
2:B:3020:G:O2'	2:B:3021:G:H5'	1.91	0.71
14:N:152:ARG:HG3	37:N:8557:HOH:O	1.91	0.71
1:A:2421:G:H3'	1:A:2422:U:H5''	1.71	0.71
18:R:25:PRO:HB2	37:R:4350:HOH:O	1.91	0.71
1:A:214:U:H5'	37:A:6109:HOH:O	1.91	0.71
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.71	0.71
1:A:1918:U:OP2	37:A:3997:HOH:O	2.07	0.71
14:N:85:ARG:HA	14:N:87:MET:HE2	1.72	0.71
26:Z:186:ARG:HG2	26:Z:186:ARG:HH11	1.56	0.71
1:A:1209:C:H2'	1:A:1210:G:H8	1.55	0.71
7:G:11:VAL:HG12	7:G:12:ASP:N	2.04	0.71
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.72	0.71
10:J:59:ASN:HD22	10:J:59:ASN:H	1.38	0.71
11:K:131:THR:HG22	11:K:134:GLU:H	1.53	0.71
27:1:10:ARG:HA	37:1:8416:HOH:O	1.89	0.71
27:1:42:CYS:SG	27:1:44:PHE:N	2.59	0.71
1:A:338:C:H4'	5:E:174:ILE:HD11	1.71	0.71
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.72	0.70
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.06	0.70
12:L:55:VAL:HG12	12:L:56:SER:N	2.06	0.70
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.72	0.70
18:R:23:THR:HA	37:R:4792:HOH:O	1.91	0.70
1:A:1019:C:OP1	37:A:3922:HOH:O	2.08	0.70
1:A:1119:G:H2'	11:K:52:GLN:HE22	1.54	0.70
1:A:2119:C:O2'	1:A:2120:U:H5'	1.91	0.70
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.54	0.70
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.73	0.70
6:F:23:VAL:HG23	6:F:23:VAL:O	1.91	0.70
1:A:2276:U:H2'	1:A:2277:U:C6	2.26	0.70
1:A:2638:G:H1'	37:A:7742:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2768:A:H2'	1:A:2769:C:O4'	1.90	0.70
5:E:39:GLN:O	5:E:43:LYS:HD3	1.92	0.70
23:W:39:ALA:N	23:W:40:PRO:HD2	2.07	0.70
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.72	0.70
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.72	0.70
1:A:544:G:C2'	1:A:545:G:H5''	2.21	0.70
32:A:8054:MG:MG	37:A:7819:HOH:O	1.33	0.70
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.57	0.70
3:C:53:ALA:HB3	37:C:8610:HOH:O	1.91	0.70
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.20	0.70
18:R:24:SER:O	37:R:2847:HOH:O	2.10	0.70
1:A:877:G:H5'	1:A:878:G:OP1	1.92	0.70
3:C:121:ALA:O	3:C:124:VAL:HG22	1.90	0.70
4:D:179:LEU:O	4:D:183:GLU:HG2	1.92	0.70
8:H:2:VAL:HG22	8:H:57:GLU:OE1	1.92	0.70
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.91	0.70
19:S:132:ARG:CZ	37:S:8582:HOH:O	2.40	0.70
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.22	0.70
37:A:4554:HOH:O	14:N:87:MET:HE1	1.91	0.69
1:A:1191:A:H3'	1:A:1192:A:H5''	1.72	0.69
1:A:2827:A:H2'	1:A:2828:G:O4'	1.91	0.69
6:F:19:GLU:O	6:F:20:LYS:HG2	1.92	0.69
14:N:89:ASN:HA	37:N:8554:HOH:O	1.91	0.69
1:A:603:A:H5''	1:A:604:G:OP1	1.92	0.69
1:A:1406:A:N1	37:A:6004:HOH:O	2.25	0.69
1:A:1810:C:OP1	22:V:44:ARG:NE	2.16	0.69
3:C:36:ASP:OD2	3:C:85:ASP:HB2	1.91	0.69
24:X:5:VAL:HG11	24:X:153:MET:HE1	1.73	0.69
27:1:30:GLU:HA	27:1:33:HIS:CB	2.22	0.69
1:A:1080:C:H4'	1:A:1081:A:OP1	1.91	0.69
4:D:145:HIS:HD2	4:D:146:THR:O	1.76	0.69
9:I:63:ARG:N	37:I:2569:HOH:O	2.25	0.69
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.75	0.69
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.75	0.69
5:E:115:LEU:O	5:E:118:THR:HB	1.90	0.69
8:H:99:THR:HA	37:H:3461:HOH:O	1.93	0.69
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.22	0.69
7:G:84:MET:HE1	7:G:148:ILE:HD12	1.74	0.69
10:J:57:ARG:HG3	37:J:8341:HOH:O	1.92	0.69
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.57	0.69
1:A:134:U:C2	1:A:145:A:C2	2.81	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.22	0.69
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.73	0.69
23:W:12:THR:HG22	23:W:15:GLU:CG	2.22	0.69
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.01	0.69
1:A:821:U:H2'	1:A:822:C:H6	1.58	0.69
11:K:45:VAL:HG23	11:K:130:VAL:O	1.93	0.69
1:A:31:C:H2'	37:A:7669:HOH:O	1.92	0.69
3:C:88:ILE:HG22	3:C:88:ILE:O	1.90	0.69
4:D:85:ARG:NH1	37:D:8637:HOH:O	2.26	0.69
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.75	0.69
1:A:1625:U:H4'	37:A:4637:HOH:O	1.90	0.68
1:A:2291:A:C8	1:A:2309:C:H5'	2.28	0.68
6:F:55:LYS:HA	37:F:6752:HOH:O	1.93	0.68
11:K:107:ASN:ND2	11:K:109:TYR:H	1.91	0.68
16:P:47:ARG:HH11	16:P:47:ARG:HG3	1.57	0.68
5:E:1:MET:HG2	5:E:2:GLN:H	1.57	0.68
22:V:9:CYS:CA	22:V:52:THR:HG23	2.22	0.68
1:A:281:U:H2'	1:A:282:C:O4'	1.93	0.68
1:A:516:A:OP2	37:A:5618:HOH:O	2.12	0.68
1:A:1119:G:H22	1:A:1246:A:H2	1.39	0.68
1:A:1151:G:OP1	9:I:16:LYS:NZ	2.25	0.68
7:G:84:MET:HE1	7:G:148:ILE:CD1	2.24	0.68
6:F:69:ILE:HG22	6:F:69:ILE:O	1.92	0.68
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.73	0.68
12:L:81:ARG:HB2	12:L:87:ARG:NH1	2.05	0.68
1:A:2434:A:O3'	30:4:28:GLY:HA3	1.92	0.68
3:C:101:GLU:OE2	3:C:131:HIS:HB2	1.94	0.68
4:D:138:GLY:O	4:D:139:ASP:O	2.11	0.68
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.75	0.68
10:J:162:SER:CB	10:J:163:PRO:HD3	2.22	0.68
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.91	0.68
1:A:1086:A:N6	24:X:11:VAL:HG11	2.08	0.68
1:A:2748:G:H2'	37:A:7521:HOH:O	1.94	0.68
1:A:2862:G:H4'	4:D:336:GLN:O	1.93	0.68
7:G:84:MET:HE2	7:G:133:VAL:CG2	2.24	0.68
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.09	0.68
26:Z:235:GLU:H	26:Z:235:GLU:CD	2.01	0.68
37:A:4639:HOH:O	20:T:23:LYS:HE2	1.94	0.68
1:A:1185:U:H2'	1:A:1186:C:C6	2.29	0.68
1:A:2054:A:N3	19:S:128:ARG:NH2	2.42	0.68
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:18:TYR:HB3	27:1:22:ILE:HG21	1.76	0.68
1:A:1422:U:H2'	1:A:1423:C:C6	2.28	0.68
1:A:2533:C:H5'	1:A:2533:C:C6	2.26	0.68
30:4:65:THR:HG23	30:4:67:LEU:HG	1.75	0.68
1:A:20:G:H21	19:S:117:HIS:HD2	1.41	0.68
12:L:115:ARG:HG3	12:L:116:GLU:N	2.09	0.68
19:S:99:ALA:CB	19:S:109:MET:HE1	2.17	0.68
24:X:88:THR:HG22	24:X:89:ASP:N	2.09	0.68
26:Z:189:ASN:ND2	26:Z:192:ASP:H	1.92	0.68
1:A:677:C:H4'	5:E:246:ARG:NH2	2.09	0.67
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.56	0.67
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.76	0.67
1:A:1666:C:H2'	1:A:1667:A:H5'	1.74	0.67
37:A:3737:HOH:O	21:U:9:LYS:CD	2.42	0.67
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.59	0.67
1:A:1041:U:H2'	1:A:1042:U:H5'	1.76	0.67
4:D:41:PHE:HB3	4:D:190:MET:HE1	1.76	0.67
34:A:8514:CL:CL	37:A:7720:HOH:O	2.50	0.67
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.26	0.67
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.09	0.67
19:S:29:LYS:HB3	37:S:8532:HOH:O	1.93	0.67
24:X:65:VAL:HA	24:X:68:THR:HG22	1.76	0.67
27:1:34:LYS:HE2	37:1:8428:HOH:O	1.94	0.67
1:A:1459:A:OP2	37:A:9224:HOH:O	2.12	0.67
37:A:6996:HOH:O	3:C:211:LYS:HG2	1.94	0.67
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.10	0.67
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.92	0.67
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.24	0.67
15:O:169:PRO:O	15:O:172:PHE:HB3	1.94	0.67
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.77	0.67
37:A:3737:HOH:O	21:U:9:LYS:HD2	1.92	0.67
6:F:105:SER:CB	6:F:131:THR:HG23	2.24	0.67
10:J:28:ILE:HA	10:J:62:GLU:OE1	1.95	0.67
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.77	0.67
15:O:89:GLY:O	15:O:92:ALA:HB3	1.95	0.67
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.09	0.67
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.10	0.67
15:O:164:ASP:CG	15:O:167:ASP:HA	2.20	0.67
23:W:4:HIS:HB3	37:W:6622:HOH:O	1.95	0.67
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.59	0.67
10:J:127:GLY:O	10:J:128:ALA:HB3	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:ARG:O	11:K:78:ILE:HG12	1.95	0.67
23:W:39:ALA:C	23:W:41:GLU:H	2.03	0.67
1:A:447:A:OP1	21:U:2:LYS:HG2	1.95	0.67
1:A:871:G:C8	1:A:871:G:C5'	2.67	0.67
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.59	0.67
37:A:7400:HOH:O	21:U:9:LYS:HB2	1.94	0.67
3:C:2:ARG:NH1	37:C:8515:HOH:O	2.08	0.67
4:D:175:LEU:HD23	4:D:175:LEU:C	2.20	0.67
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.76	0.67
28:2:10:LYS:HG3	37:2:8432:HOH:O	1.93	0.67
1:A:2346:C:O2'	6:F:52:THR:HG21	1.95	0.67
5:E:139:VAL:HG13	37:E:8447:HOH:O	1.94	0.67
14:N:164:THR:CG2	14:N:165:SER:N	2.57	0.67
27:1:47:LEU:HD23	27:1:57:CYS:HB2	1.76	0.67
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.95	0.66
1:A:1751:G:C2'	1:A:1752:G:H5''	2.25	0.66
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.28	0.66
3:C:194:MET:HE3	3:C:199:HIS:HB2	1.77	0.66
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.25	0.66
10:J:5:MET:HG3	37:J:8354:HOH:O	1.94	0.66
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.58	0.66
21:U:47:THR:HB	21:U:100:ASP:HB3	1.75	0.66
1:A:1160:G:N3	37:A:5605:HOH:O	2.28	0.66
14:N:139:PRO:O	14:N:140:ALA:HB3	1.93	0.66
15:O:107:ASN:OD1	34:O:8507:CL:CL	2.50	0.66
2:B:3026:C:OP2	37:B:3472:HOH:O	2.13	0.66
11:K:103:VAL:HG12	37:K:8565:HOH:O	1.96	0.66
27:1:46:LYS:HB2	27:1:57:CYS:SG	2.34	0.66
1:A:154:C:H2'	1:A:155:C:H6	1.60	0.66
1:A:157:G:H4'	14:N:95:LYS:HE3	1.78	0.66
1:A:2000:G:O2'	1:A:2001:G:H5'	1.96	0.66
1:A:2578:G:H5'	1:A:2578:G:H8	1.60	0.66
14:N:74:ARG:NH2	37:N:8631:HOH:O	2.27	0.66
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.77	0.66
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	1.77	0.66
1:A:2710:U:H1'	37:A:7602:HOH:O	1.96	0.66
2:B:3049:G:H5''	37:B:4707:HOH:O	1.94	0.66
14:N:87:MET:HE1	37:N:8531:HOH:O	1.96	0.66
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.11	0.66
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.30	0.66
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:27:LYS:N	10:J:58:HIS:HD2	1.91	0.66
19:S:132:ARG:HG2	19:S:133:ALA:N	2.10	0.66
1:A:400:C:O3'	37:A:5766:HOH:O	2.13	0.66
2:B:3001:U:O3'	2:B:3003:A:H5''	1.96	0.66
2:B:3039:U:H1'	2:B:3044:A:N6	2.09	0.66
11:K:93:ARG:HB3	11:K:93:ARG:HH11	1.58	0.66
1:A:553:G:P	26:Z:204:ARG:HH22	2.19	0.66
1:A:739:G:C5	37:A:7523:HOH:O	2.49	0.66
5:E:12:THR:HB	37:E:8440:HOH:O	1.95	0.66
10:J:141:ASN:HA	37:J:8356:HOH:O	1.94	0.66
3:C:94:LEU:N	3:C:94:LEU:HD23	2.10	0.66
3:C:191:GLY:HA2	3:C:194:MET:HE2	1.77	0.66
7:G:93:MET:HE1	7:G:165:GLY:N	2.10	0.66
24:X:13:MET:HE2	24:X:18:GLN:HA	1.77	0.66
1:A:396:U:H4'	37:A:4403:HOH:O	1.96	0.66
6:F:97:GLN:HG2	6:F:97:GLN:O	1.95	0.66
10:J:140:PRO:HB3	37:J:8370:HOH:O	1.95	0.66
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.21	0.65
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.77	0.65
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.78	0.65
1:A:1909:A:N1	1:A:2128:G:H1'	2.11	0.65
9:I:12:ILE:N	9:I:13:PRO:CD	2.60	0.65
26:Z:155:ARG:NH1	37:Z:8558:HOH:O	2.27	0.65
1:A:2472:C:O2'	1:A:2634:G:H4'	1.96	0.65
32:A:8034:MG:MG	37:A:4868:HOH:O	1.37	0.65
25:Y:41:PHE:O	25:Y:43:VAL:HG23	1.96	0.65
28:2:25:LYS:HG2	28:2:25:LYS:O	1.96	0.65
1:A:2036:C:OP1	37:A:6671:HOH:O	2.14	0.65
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.31	0.65
25:Y:30:MET:HE3	25:Y:55:ASN:OD1	1.96	0.65
2:B:3003:A:H2'	37:B:2430:HOH:O	1.95	0.65
2:B:3023:U:C4'	2:B:3024:U:OP2	2.41	0.65
6:F:174:VAL:HG13	37:F:6555:HOH:O	1.96	0.65
21:U:37:GLN:OE1	21:U:118:SER:HA	1.95	0.65
25:Y:25:ARG:CZ	37:Y:3861:HOH:O	2.42	0.65
1:A:1634:G:H3'	37:A:3869:HOH:O	1.96	0.65
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.79	0.65
23:W:8:ILE:HA	23:W:11:MET:HE3	1.77	0.65
1:A:188:C:H5''	14:N:163:LEU:HD21	1.77	0.65
1:A:282:C:H1'	1:A:368:C:H42	1.60	0.65
37:A:3754:HOH:O	22:V:17:THR:CG2	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.78	0.65
1:A:2320:U:H4'	1:A:2321:A:O4'	1.96	0.65
2:B:3014:G:H5'	2:B:3014:G:C8	2.30	0.65
6:F:95:THR:O	6:F:97:GLN:N	2.27	0.65
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.77	0.65
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.32	0.65
1:A:1477:C:O2'	1:A:1478:U:H5'	1.96	0.65
1:A:2769:C:H2'	1:A:2770:G:O4'	1.97	0.65
1:A:2908:A:H2'	1:A:2909:G:O4'	1.96	0.65
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.79	0.65
11:K:19:MET:HE2	11:K:79:PHE:HA	1.76	0.65
24:X:110:GLN:NE2	24:X:110:GLN:HA	2.12	0.65
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.26	0.65
1:A:1741:U:H5'	1:A:1742:A:OP1	1.96	0.65
1:A:1878:G:H1'	37:A:6090:HOH:O	1.97	0.65
2:B:3028:U:H2'	2:B:3029:C:C6	2.32	0.65
4:D:2:GLN:CD	37:D:8622:HOH:O	2.40	0.65
6:F:135:VAL:HG22	6:F:136:ARG:N	2.11	0.65
6:F:140:ARG:O	6:F:144:ARG:HG2	1.96	0.65
13:M:148:GLU:HA	37:M:8571:HOH:O	1.96	0.65
1:A:338:C:H5''	37:E:8419:HOH:O	1.97	0.64
3:C:33:GLU:O	3:C:34:ASP:HB2	1.96	0.64
5:E:236:THR:H	5:E:239:ALA:HB3	1.62	0.64
14:N:138:HIS:ND1	14:N:139:PRO:O	2.23	0.64
1:A:485:A:N3	1:A:487:G:H5''	2.12	0.64
1:A:2323:G:H5'	37:A:6990:HOH:O	1.98	0.64
4:D:238:ASN:HD22	4:D:240:GLY:N	1.95	0.64
8:H:110:GLU:HG2	37:H:6926:HOH:O	1.96	0.64
11:K:46:ILE:HA	37:K:8528:HOH:O	1.97	0.64
13:M:143:THR:HG22	13:M:145:LEU:H	1.60	0.64
15:O:163:PHE:HA	37:O:8519:HOH:O	1.96	0.64
5:E:103:ASN:HB3	37:E:8309:HOH:O	1.97	0.64
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.79	0.64
1:A:539:G:H2'	1:A:540:A:C8	2.32	0.64
6:F:95:THR:C	6:F:97:GLN:H	2.05	0.64
7:G:79:GLY:HA3	37:G:7046:HOH:O	1.98	0.64
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.62	0.64
1:A:282:C:O2'	1:A:283:U:H5'	1.98	0.64
1:A:1329:A:C2	37:A:4655:HOH:O	2.48	0.64
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.62	0.64
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:GLU:HG3	8:H:61:MET:HE2	1.79	0.64
1:A:182:G:H4'	14:N:157:LEU:HD13	1.78	0.64
1:A:240:C:H4'	14:N:146:GLN:NE2	2.13	0.64
1:A:1303:C:OP2	37:A:4492:HOH:O	2.14	0.64
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.28	0.64
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.79	0.64
1:A:2421:G:H3'	1:A:2422:U:C5'	2.28	0.64
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.80	0.64
15:O:141:ARG:N	37:O:8571:HOH:O	2.31	0.64
22:V:14:GLU:O	22:V:17:THR:HB	1.96	0.64
2:B:3009:C:OP2	37:B:466:HOH:O	2.15	0.64
10:J:27:LYS:H	10:J:58:HIS:CD2	2.09	0.64
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.63	0.64
1:A:160:A:C4	1:A:177:A:C2	2.86	0.63
3:C:131:HIS:O	3:C:132:ASP:HB2	1.96	0.63
11:K:74:ARG:HH11	11:K:74:ARG:CB	2.11	0.63
20:T:43:GLU:HB3	37:T:8344:HOH:O	1.98	0.63
23:W:64:GLY:O	23:W:65:ASP:HB2	1.96	0.63
28:2:8:GLN:HE22	28:2:11:LYS:NZ	1.96	0.63
1:A:263:U:O4'	8:H:59:ILE:HD13	1.98	0.63
1:A:926:A:O2'	13:M:41:HIS:HD2	1.81	0.63
1:A:1086:A:C6	24:X:11:VAL:HG11	2.33	0.63
1:A:1857:A:N6	1:A:2247:C:H1'	2.13	0.63
1:A:2050:G:H5''	19:S:80:TYR:O	1.98	0.63
1:A:2123:A:H5'	14:N:89:ASN:HD21	1.63	0.63
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.13	0.63
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.81	0.63
37:A:5493:HOH:O	4:D:298:LYS:HD3	1.98	0.63
1:A:558:C:H5'	37:A:5235:HOH:O	1.99	0.63
1:A:2432:C:O2'	1:A:2433:A:H5'	1.98	0.63
32:A:8023:MG:MG	37:A:7787:HOH:O	1.41	0.63
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.13	0.63
30:4:74:CYS:SG	30:4:76:LYS:CB	2.86	0.63
1:A:2281:C:C2'	1:A:2282:U:H5'	2.27	0.63
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.34	0.63
37:A:6676:HOH:O	26:Z:165:GLU:HB3	1.98	0.63
1:A:1213:C:O2'	1:A:1214:G:H5'	1.98	0.63
6:F:25:MET:HE1	6:F:37:ALA:O	1.98	0.63
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.33	0.63
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.81	0.63
1:A:1766:U:O2	1:A:1778:A:H5'	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:46:VAL:O	10:J:146:TRP:HH2	1.82	0.63
1:A:299:U:H5'	37:A:7314:HOH:O	1.98	0.63
1:A:952:G:H4'	37:A:4003:HOH:O	1.99	0.63
1:A:2637:A:H5'	37:A:9260:HOH:O	1.98	0.63
1:A:2690:U:O2'	7:G:111:LYS:HE3	1.99	0.63
5:E:16:VAL:HG12	5:E:17:ASP:N	2.13	0.63
6:F:99:ASP:CB	6:F:103:ASN:H	2.12	0.63
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.81	0.63
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.28	0.63
18:R:32:GLU:HA	18:R:71:TYR:OH	1.99	0.63
20:T:51:GLN:HE21	20:T:53:ASN:ND2	1.97	0.63
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	1.98	0.63
29:3:41:HIS:N	29:3:45:ASN:HD22	1.94	0.63
1:A:1679:C:H5'	37:A:9311:HOH:O	1.99	0.63
1:A:113:A:H3'	1:A:114:A:H5''	1.82	0.62
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.63	0.62
37:L:408:HOH:O	22:V:37:GLU:HB3	1.99	0.62
13:M:145:LEU:O	13:M:148:GLU:HG3	1.98	0.62
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.67	0.62
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.79	0.62
1:A:926:A:O2'	13:M:41:HIS:CD2	2.51	0.62
5:E:25:PRO:HG2	37:E:8325:HOH:O	1.98	0.62
15:O:73:ALA:N	37:O:8568:HOH:O	2.32	0.62
20:T:51:GLN:NE2	20:T:53:ASN:HD21	1.97	0.62
1:A:21:G:C5'	19:S:2:ILE:HA	2.28	0.62
1:A:631:A:N3	1:A:2073:G:O2'	2.32	0.62
1:A:1159:G:P	37:A:4266:HOH:O	2.57	0.62
1:A:1377:C:H6	1:A:1377:C:H5'	1.63	0.62
1:A:2314:G:C2'	1:A:2315:C:H5'	2.29	0.62
32:A:8054:MG:MG	37:A:7765:HOH:O	1.42	0.62
5:E:233:THR:HG22	5:E:234:VAL:N	2.12	0.62
30:4:40:ARG:HD2	37:4:8552:HOH:O	1.99	0.62
1:A:1119:G:N2	1:A:1246:A:C2	2.61	0.62
1:A:1134:G:C5'	10:J:151:MET:HE1	2.28	0.62
37:A:6162:HOH:O	29:3:44:ARG:HG2	2.00	0.62
2:B:3003:A:N6	2:B:3022:G:H1'	2.15	0.62
5:E:236:THR:HA	37:E:8450:HOH:O	1.99	0.62
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.34	0.62
1:A:1293:U:O2'	26:Z:149:GLN:NE2	2.29	0.62
1:A:2346:C:O5'	1:A:2346:C:H6	1.82	0.62
1:A:2635:A:O2'	1:A:2636:C:H5'	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:87:THR:O	16:P:91:GLN:HG3	1.99	0.62
19:S:39:THR:HG23	19:S:107:GLU:O	2.00	0.62
4:D:258:GLY:H	4:D:260:HIS:CE1	2.17	0.62
24:X:26:ILE:HG13	24:X:26:ILE:O	1.99	0.62
1:A:2324:G:H4'	1:A:2418:G:O2'	2.00	0.62
6:F:101:THR:HG22	37:F:7400:HOH:O	1.99	0.62
14:N:87:MET:CB	30:4:46:ILE:HD13	2.30	0.62
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.81	0.62
1:A:2878:U:H2'	1:A:2879:A:O4'	2.00	0.62
37:A:7432:HOH:O	4:D:211:THR:HG21	1.99	0.62
37:B:5071:HOH:O	15:O:23:ARG:HD3	1.99	0.62
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.64	0.62
5:E:107:ARG:NH1	5:E:107:ARG:HB3	2.15	0.62
14:N:91:ILE:HA	37:N:8645:HOH:O	1.98	0.62
21:U:55:PHE:HB2	37:U:6384:HOH:O	1.99	0.62
1:A:251:C:O2'	1:A:252:C:H5'	2.00	0.62
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.15	0.62
21:U:9:LYS:HE3	21:U:13:ARG:NH1	2.15	0.62
27:1:29:VAL:O	27:1:33:HIS:HB2	2.00	0.62
1:A:714:U:H3'	37:A:6912:HOH:O	1.99	0.62
1:A:2779:G:H21	7:G:143:GLN:NE2	1.98	0.62
37:B:5071:HOH:O	15:O:20:TYR:CE2	2.50	0.62
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.30	0.62
14:N:172:GLY:C	14:N:183:VAL:HG11	2.25	0.62
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.81	0.62
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.29	0.62
5:E:242:GLU:HG3	37:E:8380:HOH:O	1.99	0.61
7:G:7:ILE:HD11	7:G:11:VAL:C	2.25	0.61
14:N:72:SER:OG	14:N:74:ARG:HB2	1.99	0.61
1:A:1119:G:H8	11:K:52:GLN:NE2	1.98	0.61
1:A:1919:A:H4'	37:A:4823:HOH:O	1.99	0.61
1:A:2094:G:H4'	4:D:245:SER:HB3	1.81	0.61
10:J:75:SER:O	10:J:79:ALA:HB2	2.00	0.61
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.15	0.61
3:C:72:GLU:HG3	27:1:66:GLY:HA2	1.82	0.61
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.82	0.61
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.98	0.61
14:N:68:ARG:O	14:N:68:ARG:HD3	2.00	0.61
1:A:56:G:H5''	23:W:50:ARG:NH1	2.15	0.61
1:A:1441:G:O2'	1:A:1442:A:H5'	2.00	0.61
1:A:2502:C:C2'	1:A:2503:A:H5'	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2729:C:O2'	1:A:2730:G:H5'	2.00	0.61
1:A:2780:C:H2'	1:A:2781:U:C6	2.35	0.61
23:W:58:THR:O	23:W:62:GLU:HG3	2.01	0.61
27:1:53:GLY:HA2	27:1:67:GLY:O	2.00	0.61
1:A:281:U:H3'	37:A:7182:HOH:O	2.00	0.61
13:M:114:VAL:HG11	37:M:8572:HOH:O	2.01	0.61
15:O:80:SER:HB2	37:O:8537:HOH:O	2.00	0.61
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.80	0.61
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.34	0.61
1:A:2419:U:H5''	1:A:2420:G:H5'	1.81	0.61
1:A:2502:C:H2'	1:A:2503:A:H5'	1.82	0.61
4:D:36:PRO:HA	4:D:168:GLY:CA	2.31	0.61
15:O:12:ARG:HD3	15:O:18:THR:OG1	2.01	0.61
27:1:31:ILE:O	27:1:35:LYS:HG3	2.00	0.61
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.81	0.61
7:G:6:GLU:HA	7:G:46:THR:HG22	1.82	0.61
1:A:1505:U:H6	1:A:1505:U:H5'	1.63	0.61
5:E:118:THR:O	5:E:136:VAL:HG13	2.00	0.61
27:1:28:ASP:O	27:1:31:ILE:HG22	2.01	0.61
1:A:121:U:OP2	29:3:10:ARG:NH2	2.33	0.61
1:A:820:G:O2'	1:A:856:G:H4'	2.01	0.61
1:A:2281:C:H2'	1:A:2282:U:H5'	1.82	0.61
3:C:179:MET:HG2	3:C:186:TRP:CB	2.30	0.61
4:D:248:ARG:HG2	37:K:8541:HOH:O	1.99	0.61
6:F:25:MET:CE	6:F:37:ALA:HB1	2.31	0.61
14:N:59:GLY:HA3	14:N:141:ILE:HD11	1.83	0.61
21:U:48:VAL:HG22	21:U:97:ARG:C	2.25	0.61
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.01	0.61
29:3:35:ARG:HB2	37:3:2691:HOH:O	1.99	0.61
1:A:1393:A:H2'	1:A:1394:C:C6	2.36	0.61
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.66	0.61
10:J:166:ASN:N	10:J:166:ASN:HD22	1.98	0.61
11:K:90:LYS:HB2	34:K:8502:CL:CL	2.38	0.61
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.83	0.61
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.36	0.61
1:A:431:G:P	14:N:48:ARG:HH12	2.24	0.60
1:A:1773:G:C8	27:1:16:PRO:HA	2.35	0.60
2:B:3054:A:O2'	2:B:3055:U:H5'	2.01	0.60
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.83	0.60
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.83	0.60
24:X:22:GLU:HG2	24:X:27:HIS:CD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:A:H4'	37:A:5304:HOH:O	2.00	0.60
1:A:929:A:H8	1:A:929:A:O5'	1.84	0.60
1:A:1847:A:OP1	3:C:175:LYS:HG3	2.00	0.60
1:A:2432:C:C4'	37:A:9718:HOH:O	2.43	0.60
5:E:237:GLU:HB2	37:E:8429:HOH:O	2.00	0.60
6:F:36:ASN:HA	37:F:7500:HOH:O	2.00	0.60
14:N:186:SER:O	14:N:189:VAL:HG12	2.01	0.60
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.84	0.60
15:O:154:LEU:O	15:O:155:GLU:HB3	1.99	0.60
1:A:69:A:H5'	1:A:69:A:C8	2.36	0.60
4:D:305:ASP:O	4:D:306:LYS:HB2	2.02	0.60
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.64	0.60
15:O:37:ARG:CD	34:O:8507:CL:CL	2.86	0.60
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.83	0.60
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.83	0.60
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.30	0.60
1:A:797:A:O4'	27:1:10:ARG:N	2.33	0.60
1:A:2241:C:O2'	1:A:2242:U:H5'	2.01	0.60
1:A:2310:G:OP2	10:J:114:PRO:HD2	2.00	0.60
6:F:136:ARG:HD2	6:F:155:HIS:O	2.01	0.60
8:H:46:GLU:O	8:H:73:PRO:HD2	2.02	0.60
14:N:30:GLU:O	14:N:34:GLU:HG3	2.01	0.60
19:S:39:THR:HB	19:S:42:GLU:HG3	1.83	0.60
24:X:4:LEU:O	24:X:32:CYS:HA	2.01	0.60
30:4:73:GLU:HB3	37:4:8564:HOH:O	2.00	0.60
1:A:125:U:H2'	37:A:3747:HOH:O	2.02	0.60
1:A:821:U:O2'	1:A:822:C:H5'	2.01	0.60
1:A:1311:G:C2	1:A:1312:G:C8	2.90	0.60
1:A:2249:G:OP2	37:A:5416:HOH:O	2.16	0.60
6:F:35:ALA:N	37:F:5576:HOH:O	2.35	0.60
1:A:280:C:H2'	1:A:281:U:O4'	2.02	0.60
1:A:941:G:O2'	1:A:942:U:H5'	2.01	0.60
1:A:948:G:N7	37:A:5820:HOH:O	2.31	0.60
1:A:1205:U:H2'	1:A:1206:U:C5'	2.30	0.60
1:A:2388:C:OP1	37:A:4572:HOH:O	2.16	0.60
37:A:4037:HOH:O	4:D:27:ASN:HB2	2.01	0.60
7:G:11:VAL:HG13	7:G:23:GLU:O	2.01	0.60
1:A:886:A:OP1	37:A:3652:HOH:O	2.17	0.60
2:B:3035:C:H5''	37:B:4078:HOH:O	2.00	0.60
3:C:1:GLY:N	37:C:8612:HOH:O	2.29	0.60
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.67	0.60
15:O:141:ARG:HB3	37:O:8571:HOH:O	2.00	0.60
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.02	0.60
23:W:39:ALA:O	23:W:41:GLU:N	2.35	0.60
27:1:75:ALA:HB3	37:1:8440:HOH:O	2.01	0.60
1:A:1741:U:O2'	1:A:2723:G:H4'	2.01	0.60
1:A:1982:C:OP2	37:A:4252:HOH:O	2.16	0.60
15:O:119:GLN:O	15:O:123:ILE:HG13	2.01	0.60
33:A:8313:NA:NA	37:A:5123:HOH:O	1.74	0.60
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.84	0.60
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.32	0.60
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.13	0.60
26:Z:216:ARG:CD	37:Z:8569:HOH:O	2.39	0.60
1:A:1165:G:OP1	1:A:1165:G:H3'	2.02	0.59
1:A:1187:U:O2'	1:A:1189:A:H2	1.85	0.59
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.01	0.59
5:E:246:ARG:HB3	5:E:246:ARG:NH1	2.16	0.59
10:J:75:SER:C	10:J:79:ALA:HB2	2.27	0.59
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.82	0.59
14:N:139:PRO:O	14:N:140:ALA:CB	2.50	0.59
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.84	0.59
15:O:82:TYR:C	15:O:82:TYR:CD2	2.80	0.59
26:Z:115:ARG:NE	37:Z:8556:HOH:O	2.34	0.59
15:O:164:ASP:OD2	15:O:167:ASP:HA	2.02	0.59
22:V:47:ARG:HG3	37:V:4381:HOH:O	2.01	0.59
24:X:38:THR:HG22	37:X:3580:HOH:O	2.01	0.59
1:A:558:C:C2'	1:A:559:U:H5''	2.33	0.59
10:J:111:MET:O	10:J:114:PRO:HD3	2.02	0.59
15:O:152:GLU:C	15:O:154:LEU:H	2.08	0.59
1:A:182:G:H5'	37:A:5135:HOH:O	2.02	0.59
1:A:349:U:O2'	1:A:350:C:H5'	2.02	0.59
1:A:2505:G:O2'	1:A:2506:A:H5'	2.01	0.59
2:B:3055:U:H4'	2:B:3056:A:C8	2.38	0.59
4:D:312:ARG:HD3	4:D:315:VAL:HG13	1.84	0.59
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.31	0.59
1:A:703:G:O2'	1:A:704:C:H5'	2.02	0.59
1:A:1119:G:H8	11:K:52:GLN:HE22	1.49	0.59
1:A:1523:G:H2'	1:A:1524:U:C6	2.38	0.59
3:C:166:ASP:OD1	37:C:8621:HOH:O	2.16	0.59
24:X:13:MET:HE2	24:X:18:GLN:CA	2.33	0.59
1:A:1669:A:H2'	1:A:1670:G:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:15:ARG:HB3	25:Y:15:ARG:NH1	2.16	0.59
29:3:1:GLY:HA3	37:3:5969:HOH:O	2.02	0.59
37:A:9678:HOH:O	4:D:254:GLN:HG3	2.02	0.59
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.84	0.59
10:J:71:TYR:C	10:J:73:GLN:N	2.58	0.59
1:A:820:G:OP1	27:1:17:ARG:NH2	2.31	0.59
1:A:1972:U:H2'	1:A:1973:A:H5'	1.85	0.59
1:A:2001:G:O2'	1:A:2002:C:H5'	2.03	0.59
1:A:2783:A:H3'	37:A:5210:HOH:O	2.00	0.59
2:B:3002:U:OP2	2:B:3002:U:H4'	2.01	0.59
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.83	0.59
5:E:84:VAL:O	5:E:85:LYS:HB2	2.02	0.59
15:O:151:ASP:O	15:O:154:LEU:HB2	2.03	0.59
26:Z:144:ARG:NE	37:Z:8610:HOH:O	2.35	0.59
1:A:681:G:H5'	1:A:681:G:N3	2.18	0.59
1:A:962:C:C1'	15:O:5:ARG:NH1	2.63	0.59
1:A:2064:U:OP1	37:A:3329:HOH:O	2.17	0.59
1:A:2382:A:OP1	30:4:80:ARG:HG2	2.03	0.59
7:G:69:ILE:HA	7:G:72:MET:CE	2.33	0.59
8:H:58:GLU:HA	8:H:61:MET:HG3	1.85	0.59
30:4:7:PHE:HE2	30:4:22:VAL:HG21	1.67	0.59
1:A:960:G:H2'	1:A:960:G:N3	2.18	0.59
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.84	0.59
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.32	0.59
16:P:26:TRP:N	37:P:3062:HOH:O	2.34	0.59
24:X:149:LEU:CG	24:X:153:MET:HE2	2.32	0.59
26:Z:112:GLU:CD	26:Z:115:ARG:NH1	2.61	0.59
1:A:1053:G:OP1	10:J:12:PRO:HG3	2.02	0.58
32:A:8011:MG:MG	37:A:3953:HOH:O	1.45	0.58
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.03	0.58
4:D:75:GLU:C	4:D:77:PRO:HD3	2.28	0.58
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.03	0.58
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.04	0.58
1:A:2064:U:H5'	1:A:2652:U:H4'	1.85	0.58
6:F:166:ILE:HD12	37:F:6326:HOH:O	2.03	0.58
14:N:123:ASP:C	14:N:123:ASP:OD1	2.46	0.58
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.86	0.58
1:A:1923:G:H4'	30:4:31:THR:O	2.03	0.58
1:A:2748:G:H5'	37:A:7521:HOH:O	2.03	0.58
1:A:2851:G:O2'	1:A:2852:A:H5'	2.03	0.58
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:168:ARG:NH2	5:E:190:ALA:O	2.36	0.58
5:E:219:ASN:O	5:E:222:ASP:OD1	2.21	0.58
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.03	0.58
16:P:39:THR:O	16:P:115:ARG:NH2	2.36	0.58
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.84	0.58
1:A:131:A:OP2	37:A:3142:HOH:O	2.17	0.58
1:A:1183:C:N4	37:A:4371:HOH:O	2.32	0.58
1:A:2121:G:O2'	1:A:2122:C:H5'	2.04	0.58
1:A:2279:G:N3	37:A:9807:HOH:O	2.32	0.58
1:A:2507:G:H2'	1:A:2510:C:H42	1.68	0.58
3:C:11:ARG:HD3	37:C:8518:HOH:O	2.02	0.58
3:C:211:LYS:NZ	37:C:8575:HOH:O	2.37	0.58
6:F:37:ALA:O	6:F:40:ILE:HG12	2.03	0.58
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.85	0.58
1:A:113:A:OP2	1:A:114:A:H2'	2.02	0.58
8:H:110:GLU:O	8:H:114:LYS:HG3	2.04	0.58
10:J:163:PRO:O	10:J:164:ALA:HB2	2.03	0.58
13:M:143:THR:CG2	13:M:144:ASP:N	2.66	0.58
15:O:43:VAL:HG13	15:O:118:ILE:HD11	1.83	0.58
19:S:44:VAL:O	19:S:48:GLU:HG3	2.03	0.58
26:Z:112:GLU:OE1	26:Z:112:GLU:HA	2.04	0.58
27:1:25:ARG:O	27:1:29:VAL:HG23	2.03	0.58
1:A:407:A:H5'	37:A:5994:HOH:O	2.03	0.58
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.86	0.58
7:G:84:MET:HE2	7:G:133:VAL:HG21	1.85	0.58
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.39	0.58
10:J:65:ARG:CZ	37:J:8374:HOH:O	2.50	0.58
13:M:48:LYS:NZ	37:M:8532:HOH:O	2.36	0.58
1:A:285:A:H2'	1:A:286:U:O4'	2.04	0.58
1:A:371:U:H2'	1:A:372:A:H8	1.68	0.58
4:D:74:ILE:HG13	37:D:8606:HOH:O	2.03	0.58
14:N:154:ARG:CZ	37:N:8643:HOH:O	2.51	0.58
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.33	0.58
1:A:1127:C:H2'	1:A:1128:U:H5'	1.85	0.58
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.38	0.58
2:B:3055:U:H4'	2:B:3056:A:H8	1.68	0.58
6:F:99:ASP:HB3	6:F:103:ASN:H	1.68	0.58
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.19	0.58
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.86	0.58
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.85	0.58
17:Q:105:LEU:CD2	17:Q:137:LEU:HD21	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:122:ARG:HH22	24:X:154:ARG:C	2.12	0.58
1:A:2329:C:O2'	1:A:2330:U:H5'	2.04	0.58
1:A:2359:G:N7	37:A:3681:HOH:O	2.32	0.58
1:A:2594:C:O2'	1:A:2595:U:H5'	2.03	0.58
1:A:2718:C:H6	1:A:2718:C:H5'	1.69	0.58
37:A:9380:HOH:O	14:N:94:LYS:HE2	2.03	0.58
5:E:27:ARG:HG3	5:E:29:ASP:OD1	2.03	0.58
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.19	0.58
22:V:9:CYS:HA	22:V:52:THR:CG2	2.30	0.58
1:A:469:G:O2'	37:A:3035:HOH:O	2.16	0.58
1:A:489:A:C8	21:U:82:THR:HG22	2.39	0.58
1:A:1829:A:H5''	37:A:3062:HOH:O	2.02	0.58
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.39	0.58
37:A:4491:HOH:O	14:N:94:LYS:HE3	2.03	0.58
13:M:143:THR:HG22	13:M:144:ASP:H	1.69	0.58
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.39	0.58
1:A:815:U:OP1	37:A:3037:HOH:O	2.17	0.57
1:A:1474:C:H6	1:A:1474:C:C5'	2.11	0.57
1:A:1535:G:H2'	1:A:1536:C:C6	2.39	0.57
1:A:1559:A:H1'	37:A:5836:HOH:O	2.03	0.57
2:B:3026:C:P	37:B:3472:HOH:O	2.62	0.57
2:B:3107:C:H5	37:B:3167:HOH:O	1.87	0.57
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.18	0.57
6:F:86:THR:O	6:F:90:LEU:HG	2.04	0.57
8:H:46:GLU:N	37:H:3461:HOH:O	2.37	0.57
8:H:53:ASP:OD1	8:H:80:GLN:HB2	2.03	0.57
11:K:107:ASN:C	11:K:107:ASN:HD22	2.11	0.57
1:A:558:C:O2'	1:A:559:U:H5''	2.05	0.57
37:A:7435:HOH:O	5:E:188:ARG:CD	2.51	0.57
4:D:125:GLU:O	4:D:129:ARG:HG3	2.03	0.57
5:E:236:THR:O	5:E:237:GLU:C	2.47	0.57
10:J:49:VAL:O	10:J:157:ILE:HG23	2.04	0.57
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.86	0.57
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.85	0.57
1:A:474:C:O3'	5:E:73:LEU:HD21	2.04	0.57
1:A:2729:C:H2'	1:A:2730:G:H8	1.68	0.57
15:O:157:PRO:HA	37:O:8526:HOH:O	2.03	0.57
1:A:272:A:H5'	1:A:273:G:OP2	2.04	0.57
1:A:920:C:H5'	1:A:921:G:C4	2.40	0.57
1:A:1422:U:H2'	1:A:1423:C:H6	1.67	0.57
1:A:2136:G:O3'	37:A:9396:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.36	0.57
9:I:64:ASN:HD22	9:I:64:ASN:N	2.01	0.57
10:J:127:GLY:O	10:J:128:ALA:CB	2.52	0.57
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.87	0.57
14:N:165:SER:HB3	37:N:8534:HOH:O	2.04	0.57
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.39	0.57
1:A:183:A:H5'	14:N:157:LEU:HD12	1.85	0.57
1:A:1819:G:H2'	1:A:1820:G:H4'	1.85	0.57
1:A:2433:A:H2'	1:A:2434:A:C8	2.40	0.57
4:D:221:GLN:HE22	12:L:42:ASN:ND2	2.02	0.57
4:D:238:ASN:ND2	4:D:240:GLY:H	1.96	0.57
22:V:52:THR:HG22	22:V:54:THR:HB	1.87	0.57
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.16	0.57
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.05	0.57
30:4:74:CYS:SG	30:4:76:LYS:CG	2.93	0.57
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.37	0.57
1:A:2577:A:O2'	37:A:5373:HOH:O	2.18	0.57
14:N:115:LEU:HD13	14:N:115:LEU:C	2.30	0.57
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.34	0.57
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.35	0.57
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.16	0.57
1:A:637:C:OP1	26:Z:136:LYS:NZ	2.33	0.57
1:A:951:A:C2'	1:A:952:G:H5'	2.35	0.57
1:A:2015:A:H2'	1:A:2016:U:O4'	2.04	0.57
1:A:2382:A:H5'	37:A:4715:HOH:O	2.04	0.57
1:A:2769:C:C2'	1:A:2770:G:H5'	2.35	0.57
23:W:39:ALA:N	23:W:40:PRO:CD	2.67	0.57
1:A:1126:C:OP2	37:A:3619:HOH:O	2.18	0.57
1:A:2256:G:H2'	1:A:2257:G:H5'	1.87	0.57
1:A:2766:A:O2'	4:D:265:LEU:O	2.22	0.57
37:A:4810:HOH:O	11:K:47:THR:HB	2.04	0.57
5:E:7:ASP:OD1	5:E:11:ASN:O	2.22	0.57
8:H:19:ALA:O	8:H:22:VAL:HG22	2.04	0.57
1:A:69:A:H5'	1:A:69:A:H8	1.70	0.57
1:A:816:G:H5'	1:A:1598:A:H4'	1.87	0.57
1:A:1118:A:C8	1:A:1118:A:C3'	2.83	0.57
1:A:1192:A:O2'	1:A:1193:A:OP1	2.22	0.57
1:A:2506:A:O2'	1:A:2507:G:O5'	2.23	0.57
37:A:5504:HOH:O	14:N:58:GLN:HG3	2.03	0.57
4:D:7:ARG:NH1	4:D:11:LEU:HD21	2.20	0.57
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:28:ALA:HB3	8:H:99:THR:O	2.03	0.57
10:J:86:ARG:NH1	10:J:130:HIS:CD2	2.73	0.57
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.04	0.57
21:U:38:ARG:HH11	21:U:38:ARG:HG3	1.69	0.57
1:A:21:G:H4'	19:S:2:ILE:HG22	1.87	0.57
1:A:1060:C:H6	1:A:1060:C:H5'	1.70	0.57
1:A:1687:C:O2	28:2:9:GLY:HA2	2.05	0.57
8:H:107:VAL:O	8:H:111:ILE:HG13	2.04	0.57
14:N:38:VAL:C	14:N:63:VAL:HG13	2.30	0.57
29:3:41:HIS:H	29:3:45:ASN:ND2	2.03	0.57
1:A:1528:A:H2'	1:A:1529:G:O4'	2.05	0.56
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.35	0.56
1:A:1820:G:C6	1:A:2030:A:C2	2.93	0.56
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.70	0.56
3:C:192:VAL:O	3:C:207:GLN:HG2	2.05	0.56
4:D:162:MET:CE	4:D:308:LEU:HD21	2.23	0.56
10:J:14:TYR:N	10:J:91:HIS:CE1	2.72	0.56
13:M:149:ARG:O	13:M:150:GLN:HB2	2.05	0.56
14:N:169:ARG:HD2	37:N:8590:HOH:O	2.05	0.56
19:S:106:GLY:HA2	19:S:109:MET:CE	2.35	0.56
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.40	0.56
1:A:315:G:C6	1:A:316:A:C6	2.93	0.56
1:A:559:U:H5'	1:A:559:U:C6	2.37	0.56
3:C:109:GLU:HG2	3:C:116:GLY:H	1.70	0.56
4:D:190:MET:HE2	4:D:194:PHE:HD1	1.68	0.56
12:L:74:VAL:HG12	12:L:74:VAL:O	2.05	0.56
14:N:18:GLY:O	14:N:21:ALA:HB3	2.05	0.56
15:O:58:LEU:HD12	15:O:58:LEU:N	2.20	0.56
20:T:6:LYS:HB2	20:T:27:ALA:O	2.03	0.56
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.85	0.56
22:V:13:ILE:HG12	22:V:32:CYS:HB3	1.86	0.56
24:X:13:MET:HE3	24:X:17:ILE:CG2	2.35	0.56
1:A:184:G:H5''	14:N:153:THR:HG22	1.87	0.56
1:A:1056:U:H2'	1:A:1057:A:O4'	2.06	0.56
1:A:1595:G:O2'	1:A:1596:U:H5'	2.05	0.56
1:A:1887:U:OP1	27:1:21:LYS:HE3	2.05	0.56
1:A:1925:G:O2'	1:A:1926:G:H5'	2.05	0.56
1:A:2276:U:H2'	1:A:2277:U:H6	1.69	0.56
1:A:2570:G:H5''	37:A:4890:HOH:O	2.06	0.56
2:B:3006:C:P	15:O:37:ARG:NH1	2.79	0.56
2:B:3103:A:O2'	2:B:3104:A:H5'	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.87	0.56
4:D:24:PRO:HG3	4:D:204:GLY:HA2	1.87	0.56
4:D:27:ASN:HB3	37:D:8630:HOH:O	2.05	0.56
4:D:168:GLY:N	4:D:174:ARG:HD3	2.20	0.56
4:D:214:PRO:HD2	37:D:8521:HOH:O	2.05	0.56
7:G:20:ILE:CD1	7:G:33:LEU:HD12	2.36	0.56
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.34	0.56
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.87	0.56
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.34	0.56
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.35	0.56
27:1:77:LYS:HA	27:1:80:MET:HE2	1.88	0.56
1:A:816:G:C6	1:A:817:G:N1	2.73	0.56
1:A:1450:C:O2'	1:A:1494:A:H5'	2.06	0.56
1:A:1641:A:H2'	1:A:1642:A:H5'	1.87	0.56
1:A:2502:C:H4'	10:J:151:MET:HG2	1.88	0.56
37:A:3822:HOH:O	10:J:11:LYS:HE2	2.04	0.56
2:B:3064:C:H2'	2:B:3065:A:H5'	1.87	0.56
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.35	0.56
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.88	0.56
7:G:93:MET:HE1	7:G:165:GLY:H	1.69	0.56
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.33	0.56
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.40	0.56
14:N:87:MET:CE	37:N:8531:HOH:O	2.53	0.56
14:N:104:ARG:O	14:N:108:LYS:HG2	2.04	0.56
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.87	0.56
24:X:13:MET:CE	24:X:17:ILE:HG22	2.35	0.56
1:A:484:A:N1	1:A:506:G:H4'	2.21	0.56
1:A:558:C:H2'	1:A:559:U:C5'	2.35	0.56
1:A:1483:C:O2'	1:A:1484:G:H5'	2.05	0.56
4:D:14:GLY:HA2	4:D:15:PRO:C	2.30	0.56
4:D:148:PRO:HD2	37:D:8582:HOH:O	2.05	0.56
4:D:240:GLY:HA3	37:D:8528:HOH:O	2.05	0.56
4:D:333:GLU:HB2	22:V:14:GLU:OE2	2.06	0.56
14:N:59:GLY:C	14:N:141:ILE:HD11	2.31	0.56
14:N:74:ARG:O	14:N:88:VAL:HG13	2.04	0.56
1:A:289:G:N2	1:A:363:A:H2	2.01	0.56
1:A:710:G:OP1	16:P:24:ALA:HB3	2.04	0.56
1:A:778:C:C4	1:A:779:U:C4	2.94	0.56
1:A:1116:U:O2'	1:A:1118:A:C2	2.50	0.56
1:A:1701:A:H4'	1:A:1702:U:C5'	2.35	0.56
1:A:2587:U:H2'	1:A:2589:U:H5''	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:304:PRO:HD2	4:D:307:ARG:HD2	1.86	0.56
8:H:100:ASP:O	8:H:101:ALA:O	2.24	0.56
26:Z:112:GLU:OE1	26:Z:115:ARG:NH1	2.38	0.56
30:4:3:MET:O	30:4:90:PHE:HA	2.06	0.56
1:A:88:G:N7	29:3:28:LYS:HD2	2.20	0.56
1:A:134:U:O2	1:A:145:A:C2	2.58	0.56
1:A:2361:A:H2'	1:A:2362:A:C8	2.40	0.56
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.39	0.56
30:4:71:CYS:SG	30:4:72:GLY:N	2.78	0.56
1:A:1174:A:C5	1:A:1201:C:H4'	2.40	0.56
1:A:1711:A:O2'	1:A:1712:A:H5'	2.05	0.56
1:A:2064:U:H5'	1:A:2652:U:O3'	2.06	0.56
1:A:2432:C:H4'	30:4:36:ILE:HG12	1.86	0.56
6:F:11:HIS:C	6:F:13:MET:H	2.13	0.56
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.06	0.56
24:X:80:ASP:O	24:X:84:VAL:HG23	2.05	0.56
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.04	0.56
1:A:1234:U:N3	4:D:244:PRO:HB3	2.21	0.56
1:A:1362:U:H5'	37:E:8342:HOH:O	2.06	0.56
1:A:1730:G:H5'	1:A:1731:C:C5	2.41	0.56
1:A:2011:A:P	37:A:5928:HOH:O	2.64	0.56
2:B:3044:A:O4'	6:F:76:ARG:NE	2.39	0.56
4:D:16:ARG:NH2	37:D:8556:HOH:O	2.28	0.56
10:J:53:PRO:HA	10:J:125:VAL:O	2.05	0.56
1:A:136:C:H2'	1:A:137:U:O4'	2.04	0.56
1:A:1733:A:H4'	4:D:212:GLN:HA	1.87	0.56
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.88	0.56
1:A:2433:A:H2'	1:A:2434:A:H8	1.70	0.56
1:A:2526:C:O2'	1:A:2527:U:H5'	2.05	0.56
4:D:141:ARG:HD2	4:D:163:GLU:OE2	2.05	0.56
5:E:133:ARG:HD2	37:E:8408:HOH:O	2.06	0.56
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.50	0.56
12:L:101:ASN:O	12:L:102:GLU:HB2	2.06	0.56
14:N:39:ARG:NH2	37:N:8623:HOH:O	2.38	0.56
14:N:52:LEU:HD21	37:N:8616:HOH:O	2.06	0.56
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.53	0.56
1:A:821:U:H2'	1:A:822:C:C6	2.39	0.55
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.71	0.55
1:A:1688:G:H4'	28:2:8:GLN:HG3	1.87	0.55
1:A:2256:G:C2'	1:A:2257:G:H5'	2.36	0.55
1:A:2314:G:H2'	1:A:2315:C:H5'	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2791:U:H1'	1:A:2792:A:H5''	1.88	0.55
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.88	0.55
6:F:59:GLY:C	6:F:61:PHE:H	2.14	0.55
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.88	0.55
10:J:44:ALA:HA	10:J:163:PRO:O	2.07	0.55
11:K:19:MET:HE1	11:K:78:ILE:HG22	1.89	0.55
14:N:91:ILE:HG23	37:N:8645:HOH:O	2.05	0.55
18:R:75:ILE:HD13	18:R:84:ILE:HD11	1.88	0.55
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.88	0.55
1:A:542:A:H2'	1:A:543:G:O4'	2.05	0.55
1:A:1168:C:H2'	1:A:1169:U:O4'	2.05	0.55
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.88	0.55
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.37	0.55
23:W:56:ILE:O	23:W:60:GLN:HG3	2.05	0.55
1:A:111:C:H2'	1:A:112:G:O4'	2.06	0.55
1:A:820:G:C6	3:C:171:LYS:HB2	2.41	0.55
1:A:1123:A:C6	1:A:1238:C:H5'	2.42	0.55
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.55
2:B:3042:C:O2	6:F:76:ARG:NH1	2.38	0.55
10:J:69:ASN:O	10:J:72:VAL:HG12	2.07	0.55
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.06	0.55
1:A:639:A:H2'	1:A:640:G:C8	2.40	0.55
1:A:2316:G:H8	37:A:5626:HOH:O	1.89	0.55
1:A:2464:C:P	37:A:9912:HOH:O	2.64	0.55
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.35	0.55
11:K:52:GLN:HG3	11:K:53:ILE:N	2.21	0.55
12:L:30:LYS:O	12:L:55:VAL:HG13	2.06	0.55
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.24	0.55
15:O:86:LEU:O	15:O:90:LEU:HG	2.06	0.55
23:W:44:GLY:O	23:W:48:GLU:HG2	2.06	0.55
1:A:283:U:H5''	1:A:284:C:P	2.47	0.55
1:A:1182:C:H1'	1:A:1192:A:H8	1.72	0.55
2:B:3029:C:C2'	2:B:3030:C:H5'	2.36	0.55
4:D:7:ARG:HD3	4:D:9:GLY:O	2.06	0.55
5:E:16:VAL:HG12	5:E:17:ASP:H	1.71	0.55
6:F:140:ARG:O	6:F:140:ARG:HG2	2.06	0.55
7:G:81:GLU:HG2	7:G:134:SER:CB	2.37	0.55
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.55	0.55
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.70	0.55
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.21	0.55
1:A:57:C:H5''	37:A:6728:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2271:G:P	37:A:9415:HOH:O	2.65	0.55
1:A:2349:G:OP1	6:F:20:LYS:NZ	2.39	0.55
1:A:2897:C:H2'	1:A:2898:G:H8	1.71	0.55
13:M:57:VAL:HG12	13:M:57:VAL:O	2.05	0.55
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.42	0.55
1:A:506:G:H22	1:A:509:A:H5''	1.68	0.55
1:A:516:A:P	37:A:5618:HOH:O	2.64	0.55
1:A:545:G:H5'	1:A:545:G:C8	2.37	0.55
1:A:671:A:O2'	1:A:672:G:H2'	2.07	0.55
1:A:2649:A:H5'	1:A:2649:A:H8	1.71	0.55
37:A:6996:HOH:O	3:C:211:LYS:CG	2.52	0.55
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.88	0.55
4:D:280:VAL:CG1	4:D:334:SER:HA	2.36	0.55
14:N:149:TRP:O	14:N:152:ARG:HG2	2.06	0.55
23:W:64:GLY:O	23:W:65:ASP:CB	2.55	0.55
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.22	0.55
26:Z:99:ALA:HB2	26:Z:233:TYR:CE2	2.42	0.55
1:A:1134:G:H4'	10:J:151:MET:CE	2.19	0.55
1:A:1825:U:O4'	1:A:1999:C:H5''	2.06	0.55
1:A:1862:C:H1'	37:A:7195:HOH:O	2.07	0.55
1:A:2897:C:O2'	1:A:2898:G:H5'	2.07	0.55
37:A:3051:HOH:O	19:S:83:LYS:HB3	2.06	0.55
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.88	0.55
15:O:22:GLN:HG2	15:O:26:LEU:HD22	1.88	0.55
15:O:64:SER:C	15:O:66:LEU:H	2.15	0.55
16:P:44:ASN:OD1	16:P:65:LEU:HB2	2.07	0.55
26:Z:144:ARG:CZ	37:Z:8610:HOH:O	2.54	0.55
28:2:25:LYS:HE2	37:3:7213:HOH:O	2.06	0.55
1:A:2326:U:H4'	1:A:2412:G:C4'	2.37	0.55
1:A:2365:G:H4'	18:R:45:PRO:O	2.06	0.55
4:D:140:LEU:HD23	37:D:8581:HOH:O	2.07	0.55
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.07	0.55
9:I:12:ILE:HG22	9:I:12:ILE:O	2.05	0.55
1:A:694:A:H2'	1:A:695:C:H5'	1.89	0.55
1:A:1079:A:N1	1:A:2068:G:O2'	2.39	0.55
1:A:1205:U:C2'	1:A:1206:U:H5'	2.32	0.55
1:A:1653:A:N6	37:A:4237:HOH:O	2.40	0.55
4:D:1:PRO:O	4:D:2:GLN:HB2	2.07	0.55
7:G:11:VAL:CG1	7:G:12:ASP:N	2.69	0.55
28:2:8:GLN:HE22	28:2:11:LYS:HZ1	1.52	0.55
1:A:902:G:N7	13:M:18:HIS:HD2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2404:G:O3'	37:A:6569:HOH:O	2.18	0.54
1:A:2679:G:H2'	1:A:2681:A:OP2	2.07	0.54
3:C:105:VAL:HG12	3:C:106:CYS:N	2.22	0.54
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.07	0.54
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.89	0.54
12:L:37:TYR:CD2	37:L:7169:HOH:O	2.53	0.54
17:Q:13:VAL:HG11	17:Q:40:VAL:HG11	1.87	0.54
26:Z:107:PRO:HB3	26:Z:182:PHE:CD2	2.43	0.54
1:A:2760:C:H5''	37:A:5303:HOH:O	2.07	0.54
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.88	0.54
5:E:85:LYS:NZ	37:E:8328:HOH:O	2.13	0.54
8:H:91:VAL:CG1	8:H:92:GLY:H	2.17	0.54
14:N:154:ARG:HG3	37:N:8613:HOH:O	2.07	0.54
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.65	0.54
29:3:18:ASN:HD21	29:3:40:ARG:H	1.53	0.54
1:A:281:U:O2'	1:A:282:C:H5'	2.08	0.54
1:A:401:C:P	37:A:5766:HOH:O	2.66	0.54
1:A:739:G:N7	37:A:7523:HOH:O	2.38	0.54
1:A:1159:G:H21	1:A:1189:A:H8	1.53	0.54
1:A:1269:G:H2'	1:A:1270:U:C6	2.43	0.54
1:A:1562:C:O2	1:A:1562:C:H2'	2.07	0.54
1:A:1882:C:O2'	1:A:2012:U:OP2	2.23	0.54
31:A:9001:SPR:H6A3	31:A:9001:SPR:C2B	2.22	0.54
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.88	0.54
6:F:50:VAL:O	6:F:71:ALA:HA	2.07	0.54
8:H:21:GLU:O	8:H:24:ARG:HG3	2.06	0.54
21:U:106:GLU:HG3	37:U:4913:HOH:O	2.06	0.54
23:W:49:LEU:O	23:W:53:ILE:HG13	2.06	0.54
1:A:175:G:H2'	14:N:192:ALA:HB3	1.88	0.54
1:A:1164:U:O4'	1:A:1165:G:OP1	2.25	0.54
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.08	0.54
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.72	0.54
15:O:91:ARG:HG3	15:O:186:LEU:HD23	1.89	0.54
1:A:2359:G:H3'	37:A:5662:HOH:O	2.08	0.54
4:D:305:ASP:O	4:D:306:LYS:CB	2.55	0.54
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.72	0.54
6:F:170:TYR:O	6:F:171:ASP:HB3	2.06	0.54
10:J:71:TYR:O	10:J:73:GLN:N	2.40	0.54
10:J:147:ARG:HA	10:J:150:LYS:HZ2	1.73	0.54
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.90	0.54
15:O:67:ALA:C	15:O:69:TYR:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:39:CYS:HA	27:1:47:LEU:CD1	2.34	0.54
1:A:2894:C:O2'	1:A:2895:C:H5'	2.07	0.54
10:J:136:VAL:HG22	10:J:137:ASN:O	2.07	0.54
13:M:104:ASP:O	13:M:105:TYR:HB3	2.05	0.54
15:O:155:GLU:O	15:O:156:GLU:HG3	2.08	0.54
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.36	0.54
1:A:204:A:H2'	1:A:205:U:H5'	1.89	0.54
1:A:661:G:C5	1:A:686:A:C2	2.95	0.54
1:A:1330:A:H5''	1:A:1331:A:OP2	2.08	0.54
1:A:1847:A:OP1	3:C:175:LYS:NZ	2.41	0.54
5:E:154:VAL:O	5:E:158:GLU:HG3	2.07	0.54
6:F:86:THR:C	6:F:89:PRO:HD2	2.32	0.54
7:G:32:ARG:O	7:G:33:LEU:HD23	2.07	0.54
10:J:13:ALA:HA	10:J:91:HIS:HE1	1.72	0.54
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.90	0.54
22:V:13:ILE:HG12	22:V:32:CYS:HB2	1.89	0.54
22:V:52:THR:CG2	22:V:54:THR:HB	2.38	0.54
1:A:338:C:H4'	5:E:174:ILE:HD12	1.86	0.54
1:A:470:U:O2'	28:2:16:HIS:HD2	1.90	0.54
1:A:541:C:O2'	1:A:542:A:H5''	2.07	0.54
1:A:775:G:OP1	28:2:16:HIS:HE1	1.91	0.54
1:A:1878:G:C1'	37:A:6090:HOH:O	2.54	0.54
1:A:1887:U:OP1	27:1:21:LYS:HG3	2.07	0.54
1:A:2082:G:O2'	1:A:2083:A:H5'	2.07	0.54
3:C:175:LYS:HE2	37:C:8579:HOH:O	2.07	0.54
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.07	0.54
6:F:163:VAL:HA	37:F:6326:HOH:O	2.07	0.54
10:J:139:ASP:N	10:J:140:PRO:CD	2.69	0.54
12:L:125:ALA:C	12:L:127:ALA:H	2.15	0.54
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.71	0.54
1:A:1268:C:H2'	1:A:1269:G:H8	1.73	0.54
37:A:5766:HOH:O	14:N:170:CYS:SG	2.59	0.54
6:F:10:PHE:CG	6:F:11:HIS:N	2.76	0.54
10:J:26:LYS:HD3	10:J:89:PRO:CG	2.38	0.54
14:N:154:ARG:HD3	37:N:8643:HOH:O	2.07	0.54
15:O:182:GLY:N	37:O:8572:HOH:O	2.39	0.54
1:A:921:G:H4'	1:A:924:G:N1	2.23	0.54
1:A:963:C:O5'	1:A:963:C:H6	1.91	0.54
1:A:1695:G:C6	1:A:1696:U:C4	2.96	0.54
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.88	0.54
4:D:55:ASN:HB3	4:D:64:GLY:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:251:VAL:HG23	4:D:252:PRO:HD2	1.89	0.54
5:E:43:LYS:NZ	37:E:8387:HOH:O	2.36	0.54
6:F:154:LYS:H	6:F:154:LYS:CD	2.15	0.54
11:K:22:VAL:O	11:K:26:VAL:HG23	2.08	0.54
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.08	0.54
30:4:48:ASN:ND2	30:4:50:GLY:H	2.06	0.54
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.91	0.53
10:J:45:GLN:HE21	10:J:135:TRP:NE1	2.06	0.53
10:J:139:ASP:H	10:J:140:PRO:HD3	1.68	0.53
13:M:104:ASP:HB3	37:M:8564:HOH:O	2.08	0.53
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.08	0.53
24:X:26:ILE:O	24:X:26:ILE:CG1	2.56	0.53
26:Z:187:VAL:HB	37:Z:8570:HOH:O	2.08	0.53
1:A:119:A:H2'	1:A:120:A:H5'	1.89	0.53
1:A:217:C:OP1	1:A:395:A:O2'	2.25	0.53
1:A:558:C:H2'	1:A:559:U:H5'	1.90	0.53
1:A:922:A:N7	1:A:2281:C:H5'	2.23	0.53
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.44	0.53
8:H:99:THR:O	8:H:99:THR:HG23	2.07	0.53
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.37	0.53
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.43	0.53
13:M:133:VAL:HB	37:M:8558:HOH:O	2.08	0.53
22:V:49:LEU:CD1	37:V:3805:HOH:O	2.56	0.53
1:A:39:G:N2	1:A:444:C:C2	2.77	0.53
1:A:1176:C:H1'	37:A:3905:HOH:O	2.08	0.53
1:A:1636:G:O2'	1:A:1637:A:H5'	2.08	0.53
2:B:3041:C:C6	6:F:50:VAL:HG21	2.43	0.53
10:J:117:LYS:HB2	37:J:8326:HOH:O	2.08	0.53
11:K:4:ALA:N	37:K:8572:HOH:O	2.41	0.53
16:P:59:VAL:HG23	16:P:111:VAL:HG23	1.89	0.53
22:V:47:ARG:CG	37:V:4381:HOH:O	2.55	0.53
27:1:39:CYS:CB	27:1:47:LEU:HD21	2.37	0.53
1:A:154:C:H2'	1:A:155:C:C6	2.42	0.53
1:A:553:G:O4'	1:A:1325:G:H5'	2.08	0.53
1:A:1308:A:H5'	37:A:6904:HOH:O	2.08	0.53
1:A:2055:A:H5'	19:S:134:SER:HB2	1.90	0.53
1:A:2073:G:OP2	1:A:2490:A:H5'	2.08	0.53
4:D:275:GLY:O	4:D:291:ASP:HA	2.08	0.53
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.09	0.53
20:T:81:ILE:HG23	37:T:8336:HOH:O	2.07	0.53
21:U:38:ARG:HG3	21:U:38:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:46:LYS:O	27:1:57:CYS:HA	2.08	0.53
1:A:657:G:OP1	5:E:27:ARG:NH2	2.29	0.53
1:A:2459:G:OP2	30:4:64:LYS:HD2	2.07	0.53
37:A:6290:HOH:O	6:F:55:LYS:HB2	2.08	0.53
37:A:9544:HOH:O	4:D:267:LYS:HD3	2.07	0.53
3:C:93:THR:C	3:C:94:LEU:HD23	2.33	0.53
4:D:243:ASN:HA	4:D:244:PRO:C	2.32	0.53
7:G:21:THR:HG23	7:G:30:THR:OG1	2.09	0.53
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.09	0.53
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.89	0.53
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.23	0.53
11:K:107:ASN:HD22	11:K:109:TYR:H	1.54	0.53
14:N:87:MET:SD	37:N:8533:HOH:O	2.58	0.53
14:N:154:ARG:NE	37:N:8643:HOH:O	2.42	0.53
24:X:41:TYR:HA	24:X:44:MET:HE3	1.91	0.53
1:A:396:U:OP2	30:4:38:ARG:NH1	2.42	0.53
1:A:1189:A:H1'	1:A:1209:C:C1'	2.39	0.53
1:A:1209:C:H2'	1:A:1210:G:C8	2.40	0.53
1:A:1250:C:O2'	1:A:1251:C:H5'	2.08	0.53
1:A:2121:G:C2'	1:A:2122:C:H5'	2.38	0.53
1:A:2414:A:H2'	1:A:2415:A:C8	2.43	0.53
3:C:217:ARG:HH11	3:C:217:ARG:CG	2.21	0.53
6:F:23:VAL:O	6:F:23:VAL:CG2	2.55	0.53
14:N:87:MET:HB2	14:N:91:ILE:CD1	2.39	0.53
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.09	0.53
17:Q:115:SER:O	17:Q:117:SER:N	2.42	0.53
1:A:1527:A:H1'	1:A:1528:A:C8	2.43	0.53
1:A:2613:G:O2'	1:A:2614:C:H5'	2.08	0.53
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.71	0.53
3:C:109:GLU:HG2	3:C:116:GLY:N	2.24	0.53
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.91	0.53
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.90	0.53
6:F:84:LEU:C	6:F:86:THR:H	2.16	0.53
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.39	0.53
1:A:327:A:OP1	5:E:149:LYS:NZ	2.27	0.53
1:A:329:A:OP1	5:E:205:ARG:NE	2.37	0.53
1:A:1164:U:C4'	1:A:1165:G:OP1	2.50	0.53
1:A:1166:A:H1'	1:A:1192:A:N1	2.23	0.53
1:A:1947:G:N2	1:A:1966:U:C2	2.77	0.53
7:G:20:ILE:HD12	7:G:33:LEU:HD12	1.90	0.53
8:H:117:GLU:C	8:H:119:ARG:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ARG:C	10:J:59:ASN:N	2.65	0.53
22:V:14:GLU:OE1	22:V:15:PRO:HD2	2.09	0.53
25:Y:73:ARG:O	25:Y:85:VAL:HG13	2.09	0.53
1:A:449:A:N7	5:E:43:LYS:HG2	2.23	0.53
1:A:2634:G:O2'	1:A:2635:A:H5'	2.09	0.53
37:A:7435:HOH:O	5:E:188:ARG:HD2	2.09	0.53
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.90	0.53
19:S:115:ALA:O	19:S:143:VAL:HG23	2.09	0.53
21:U:48:VAL:HG22	21:U:97:ARG:O	2.09	0.53
1:A:1185:U:H5'	37:A:7445:HOH:O	2.08	0.53
1:A:1525:G:H5'	1:A:1526:A:OP2	2.09	0.53
1:A:2405:C:P	37:A:6569:HOH:O	2.66	0.53
4:D:7:ARG:CD	4:D:9:GLY:O	2.57	0.53
4:D:82:VAL:O	4:D:82:VAL:HG12	2.09	0.53
7:G:15:GLN:HG2	7:G:19:ASP:O	2.09	0.53
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.91	0.53
17:Q:58:SER:HB3	37:Q:4744:HOH:O	2.08	0.53
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.44	0.53
1:A:1667:A:H2'	1:A:1668:U:C6	2.44	0.52
1:A:2326:U:H4'	1:A:2412:G:H4'	1.90	0.52
3:C:164:ARG:NE	37:C:8593:HOH:O	2.41	0.52
7:G:43:ASP:HA	37:G:5864:HOH:O	2.08	0.52
7:G:69:ILE:HA	7:G:72:MET:HE3	1.91	0.52
1:A:88:G:H5'	1:A:88:G:H8	1.74	0.52
1:A:656:G:OP2	16:P:37:ARG:HD2	2.09	0.52
1:A:1733:A:C6	1:A:1734:C:C2	2.97	0.52
3:C:37:VAL:HG22	37:C:8600:HOH:O	2.09	0.52
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.08	0.52
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.73	0.52
24:X:38:THR:HG22	24:X:39:ASP:N	2.25	0.52
1:A:820:G:H5'	1:A:821:U:H5'	1.91	0.52
1:A:1041:U:C2'	1:A:1042:U:H5'	2.39	0.52
1:A:1200:A:C4'	37:A:7318:HOH:O	2.57	0.52
1:A:1375:A:O2'	1:A:1376:G:H5'	2.10	0.52
1:A:1490:G:OP2	37:A:3628:HOH:O	2.18	0.52
1:A:2735:U:H2'	1:A:2736:U:C6	2.45	0.52
37:A:3737:HOH:O	21:U:9:LYS:HD3	2.09	0.52
2:B:3020:G:H3'	37:B:2984:HOH:O	2.09	0.52
2:B:3092:G:H2'	2:B:3093:A:C8	2.45	0.52
5:E:1:MET:HG2	5:E:2:GLN:N	2.23	0.52
6:F:64:ARG:O	6:F:67:ASP:OD2	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:128:LEU:HD23	6:F:128:LEU:C	2.35	0.52
10:J:117:LYS:O	10:J:119:VAL:HG13	2.09	0.52
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.92	0.52
14:N:61:ILE:HD12	14:N:61:ILE:N	2.24	0.52
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.39	0.52
15:O:170:GLU:O	15:O:174:GLU:HG3	2.09	0.52
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.20	0.52
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.44	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.09	0.52
1:A:628:A:C8	1:A:2071:C:N4	2.78	0.52
1:A:738:G:H3'	37:A:7019:HOH:O	2.08	0.52
1:A:1197:G:N2	37:A:6202:HOH:O	2.42	0.52
1:A:2787:C:H5	37:A:4602:HOH:O	1.91	0.52
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.22	0.52
10:J:65:ARG:NH1	37:J:8374:HOH:O	2.42	0.52
11:K:77:GLY:O	11:K:78:ILE:C	2.52	0.52
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.90	0.52
19:S:39:THR:HB	19:S:42:GLU:CD	2.34	0.52
28:2:37:CYS:SG	28:2:39:PHE:HB2	2.49	0.52
1:A:1127:C:C5	1:A:1128:U:C4	2.97	0.52
1:A:1166:A:H61	1:A:1180:U:H3	1.55	0.52
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.24	0.52
37:A:9079:HOH:O	14:N:172:GLY:HA2	2.09	0.52
2:B:3044:A:H1'	6:F:76:ARG:NH2	2.24	0.52
7:G:7:ILE:HD11	7:G:11:VAL:O	2.09	0.52
7:G:23:GLU:HG2	7:G:28:SER:CB	2.40	0.52
13:M:143:THR:CG2	13:M:144:ASP:H	2.22	0.52
27:1:30:GLU:HB3	27:1:34:LYS:HE3	1.92	0.52
1:A:82:C:OP1	21:U:67:LEU:HB2	2.09	0.52
1:A:381:G:H5''	37:A:4291:HOH:O	2.08	0.52
1:A:1861:C:H4'	3:C:6:GLY:O	2.10	0.52
37:A:4332:HOH:O	16:P:37:ARG:HG3	2.10	0.52
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.09	0.52
7:G:11:VAL:HG12	7:G:12:ASP:H	1.74	0.52
10:J:151:MET:HA	10:J:151:MET:HE3	1.92	0.52
12:L:101:ASN:O	12:L:102:GLU:CB	2.58	0.52
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.91	0.52
19:S:39:THR:O	19:S:40:ALA:C	2.51	0.52
27:1:59:HIS:HA	37:1:8444:HOH:O	2.10	0.52
1:A:432:G:O2'	1:A:433:C:H5'	2.09	0.52
1:A:921:G:H4'	1:A:924:G:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2768:A:O2'	1:A:2769:C:H5'	2.10	0.52
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.10	0.52
8:H:28:ALA:CB	8:H:99:THR:HG23	2.40	0.52
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.43	0.52
10:J:132:PHE:O	10:J:133:ILE:HD13	2.10	0.52
15:O:113:SER:C	37:O:8560:HOH:O	2.53	0.52
1:A:316:A:N3	1:A:336:G:O2'	2.41	0.52
1:A:1180:U:H2'	1:A:1181:A:O4'	2.10	0.52
1:A:1205:U:C2'	1:A:1206:U:C5'	2.88	0.52
1:A:2123:A:H5'	14:N:89:ASN:ND2	2.25	0.52
1:A:2435:U:H1'	37:A:5404:HOH:O	2.09	0.52
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.19	0.52
5:E:104:ASP:O	5:E:108:GLN:HG3	2.09	0.52
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.08	0.52
8:H:91:VAL:CG1	8:H:92:GLY:N	2.70	0.52
10:J:53:PRO:HG3	10:J:127:GLY:H	1.75	0.52
14:N:115:LEU:HD13	14:N:116:ASN:HB2	1.91	0.52
15:O:110:THR:HB	15:O:113:SER:OG	2.10	0.52
17:Q:98:ILE:O	17:Q:98:ILE:HD13	2.10	0.52
29:3:48:ASP:O	29:3:49:GLU:HB2	2.10	0.52
1:A:564:G:H1'	37:A:6280:HOH:O	2.10	0.52
1:A:1398:G:H2'	1:A:1399:A:C8	2.45	0.52
4:D:27:ASN:HD22	4:D:27:ASN:H	1.57	0.52
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.91	0.52
14:N:59:GLY:CA	14:N:141:ILE:HD11	2.39	0.52
15:O:67:ALA:C	15:O:69:TYR:N	2.68	0.52
27:1:47:LEU:CD2	27:1:57:CYS:HB2	2.40	0.52
1:A:105:G:O2'	1:A:106:A:H5'	2.10	0.52
1:A:151:A:C2	1:A:442:A:C8	2.98	0.52
1:A:820:G:C5	3:C:171:LYS:HB2	2.45	0.52
1:A:1189:A:O2'	1:A:1208:C:H2'	2.10	0.52
1:A:2256:G:H2'	1:A:2257:G:C5'	2.40	0.52
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.40	0.52
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.34	0.52
10:J:56:ILE:HG21	10:J:61:LEU:HD13	1.91	0.52
1:A:283:U:H5''	1:A:284:C:OP2	2.11	0.51
1:A:2638:G:H5'	37:A:4906:HOH:O	2.09	0.51
37:A:4675:HOH:O	27:1:54:ILE:HD12	2.09	0.51
5:E:109:LEU:HD12	5:E:109:LEU:O	2.10	0.51
9:I:16:LYS:O	9:I:20:VAL:HG23	2.10	0.51
12:L:10:GLN:NE2	12:L:10:GLN:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:87:LEU:CD1	15:O:186:LEU:HD21	2.34	0.51
17:Q:143:ALA:HA	37:Q:5521:HOH:O	2.08	0.51
18:R:40:HIS:HD2	18:R:60:THR:OG1	1.93	0.51
24:X:28:HIS:HD2	24:X:31:HIS:CE1	2.27	0.51
1:A:2468:A:H61	30:4:48:ASN:ND2	2.03	0.51
1:A:2672:C:H1'	37:D:8637:HOH:O	2.10	0.51
1:A:2812:A:C2	1:A:2814:A:N6	2.74	0.51
10:J:39:GLY:O	10:J:41:THR:N	2.44	0.51
10:J:150:LYS:HE2	37:J:8368:HOH:O	2.09	0.51
12:L:55:VAL:CG1	12:L:56:SER:N	2.74	0.51
14:N:67:ILE:HG21	14:N:97:ILE:HG23	1.93	0.51
16:P:42:GLU:HB2	37:P:2176:HOH:O	2.09	0.51
24:X:76:ASP:O	24:X:77:ALA:C	2.53	0.51
1:A:514:G:OP1	1:A:514:G:H2'	2.10	0.51
1:A:2429:A:H2'	1:A:2430:A:C8	2.45	0.51
37:A:4163:HOH:O	26:Z:186:ARG:HD2	2.10	0.51
3:C:8:ARG:NH1	37:C:8554:HOH:O	2.30	0.51
4:D:79:MET:HE3	4:D:144:THR:HG21	1.93	0.51
5:E:85:LYS:CE	37:E:8328:HOH:O	2.55	0.51
5:E:246:ARG:HB3	5:E:246:ARG:HH11	1.73	0.51
21:U:69:LYS:O	21:U:71:VAL:HG23	2.11	0.51
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.10	0.51
26:Z:186:ARG:HG2	26:Z:186:ARG:NH1	2.22	0.51
1:A:371:U:H2'	1:A:372:A:C8	2.44	0.51
1:A:603:A:H4'	1:A:604:G:O5'	2.09	0.51
3:C:132:ASP:OD1	3:C:133:ARG:N	2.42	0.51
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.23	0.51
5:E:162:VAL:HG12	5:E:162:VAL:O	2.09	0.51
8:H:58:GLU:HA	8:H:61:MET:HE2	1.92	0.51
22:V:9:CYS:SG	37:V:6796:HOH:O	2.59	0.51
24:X:119:HIS:HD2	24:X:120:PRO:O	1.92	0.51
26:Z:142:SER:OG	37:Z:8610:HOH:O	2.18	0.51
1:A:424:C:H2'	1:A:425:U:C6	2.44	0.51
1:A:1450:C:C4'	1:A:1451:C:OP2	2.58	0.51
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.46	0.51
1:A:2284:G:H5'	37:A:9437:HOH:O	2.11	0.51
1:A:2392:C:N3	37:A:4825:HOH:O	2.34	0.51
1:A:2408:A:H2	37:A:3080:HOH:O	1.92	0.51
1:A:2466:G:C5'	37:A:3625:HOH:O	2.50	0.51
1:A:2478:U:O2'	1:A:2479:A:H5'	2.10	0.51
1:A:2724:U:H2'	1:A:2725:G:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:4543:HOH:O	14:N:83:SER:HA	2.10	0.51
37:A:7116:HOH:O	28:2:1:THR:HB	2.09	0.51
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.93	0.51
3:C:211:LYS:NZ	37:C:8623:HOH:O	2.32	0.51
4:D:63:GLU:O	4:D:63:GLU:HG3	2.11	0.51
8:H:60:VAL:O	8:H:61:MET:C	2.53	0.51
16:P:63:LYS:NZ	37:P:2363:HOH:O	2.43	0.51
16:P:96:VAL:HA	37:P:4258:HOH:O	2.10	0.51
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.44	0.51
21:U:48:VAL:CG1	21:U:96:VAL:HG13	2.41	0.51
25:Y:25:ARG:CD	37:Y:3861:HOH:O	2.50	0.51
27:1:61:GLY:HA3	37:1:8429:HOH:O	2.09	0.51
1:A:538:C:OP2	26:Z:134:HIS:HE1	1.93	0.51
1:A:1850:U:H2'	1:A:1851:G:H8	1.75	0.51
1:A:2269:C:H2'	1:A:2270:G:H5'	1.92	0.51
4:D:119:HIS:O	4:D:121:PRO:HD3	2.10	0.51
4:D:144:THR:HG22	4:D:145:HIS:N	2.25	0.51
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.10	0.51
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.58	0.51
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.41	0.51
14:N:114:VAL:HB	14:N:159:THR:HG23	1.93	0.51
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.89	0.51
1:A:56:G:H5''	23:W:50:ARG:HH12	1.74	0.51
1:A:1669:A:H2'	1:A:1670:G:H8	1.75	0.51
1:A:2315:C:H4'	1:A:2425:A:C6	2.46	0.51
4:D:43:GLY:O	4:D:308:LEU:HD12	2.11	0.51
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.92	0.51
1:A:1189:A:H1'	1:A:1209:C:O4'	2.11	0.51
1:A:1299:G:O6	13:M:6:ARG:HD3	2.11	0.51
1:A:1329:A:N1	34:A:8513:CL:CL	2.81	0.51
4:D:103:ASP:HB2	37:D:8593:HOH:O	2.10	0.51
4:D:146:THR:O	4:D:159:PRO:HB3	2.10	0.51
11:K:6:PHE:O	11:K:8:ALA:N	2.43	0.51
17:Q:21:VAL:HG23	17:Q:21:VAL:O	2.09	0.51
27:1:26:VAL:O	27:1:30:GLU:HG3	2.10	0.51
27:1:42:CYS:SG	27:1:43:GLY:N	2.84	0.51
1:A:382:U:C5	1:A:406:G:N2	2.78	0.51
1:A:489:A:C8	21:U:82:THR:CG2	2.94	0.51
1:A:2247:C:H5''	37:A:7322:HOH:O	2.11	0.51
1:A:2756:U:H3	1:A:2896:A:H2	1.55	0.51
1:A:2769:C:O2'	1:A:2770:G:H5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:GLN:NE2	37:D:8622:HOH:O	2.44	0.51
5:E:212:VAL:HG23	5:E:212:VAL:O	2.11	0.51
6:F:57:THR:HG23	6:F:63:ILE:CB	2.41	0.51
7:G:68:HIS:O	7:G:72:MET:HG3	2.11	0.51
12:L:118:ALA:C	12:L:120:ARG:H	2.19	0.51
13:M:21:ARG:N	37:M:8535:HOH:O	2.44	0.51
24:X:122:ARG:HH11	24:X:122:ARG:CG	2.15	0.51
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.26	0.51
1:A:113:A:H3'	1:A:114:A:C5'	2.41	0.51
1:A:461:C:H2'	37:A:3974:HOH:O	2.11	0.51
1:A:1119:G:C8	11:K:52:GLN:NE2	2.79	0.51
1:A:1192:A:H3'	1:A:1193:A:H5'	1.92	0.51
4:D:297:VAL:HB	37:D:8606:HOH:O	2.11	0.51
7:G:157:LYS:NZ	37:G:2401:HOH:O	2.44	0.51
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.26	0.51
10:J:57:ARG:HG3	10:J:57:ARG:HH11	1.76	0.51
12:L:29:LEU:HB3	12:L:55:VAL:CG1	2.28	0.51
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.11	0.51
13:M:146:GLY:C	13:M:148:GLU:H	2.19	0.51
14:N:138:HIS:C	14:N:139:PRO:O	2.47	0.51
1:A:154:C:P	14:N:188:ARG:HH12	2.34	0.50
1:A:639:A:C2	1:A:1363:G:C2	2.99	0.50
1:A:1209:C:C2	1:A:1210:G:C8	2.99	0.50
1:A:2321:A:O2'	1:A:2322:U:H3'	2.11	0.50
1:A:2453:G:H4'	13:M:50:GLY:C	2.36	0.50
3:C:191:GLY:HA2	3:C:194:MET:CE	2.41	0.50
4:D:16:ARG:NE	37:D:8556:HOH:O	2.28	0.50
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.74	0.50
8:H:47:LEU:HD22	8:H:108:LEU:CD1	2.41	0.50
12:L:34:VAL:HB	37:L:7169:HOH:O	2.11	0.50
12:L:109:LEU:HD13	12:L:113:ILE:HD11	1.93	0.50
16:P:98:LEU:O	16:P:102:ILE:HG13	2.11	0.50
21:U:75:GLU:O	21:U:76:ASP:HB2	2.10	0.50
29:3:40:ARG:HG2	29:3:40:ARG:HH11	1.76	0.50
1:A:344:C:H2'	1:A:345:G:O4'	2.10	0.50
1:A:445:U:H1'	37:A:7314:HOH:O	2.12	0.50
1:A:790:A:H1'	1:A:1710:A:H2'	1.92	0.50
1:A:1041:U:H2'	1:A:1042:U:C5'	2.41	0.50
1:A:1189:A:H1'	1:A:1209:C:H1'	1.93	0.50
1:A:1200:A:H4'	37:A:7318:HOH:O	2.11	0.50
1:A:2912:C:OP2	37:A:5528:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:58:GLU:OE1	14:N:27:ARG:NH2	2.41	0.50
11:K:130:VAL:HG12	11:K:131:THR:N	2.24	0.50
24:X:38:THR:HG22	24:X:39:ASP:H	1.77	0.50
1:A:204:A:C2'	1:A:205:U:H5'	2.41	0.50
1:A:244:C:OP2	8:H:38:LYS:HE3	2.12	0.50
1:A:1353:C:OP2	37:A:4516:HOH:O	2.19	0.50
1:A:1690:C:C5	1:A:1692:C:C4	2.99	0.50
1:A:1700:C:OP2	37:A:6004:HOH:O	2.19	0.50
1:A:2064:U:H4'	1:A:2653:A:P	2.51	0.50
37:A:3641:HOH:O	14:N:79:LYS:HD2	2.11	0.50
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.35	0.50
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.79	0.50
7:G:15:GLN:NE2	7:G:40:VAL:O	2.44	0.50
21:U:20:HIS:ND1	21:U:41:ARG:NE	2.54	0.50
25:Y:71:ARG:CD	37:Y:2171:HOH:O	2.59	0.50
1:A:454:U:O4	37:A:9151:HOH:O	2.19	0.50
1:A:778:C:OP1	37:A:5516:HOH:O	2.20	0.50
1:A:1370:G:OP1	19:S:64:SER:OG	2.29	0.50
1:A:1787:C:H4'	1:A:2883:A:O4'	2.11	0.50
1:A:2271:G:H2'	1:A:2271:G:N3	2.27	0.50
1:A:2314:G:O2'	1:A:2315:C:H5'	2.10	0.50
1:A:2361:A:H5''	37:A:9002:HOH:O	2.11	0.50
3:C:51:ARG:HB2	37:C:8610:HOH:O	2.11	0.50
5:E:234:VAL:HG22	5:E:234:VAL:O	2.11	0.50
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.86	0.50
10:J:166:ASN:N	10:J:166:ASN:ND2	2.59	0.50
14:N:84:LYS:O	14:N:87:MET:HG2	2.10	0.50
15:O:37:ARG:NH2	37:O:8534:HOH:O	2.44	0.50
20:T:57:THR:C	20:T:59:ASP:H	2.17	0.50
30:4:57:GLY:HA2	37:4:8528:HOH:O	2.10	0.50
1:A:2464:C:H5''	1:A:2465:A:OP1	2.11	0.50
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.76	0.50
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.42	0.50
6:F:40:ILE:HG23	37:F:5583:HOH:O	2.10	0.50
13:M:134:GLU:HA	13:M:138:GLY:O	2.12	0.50
14:N:134:ILE:O	14:N:136:PRO:HD3	2.12	0.50
15:O:34:LEU:HD22	15:O:129:ILE:HD13	1.93	0.50
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.47	0.50
1:A:88:G:C8	29:3:28:LYS:HB2	2.46	0.50
1:A:1666:C:C2'	1:A:1667:A:C5'	2.90	0.50
3:C:36:ASP:O	3:C:38:ILE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:11:HIS:O	6:F:12:GLU:HB3	2.10	0.50
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.41	0.50
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.60	0.50
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.27	0.50
19:S:17:MET:HE1	19:S:19:ARG:NH2	2.27	0.50
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.93	0.50
27:1:59:HIS:CE1	37:1:8441:HOH:O	2.64	0.50
1:A:424:C:H2'	1:A:425:U:H6	1.77	0.50
1:A:559:U:H2'	1:A:560:C:O4'	2.12	0.50
1:A:1834:C:H2'	1:A:1840:A:H62	1.75	0.50
3:C:149:ASP:OD1	3:C:151:GLN:HB2	2.11	0.50
4:D:248:ARG:NH2	37:D:8525:HOH:O	2.44	0.50
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.47	0.50
10:J:118:PRO:HD2	37:J:8326:HOH:O	2.10	0.50
24:X:88:THR:CG2	24:X:110:GLN:NE2	2.70	0.50
27:1:42:CYS:HG	27:1:44:PHE:HB2	1.76	0.50
29:3:49:GLU:CD	37:3:719:HOH:O	2.54	0.50
1:A:415:A:O2'	1:A:416:G:H5'	2.12	0.50
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.43	0.50
1:A:2265:U:H2'	1:A:2266:A:C8	2.47	0.50
1:A:2505:G:C2'	1:A:2506:A:H5'	2.41	0.50
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.42	0.50
6:F:25:MET:HE2	6:F:41:LEU:CG	2.21	0.50
8:H:99:THR:O	8:H:100:ASP:HB2	2.11	0.50
14:N:85:ARG:NE	37:N:8519:HOH:O	2.14	0.50
21:U:19:ARG:NH1	21:U:68:ASP:O	2.44	0.50
24:X:48:VAL:CG1	24:X:48:VAL:O	2.58	0.50
1:A:402:U:H2'	1:A:403:C:C6	2.47	0.50
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.77	0.50
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.46	0.50
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.42	0.50
7:G:80:TRP:O	7:G:134:SER:HA	2.11	0.50
10:J:62:GLU:O	10:J:66:VAL:HG23	2.11	0.50
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.77	0.50
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.77	0.50
21:U:48:VAL:HG23	21:U:98:VAL:HA	1.93	0.50
1:A:1003:U:O2	10:J:90:PHE:CZ	2.65	0.49
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.75	0.49
1:A:1123:A:C2	1:A:1129:C:H4'	2.47	0.49
1:A:1589:G:N2	1:A:1605:G:H1'	2.27	0.49
1:A:1682:A:H5''	37:A:9436:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2763:G:OP1	12:L:9:THR:OG1	2.16	0.49
5:E:133:ARG:NH2	37:E:8424:HOH:O	2.45	0.49
10:J:95:GLU:HB3	10:J:119:VAL:HG11	1.93	0.49
16:P:25:VAL:HG23	16:P:26:TRP:N	2.27	0.49
20:T:80:ARG:HG2	37:T:8336:HOH:O	2.11	0.49
1:A:453:A:H4'	1:A:455:A:N7	2.27	0.49
1:A:1804:A:H2'	1:A:1805:G:C8	2.46	0.49
1:A:2094:G:C2	1:A:2652:U:O2	2.65	0.49
1:A:2506:A:H1'	37:A:6024:HOH:O	2.13	0.49
1:A:2563:U:H2'	1:A:2565:C:O5'	2.11	0.49
1:A:2719:A:C2	4:D:70:PRO:HG3	2.48	0.49
1:A:2906:A:H5'	1:A:2907:C:O4'	2.12	0.49
8:H:57:GLU:O	8:H:61:MET:HG3	2.12	0.49
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.47	0.49
14:N:25:TRP:HE3	14:N:26:HIS:HD2	1.59	0.49
14:N:39:ARG:NE	37:N:8623:HOH:O	2.45	0.49
14:N:107:ARG:NH1	37:N:8579:HOH:O	2.45	0.49
18:R:33:PHE:N	18:R:71:TYR:OH	2.38	0.49
20:T:57:THR:HG22	20:T:59:ASP:HB2	1.94	0.49
24:X:88:THR:CG2	24:X:89:ASP:H	2.21	0.49
26:Z:148:GLY:O	26:Z:154:ARG:HD3	2.12	0.49
28:2:25:LYS:NZ	37:2:8433:HOH:O	2.45	0.49
30:4:74:CYS:SG	30:4:76:LYS:HG3	2.51	0.49
1:A:92:G:H4'	23:W:44:GLY:HA3	1.93	0.49
1:A:221:G:H2'	1:A:222:A:C8	2.46	0.49
1:A:241:A:C2	1:A:378:A:H4'	2.47	0.49
3:C:109:GLU:CD	3:C:113:GLY:H	2.20	0.49
4:D:88:GLU:O	4:D:88:GLU:HG3	2.11	0.49
4:D:248:ARG:O	4:D:251:VAL:CG1	2.60	0.49
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.75	0.49
5:E:184:ARG:HB3	37:E:8362:HOH:O	2.12	0.49
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.47	0.49
13:M:101:ASP:C	13:M:103:ALA:H	2.18	0.49
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.27	0.49
19:S:27:HIS:O	19:S:31:ILE:HG13	2.11	0.49
24:X:11:VAL:O	24:X:12:ASN:HB2	2.12	0.49
25:Y:71:ARG:HD3	37:Y:2171:HOH:O	2.12	0.49
29:3:18:ASN:ND2	29:3:40:ARG:H	2.10	0.49
1:A:159:G:H2'	1:A:175:G:N2	2.27	0.49
1:A:539:G:H2'	1:A:540:A:H8	1.76	0.49
1:A:2099:G:H1	31:A:9001:SPR:HO2A	1.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2559:C:H4'	37:A:7232:HOH:O	2.12	0.49
2:B:3031:C:H2'	2:B:3032:G:O4'	2.12	0.49
4:D:4:SER:O	4:D:5:ARG:HB2	2.13	0.49
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.30	0.49
7:G:132:THR:HB	37:G:2227:HOH:O	2.11	0.49
10:J:81:TYR:CD1	10:J:81:TYR:C	2.89	0.49
10:J:144:GLU:OE1	10:J:144:GLU:HA	2.12	0.49
12:L:99:ASP:OD1	12:L:101:ASN:N	2.44	0.49
13:M:122:ALA:HB3	13:M:125:PHE:CZ	2.48	0.49
21:U:19:ARG:HD3	21:U:67:LEU:O	2.12	0.49
24:X:65:VAL:HA	24:X:68:THR:CG2	2.41	0.49
1:A:1699:C:H4'	37:A:6415:HOH:O	2.12	0.49
1:A:1768:C:H2'	1:A:1769:C:O4'	2.12	0.49
1:A:1827:G:C6	1:A:1828:G:C6	3.01	0.49
1:A:2251:G:H2'	1:A:2252:A:C8	2.48	0.49
37:A:6218:HOH:O	22:V:56:ARG:HB3	2.11	0.49
4:D:16:ARG:NH1	37:D:8617:HOH:O	2.45	0.49
5:E:127:ARG:HG2	5:E:127:ARG:HH11	1.77	0.49
1:A:1840:A:H4'	1:A:1841:C:O5'	2.13	0.49
1:A:2353:A:H4'	1:A:2354:A:O5'	2.12	0.49
37:A:7661:HOH:O	14:N:154:ARG:HB2	2.12	0.49
6:F:58:VAL:HG12	6:F:59:GLY:N	2.26	0.49
8:H:113:ASP:O	8:H:117:GLU:HG3	2.12	0.49
13:M:72:ASN:HB2	37:M:8580:HOH:O	2.12	0.49
17:Q:27:ARG:O	17:Q:31:ILE:HG13	2.12	0.49
24:X:122:ARG:HG2	24:X:122:ARG:NH1	2.21	0.49
1:A:333:G:O2'	1:A:334:G:H5'	2.12	0.49
1:A:710:G:P	16:P:24:ALA:HB3	2.53	0.49
1:A:2577:A:H5'	37:A:7734:HOH:O	2.13	0.49
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.93	0.49
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.47	0.49
19:S:39:THR:HB	19:S:42:GLU:CG	2.41	0.49
24:X:28:HIS:CD2	24:X:31:HIS:CE1	3.01	0.49
24:X:69:ARG:HD2	24:X:117:ARG:O	2.12	0.49
1:A:470:U:H2'	1:A:471:G:O4'	2.13	0.49
1:A:536:A:H3'	37:A:5025:HOH:O	2.13	0.49
1:A:926:A:H1'	13:M:38:HIS:O	2.13	0.49
1:A:1741:U:HO2'	1:A:2723:G:H4'	1.78	0.49
2:B:3064:C:C2'	2:B:3065:A:H5'	2.43	0.49
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.94	0.49
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:64:ASN:O	9:I:68:GLU:HG3	2.13	0.49
10:J:59:ASN:H	10:J:59:ASN:ND2	2.10	0.49
13:M:65:ASP:HA	13:M:109:LEU:O	2.12	0.49
16:P:10:LEU:HD13	16:P:99:GLU:HG3	1.95	0.49
18:R:28:ARG:NH1	37:R:6206:HOH:O	2.39	0.49
19:S:39:THR:CG2	19:S:42:GLU:HG3	2.42	0.49
1:A:107:U:H2'	1:A:108:U:H5'	1.95	0.49
1:A:660:A:H4'	1:A:661:G:O5'	2.13	0.49
1:A:669:G:O2'	1:A:670:G:H5'	2.13	0.49
1:A:1609:C:H2'	1:A:1610:G:H8	1.77	0.49
1:A:2780:C:H2'	1:A:2781:U:H6	1.76	0.49
5:E:111:VAL:HB	37:E:8324:HOH:O	2.13	0.49
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.95	0.49
7:G:18:LEU:HD13	7:G:34:TRP:CG	2.47	0.49
7:G:20:ILE:HD12	7:G:33:LEU:CD1	2.43	0.49
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.95	0.49
10:J:129:ASN:HD22	10:J:129:ASN:N	2.10	0.49
14:N:78:ASN:ND2	37:N:8647:HOH:O	2.40	0.49
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.95	0.49
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.27	0.49
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.41	0.49
1:A:159:G:H2'	1:A:175:G:H22	1.77	0.49
1:A:380:A:C2	14:N:13:LYS:HB3	2.48	0.49
1:A:538:C:H5''	1:A:539:G:C8	2.48	0.49
1:A:737:A:H2'	1:A:738:G:O4'	2.13	0.49
1:A:1477:C:H5'	1:A:1868:G:C5'	2.43	0.49
1:A:1593:C:O2'	1:A:1594:C:H5'	2.13	0.49
1:A:2649:A:H5'	1:A:2649:A:C8	2.48	0.49
1:A:2896:A:H2'	1:A:2896:A:N3	2.28	0.49
4:D:202:VAL:HG11	4:D:301:VAL:HG13	1.95	0.49
4:D:279:THR:CG2	4:D:280:VAL:N	2.75	0.49
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.42	0.49
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.95	0.49
17:Q:2:ASP:C	17:Q:2:ASP:OD1	2.55	0.49
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.39	0.49
1:A:13:G:H2'	1:A:14:C:H6	1.78	0.48
1:A:182:G:O3'	14:N:157:LEU:HD13	2.13	0.48
1:A:1209:C:O2	1:A:1210:G:C8	2.66	0.48
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.13	0.48
1:A:2004:U:H1'	37:A:3178:HOH:O	2.12	0.48
1:A:2502:C:C4'	10:J:151:MET:HG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:27:ILE:HG22	6:F:28:GLY:N	2.22	0.48
10:J:154:THR:HB	10:J:155:PRO:HD3	1.95	0.48
13:M:72:ASN:O	13:M:76:LEU:HG	2.13	0.48
15:O:77:ASN:OD1	15:O:80:SER:HB2	2.13	0.48
20:T:29:ASP:OD2	20:T:31:ARG:NH1	2.45	0.48
27:1:11:THR:HG21	27:1:23:ARG:HB2	1.94	0.48
27:1:57:CYS:O	27:1:61:GLY:N	2.44	0.48
1:A:584:U:H3'	37:A:6064:HOH:O	2.12	0.48
1:A:734:U:O2'	1:A:737:A:N6	2.45	0.48
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.13	0.48
7:G:18:LEU:HD13	7:G:34:TRP:CD1	2.49	0.48
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.43	0.48
12:L:40:THR:O	12:L:41:LYS:C	2.55	0.48
13:M:73:VAL:HG23	13:M:74:THR:H	1.76	0.48
16:P:47:ARG:HG3	16:P:47:ARG:NH1	2.27	0.48
17:Q:115:SER:C	17:Q:117:SER:H	2.22	0.48
1:A:81:G:N3	1:A:98:A:C2	2.81	0.48
1:A:101:C:H2'	1:A:102:A:H8	1.78	0.48
1:A:625:U:H5''	1:A:1044:C:N4	2.28	0.48
1:A:1044:C:H5''	37:A:9022:HOH:O	2.13	0.48
1:A:1268:C:O2'	1:A:1269:G:H5'	2.13	0.48
1:A:1383:U:H5''	37:A:6631:HOH:O	2.12	0.48
1:A:2584:G:C2	1:A:2585:G:N7	2.81	0.48
3:C:18:ALA:O	3:C:20:SER:N	2.43	0.48
3:C:194:MET:HE3	3:C:199:HIS:CB	2.42	0.48
5:E:214:THR:HG23	37:E:8436:HOH:O	2.12	0.48
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.82	0.48
9:I:71:LEU:C	9:I:73:ASP:H	2.21	0.48
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.25	0.48
13:M:126:SER:O	13:M:127:GLU:C	2.54	0.48
14:N:52:LEU:HD13	14:N:116:ASN:CB	2.42	0.48
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.12	0.48
17:Q:83:LYS:O	17:Q:86:ALA:HB3	2.12	0.48
24:X:90:TYR:N	24:X:90:TYR:CD1	2.80	0.48
1:A:581:G:H5'	37:A:7664:HOH:O	2.13	0.48
1:A:1743:G:H1'	37:A:4867:HOH:O	2.12	0.48
1:A:2256:G:O2'	1:A:2257:G:H5'	2.12	0.48
1:A:2657:G:OP1	4:D:17:LYS:HB2	2.13	0.48
2:B:3042:C:H5'	2:B:3043:G:OP2	2.13	0.48
4:D:76:THR:N	4:D:77:PRO:HD3	2.29	0.48
5:E:218:VAL:HG12	37:E:8422:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:GLU:HB2	7:G:116:THR:O	2.13	0.48
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.47	0.48
24:X:110:GLN:HE21	24:X:110:GLN:HA	1.78	0.48
1:A:485:A:O2'	1:A:487:G:H5'	2.13	0.48
1:A:832:U:H2'	1:A:833:G:C8	2.49	0.48
1:A:1333:U:H2'	1:A:1334:C:C6	2.48	0.48
1:A:1850:U:H2'	1:A:1851:G:C8	2.48	0.48
1:A:2019:A:H5'	37:A:4508:HOH:O	2.13	0.48
1:A:2459:G:P	30:4:64:LYS:HB2	2.54	0.48
1:A:2866:U:H4'	1:A:2867:G:H5'	1.95	0.48
37:A:7382:HOH:O	21:U:2:LYS:HE2	2.13	0.48
5:E:184:ARG:NE	37:E:8409:HOH:O	2.41	0.48
5:E:236:THR:CG2	5:E:239:ALA:H	2.00	0.48
6:F:84:LEU:HA	6:F:87:ALA:HB3	1.96	0.48
10:J:35:ASN:ND2	10:J:79:ALA:O	2.46	0.48
10:J:48:LEU:CG	10:J:157:ILE:HG21	2.43	0.48
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.43	0.48
19:S:82:GLU:HG3	19:S:83:LYS:N	2.28	0.48
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.79	0.48
24:X:4:LEU:HD22	24:X:52:VAL:HG22	1.93	0.48
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.74	0.48
26:Z:151:SER:HB3	26:Z:154:ARG:HB3	1.96	0.48
26:Z:187:VAL:HG23	26:Z:192:ASP:HB3	1.94	0.48
30:4:62:THR:HB	37:4:8554:HOH:O	2.12	0.48
30:4:69:TYR:CB	30:4:78:HIS:CE1	2.96	0.48
1:A:394:G:H1	14:N:181:GLU:CD	2.22	0.48
1:A:1241:G:N2	11:K:86:MET:HE2	2.28	0.48
1:A:1361:C:O3'	5:E:77:ALA:HB3	2.14	0.48
1:A:2251:G:H4'	37:A:7385:HOH:O	2.14	0.48
2:B:3038:A:H2	2:B:3043:G:H5''	1.78	0.48
2:B:3080:A:C2	2:B:3103:A:C4	3.02	0.48
6:F:51:ARG:HD3	37:F:7636:HOH:O	2.14	0.48
17:Q:141:ILE:C	17:Q:143:ALA:H	2.22	0.48
1:A:288:A:H2'	1:A:289:G:C8	2.49	0.48
1:A:380:A:H5''	14:N:48:ARG:NH2	2.29	0.48
1:A:2730:G:O2'	1:A:2731:G:H5'	2.14	0.48
37:A:4700:HOH:O	15:O:21:HIS:HD2	1.96	0.48
10:J:26:LYS:HG2	10:J:28:ILE:N	2.23	0.48
10:J:157:ILE:CG2	10:J:158:ASN:N	2.76	0.48
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.43	0.48
23:W:1:THR:HG23	23:W:2:VAL:N	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:75:GLY:HA3	37:X:5763:HOH:O	2.13	0.48
25:Y:27:ASP:OD2	25:Y:27:ASP:N	2.47	0.48
1:A:639:A:H2'	1:A:640:G:H8	1.79	0.48
1:A:1380:U:H5'	37:A:9206:HOH:O	2.14	0.48
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.78	0.48
5:E:79:ARG:O	5:E:87:ARG:N	2.42	0.48
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.27	0.48
14:N:47:ASP:CG	14:N:48:ARG:N	2.72	0.48
1:A:1075:G:C2	1:A:1085:C:C2	3.02	0.48
1:A:1316:G:H1'	1:A:1340:G:N2	2.29	0.48
1:A:1666:C:H2'	1:A:1667:A:C5'	2.44	0.48
1:A:2073:G:C6	1:A:2607:U:C2	3.01	0.48
1:A:2269:C:C2'	1:A:2270:G:H5'	2.44	0.48
1:A:2755:G:H1'	37:A:4654:HOH:O	2.13	0.48
37:A:4849:HOH:O	14:N:174:ARG:HG2	2.13	0.48
3:C:212:PRO:HB2	37:C:8562:HOH:O	2.14	0.48
4:D:84:LEU:O	4:D:84:LEU:HD13	2.13	0.48
10:J:45:GLN:HE21	10:J:135:TRP:HE1	1.62	0.48
14:N:154:ARG:CD	37:N:8643:HOH:O	2.62	0.48
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.95	0.48
1:A:138:U:H5''	1:A:139:C:OP2	2.14	0.48
1:A:244:C:O5'	1:A:244:C:H6	1.96	0.48
1:A:1377:C:H5'	1:A:1377:C:C6	2.45	0.48
1:A:1735:C:HO2'	1:A:1736:A:H5'	1.76	0.48
1:A:2781:U:C2'	1:A:2782:G:H5'	2.44	0.48
2:B:3092:G:H22	10:J:52:LYS:NZ	2.12	0.48
7:G:92:PRO:HB2	37:G:4917:HOH:O	2.13	0.48
11:K:131:THR:HG22	11:K:133:GLY:N	2.29	0.48
1:A:182:G:O3'	14:N:157:LEU:CD1	2.62	0.47
1:A:212:A:O4'	1:A:214:U:C6	2.67	0.47
1:A:861:A:H2'	1:A:862:U:C6	2.48	0.47
1:A:894:A:C2	5:E:87:ARG:NH2	2.82	0.47
1:A:1052:G:N3	1:A:1052:G:H2'	2.28	0.47
1:A:1249:U:H2'	1:A:1250:C:C6	2.49	0.47
1:A:1352:A:N1	5:E:48:SER:HB3	2.29	0.47
1:A:1407:A:O2'	1:A:1408:U:H3'	2.14	0.47
1:A:2001:G:C2'	1:A:2002:C:H5'	2.44	0.47
1:A:2055:A:H4'	19:S:132:ARG:NH2	2.29	0.47
31:A:9001:SPR:C7C	31:A:9001:SPR:H6C3	2.43	0.47
5:E:107:ARG:HB3	5:E:107:ARG:HH11	1.77	0.47
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:74:VAL:CG1	12:L:74:VAL:O	2.60	0.47
14:N:104:ARG:O	14:N:108:LYS:HE2	2.14	0.47
1:A:682:A:H2'	1:A:683:G:O4'	2.14	0.47
1:A:1164:U:C1'	1:A:1165:G:OP1	2.62	0.47
1:A:1934:A:C8	1:A:1935:C:C5	3.01	0.47
1:A:2670:G:O2'	1:A:2671:U:H5'	2.14	0.47
37:A:7435:HOH:O	5:E:188:ARG:HD3	2.12	0.47
4:D:168:GLY:O	4:D:169:GLY:O	2.32	0.47
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.96	0.47
12:L:22:ASP:C	12:L:22:ASP:OD1	2.56	0.47
15:O:34:LEU:HD13	15:O:47:LEU:HD21	1.96	0.47
21:U:32:ARG:NH1	21:U:38:ARG:NH1	2.56	0.47
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.13	0.47
1:A:558:C:C2'	1:A:559:U:C5'	2.92	0.47
1:A:920:C:H4'	1:A:921:G:C2	2.49	0.47
1:A:952:G:OP1	18:R:42:LYS:HE2	2.14	0.47
1:A:1003:U:O2'	10:J:90:PHE:HE1	1.97	0.47
1:A:1097:A:H5''	24:X:125:HIS:NE2	2.30	0.47
1:A:2443:C:H3'	37:A:3456:HOH:O	2.14	0.47
4:D:279:THR:OG1	4:D:290:VAL:HB	2.14	0.47
5:E:65:ARG:HG3	5:E:67:GLN:HB2	1.97	0.47
9:I:23:ILE:O	9:I:27:ILE:HG13	2.13	0.47
11:K:142:ASN:O	11:K:144:THR:N	2.47	0.47
12:L:55:VAL:HG12	12:L:56:SER:H	1.77	0.47
15:O:154:LEU:HG	15:O:155:GLU:H	1.78	0.47
23:W:16:ARG:NH2	23:W:63:GLU:HG3	2.28	0.47
1:A:1119:G:N2	1:A:1246:A:H2	2.08	0.47
1:A:1504:A:H5'	37:A:4384:HOH:O	2.14	0.47
1:A:1659:A:H2'	1:A:1660:G:O4'	2.15	0.47
37:A:9776:HOH:O	12:L:39:GLY:HA3	2.13	0.47
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.50	0.47
4:D:177:HIS:O	4:D:181:ILE:HG13	2.15	0.47
5:E:127:ARG:CZ	5:E:225:PRO:HG2	2.44	0.47
6:F:10:PHE:CD1	6:F:11:HIS:N	2.82	0.47
6:F:86:THR:HG23	37:F:7477:HOH:O	2.14	0.47
6:F:99:ASP:HB2	6:F:103:ASN:H	1.80	0.47
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.95	0.47
14:N:35:PRO:HD2	14:N:38:VAL:HG21	1.96	0.47
17:Q:71:LYS:HG3	17:Q:71:LYS:O	2.14	0.47
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.14	0.47
1:A:625:U:H5'	37:A:3169:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1503:U:H2'	1:A:1504:A:O4'	2.14	0.47
1:A:2430:A:O5'	1:A:2430:A:H8	1.97	0.47
1:A:2524:G:H21	1:A:2526:C:N4	2.12	0.47
1:A:2830:U:H3'	37:A:5206:HOH:O	2.13	0.47
1:A:2883:A:H2'	1:A:2884:G:O4'	2.15	0.47
37:A:3180:HOH:O	13:M:4:LYS:HG3	2.13	0.47
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.96	0.47
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.77	0.47
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.43	0.47
12:L:130:MET:SD	22:V:26:GLY:HA3	2.54	0.47
14:N:113:ARG:HH21	14:N:156:ARG:HG2	1.77	0.47
27:1:58:GLY:HA3	37:1:8442:HOH:O	2.13	0.47
1:A:151:A:H2'	1:A:152:A:O4'	2.14	0.47
1:A:1127:C:C2'	1:A:1128:U:H5'	2.44	0.47
1:A:2093:G:H5''	37:A:9462:HOH:O	2.13	0.47
1:A:2133:U:H4'	1:A:2134:G:H5'	1.97	0.47
1:A:2416:G:H2'	1:A:2417:C:C6	2.50	0.47
1:A:2488:A:H61	1:A:2534:C:H42	1.62	0.47
1:A:2812:A:H1'	37:A:5763:HOH:O	2.14	0.47
3:C:33:GLU:H	3:C:33:GLU:CD	2.22	0.47
3:C:192:VAL:O	3:C:192:VAL:HG12	2.13	0.47
4:D:62:ARG:CB	4:D:65:MET:HE3	2.43	0.47
6:F:59:GLY:C	6:F:61:PHE:N	2.73	0.47
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.96	0.47
10:J:149:ALA:C	10:J:151:MET:H	2.21	0.47
15:O:182:GLY:O	15:O:183:ASP:O	2.32	0.47
18:R:21:ARG:NH2	37:R:5853:HOH:O	2.29	0.47
24:X:65:VAL:CA	24:X:68:THR:HG22	2.44	0.47
27:1:13:ARG:NH1	27:1:14:PHE:CZ	2.82	0.47
1:A:470:U:O2'	28:2:16:HIS:CD2	2.67	0.47
1:A:790:A:H2'	1:A:791:A:O4'	2.14	0.47
1:A:1019:C:P	37:A:3922:HOH:O	2.73	0.47
1:A:1023:C:H2'	1:A:1024:G:O4'	2.14	0.47
1:A:1463:A:C6	1:A:1464:U:O4	2.68	0.47
1:A:1555:G:H4'	1:A:1630:A:H2	1.80	0.47
1:A:1694:G:H1'	37:A:9177:HOH:O	2.14	0.47
1:A:1858:A:H2'	1:A:1859:A:C8	2.50	0.47
1:A:1878:G:O2'	1:A:1879:U:C6	2.65	0.47
1:A:2005:G:O2'	1:A:2008:U:OP2	2.25	0.47
1:A:2089:A:O2'	1:A:2090:G:H5'	2.15	0.47
1:A:2456:A:H5'	37:A:5666:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2533:C:H6	1:A:2533:C:C5'	2.20	0.47
1:A:2781:U:O2'	1:A:2782:G:H5'	2.15	0.47
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.15	0.47
2:B:3031:C:O2'	2:B:3032:G:H5'	2.14	0.47
2:B:3049:G:O2'	2:B:3050:G:H5'	2.15	0.47
3:C:217:ARG:CG	3:C:217:ARG:NH1	2.76	0.47
4:D:51:VAL:HG23	4:D:329:TYR:O	2.14	0.47
4:D:84:LEU:HD13	4:D:84:LEU:C	2.40	0.47
4:D:139:ASP:HB2	4:D:165:ARG:HE	1.80	0.47
6:F:76:ARG:O	6:F:77:ASP:HB2	2.15	0.47
8:H:20:LEU:O	8:H:23:ALA:HB3	2.15	0.47
11:K:42:GLU:O	11:K:131:THR:HG23	2.14	0.47
13:M:73:VAL:HG23	13:M:74:THR:N	2.29	0.47
14:N:37:VAL:HG21	14:N:108:LYS:HG3	1.97	0.47
15:O:11:ARG:O	15:O:15:GLU:HG3	2.14	0.47
15:O:37:ARG:NE	37:O:8534:HOH:O	2.47	0.47
15:O:154:LEU:O	15:O:155:GLU:CB	2.63	0.47
17:Q:115:SER:C	17:Q:117:SER:N	2.73	0.47
18:R:10:THR:O	18:R:11:ARG:C	2.58	0.47
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.14	0.47
24:X:129:LYS:HG2	37:X:1990:HOH:O	2.15	0.47
27:1:13:ARG:NH1	27:1:14:PHE:CE2	2.83	0.47
1:A:168:C:O2'	1:A:169:A:H5'	2.15	0.47
1:A:646:G:H2'	1:A:647:U:C6	2.50	0.47
1:A:2383:G:N3	37:A:6675:HOH:O	2.35	0.47
1:A:2723:G:H1'	37:A:4815:HOH:O	2.14	0.47
37:A:5324:HOH:O	21:U:3:GLN:HG2	2.14	0.47
37:A:7202:HOH:O	14:N:13:LYS:HE2	2.14	0.47
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.30	0.47
6:F:35:ALA:C	6:F:37:ALA:N	2.72	0.47
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.96	0.47
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.29	0.47
1:A:825:U:H5''	1:A:826:U:OP1	2.15	0.47
1:A:843:A:C2	1:A:846:A:C8	3.03	0.47
1:A:1702:U:H5''	37:A:7193:HOH:O	2.14	0.47
1:A:1759:A:N3	1:A:1818:C:H2'	2.30	0.47
1:A:2421:G:H4'	37:A:4754:HOH:O	2.15	0.47
1:A:2431:C:O2'	1:A:2432:C:H5'	2.15	0.47
1:A:2481:G:C3'	1:A:2482:G:H5''	2.44	0.47
37:A:5995:HOH:O	18:R:50:GLY:HA2	2.15	0.47
2:B:3008:G:O6	15:O:11:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:ARG:HH11	3:C:217:ARG:HG3	1.80	0.47
13:M:73:VAL:HG11	13:M:118:LEU:HD21	1.97	0.47
15:O:154:LEU:HD12	15:O:156:GLU:O	2.15	0.47
29:3:40:ARG:HG2	29:3:40:ARG:NH1	2.30	0.47
1:A:13:G:H2'	1:A:14:C:C6	2.50	0.47
1:A:128:A:H3'	1:A:128:A:C8	2.50	0.47
1:A:283:U:H5	1:A:284:C:N4	2.13	0.47
1:A:426:G:H2'	1:A:427:C:O4'	2.14	0.47
1:A:512:G:O3'	1:A:513:A:H8	1.98	0.47
1:A:581:G:O2'	1:A:582:C:H5'	2.15	0.47
1:A:625:U:O2'	1:A:627:G:N7	2.42	0.47
1:A:1268:C:H2'	1:A:1269:G:C8	2.49	0.47
1:A:1609:C:H2'	1:A:1610:G:C8	2.50	0.47
1:A:2072:G:C6	1:A:2533:C:H1'	2.50	0.47
1:A:2840:A:OP1	4:D:211:THR:HG23	2.15	0.47
3:C:192:VAL:HB	37:C:8598:HOH:O	2.14	0.47
4:D:60:SER:C	4:D:62:ARG:H	2.23	0.47
7:G:34:TRP:O	11:K:127:ILE:HD11	2.14	0.47
8:H:34:ASN:O	8:H:38:LYS:HG3	2.15	0.47
10:J:84:ARG:CZ	10:J:135:TRP:CH2	2.98	0.47
15:O:67:ALA:HA	15:O:71:TRP:H	1.80	0.47
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.80	0.47
22:V:33:SER:O	22:V:37:GLU:HG3	2.15	0.47
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.97	0.47
24:X:126:ASP:HB3	24:X:135:GLY:O	2.15	0.47
1:A:317:A:H5''	21:U:52:ARG:HD2	1.97	0.46
1:A:869:G:OP1	14:N:79:LYS:HE2	2.13	0.46
1:A:1114:A:H2'	1:A:1115:U:H6	1.80	0.46
1:A:1130:U:H5'	37:A:7653:HOH:O	2.15	0.46
1:A:2598:U:H5''	12:L:36:GLY:HA2	1.96	0.46
3:C:153:ARG:HH11	3:C:153:ARG:CB	2.27	0.46
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.97	0.46
5:E:107:ARG:HH11	5:E:107:ARG:CB	2.28	0.46
6:F:19:GLU:O	6:F:133:ASN:HB3	2.15	0.46
10:J:29:ALA:N	10:J:62:GLU:OE1	2.45	0.46
10:J:57:ARG:C	10:J:59:ASN:H	2.21	0.46
11:K:131:THR:HB	11:K:134:GLU:HG3	1.97	0.46
21:U:41:ARG:NH1	21:U:42:VAL:O	2.49	0.46
24:X:122:ARG:CG	24:X:152:ALA:O	2.63	0.46
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.44	0.46
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:189:ASN:C	26:Z:189:ASN:ND2	2.71	0.46
1:A:308:U:C4	1:A:342:C:H1'	2.50	0.46
1:A:514:G:H8	1:A:514:G:O5'	1.98	0.46
1:A:832:U:H2'	1:A:833:G:H8	1.80	0.46
1:A:1334:C:H2'	1:A:1335:C:H6	1.79	0.46
1:A:1506:U:H6	1:A:1506:U:H5'	1.80	0.46
1:A:2010:A:H5''	37:A:4144:HOH:O	2.14	0.46
1:A:2089:A:C2'	1:A:2090:G:H5'	2.45	0.46
37:A:9966:HOH:O	13:M:22:ARG:HG2	2.14	0.46
37:E:8355:HOH:O	16:P:3:THR:HG21	2.14	0.46
7:G:158:ASP:OD1	7:G:160:ARG:HB2	2.14	0.46
14:N:49:ALA:C	14:N:54:TYR:HB3	2.39	0.46
18:R:31:GLU:CD	18:R:93:ARG:HH12	2.24	0.46
19:S:22:GLN:HA	19:S:139:PRO:O	2.15	0.46
21:U:48:VAL:CG2	21:U:98:VAL:HA	2.44	0.46
1:A:60:A:C2	1:A:61:G:C8	3.04	0.46
1:A:200:U:H2'	37:A:3428:HOH:O	2.14	0.46
1:A:447:A:O2'	1:A:448:G:H5'	2.16	0.46
1:A:1162:G:H2'	37:A:6556:HOH:O	2.15	0.46
1:A:2090:G:H2'	1:A:2091:G:C8	2.49	0.46
1:A:2494:G:H4'	10:J:5:MET:SD	2.55	0.46
1:A:2898:G:O2'	1:A:2899:A:H5'	2.16	0.46
3:C:97:ALA:HB2	3:C:150:PRO:HB2	1.97	0.46
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.50	0.46
4:D:234:ARG:NH1	37:D:8620:HOH:O	2.37	0.46
5:E:33:LYS:HE2	37:E:8358:HOH:O	2.14	0.46
6:F:25:MET:HE3	6:F:37:ALA:HB1	1.97	0.46
11:K:45:VAL:HG22	11:K:46:ILE:N	2.30	0.46
15:O:180:LEU:O	15:O:181:ASP:HB3	2.15	0.46
16:P:25:VAL:O	16:P:29:VAL:HG23	2.14	0.46
17:Q:41:ARG:O	17:Q:44:VAL:HB	2.15	0.46
18:R:50:GLY:HA3	18:R:87:THR:OG1	2.15	0.46
30:4:23:GLU:HG2	30:4:24:LYS:O	2.15	0.46
1:A:160:A:C5	1:A:177:A:C2	3.03	0.46
1:A:396:U:H1'	37:A:7610:HOH:O	2.14	0.46
1:A:500:G:O2'	1:A:501:G:H5'	2.16	0.46
1:A:1513:C:O2'	1:A:1514:C:H5'	2.15	0.46
1:A:2010:A:H2'	37:A:5928:HOH:O	2.15	0.46
1:A:2445:U:H2'	1:A:2446:G:C8	2.50	0.46
1:A:2506:A:C1'	37:A:6024:HOH:O	2.62	0.46
1:A:2630:G:O6	3:C:206:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.84	0.46
4:D:204:GLY:HA3	37:D:8655:HOH:O	2.15	0.46
4:D:221:GLN:NE2	12:L:42:ASN:HD22	2.09	0.46
5:E:115:LEU:HD12	5:E:115:LEU:HA	1.80	0.46
6:F:59:GLY:O	6:F:61:PHE:N	2.37	0.46
7:G:69:ILE:HA	7:G:72:MET:HE2	1.96	0.46
10:J:157:ILE:HG22	10:J:158:ASN:N	2.30	0.46
13:M:12:THR:HG21	13:M:16:GLY:O	2.16	0.46
14:N:57:LYS:HE2	14:N:140:ALA:O	2.15	0.46
14:N:95:LYS:HG2	14:N:99:ARG:HB3	1.97	0.46
14:N:169:ARG:NH1	37:N:8573:HOH:O	2.49	0.46
24:X:88:THR:O	37:X:2374:HOH:O	2.21	0.46
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.78	0.46
27:1:30:GLU:CA	27:1:33:HIS:HB3	2.41	0.46
27:1:39:CYS:SG	27:1:40:PRO:HD2	2.55	0.46
1:A:858:U:H2'	1:A:859:C:C6	2.49	0.46
1:A:1064:U:H2'	1:A:1065:G:C8	2.51	0.46
1:A:2099:G:O6	31:A:9001:SPR:H8A2	2.16	0.46
2:B:3065:A:O2'	2:B:3066:G:P	2.72	0.46
3:C:8:ARG:HG2	37:C:8554:HOH:O	2.14	0.46
3:C:186:TRP:CG	3:C:187:PRO:HA	2.51	0.46
6:F:95:THR:C	6:F:97:GLN:N	2.70	0.46
7:G:7:ILE:HG22	7:G:45:ASP:O	2.15	0.46
7:G:93:MET:HE2	7:G:107:PHE:CD1	2.50	0.46
14:N:69:LYS:O	14:N:73:ARG:CZ	2.64	0.46
15:O:143:ARG:HH12	15:O:173:ASP:CG	2.21	0.46
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.79	0.46
28:2:10:LYS:CG	37:2:8432:HOH:O	2.58	0.46
1:A:79:G:H22	1:A:97:G:H1'	1.80	0.46
1:A:278:A:H2'	1:A:279:C:O4'	2.16	0.46
1:A:820:G:H5'	1:A:821:U:C5'	2.45	0.46
1:A:849:C:O2'	1:A:850:U:H5'	2.16	0.46
1:A:1218:U:H2'	1:A:1219:U:C6	2.50	0.46
4:D:162:MET:HE2	4:D:310:ARG:CG	2.45	0.46
4:D:175:LEU:C	4:D:175:LEU:CD2	2.88	0.46
5:E:61:PHE:HD1	37:E:8377:HOH:O	1.98	0.46
21:U:48:VAL:HG13	21:U:49:GLU:N	2.30	0.46
25:Y:12:ILE:HG23	25:Y:36:HIS:CG	2.50	0.46
26:Z:130:ARG:HB2	26:Z:142:SER:O	2.16	0.46
27:1:38:LYS:HG3	37:1:8432:HOH:O	2.14	0.46
1:A:101:C:O2'	1:A:102:A:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:A:H4'	1:A:338:C:C4	2.51	0.46
1:A:679:G:OP2	37:A:4409:HOH:O	2.20	0.46
1:A:1015:C:H2'	1:A:1016:U:C6	2.51	0.46
1:A:1855:G:H8	3:C:144:GLU:OE2	1.99	0.46
37:A:4055:HOH:O	8:H:31:LYS:HE3	2.16	0.46
3:C:192:VAL:O	3:C:192:VAL:CG1	2.63	0.46
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.15	0.46
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.45	0.46
9:I:12:ILE:O	9:I:13:PRO:C	2.58	0.46
12:L:37:TYR:HD2	37:L:7169:HOH:O	1.96	0.46
13:M:77:ALA:HB3	37:M:8534:HOH:O	2.15	0.46
15:O:115:VAL:O	15:O:118:ILE:HB	2.14	0.46
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.46	0.46
24:X:14:HIS:HB2	24:X:17:ILE:HG13	1.98	0.46
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.97	0.46
1:A:190:G:OP2	37:A:3713:HOH:O	2.21	0.46
1:A:331:A:C6	1:A:332:G:C4	3.03	0.46
1:A:1534:C:N3	37:A:9465:HOH:O	2.36	0.46
1:A:1613:C:H2'	1:A:1614:G:O4'	2.15	0.46
1:A:2016:U:O5'	1:A:2016:U:H6	1.99	0.46
2:B:3057:A:C8	6:F:141:VAL:HG21	2.51	0.46
10:J:141:ASN:CA	37:J:8356:HOH:O	2.59	0.46
12:L:9:THR:O	12:L:10:GLN:C	2.59	0.46
14:N:133:LEU:O	14:N:134:ILE:HD13	2.16	0.46
16:P:105:ASN:HD21	16:P:109:SER:H	1.62	0.46
19:S:15:LYS:HE3	37:S:8578:HOH:O	2.16	0.46
1:A:450:C:H4'	5:E:46:TYR:CE1	2.51	0.46
1:A:1003:U:O2	10:J:90:PHE:HZ	1.99	0.46
1:A:2873:C:N4	1:A:2874:G:C6	2.84	0.46
37:A:7400:HOH:O	21:U:9:LYS:HD2	2.16	0.46
2:B:3078:G:O2'	2:B:3079:U:P	2.74	0.46
4:D:138:GLY:O	4:D:139:ASP:C	2.58	0.46
4:D:154:VAL:CG1	4:D:156:LYS:HG2	2.46	0.46
7:G:11:VAL:CG1	7:G:12:ASP:H	2.29	0.46
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.16	0.46
1:A:289:G:O2'	1:A:290:C:H5'	2.15	0.46
1:A:392:U:C5'	14:N:193:LYS:HB3	2.46	0.46
1:A:1497:G:H4'	1:A:1627:G:O2'	2.16	0.46
1:A:1603:A:H5'	1:A:1605:G:C4'	2.46	0.46
1:A:1657:A:H2'	1:A:1658:A:C8	2.51	0.46
1:A:1909:A:H2'	1:A:1910:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2045:G:H2'	1:A:2046:G:O4'	2.16	0.46
1:A:2604:A:H5'	37:A:5764:HOH:O	2.16	0.46
37:A:9939:HOH:O	30:4:84:ARG:HB2	2.16	0.46
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.50	0.46
5:E:142:ASP:OD1	5:E:236:THR:HG23	2.15	0.46
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.15	0.46
6:F:94:ALA:O	6:F:95:THR:O	2.33	0.46
10:J:4:ALA:HB3	37:J:8354:HOH:O	2.16	0.46
12:L:99:ASP:OD1	12:L:99:ASP:C	2.58	0.46
14:N:155:HIS:O	14:N:158:ARG:HG2	2.16	0.46
15:O:50:LEU:HB2	37:O:8523:HOH:O	2.16	0.46
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.98	0.46
1:A:251:C:HO2'	1:A:252:C:H5'	1.80	0.45
1:A:566:A:H2'	1:A:567:U:O4'	2.16	0.45
1:A:1004:C:O2'	1:A:1005:A:H5'	2.16	0.45
1:A:1191:A:C3'	1:A:1192:A:H5''	2.42	0.45
1:A:1420:C:C2	1:A:1445:G:N2	2.84	0.45
1:A:1562:C:H42	1:A:2738:G:H1	1.63	0.45
1:A:1603:A:C5'	1:A:1605:G:H5'	2.46	0.45
1:A:1624:A:H5'	1:A:1626:A:O4'	2.17	0.45
1:A:2460:A:OP1	30:4:60:LYS:N	2.46	0.45
1:A:2697:A:H2'	1:A:2698:G:O4'	2.15	0.45
1:A:2833:C:C2	1:A:2848:G:N2	2.84	0.45
2:B:3042:C:H2'	37:B:6700:HOH:O	2.14	0.45
3:C:57:ALA:HA	3:C:67:LEU:HD23	1.97	0.45
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.46	0.45
5:E:142:ASP:OD1	5:E:237:GLU:HB3	2.16	0.45
6:F:93:LEU:HG	37:F:3862:HOH:O	2.16	0.45
7:G:101:GLU:OE2	7:G:115:ARG:NH1	2.49	0.45
7:G:145:ALA:HB1	7:G:168:ILE:CD1	2.46	0.45
13:M:35:ARG:NH1	13:M:35:ARG:O	2.49	0.45
1:A:960:G:N3	1:A:960:G:C2'	2.78	0.45
1:A:1057:A:C6	1:A:1058:A:C6	3.04	0.45
1:A:1753:C:O2	4:D:229:ARG:NH2	2.47	0.45
1:A:2478:U:H2'	1:A:2479:A:C8	2.51	0.45
1:A:2821:C:H4'	4:D:116:PRO:CB	2.46	0.45
3:C:94:LEU:N	3:C:94:LEU:CD2	2.79	0.45
3:C:129:LEU:CD1	3:C:145:MET:HE1	2.47	0.45
5:E:200:PRO:HB3	5:E:212:VAL:HG23	1.98	0.45
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.51	0.45
1:A:316:A:H5'	21:U:54:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:C:N4	1:A:2467:A:C8	2.84	0.45
1:A:949:U:O2'	18:R:40:HIS:HE1	1.99	0.45
1:A:970:U:H2'	37:A:6298:HOH:O	2.16	0.45
1:A:1552:G:H2'	1:A:1553:C:C6	2.50	0.45
1:A:1603:A:H5''	1:A:1605:G:H5'	1.97	0.45
1:A:1730:G:C5'	1:A:1731:C:C6	2.99	0.45
1:A:2004:U:O2	1:A:2004:U:H2'	2.15	0.45
1:A:2467:A:P	37:A:9038:HOH:O	2.73	0.45
4:D:53:LEU:HD11	4:D:327:VAL:HG22	1.99	0.45
5:E:34:ALA:HB3	5:E:220:THR:HG21	1.99	0.45
5:E:233:THR:CG2	5:E:234:VAL:N	2.77	0.45
13:M:30:ARG:NH2	37:M:8524:HOH:O	2.37	0.45
37:N:8533:HOH:O	30:4:46:ILE:HB	2.16	0.45
1:A:558:C:H2'	1:A:559:U:H5''	1.97	0.45
1:A:695:C:H2'	1:A:696:C:C6	2.51	0.45
1:A:716:G:H2'	1:A:717:C:O5'	2.17	0.45
1:A:1172:G:H1'	37:A:4951:HOH:O	2.15	0.45
1:A:1500:U:P	17:Q:41:ARG:HH22	2.38	0.45
1:A:2107:U:O2'	1:A:2108:A:H5'	2.16	0.45
1:A:2300:A:C2	1:A:2306:U:C5	3.03	0.45
1:A:2450:C:O5'	1:A:2450:C:H6	2.00	0.45
1:A:2487:C:H5	37:A:4863:HOH:O	2.00	0.45
1:A:2533:C:O2'	1:A:2534:C:H5'	2.17	0.45
37:A:3444:HOH:O	11:K:46:ILE:HD12	2.16	0.45
2:B:3006:C:P	15:O:37:ARG:HH11	2.40	0.45
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.15	0.45
11:K:39:VAL:CG1	11:K:107:ASN:HB2	2.47	0.45
12:L:30:LYS:C	12:L:55:VAL:HG13	2.42	0.45
14:N:68:ARG:O	14:N:68:ARG:CG	2.61	0.45
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.80	0.45
24:X:88:THR:CG2	24:X:89:ASP:N	2.79	0.45
26:Z:109:LEU:HA	37:Z:8571:HOH:O	2.16	0.45
1:A:21:G:H5''	19:S:1:GLY:O	2.17	0.45
1:A:711:G:C2	1:A:718:C:C2	3.04	0.45
1:A:1328:A:OP1	26:Z:169:ARG:HD2	2.17	0.45
1:A:1593:C:OP1	17:Q:117:SER:CB	2.65	0.45
1:A:1778:A:H2'	1:A:1779:A:H5'	1.98	0.45
1:A:1805:G:H2'	1:A:1806:G:H8	1.81	0.45
1:A:1896:G:H1'	37:A:4232:HOH:O	2.15	0.45
1:A:2437:A:H2'	1:A:2438:G:C8	2.52	0.45
1:A:2769:C:H2'	1:A:2770:G:C5'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3057:A:N6	37:B:3535:HOH:O	2.44	0.45
4:D:274:GLU:HA	4:D:292:GLY:O	2.16	0.45
6:F:65:GLU:HA	37:F:6752:HOH:O	2.16	0.45
10:J:58:HIS:CE1	10:J:59:ASN:ND2	2.84	0.45
10:J:109:ASP:HB2	37:J:8333:HOH:O	2.15	0.45
12:L:14:LYS:HD2	12:L:45:PRO:HG3	1.99	0.45
13:M:143:THR:HG21	37:M:8542:HOH:O	2.17	0.45
15:O:5:ARG:HG3	18:R:18:PRO:HB3	1.98	0.45
15:O:154:LEU:HG	15:O:155:GLU:N	2.30	0.45
21:U:43:ASN:C	21:U:45:GLY:H	2.25	0.45
1:A:328:U:O4'	5:E:202:THR:HG22	2.17	0.45
1:A:1008:C:OP1	10:J:16:ARG:NH2	2.47	0.45
1:A:1161:A:H8	1:A:1161:A:O5'	2.00	0.45
1:A:1241:G:C2	11:K:86:MET:HE2	2.52	0.45
1:A:2038:A:OP2	4:D:224:LYS:NZ	2.43	0.45
37:A:5657:HOH:O	15:O:21:HIS:HE1	1.99	0.45
2:B:3049:G:H2'	2:B:3050:G:O4'	2.16	0.45
3:C:211:LYS:HD3	37:C:8615:HOH:O	2.16	0.45
4:D:72:THR:HB	37:D:8606:HOH:O	2.15	0.45
5:E:85:LYS:HE2	37:E:8328:HOH:O	2.16	0.45
6:F:25:MET:SD	6:F:40:ILE:HD11	2.57	0.45
10:J:46:VAL:O	10:J:146:TRP:CH2	2.66	0.45
14:N:77:PHE:CD2	14:N:86:MET:HA	2.52	0.45
15:O:161:GLY:O	15:O:162:ASP:C	2.59	0.45
1:A:422:G:C6	1:A:2446:G:C6	3.04	0.45
1:A:457:U:H5	1:A:460:A:OP2	2.00	0.45
1:A:920:C:H5'	1:A:921:G:N3	2.31	0.45
1:A:1188:A:C5	1:A:1189:A:C2	3.05	0.45
1:A:1745:G:H5'	37:A:4303:HOH:O	2.17	0.45
1:A:1827:G:H2'	1:A:1828:G:C8	2.51	0.45
1:A:1862:C:O2'	1:A:1863:G:H5'	2.16	0.45
1:A:2428:G:O6	1:A:2464:C:H1'	2.17	0.45
1:A:2909:G:H2'	1:A:2910:A:H8	1.82	0.45
2:B:3008:G:C6	2:B:3009:C:C4	3.04	0.45
4:D:7:ARG:HH12	4:D:11:LEU:HD21	1.81	0.45
4:D:55:ASN:HB3	4:D:64:GLY:N	2.31	0.45
5:E:80:VAL:HA	5:E:81:PRO:HD3	1.82	0.45
5:E:187:ARG:O	5:E:187:ARG:HG3	2.15	0.45
5:E:236:THR:C	37:E:8447:HOH:O	2.59	0.45
11:K:126:ASN:O	11:K:129:PHE:HE2	1.99	0.45
14:N:38:VAL:O	14:N:63:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:173:LEU:HD23	14:N:183:VAL:CG1	2.46	0.45
19:S:61:GLN:CD	37:S:8541:HOH:O	2.59	0.45
23:W:42:ASN:O	23:W:44:GLY:N	2.49	0.45
25:Y:21:PRO:HD3	37:Y:6179:HOH:O	2.16	0.45
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.50	0.45
30:4:7:PHE:HE2	30:4:22:VAL:CG2	2.27	0.45
1:A:158:A:O2'	1:A:159:G:H5'	2.17	0.45
1:A:168:C:C2'	1:A:169:A:H5'	2.46	0.45
1:A:426:G:C2	1:A:427:C:C2	3.05	0.45
1:A:958:G:H2'	1:A:959:C:C6	2.51	0.45
1:A:1301:C:O2'	1:A:1331:A:H4'	2.17	0.45
1:A:1335:C:OP2	26:Z:207:SER:CB	2.64	0.45
1:A:1614:G:H2'	37:A:4597:HOH:O	2.16	0.45
1:A:2032:U:O2'	1:A:2033:G:H5''	2.15	0.45
1:A:2290:U:H4'	1:A:2291:A:OP1	2.17	0.45
1:A:2379:G:H4'	1:A:2380:A:H5''	1.99	0.45
1:A:2420:G:H4'	37:A:4068:HOH:O	2.17	0.45
1:A:2667:G:H1'	1:A:2914:A:N3	2.31	0.45
1:A:2904:U:H4'	25:Y:8:ARG:NH1	2.32	0.45
3:C:164:ARG:HA	27:1:69:TYR:CE1	2.52	0.45
5:E:51:TYR:CE2	28:2:53:LYS:HB3	2.52	0.45
7:G:12:ASP:HA	37:G:1750:HOH:O	2.17	0.45
16:P:60:VAL:O	16:P:62:GLY:N	2.39	0.45
17:Q:28:GLN:N	37:Q:6051:HOH:O	2.50	0.45
19:S:89:LEU:HD23	19:S:89:LEU:HA	1.82	0.45
21:U:113:GLU:O	21:U:114:SER:C	2.59	0.45
24:X:64:THR:O	24:X:68:THR:HG22	2.16	0.45
24:X:122:ARG:HG2	24:X:152:ALA:O	2.15	0.45
24:X:142:ASP:HB3	24:X:145:GLY:H	1.81	0.45
25:Y:73:ARG:C	25:Y:85:VAL:HG13	2.42	0.45
26:Z:129:ASN:OD1	26:Z:141:THR:OG1	2.35	0.45
1:A:644:G:N3	1:A:644:G:H5'	2.32	0.45
1:A:653:C:H2'	1:A:654:A:C8	2.51	0.45
1:A:1293:U:HO2'	26:Z:149:GLN:HE22	1.60	0.45
1:A:1656:A:H2'	1:A:1657:A:O4'	2.17	0.45
1:A:1706:G:C5	1:A:1707:G:C6	3.05	0.45
1:A:2547:C:H2'	1:A:2548:C:H6	1.81	0.45
1:A:2569:A:H8	1:A:2569:A:O5'	2.00	0.45
1:A:2761:A:C4	1:A:2763:G:C8	3.05	0.45
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.46	0.45
7:G:162:PHE:CD1	7:G:162:PHE:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:58:LEU:N	15:O:58:LEU:CD1	2.80	0.45
15:O:71:TRP:N	37:O:8540:HOH:O	2.49	0.45
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.52	0.45
27:1:47:LEU:HD23	27:1:57:CYS:CB	2.45	0.45
1:A:846:A:O2'	1:A:847:C:H5'	2.17	0.45
1:A:1477:C:H5'	1:A:1868:G:H5''	1.98	0.45
1:A:1880:C:C2	1:A:1881:A:C8	3.05	0.45
1:A:2011:A:H4'	1:A:2012:U:O5'	2.17	0.45
1:A:2434:A:O3'	30:4:28:GLY:CA	2.65	0.45
1:A:2909:G:O2'	1:A:2910:A:H5'	2.17	0.45
2:B:3114:G:H2'	2:B:3115:C:C6	2.52	0.45
3:C:36:ASP:O	3:C:37:VAL:C	2.60	0.45
3:C:105:VAL:HG13	3:C:155:THR:O	2.16	0.45
3:C:125:ASN:ND2	37:C:8538:HOH:O	2.41	0.45
5:E:27:ARG:HD2	5:E:29:ASP:OD1	2.16	0.45
6:F:58:VAL:CG1	6:F:59:GLY:N	2.78	0.45
10:J:30:GLN:H	10:J:65:ARG:NH1	2.15	0.45
11:K:70:PHE:CD2	11:K:70:PHE:O	2.70	0.45
12:L:14:LYS:CB	12:L:45:PRO:HG2	2.41	0.45
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.32	0.45
15:O:25:ARG:HA	15:O:28:LYS:HG3	1.98	0.45
19:S:28:SER:O	19:S:29:LYS:C	2.59	0.45
25:Y:51:ASP:OD2	25:Y:52:PRO:HD2	2.17	0.45
26:Z:144:ARG:NH2	37:Z:8610:HOH:O	2.50	0.45
27:1:11:THR:O	27:1:14:PHE:HB2	2.17	0.45
1:A:401:C:H2'	1:A:402:U:C6	2.52	0.44
1:A:596:C:H2'	1:A:597:A:C8	2.52	0.44
1:A:711:G:N2	1:A:718:C:C2	2.85	0.44
1:A:2325:C:H1'	37:A:4120:HOH:O	2.18	0.44
1:A:2362:A:H2'	1:A:2363:G:C8	2.52	0.44
1:A:2435:U:P	30:4:28:GLY:HA3	2.56	0.44
3:C:179:MET:HA	3:C:179:MET:HE3	1.98	0.44
4:D:23:THR:CG2	4:D:162:MET:HE3	2.47	0.44
4:D:316:ARG:N	4:D:317:PRO:HD3	2.33	0.44
5:E:173:LYS:NZ	37:E:8319:HOH:O	2.49	0.44
10:J:1:LYS:HA	10:J:2:PRO:HD3	1.68	0.44
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.47	0.44
15:O:143:ARG:NH1	15:O:173:ASP:OD2	2.40	0.44
19:S:29:LYS:HD3	37:S:8532:HOH:O	2.15	0.44
24:X:48:VAL:O	24:X:48:VAL:HG12	2.16	0.44
26:Z:117:LEU:HD12	26:Z:174:VAL:CG1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:A:C6	16:P:65:LEU:HD13	2.52	0.44
1:A:1384:C:H5'	25:Y:30:MET:HG2	1.99	0.44
1:A:1434:A:H2'	1:A:1436:C:C5	2.51	0.44
1:A:1543:G:N1	1:A:1641:A:OP2	2.39	0.44
1:A:1592:G:O2'	1:A:1593:C:O5'	2.35	0.44
1:A:1596:U:H2'	1:A:1598:A:OP2	2.16	0.44
1:A:1701:A:H5''	1:A:1702:U:H3'	1.99	0.44
1:A:1771:U:O2'	27:1:23:ARG:NH2	2.49	0.44
1:A:1886:A:O2'	27:1:20:LEU:HB2	2.17	0.44
1:A:2044:G:OP1	25:Y:23:HIS:HE1	1.99	0.44
1:A:2099:G:N1	31:A:9001:SPR:O2A	2.47	0.44
1:A:2467:A:O2'	1:A:2468:A:H2'	2.17	0.44
1:A:2598:U:O2	1:A:2600:A:H8	2.00	0.44
2:B:3076:G:C3'	2:B:3077:A:H5''	2.38	0.44
3:C:105:VAL:CG1	3:C:106:CYS:N	2.80	0.44
5:E:13:ASP:N	37:E:8440:HOH:O	2.51	0.44
5:E:20:ASP:O	5:E:23:GLU:HB2	2.17	0.44
5:E:173:LYS:HB3	5:E:187:ARG:HG3	1.98	0.44
7:G:77:THR:OG1	7:G:78:GLU:N	2.49	0.44
15:O:113:SER:CB	37:O:8560:HOH:O	2.58	0.44
15:O:120:GLU:HG3	15:O:136:LEU:HD13	1.99	0.44
17:Q:59:ARG:HH22	17:Q:66:GLN:HE22	1.62	0.44
19:S:79:ARG:C	19:S:81:PRO:HD3	2.42	0.44
23:W:12:THR:HG23	23:W:14:ALA:H	1.81	0.44
1:A:240:C:O2	1:A:240:C:H2'	2.17	0.44
1:A:533:U:C5	1:A:2084:C:H5'	2.53	0.44
1:A:818:A:C2	27:1:13:ARG:HA	2.52	0.44
1:A:920:C:H5''	1:A:921:G:O5'	2.17	0.44
1:A:958:G:O2'	1:A:959:C:H5'	2.17	0.44
1:A:1114:A:H2'	1:A:1115:U:C6	2.53	0.44
1:A:1269:G:O2'	1:A:1270:U:H5'	2.17	0.44
1:A:2715:G:N2	4:D:264:GLU:OE1	2.51	0.44
1:A:2791:U:C1'	1:A:2792:A:H5''	2.47	0.44
37:A:3671:HOH:O	7:G:143:GLN:HG2	2.17	0.44
5:E:55:ARG:HB2	37:E:8311:HOH:O	2.16	0.44
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.46	0.44
6:F:101:THR:HG22	6:F:101:THR:O	2.17	0.44
7:G:81:GLU:HA	7:G:133:VAL:O	2.17	0.44
10:J:82:LYS:HB2	10:J:82:LYS:NZ	2.32	0.44
20:T:37:VAL:O	20:T:41:VAL:HG23	2.18	0.44
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:10:ARG:HG3	27:1:11:THR:N	2.33	0.44
28:2:28:HIS:HD2	28:2:30:LYS:H	1.64	0.44
1:A:10:U:H5'	37:A:6007:HOH:O	2.17	0.44
1:A:157:G:H4'	14:N:95:LYS:CE	2.44	0.44
1:A:195:C:H2'	1:A:196:G:H5'	1.99	0.44
1:A:226:A:H1'	1:A:393:G:C5	2.52	0.44
1:A:602:A:O2'	1:A:605:C:H4'	2.17	0.44
1:A:1236:A:H2'	1:A:1237:U:O4'	2.17	0.44
1:A:1353:C:O5'	37:A:4650:HOH:O	2.19	0.44
1:A:1423:C:O2'	1:A:1424:A:H5'	2.17	0.44
1:A:1440:U:OP2	37:A:4435:HOH:O	2.21	0.44
1:A:1685:A:H4'	1:A:1686:C:OP2	2.17	0.44
1:A:1979:G:O2'	1:A:1980:U:OP1	2.32	0.44
1:A:2284:G:H1'	37:A:9552:HOH:O	2.18	0.44
1:A:2851:G:C2'	1:A:2852:A:H5'	2.48	0.44
4:D:41:PHE:CE1	4:D:79:MET:HG3	2.51	0.44
7:G:126:ILE:HB	7:G:131:LEU:HD23	1.98	0.44
10:J:72:VAL:CG1	10:J:81:TYR:CZ	3.01	0.44
15:O:152:GLU:C	15:O:154:LEU:N	2.75	0.44
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.18	0.44
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.99	0.44
26:Z:136:LYS:HE2	26:Z:138:ARG:NH1	2.31	0.44
30:4:38:ARG:O	30:4:42:ARG:HB2	2.17	0.44
1:A:1517:U:C2	1:A:1670:G:N2	2.85	0.44
1:A:2428:G:C6	1:A:2464:C:H1'	2.53	0.44
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.44	0.44
1:A:2777:G:O2'	1:A:2778:A:H5'	2.17	0.44
4:D:195:ARG:NH1	4:D:324:ASP:OD1	2.48	0.44
5:E:59:GLU:C	5:E:71:PRO:HA	2.43	0.44
5:E:84:VAL:O	5:E:85:LYS:CB	2.65	0.44
6:F:36:ASN:CA	37:F:7500:HOH:O	2.62	0.44
7:G:22:VAL:O	7:G:28:SER:HA	2.18	0.44
9:I:12:ILE:HD12	37:I:692:HOH:O	2.16	0.44
10:J:112:ARG:O	10:J:113:ALA:C	2.60	0.44
10:J:150:LYS:HG2	37:J:8372:HOH:O	2.17	0.44
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.48	0.44
13:M:93:VAL:HG12	13:M:97:VAL:HG23	2.00	0.44
15:O:132:ASN:O	15:O:135:VAL:HG12	2.18	0.44
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.53	0.44
26:Z:235:GLU:CD	26:Z:235:GLU:N	2.73	0.44
27:1:22:ILE:O	27:1:26:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:C:H4'	21:U:16:LEU:HB2	2.00	0.44
1:A:160:A:C8	1:A:177:A:C6	3.05	0.44
1:A:534:C:N4	37:A:7556:HOH:O	2.47	0.44
1:A:818:A:H2	27:1:13:ARG:HA	1.81	0.44
1:A:920:C:C4	1:A:2467:A:C5	3.05	0.44
1:A:1414:A:H2'	1:A:1415:G:O4'	2.17	0.44
1:A:2363:G:O2'	18:R:11:ARG:HG3	2.18	0.44
1:A:2443:C:O3'	13:M:56:LYS:HE3	2.17	0.44
4:D:23:THR:HG23	4:D:162:MET:HE3	2.00	0.44
4:D:248:ARG:NH1	37:D:8616:HOH:O	2.49	0.44
7:G:36:PRO:HD3	11:K:127:ILE:HD12	1.99	0.44
20:T:11:THR:O	20:T:12:GLU:C	2.60	0.44
30:4:69:TYR:O	30:4:77:ALA:HA	2.17	0.44
1:A:236:A:H2'	1:A:236:A:O5'	2.17	0.44
1:A:1137:G:H1'	37:A:3854:HOH:O	2.18	0.44
1:A:1158:G:O2'	1:A:1159:G:H5'	2.17	0.44
1:A:1992:U:H2'	1:A:1994:A:OP2	2.17	0.44
37:A:6516:HOH:O	27:1:22:ILE:HG13	2.16	0.44
2:B:3092:G:H22	10:J:52:LYS:HZ2	1.63	0.44
4:D:2:GLN:HA	37:D:8622:HOH:O	2.18	0.44
4:D:304:PRO:HD2	4:D:307:ARG:CD	2.48	0.44
5:E:21:VAL:C	5:E:23:GLU:H	2.26	0.44
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.48	0.44
9:I:64:ASN:N	9:I:64:ASN:ND2	2.65	0.44
10:J:85:ILE:HG23	10:J:85:ILE:O	2.18	0.44
12:L:28:GLU:OE2	12:L:58:THR:HG21	2.17	0.44
14:N:81:ARG:O	14:N:86:MET:HE2	2.17	0.44
23:W:1:THR:C	23:W:3:LEU:N	2.75	0.44
24:X:4:LEU:HD21	24:X:52:VAL:HG11	1.99	0.44
1:A:155:C:OP1	14:N:186:SER:OG	2.26	0.44
1:A:236:A:H4'	1:A:237:G:OP1	2.18	0.44
1:A:628:A:C4	1:A:2071:C:C4	3.06	0.44
1:A:731:U:O2'	1:A:732:C:H5'	2.18	0.44
1:A:920:C:H4'	1:A:921:G:N2	2.32	0.44
1:A:1135:G:H5'	37:A:5898:HOH:O	2.17	0.44
1:A:2265:U:H2'	1:A:2266:A:H8	1.83	0.44
1:A:2547:C:C2	1:A:2548:C:C5	3.05	0.44
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.99	0.44
5:E:35:VAL:HG21	5:E:227:GLY:HA2	1.99	0.44
5:E:150:THR:HA	5:E:203:ALA:O	2.17	0.44
5:E:191:SER:OG	5:E:192:ILE:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:63:ARG:O	9:I:67:LEU:HG	2.18	0.44
13:M:54:PRO:HG2	13:M:57:VAL:HG21	1.99	0.44
18:R:93:ARG:HH11	18:R:93:ARG:HG3	1.82	0.44
24:X:5:VAL:O	24:X:52:VAL:HG22	2.17	0.44
24:X:6:GLN:HA	24:X:52:VAL:HG23	1.98	0.44
24:X:85:ALA:HB2	24:X:91:ASP:O	2.18	0.44
1:A:148:A:H5''	28:2:44:LYS:HG2	2.00	0.44
1:A:513:A:N3	37:A:3639:HOH:O	2.36	0.44
1:A:716:G:C2'	1:A:717:C:O5'	2.66	0.44
1:A:797:A:H5'	27:1:10:ARG:HG2	2.00	0.44
1:A:834:G:H5''	1:A:835:U:O5'	2.18	0.44
1:A:1819:G:H2'	1:A:1820:G:C5'	2.48	0.44
1:A:1855:G:O6	3:C:142:SER:HB3	2.18	0.44
1:A:2010:A:C2'	37:A:5928:HOH:O	2.66	0.44
37:A:7559:HOH:O	27:1:31:ILE:HG13	2.18	0.44
3:C:99:ILE:O	3:C:131:HIS:CE1	2.71	0.44
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.47	0.44
10:J:139:ASP:O	10:J:139:ASP:CG	2.60	0.44
10:J:165:GLY:C	10:J:166:ASN:HD22	2.26	0.44
14:N:61:ILE:HA	37:N:8623:HOH:O	2.18	0.44
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.47	0.44
15:O:171:HIS:CE1	37:O:8568:HOH:O	2.70	0.44
19:S:39:THR:CB	19:S:42:GLU:HG3	2.48	0.44
22:V:49:LEU:O	22:V:55:ALA:CB	2.66	0.44
23:W:45:ARG:C	23:W:47:LYS:N	2.74	0.44
24:X:154:ARG:HE	24:X:154:ARG:HB3	1.59	0.44
30:4:17:HIS:O	30:4:18:GLN:HG3	2.18	0.44
1:A:585:C:H6	37:A:6064:HOH:O	1.99	0.43
1:A:1348:A:N3	37:A:9951:HOH:O	2.36	0.43
1:A:1375:A:C2'	1:A:1376:G:H5'	2.48	0.43
1:A:1594:C:O2'	1:A:1607:A:H4'	2.18	0.43
1:A:1730:G:C5'	1:A:1731:C:H6	2.30	0.43
1:A:1878:G:C4'	37:A:6090:HOH:O	2.65	0.43
1:A:1881:A:OP1	3:C:199:HIS:HE1	2.01	0.43
1:A:2453:G:H5'	37:A:4663:HOH:O	2.17	0.43
1:A:2715:G:O2'	4:D:262:ARG:HD2	2.18	0.43
2:B:3103:A:HO2'	2:B:3104:A:H5'	1.83	0.43
3:C:81:GLN:CB	3:C:92:ASN:ND2	2.80	0.43
3:C:103:VAL:HA	3:C:104:PRO:HD3	1.85	0.43
4:D:132:HIS:HB2	4:D:137:LEU:HD22	2.00	0.43
4:D:314:ALA:CB	4:D:317:PRO:HG3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:165:ASP:O	5:E:168:ARG:HB3	2.18	0.43
6:F:99:ASP:O	6:F:159:PRO:HG3	2.17	0.43
7:G:107:PHE:CZ	7:G:108:LEU:HD13	2.52	0.43
7:G:139:GLU:CD	37:G:5919:HOH:O	2.61	0.43
8:H:117:GLU:C	8:H:119:ARG:N	2.76	0.43
10:J:65:ARG:HD3	37:J:8374:HOH:O	2.17	0.43
10:J:113:ALA:N	10:J:114:PRO:CD	2.81	0.43
15:O:24:LEU:HD13	18:R:26:PRO:HB3	2.00	0.43
19:S:125:ARG:HG2	37:S:8543:HOH:O	2.18	0.43
20:T:10:VAL:HG11	23:W:36:ALA:HA	1.99	0.43
1:A:177:A:H2'	1:A:178:U:O4'	2.18	0.43
1:A:707:C:H2'	1:A:708:A:H8	1.82	0.43
1:A:920:C:N4	1:A:2467:A:C4	2.86	0.43
1:A:1185:U:C5'	37:A:7445:HOH:O	2.65	0.43
1:A:1545:C:O2'	1:A:1546:G:H5'	2.18	0.43
1:A:1819:G:H2'	1:A:1820:G:C4'	2.48	0.43
3:C:199:HIS:HD2	3:C:201:PHE:N	2.06	0.43
5:E:140:VAL:HG12	5:E:141:SER:N	2.33	0.43
5:E:180:SER:HB2	37:E:8444:HOH:O	2.18	0.43
7:G:20:ILE:O	7:G:30:THR:HA	2.18	0.43
7:G:139:GLU:CG	37:G:5919:HOH:O	2.65	0.43
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.17	0.43
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.33	0.43
11:K:130:VAL:CG1	11:K:131:THR:N	2.81	0.43
12:L:14:LYS:HB2	12:L:45:PRO:CG	2.41	0.43
13:M:38:HIS:H	13:M:38:HIS:HD1	1.67	0.43
13:M:148:GLU:HB2	37:M:8587:HOH:O	2.17	0.43
14:N:127:LYS:NZ	37:N:8568:HOH:O	2.50	0.43
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.45	0.43
20:T:57:THR:CG2	20:T:59:ASP:HB2	2.49	0.43
22:V:17:THR:HG22	22:V:18:GLY:N	2.33	0.43
27:1:56:MET:HA	27:1:62:TYR:O	2.18	0.43
30:4:3:MET:HG3	30:4:4:PRO:HD2	2.00	0.43
1:A:255:A:H2'	1:A:256:C:C6	2.53	0.43
1:A:303:C:H2'	1:A:304:G:O4'	2.19	0.43
1:A:340:A:C2	1:A:341:C:C6	3.06	0.43
1:A:694:A:C2'	1:A:695:C:H5'	2.48	0.43
1:A:827:A:H2'	1:A:828:G:O4'	2.17	0.43
1:A:1215:A:O3'	1:A:1216:G:C4'	2.66	0.43
1:A:1973:A:H2'	1:A:1974:G:O4'	2.18	0.43
1:A:2004:U:H5''	1:A:2005:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2084:C:O2'	1:A:2085:A:H5'	2.18	0.43
2:B:3007:G:OP1	15:O:23:ARG:HD2	2.18	0.43
3:C:58:VAL:O	3:C:65:ARG:HD2	2.18	0.43
3:C:179:MET:HG2	3:C:186:TRP:HB3	1.99	0.43
5:E:5:ILE:CD1	5:E:16:VAL:HG23	2.28	0.43
6:F:52:THR:N	6:F:70:GLY:O	2.51	0.43
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.54	0.43
12:L:72:VAL:HG11	12:L:121:PHE:CD1	2.53	0.43
13:M:98:GLU:O	13:M:99:GLU:CB	2.66	0.43
14:N:62:VAL:C	14:N:63:VAL:HG23	2.43	0.43
14:N:139:PRO:HA	14:N:142:LYS:HB2	2.00	0.43
14:N:158:ARG:N	34:N:8518:CL:CL	2.88	0.43
25:Y:20:GLU:CD	25:Y:21:PRO:HD2	2.43	0.43
26:Z:107:PRO:HD3	26:Z:182:PHE:CE1	2.54	0.43
27:1:47:LEU:HA	27:1:56:MET:O	2.18	0.43
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.33	0.43
1:A:10:U:HO2'	1:A:11:A:P	2.42	0.43
1:A:95:A:H5''	1:A:97:G:O4'	2.18	0.43
1:A:206:G:O2'	1:A:438:C:N3	2.48	0.43
1:A:392:U:H4'	14:N:193:LYS:HB3	2.00	0.43
1:A:621:C:H5'	26:Z:132:ASP:OD2	2.19	0.43
1:A:629:A:N7	37:A:9835:HOH:O	2.37	0.43
1:A:907:A:H4'	1:A:1328:A:C2	2.53	0.43
1:A:911:G:H5'	1:A:932:U:OP1	2.18	0.43
1:A:1069:C:H4'	1:A:1081:A:O2'	2.18	0.43
1:A:2419:U:H5''	1:A:2420:G:C5'	2.48	0.43
37:B:4707:HOH:O	15:O:147:ILE:HB	2.19	0.43
3:C:93:THR:HG23	3:C:154:ALA:O	2.19	0.43
4:D:108:GLU:HB3	4:D:111:ARG:HD2	2.00	0.43
5:E:136:VAL:HG22	5:E:137:PRO:HA	1.99	0.43
7:G:107:PHE:CD2	7:G:108:LEU:HD13	2.51	0.43
8:H:105:ALA:HB2	37:H:5522:HOH:O	2.19	0.43
11:K:72:PRO:O	11:K:78:ILE:CD1	2.67	0.43
16:P:96:VAL:HG13	16:P:100:GLN:HB2	2.01	0.43
20:T:23:LYS:HD3	20:T:65:VAL:HG12	2.00	0.43
21:U:96:VAL:HG13	21:U:97:ARG:N	2.33	0.43
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.82	0.43
24:X:35:VAL:HG23	24:X:41:TYR:CD2	2.53	0.43
30:4:1:MET:N	30:4:87:ARG:O	2.47	0.43
1:A:183:A:C5'	14:N:157:LEU:HD12	2.48	0.43
1:A:297:U:H1'	37:A:3911:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:U:C5'	37:A:7314:HOH:O	2.62	0.43
1:A:440:C:C4	1:A:441:A:C6	3.06	0.43
1:A:899:C:OP2	13:M:22:ARG:NH1	2.51	0.43
1:A:1894:C:C2	1:A:1939:U:C4	3.05	0.43
1:A:2478:U:H2'	1:A:2479:A:H8	1.83	0.43
1:A:2484:U:C2	37:A:9600:HOH:O	2.57	0.43
1:A:2783:A:O2'	1:A:2784:A:H5'	2.18	0.43
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.48	0.43
4:D:54:VAL:O	4:D:55:ASN:C	2.60	0.43
6:F:92:GLU:O	6:F:93:LEU:O	2.36	0.43
8:H:6:PHE:CD1	8:H:6:PHE:C	2.97	0.43
14:N:186:SER:OG	14:N:189:VAL:HG12	2.19	0.43
16:P:14:LEU:CD2	16:P:102:ILE:HD11	2.48	0.43
20:T:10:VAL:HG13	23:W:35:ALA:O	2.18	0.43
27:1:48:LYS:HG2	37:1:8434:HOH:O	2.18	0.43
1:A:282:C:H2'	1:A:283:U:O4'	2.17	0.43
1:A:628:A:C4	1:A:2071:C:N4	2.86	0.43
1:A:772:G:H2'	1:A:773:A:O4'	2.19	0.43
1:A:943:A:C5	24:X:23:MET:HE2	2.54	0.43
1:A:1098:A:H2'	1:A:1099:G:O4'	2.19	0.43
1:A:1730:G:H5'	1:A:1731:C:C6	2.54	0.43
1:A:2769:C:H2'	1:A:2770:G:H5'	2.01	0.43
37:A:5056:HOH:O	4:D:216:LYS:HA	2.18	0.43
4:D:86:ALA:HB2	4:D:128:ILE:HD13	2.01	0.43
4:D:185:GLY:HA2	37:D:8636:HOH:O	2.19	0.43
4:D:280:VAL:HG13	4:D:334:SER:HA	1.99	0.43
5:E:54:LEU:HD21	5:E:87:ARG:HD2	1.99	0.43
5:E:218:VAL:CG1	37:E:8422:HOH:O	2.67	0.43
7:G:9:GLU:HG3	7:G:10:ASP:N	2.34	0.43
8:H:27:GLY:HA3	37:H:5413:HOH:O	2.18	0.43
8:H:36:THR:HG23	8:H:97:ALA:HB2	2.00	0.43
8:H:104:ALA:HA	37:H:6617:HOH:O	2.18	0.43
12:L:103:ASP:O	12:L:104:PRO:C	2.60	0.43
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.34	0.43
14:N:115:LEU:HD13	14:N:115:LEU:O	2.19	0.43
15:O:73:ALA:CB	37:O:8568:HOH:O	2.66	0.43
18:R:8:GLU:CD	18:R:8:GLU:C	2.85	0.43
21:U:48:VAL:HG11	21:U:96:VAL:CG1	2.48	0.43
26:Z:115:ARG:CZ	37:Z:8556:HOH:O	2.67	0.43
1:A:245:C:H2'	1:A:246:G:H5'	1.99	0.43
1:A:1066:U:H2'	1:A:1067:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:G:H1	1:A:1208:C:H42	1.67	0.43
1:A:1308:A:O4'	5:E:226:GLY:HA3	2.19	0.43
1:A:1495:C:H1'	1:A:1573:A:H1'	2.01	0.43
1:A:1545:C:H2'	1:A:1546:G:O4'	2.18	0.43
1:A:1666:C:C2'	1:A:1667:A:H5'	2.46	0.43
1:A:1732:A:O5'	1:A:1732:A:H8	2.02	0.43
1:A:1790:C:H2'	1:A:1791:U:H6	1.83	0.43
1:A:1815:A:H4'	1:A:2751:C:O4'	2.18	0.43
1:A:2269:C:H2'	1:A:2270:G:C5'	2.49	0.43
1:A:2403:C:H5'	37:A:5995:HOH:O	2.19	0.43
1:A:2405:C:H5'	37:A:6569:HOH:O	2.19	0.43
1:A:2728:C:H6	1:A:2728:C:O5'	2.01	0.43
1:A:2737:C:OP2	17:Q:58:SER:HB2	2.19	0.43
1:A:2781:U:H2'	1:A:2782:G:H5'	2.00	0.43
37:A:9185:HOH:O	5:E:107:ARG:NH2	2.51	0.43
4:D:258:GLY:N	4:D:260:HIS:CE1	2.86	0.43
6:F:23:VAL:HG23	6:F:41:LEU:HD22	2.00	0.43
10:J:26:LYS:HG3	10:J:58:HIS:HB2	2.01	0.43
10:J:62:GLU:OE2	10:J:66:VAL:CG2	2.67	0.43
12:L:37:TYR:CE2	12:L:45:PRO:HA	2.54	0.43
14:N:68:ARG:O	14:N:68:ARG:CD	2.65	0.43
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.01	0.43
22:V:52:THR:HG22	22:V:54:THR:H	1.84	0.43
29:3:19:SER:O	29:3:36:ASN:ND2	2.52	0.43
1:A:377:C:H5	37:A:3291:HOH:O	2.01	0.43
1:A:830:G:O2'	1:A:831:U:H5'	2.19	0.43
1:A:890:C:OP1	5:E:57:PRO:HG3	2.18	0.43
1:A:962:C:H5''	37:A:4892:HOH:O	2.18	0.43
1:A:1187:U:C2'	37:A:6864:HOH:O	2.55	0.43
1:A:1221:G:C8	37:A:5958:HOH:O	2.69	0.43
1:A:1332:C:O2'	1:A:1333:U:H5'	2.19	0.43
1:A:1773:G:H2'	1:A:1774:G:H5'	2.00	0.43
1:A:1862:C:C2'	1:A:1863:G:H5'	2.49	0.43
1:A:2246:U:N3	1:A:2256:G:C2	2.87	0.43
1:A:2300:A:H4'	1:A:2301:A:O5'	2.19	0.43
1:A:2456:A:H2'	1:A:2457:U:C6	2.54	0.43
1:A:2911:C:H2'	1:A:2912:C:C6	2.54	0.43
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.48	0.43
10:J:14:TYR:N	10:J:91:HIS:HE1	2.15	0.43
13:M:130:ARG:NH2	37:M:8547:HOH:O	2.51	0.43
14:N:84:LYS:O	14:N:87:MET:CG	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:40:ALA:O	19:S:44:VAL:HG23	2.18	0.43
19:S:82:GLU:HG3	19:S:83:LYS:H	1.84	0.43
19:S:141:VAL:HG12	19:S:142:ASP:O	2.19	0.43
21:U:12:ARG:NH1	37:U:3035:HOH:O	2.51	0.43
21:U:105:ASP:OD1	21:U:107:LYS:N	2.51	0.43
28:2:52:SER:HA	37:2:8442:HOH:O	2.19	0.43
1:A:101:C:H2'	1:A:102:A:C8	2.53	0.43
1:A:201:G:N2	1:A:202:U:C2	2.87	0.43
1:A:451:C:N4	1:A:452:G:C6	2.87	0.43
1:A:684:G:H2'	1:A:685:C:C6	2.53	0.43
1:A:696:C:O2'	1:A:697:G:H5'	2.18	0.43
1:A:1262:C:H1'	24:X:120:PRO:HG3	2.00	0.43
1:A:1299:G:N2	37:A:4655:HOH:O	2.51	0.43
1:A:1463:A:C6	1:A:1464:U:C4	3.07	0.43
1:A:1940:C:H4'	37:A:7324:HOH:O	2.18	0.43
1:A:2296:C:H5	37:R:5998:HOH:O	2.02	0.43
1:A:2415:A:N3	15:O:26:LEU:HD13	2.33	0.43
1:A:2672:C:O2'	1:A:2673:U:H5'	2.19	0.43
2:B:3056:A:C3'	2:B:3057:A:H5''	2.49	0.43
3:C:55:VAL:HG22	3:C:68:ILE:O	2.19	0.43
4:D:279:THR:HG22	4:D:280:VAL:N	2.32	0.43
5:E:78:ARG:HG2	37:E:8307:HOH:O	2.19	0.43
5:E:193:LEU:O	5:E:233:THR:HG23	2.18	0.43
7:G:132:THR:O	7:G:132:THR:HG23	2.19	0.43
10:J:136:VAL:CG2	37:J:8330:HOH:O	2.56	0.43
12:L:90:PHE:N	12:L:90:PHE:CD1	2.87	0.43
13:M:65:ASP:CG	13:M:111:ALA:HB3	2.43	0.43
14:N:69:LYS:HG2	14:N:127:LYS:HG3	2.01	0.43
18:R:41:LEU:N	18:R:41:LEU:HD12	2.33	0.43
25:Y:76:ARG:HA	25:Y:82:GLU:O	2.19	0.43
1:A:794:U:H3	1:A:819:A:H61	1.66	0.43
1:A:812:A:H2'	1:A:813:C:O4'	2.18	0.43
1:A:1044:C:C5'	37:A:9022:HOH:O	2.66	0.43
1:A:1103:C:O2'	11:K:86:MET:HB3	2.19	0.43
1:A:1634:G:H2'	1:A:1635:U:C6	2.53	0.43
37:A:7121:HOH:O	29:3:24:TRP:CD1	2.72	0.43
5:E:127:ARG:HG2	5:E:127:ARG:NH1	2.33	0.43
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.49	0.43
11:K:17:CYS:O	11:K:45:VAL:HG12	2.18	0.43
14:N:42:ARG:HA	14:N:43:PRO:HD3	1.75	0.43
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:48:VAL:HG13	21:U:96:VAL:HG13	2.01	0.43
27:1:38:LYS:HA	27:1:45:LYS:HA	2.01	0.43
1:A:80:A:H3'	21:U:43:ASN:OD1	2.19	0.42
1:A:290:C:H2'	1:A:291:C:O4'	2.19	0.42
1:A:445:U:C1'	37:A:7314:HOH:O	2.66	0.42
1:A:517:U:H1'	37:A:7554:HOH:O	2.19	0.42
1:A:1279:U:H5''	37:A:9572:HOH:O	2.19	0.42
1:A:1391:G:H2'	1:A:1392:A:H5'	2.01	0.42
1:A:2460:A:OP1	30:4:60:LYS:HB2	2.19	0.42
1:A:2500:C:O2'	1:A:2501:G:H5'	2.18	0.42
1:A:2621:U:H5	37:A:9961:HOH:O	2.01	0.42
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.29	0.42
3:C:69:LEU:C	3:C:69:LEU:HD12	2.44	0.42
4:D:60:SER:C	4:D:62:ARG:N	2.76	0.42
5:E:77:ALA:O	5:E:78:ARG:HG3	2.19	0.42
6:F:166:ILE:O	6:F:169:THR:N	2.52	0.42
6:F:173:GLU:HG3	6:F:174:VAL:N	2.34	0.42
12:L:130:MET:SD	22:V:25:ASP:O	2.77	0.42
15:O:24:LEU:O	15:O:28:LYS:HG2	2.19	0.42
15:O:32:PRO:HD2	15:O:99:GLU:O	2.19	0.42
15:O:143:ARG:NH1	15:O:173:ASP:OD1	2.52	0.42
21:U:55:PHE:CD2	21:U:77:VAL:HG13	2.54	0.42
22:V:35:LYS:NZ	37:V:6621:HOH:O	2.17	0.42
25:Y:21:PRO:HG2	25:Y:24:LYS:HD3	2.01	0.42
26:Z:112:GLU:CD	26:Z:115:ARG:HH12	2.27	0.42
1:A:291:C:H2'	1:A:292:G:O4'	2.19	0.42
1:A:567:U:H5''	37:A:6375:HOH:O	2.19	0.42
1:A:636:G:H5'	1:A:2059:U:OP2	2.19	0.42
1:A:724:G:O2'	1:A:725:C:H5'	2.19	0.42
1:A:1706:G:C6	1:A:1707:G:C6	3.07	0.42
1:A:1789:G:O6	17:Q:73:HIS:HE1	2.03	0.42
1:A:1968:A:H2'	1:A:1969:A:C8	2.54	0.42
1:A:2526:C:C6	1:A:2526:C:H5'	2.54	0.42
2:B:3034:A:H2'	2:B:3035:C:O4'	2.19	0.42
3:C:70:ALA:HA	3:C:71:PRO:HD3	1.80	0.42
5:E:13:ASP:OD1	5:E:13:ASP:O	2.37	0.42
5:E:79:ARG:O	5:E:87:ARG:HG2	2.19	0.42
12:L:86:THR:HG22	12:L:87:ARG:N	2.34	0.42
13:M:35:ARG:O	13:M:40:PHE:HA	2.18	0.42
13:M:148:GLU:HG2	37:M:8553:HOH:O	2.20	0.42
14:N:27:ARG:O	14:N:30:GLU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:35:PRO:HD2	14:N:38:VAL:CG2	2.49	0.42
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.54	0.42
16:P:47:ARG:NH2	37:P:510:HOH:O	2.51	0.42
19:S:132:ARG:NH1	37:S:8582:HOH:O	2.51	0.42
24:X:73:LEU:HD12	24:X:73:LEU:HA	1.86	0.42
1:A:1117:A:C2	1:A:1244:U:C2	3.07	0.42
1:A:1166:A:N3	1:A:1166:A:H2'	2.34	0.42
1:A:1215:A:O3'	1:A:1216:G:H4'	2.19	0.42
1:A:1611:G:O2'	1:A:1612:A:H5'	2.20	0.42
1:A:1902:G:H2'	1:A:1903:U:O4'	2.19	0.42
1:A:2247:C:C5'	37:A:7322:HOH:O	2.67	0.42
37:A:7336:HOH:O	3:C:177:HIS:HE1	2.01	0.42
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.49	0.42
6:F:169:THR:O	6:F:170:TYR:HB2	2.19	0.42
13:M:55:GLN:HA	13:M:58:GLN:NE2	2.33	0.42
14:N:74:ARG:HD3	14:N:91:ILE:HD12	2.00	0.42
14:N:87:MET:H	14:N:87:MET:HG3	1.42	0.42
15:O:47:LEU:CD1	15:O:97:VAL:HG11	2.49	0.42
15:O:154:LEU:C	15:O:156:GLU:H	2.26	0.42
19:S:119:VAL:O	19:S:119:VAL:HG12	2.18	0.42
30:4:73:GLU:HB2	37:4:8529:HOH:O	2.18	0.42
1:A:120:A:H5'	28:2:20:ARG:HH21	1.84	0.42
1:A:259:G:H21	14:N:58:GLN:NE2	2.17	0.42
1:A:553:G:P	26:Z:204:ARG:NH2	2.91	0.42
1:A:707:C:C2	1:A:708:A:C8	3.06	0.42
1:A:795:G:N3	1:A:817:G:C2	2.88	0.42
1:A:876:A:N3	1:A:876:A:H2'	2.35	0.42
1:A:1681:G:H5''	1:A:1682:A:H5'	2.00	0.42
1:A:2088:C:H1'	1:A:2841:A:N1	2.34	0.42
1:A:2241:C:H2'	1:A:2242:U:C6	2.54	0.42
37:A:9535:HOH:O	24:X:119:HIS:HE1	2.02	0.42
2:B:3030:C:OP1	6:F:137:PRO:O	2.37	0.42
6:F:53:LYS:HA	6:F:67:ASP:O	2.20	0.42
10:J:65:ARG:NH2	10:J:66:VAL:HG22	2.35	0.42
17:Q:7:LYS:CD	17:Q:21:VAL:HG21	2.49	0.42
30:4:75:GLY:HA2	37:4:8563:HOH:O	2.19	0.42
1:A:473:A:O2'	1:A:474:C:H5'	2.19	0.42
1:A:1586:G:O2'	1:A:1587:U:H5'	2.19	0.42
1:A:1886:A:H4'	37:1:8405:HOH:O	2.19	0.42
1:A:2270:G:H4'	3:C:223:ARG:NH1	2.34	0.42
1:A:2307:A:C2	1:A:2308:U:N3	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:211:LYS:HB2	37:C:8622:HOH:O	2.18	0.42
5:E:27:ARG:HG2	5:E:30:LEU:HG	2.02	0.42
5:E:78:ARG:NH1	5:E:78:ARG:CG	2.76	0.42
6:F:153:THR:HG22	37:F:5234:HOH:O	2.19	0.42
8:H:49:PHE:O	8:H:95:ALA:HA	2.19	0.42
10:J:58:HIS:CE1	10:J:59:ASN:HD21	2.37	0.42
14:N:71:SER:O	14:N:73:ARG:NH1	2.51	0.42
15:O:184:ILE:HG22	15:O:185:GLU:N	2.33	0.42
18:R:41:LEU:HB3	18:R:52:PHE:CZ	2.55	0.42
26:Z:133:HIS:CD2	37:Z:8583:HOH:O	2.52	0.42
1:A:161:A:OP1	14:N:82:ARG:HG2	2.20	0.42
1:A:269:G:C2	1:A:270:U:O4	2.72	0.42
1:A:657:G:H2'	1:A:658:C:C6	2.55	0.42
1:A:1450:C:O2'	1:A:1493:A:H2'	2.19	0.42
1:A:1616:A:H5''	1:A:1617:C:OP1	2.20	0.42
1:A:1666:C:H2'	1:A:1667:A:H8	1.84	0.42
1:A:1972:U:C2'	1:A:1973:A:H5'	2.48	0.42
1:A:2134:G:C6	1:A:2258:A:C8	3.08	0.42
1:A:2900:G:H2'	1:A:2901:C:O4'	2.20	0.42
1:A:2911:C:H3'	37:A:5528:HOH:O	2.19	0.42
37:B:4707:HOH:O	15:O:147:ILE:HD12	2.20	0.42
5:E:53:GLY:O	5:E:79:ARG:HA	2.19	0.42
8:H:56:PRO:CG	14:N:44:THR:HA	2.49	0.42
9:I:71:LEU:C	9:I:73:ASP:N	2.77	0.42
11:K:54:VAL:HG11	11:K:138:THR:HG21	2.01	0.42
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.34	0.42
16:P:14:LEU:HD23	16:P:102:ILE:HD11	2.01	0.42
19:S:5:SER:OG	19:S:144:GLU:OE1	2.33	0.42
19:S:75:TRP:CG	19:S:76:ASP:H	2.37	0.42
21:U:96:VAL:CG1	21:U:97:ARG:N	2.80	0.42
26:Z:122:ARG:NH2	37:Z:8535:HOH:O	2.52	0.42
28:2:5:THR:HB	28:2:6:PRO:CD	2.50	0.42
1:A:88:G:H2'	1:A:89:G:C8	2.53	0.42
1:A:97:G:C2	21:U:107:LYS:HD2	2.54	0.42
1:A:219:G:O5'	1:A:220:C:H5''	2.20	0.42
1:A:324:G:O2'	1:A:325:U:H5'	2.19	0.42
1:A:1139:U:H2'	1:A:1140:C:C6	2.54	0.42
1:A:1185:U:O4'	37:A:7445:HOH:O	2.22	0.42
1:A:1456:C:H2'	1:A:1457:U:C6	2.55	0.42
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.20	0.42
1:A:2820:A:H2'	1:A:2821:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2836:G:C6	1:A:2838:A:C2	3.07	0.42
3:C:72:GLU:OE1	27:1:72:GLU:HA	2.19	0.42
4:D:312:ARG:HG2	4:D:313:PRO:N	2.33	0.42
12:L:34:VAL:CG2	12:L:47:ALA:HB2	2.48	0.42
15:O:90:LEU:HB2	15:O:186:LEU:HD22	2.00	0.42
15:O:181:ASP:HA	37:O:8572:HOH:O	2.19	0.42
16:P:21:SER:OG	16:P:106:PRO:HB2	2.20	0.42
20:T:10:VAL:CG1	23:W:35:ALA:O	2.68	0.42
24:X:58:SER:O	24:X:59:GLN:C	2.61	0.42
24:X:139:GLY:O	24:X:141:HIS:HD2	2.01	0.42
25:Y:79:GLU:OE2	37:Y:5564:HOH:O	2.21	0.42
30:4:91:GLN:O	30:4:92:GLU:HB2	2.19	0.42
1:A:24:G:N2	1:A:518:G:H1'	2.34	0.42
1:A:87:C:H2'	29:3:28:LYS:O	2.19	0.42
1:A:736:A:H2'	1:A:737:A:O4'	2.19	0.42
1:A:1829:A:N6	27:1:18:TYR:HA	2.34	0.42
3:C:43:VAL:O	3:C:44:ASP:HB2	2.20	0.42
3:C:111:SER:O	3:C:112:PRO:C	2.62	0.42
4:D:71:VAL:HG11	4:D:296:LEU:HB3	2.01	0.42
4:D:87:TYR:O	4:D:138:GLY:N	2.39	0.42
6:F:35:ALA:O	6:F:37:ALA:N	2.53	0.42
14:N:39:ARG:CZ	37:N:8623:HOH:O	2.66	0.42
14:N:87:MET:SD	37:N:8531:HOH:O	2.62	0.42
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.19	0.42
21:U:65:VAL:HG22	21:U:72:ILE:HG22	2.02	0.42
24:X:101:LEU:HD23	24:X:101:LEU:HA	1.89	0.42
25:Y:76:ARG:NH1	25:Y:76:ARG:CG	2.82	0.42
1:A:67:A:H5''	1:A:69:A:C8	2.55	0.42
1:A:86:A:C2	29:3:25:VAL:HG13	2.55	0.42
1:A:391:U:OP2	14:N:84:LYS:NZ	2.48	0.42
1:A:629:A:C2	1:A:2074:A:C2	3.08	0.42
1:A:1089:G:C8	1:A:1290:G:C2	3.07	0.42
1:A:1559:A:C1'	37:A:5836:HOH:O	2.67	0.42
1:A:1890:U:H4'	1:A:2010:A:C6	2.55	0.42
1:A:2785:C:H4'	1:A:2786:G:OP2	2.20	0.42
1:A:2852:A:OP1	4:D:157:LYS:HE2	2.19	0.42
6:F:167:GLU:C	6:F:169:THR:H	2.28	0.42
10:J:46:VAL:C	10:J:146:TRP:CZ3	2.98	0.42
11:K:51:GLU:O	11:K:55:GLU:HG3	2.20	0.42
12:L:118:ALA:C	12:L:120:ARG:N	2.78	0.42
14:N:162:GLY:HA2	37:N:8520:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:176:ARG:O	15:O:180:LEU:HG	2.19	0.42
23:W:27:LEU:O	23:W:30:ALA:N	2.52	0.42
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.20	0.42
24:X:84:VAL:HG12	37:X:6679:HOH:O	2.20	0.42
24:X:90:TYR:N	37:X:6679:HOH:O	2.53	0.42
1:A:10:U:H1'	1:A:532:A:H62	1.85	0.42
1:A:99:A:H3'	1:A:100:C:C6	2.55	0.42
1:A:245:C:C2'	1:A:246:G:H5'	2.50	0.42
1:A:803:C:O2'	1:A:804:C:H5'	2.20	0.42
1:A:870:G:C3'	1:A:871:G:H5''	2.50	0.42
1:A:1051:C:H2'	1:A:1052:G:O4'	2.20	0.42
1:A:1132:A:N6	1:A:1229:C:H2'	2.35	0.42
1:A:1187:U:C3'	37:A:6864:HOH:O	2.67	0.42
1:A:1444:G:O2'	1:A:1445:G:H5'	2.20	0.42
1:A:1705:C:O2	1:A:2735:U:H5''	2.20	0.42
1:A:2453:G:H2'	1:A:2454:C:C6	2.55	0.42
1:A:2529:G:O2'	1:A:2530:C:H5'	2.20	0.42
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.34	0.42
5:E:160:LEU:O	5:E:162:VAL:HG23	2.19	0.42
6:F:41:LEU:O	6:F:44:ILE:HG22	2.20	0.42
6:F:81:GLU:C	6:F:83:PHE:N	2.76	0.42
7:G:84:MET:HB2	7:G:131:LEU:HB2	2.01	0.42
10:J:57:ARG:HG3	10:J:57:ARG:NH1	2.35	0.42
11:K:72:PRO:O	11:K:78:ILE:HD11	2.20	0.42
11:K:79:PHE:O	11:K:83:ILE:HG13	2.19	0.42
12:L:58:THR:HG22	12:L:59:LYS:HG3	2.00	0.42
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.50	0.42
14:N:83:SER:HA	14:N:86:MET:HE3	2.02	0.42
15:O:80:SER:CB	37:O:8537:HOH:O	2.63	0.42
1:A:236:A:O5'	1:A:236:A:C2'	2.68	0.41
1:A:250:C:O2'	1:A:251:C:H5'	2.20	0.41
1:A:259:G:O2'	1:A:260:C:H5'	2.20	0.41
1:A:314:G:N2	1:A:316:A:H3'	2.35	0.41
1:A:940:G:C5	1:A:1027:G:C2	3.07	0.41
1:A:1947:G:N2	1:A:1966:U:O2	2.52	0.41
1:A:2758:G:H2'	1:A:2759:C:C6	2.55	0.41
1:A:2815:G:N7	11:K:80:LYS:NZ	2.66	0.41
37:A:3671:HOH:O	7:G:143:GLN:CG	2.68	0.41
3:C:30:ARG:HE	3:C:30:ARG:HB3	1.65	0.41
3:C:46:GLU:O	3:C:55:VAL:N	2.49	0.41
3:C:192:VAL:HG12	3:C:207:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:THR:HG23	4:D:182:VAL:CG1	2.50	0.41
5:E:178:GLN:C	5:E:180:SER:N	2.75	0.41
6:F:140:ARG:HH11	6:F:140:ARG:HG3	1.85	0.41
14:N:77:PHE:HD2	37:N:8527:HOH:O	2.02	0.41
16:P:32:ARG:HG2	37:P:2336:HOH:O	2.20	0.41
16:P:44:ASN:HA	16:P:65:LEU:O	2.19	0.41
17:Q:131:PHE:CD1	17:Q:137:LEU:HD13	2.55	0.41
22:V:52:THR:HG22	22:V:54:THR:N	2.35	0.41
25:Y:7:GLU:HA	25:Y:74:ALA:O	2.20	0.41
26:Z:154:ARG:HH12	26:Z:155:ARG:HG3	1.84	0.41
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.55	0.41
28:2:21:ARG:HD2	28:2:39:PHE:HB2	2.02	0.41
1:A:951:A:H2'	1:A:952:G:H5'	2.00	0.41
1:A:1921:A:C6	1:A:1922:A:C2	3.07	0.41
1:A:1985:U:C5	1:A:1996:U:C2	3.07	0.41
1:A:2047:C:H5'	37:A:9799:HOH:O	2.19	0.41
1:A:2523:U:O2'	1:A:2524:G:H5'	2.20	0.41
1:A:2549:C:H1'	4:D:248:ARG:NH2	2.34	0.41
1:A:2739:A:N6	1:A:2740:G:C6	2.88	0.41
37:A:4537:HOH:O	5:E:50:GLU:HG2	2.20	0.41
2:B:3057:A:H8	6:F:141:VAL:HG21	1.85	0.41
2:B:3096:C:H2'	2:B:3097:U:C6	2.55	0.41
3:C:36:ASP:CB	3:C:85:ASP:H	2.32	0.41
3:C:100:PRO:HG2	3:C:103:VAL:CG2	2.48	0.41
3:C:101:GLU:HG2	3:C:131:HIS:ND1	2.34	0.41
5:E:3:ALA:HA	37:E:8451:HOH:O	2.20	0.41
6:F:60:GLU:C	6:F:62:ASP:N	2.75	0.41
6:F:101:THR:CG2	37:F:7400:HOH:O	2.65	0.41
8:H:21:GLU:HA	8:H:24:ARG:HE	1.84	0.41
10:J:48:LEU:HD11	10:J:157:ILE:HG21	2.01	0.41
10:J:56:ILE:HG21	10:J:61:LEU:CD1	2.50	0.41
11:K:4:ALA:O	11:K:5:GLU:O	2.38	0.41
11:K:46:ILE:HG12	11:K:53:ILE:HD13	2.02	0.41
14:N:96:ASN:ND2	37:N:8541:HOH:O	2.48	0.41
15:O:127:LEU:HA	15:O:127:LEU:HD12	1.84	0.41
15:O:159:TYR:CE2	15:O:163:PHE:HE2	2.34	0.41
16:P:26:TRP:HB2	37:P:3062:HOH:O	2.21	0.41
22:V:20:MET:CG	22:V:28:THR:HG23	2.50	0.41
22:V:31:PHE:CE2	22:V:37:GLU:HA	2.54	0.41
27:1:42:CYS:SG	27:1:44:PHE:CB	2.94	0.41
1:A:382:U:C5	1:A:406:G:C2	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:U:H2'	1:A:646:G:C8	2.55	0.41
1:A:883:U:O2	1:A:883:U:C2'	2.68	0.41
1:A:1014:A:H5''	2:B:3101:G:O2'	2.20	0.41
1:A:1865:A:H2'	1:A:1866:A:C8	2.55	0.41
1:A:2255:A:C6	1:A:2256:G:C5	3.08	0.41
1:A:2626:C:H2'	1:A:2627:G:C8	2.55	0.41
4:D:132:HIS:CE1	4:D:171:VAL:CG2	3.03	0.41
6:F:35:ALA:C	6:F:37:ALA:H	2.27	0.41
6:F:95:THR:HG21	6:F:174:VAL:HG22	2.02	0.41
10:J:73:GLN:OE1	10:J:73:GLN:CA	2.68	0.41
10:J:112:ARG:C	10:J:114:PRO:HD3	2.45	0.41
10:J:154:THR:HB	10:J:155:PRO:CD	2.50	0.41
15:O:163:PHE:O	15:O:164:ASP:O	2.38	0.41
16:P:25:VAL:HG23	16:P:26:TRP:H	1.85	0.41
28:2:10:LYS:CB	37:2:8432:HOH:O	2.68	0.41
1:A:306:A:H2'	1:A:341:C:O2'	2.20	0.41
1:A:419:A:H1'	1:A:1921:A:C2	2.56	0.41
1:A:764:C:H2'	1:A:765:G:O4'	2.20	0.41
1:A:1265:G:H1'	37:A:4979:HOH:O	2.19	0.41
1:A:1653:A:N7	37:A:6918:HOH:O	2.37	0.41
1:A:1825:U:O2'	1:A:1826:C:H5'	2.21	0.41
3:C:65:ARG:C	3:C:66:ARG:HG3	2.45	0.41
4:D:41:PHE:CD2	4:D:190:MET:HE3	2.55	0.41
4:D:146:THR:C	4:D:148:PRO:HD3	2.45	0.41
5:E:40:ALA:O	5:E:43:LYS:HB2	2.20	0.41
5:E:200:PRO:HB3	5:E:212:VAL:CG2	2.50	0.41
6:F:95:THR:OG1	6:F:174:VAL:HG22	2.20	0.41
6:F:173:GLU:O	6:F:174:VAL:C	2.63	0.41
7:G:49:ILE:HD11	7:G:69:ILE:HD12	2.02	0.41
10:J:136:VAL:HG22	10:J:137:ASN:N	2.36	0.41
12:L:32:ILE:O	12:L:33:SER:OG	2.38	0.41
17:Q:115:SER:HG	17:Q:118:GLN:HG3	1.83	0.41
23:W:11:MET:HB3	23:W:15:GLU:HB2	2.02	0.41
1:A:130:C:H5'	37:A:5192:HOH:O	2.19	0.41
1:A:392:U:O2'	1:A:394:G:N7	2.49	0.41
3:C:36:ASP:HB2	3:C:84:VAL:N	2.36	0.41
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.85	0.41
3:C:232:ARG:NE	37:C:8586:HOH:O	2.54	0.41
4:D:154:VAL:HA	4:D:155:PRO:HD3	1.89	0.41
5:E:93:LYS:O	5:E:98:ARG:NH2	2.53	0.41
8:H:53:ASP:CG	8:H:80:GLN:HB2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:34:LEU:HD22	15:O:129:ILE:CD1	2.51	0.41
17:Q:13:VAL:HG11	17:Q:40:VAL:HG12	2.02	0.41
24:X:122:ARG:NH2	37:X:4276:HOH:O	2.53	0.41
24:X:122:ARG:NH1	24:X:152:ALA:O	2.53	0.41
25:Y:25:ARG:NE	37:Y:3861:HOH:O	2.52	0.41
26:Z:205:ILE:O	26:Z:206:ALA:C	2.64	0.41
1:A:40:C:H6	1:A:40:C:O5'	2.04	0.41
1:A:155:C:H4'	1:A:188:C:H4'	2.03	0.41
1:A:492:C:O2'	1:A:493:U:H5'	2.21	0.41
1:A:659:A:O2'	1:A:661:G:O2'	2.37	0.41
1:A:661:G:C4	1:A:686:A:C2	3.09	0.41
1:A:849:C:C2'	1:A:850:U:H5'	2.51	0.41
1:A:1025:C:H5'	24:X:23:MET:O	2.20	0.41
1:A:1278:A:H4'	1:A:1279:U:C4	2.56	0.41
1:A:1462:C:H2'	1:A:1463:A:C8	2.56	0.41
1:A:1751:G:C3'	1:A:1752:G:H5''	2.50	0.41
1:A:2079:G:H2'	1:A:2080:G:O4'	2.20	0.41
1:A:2505:G:H8	37:A:5611:HOH:O	2.04	0.41
1:A:2607:U:O5'	1:A:2609:G:H4'	2.20	0.41
1:A:2739:A:C6	1:A:2740:G:C5	3.08	0.41
3:C:29:HIS:HB2	3:C:153:ARG:HH12	1.86	0.41
4:D:5:ARG:HA	4:D:6:PRO:HD3	1.94	0.41
6:F:17:ARG:NH2	37:F:3723:HOH:O	2.43	0.41
6:F:170:TYR:N	6:F:170:TYR:CD1	2.88	0.41
8:H:16:ALA:HA	8:H:111:ILE:HD13	2.01	0.41
10:J:26:LYS:HD2	10:J:28:ILE:HB	2.02	0.41
14:N:94:LYS:CE	37:N:8646:HOH:O	2.69	0.41
15:O:108:SER:HA	15:O:109:PRO:HD3	1.79	0.41
22:V:38:ASN:O	22:V:42:LEU:HG	2.21	0.41
22:V:44:ARG:CB	37:V:3805:HOH:O	2.67	0.41
24:X:21:LEU:HB3	24:X:26:ILE:HG12	2.02	0.41
26:Z:189:ASN:ND2	26:Z:192:ASP:N	2.65	0.41
1:A:209:G:C6	1:A:210:U:N3	2.89	0.41
1:A:304:G:H1'	1:A:347:A:N6	2.35	0.41
1:A:329:A:OP2	5:E:206:ASN:HB2	2.20	0.41
1:A:398:U:H2'	1:A:399:C:C6	2.56	0.41
1:A:542:A:H1'	37:A:4648:HOH:O	2.21	0.41
1:A:812:A:H2'	1:A:813:C:C6	2.55	0.41
1:A:1116:U:H3	1:A:1246:A:N6	2.09	0.41
1:A:1167:G:O2'	1:A:1168:C:H5'	2.21	0.41
1:A:1377:C:H6	1:A:1377:C:C5'	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:A:H2'	1:A:1516:C:C6	2.56	0.41
1:A:1888:C:N4	1:A:1889:C:C4	2.89	0.41
1:A:1912:A:O5'	1:A:1912:A:H8	2.03	0.41
1:A:2327:A:C2	1:A:2374:A:C2	3.08	0.41
37:A:4513:HOH:O	10:J:151:MET:HE2	2.20	0.41
4:D:268:ARG:NE	37:D:8608:HOH:O	2.53	0.41
4:D:280:VAL:CG1	4:D:281:ASP:N	2.83	0.41
6:F:57:THR:HA	6:F:63:ILE:HA	2.01	0.41
8:H:26:THR:HB	8:H:102:GLY:HA3	2.03	0.41
9:I:12:ILE:HB	37:I:4714:HOH:O	2.19	0.41
10:J:113:ALA:N	10:J:114:PRO:HD3	2.36	0.41
13:M:17:SER:C	13:M:19:LYS:H	2.29	0.41
14:N:63:VAL:O	14:N:130:GLU:HA	2.21	0.41
15:O:37:ARG:HD3	15:O:37:ARG:HA	1.84	0.41
15:O:37:ARG:CZ	37:O:8534:HOH:O	2.69	0.41
15:O:149:GLU:O	15:O:152:GLU:HB2	2.20	0.41
16:P:47:ARG:NH1	37:P:4564:HOH:O	2.53	0.41
19:S:132:ARG:NH1	37:S:8558:HOH:O	2.53	0.41
21:U:27:LEU:HD21	21:U:40:VAL:CG1	2.51	0.41
21:U:80:GLU:OE2	21:U:84:GLY:HA2	2.20	0.41
25:Y:12:ILE:HD12	25:Y:36:HIS:ND1	2.36	0.41
1:A:171:C:OP2	14:N:84:LYS:HG3	2.20	0.41
1:A:183:A:O2'	1:A:184:G:H5'	2.21	0.41
1:A:542:A:C8	1:A:542:A:C5'	2.99	0.41
1:A:955:A:C2	1:A:1013:A:C4	3.08	0.41
1:A:1471:A:H2'	1:A:1472:C:C6	2.56	0.41
1:A:1490:G:H4'	1:A:1533:A:OP1	2.20	0.41
1:A:1666:C:O2'	1:A:1667:A:C5'	2.65	0.41
1:A:1871:U:O4'	1:A:1873:G:C8	2.74	0.41
1:A:2118:A:H2'	1:A:2119:C:H6	1.85	0.41
1:A:2123:A:P	14:N:89:ASN:HD22	2.44	0.41
1:A:2456:A:H2'	1:A:2457:U:H6	1.86	0.41
1:A:2481:G:H3'	1:A:2482:G:H5''	2.02	0.41
2:B:3107:C:H2'	2:B:3108:C:C6	2.55	0.41
4:D:168:GLY:H	4:D:174:ARG:HD3	1.84	0.41
4:D:236:ILE:HG21	4:D:236:ILE:HD13	1.80	0.41
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.84	0.41
5:E:14:GLY:N	37:E:8440:HOH:O	2.54	0.41
7:G:34:TRP:HA	37:G:4572:HOH:O	2.20	0.41
10:J:47:GLU:HG2	10:J:133:ILE:HD12	2.02	0.41
10:J:57:ARG:O	10:J:61:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:68:GLU:O	13:M:69:ILE:C	2.64	0.41
17:Q:37:ARG:O	17:Q:41:ARG:HG3	2.20	0.41
1:A:64:G:H2'	1:A:65:C:O4'	2.21	0.41
1:A:834:G:H4'	1:A:835:U:OP2	2.20	0.41
1:A:853:C:H2'	1:A:854:G:O4'	2.20	0.41
1:A:858:U:H2'	1:A:859:C:H6	1.85	0.41
1:A:903:U:OP2	13:M:11:ARG:NH1	2.50	0.41
1:A:1021:G:O2'	1:A:1022:A:H5'	2.20	0.41
1:A:1589:G:H4'	37:A:6824:HOH:O	2.21	0.41
1:A:1744:G:N7	1:A:1745:G:C5	2.89	0.41
1:A:2111:G:H1'	37:A:9042:HOH:O	2.20	0.41
1:A:2122:C:H3'	37:A:5266:HOH:O	2.20	0.41
1:A:2246:U:C2	1:A:2256:G:N2	2.89	0.41
1:A:2263:G:C6	1:A:2264:A:C5	3.09	0.41
1:A:2473:U:O3'	1:A:2474:A:H3'	2.20	0.41
1:A:2825:C:H4'	1:A:2826:G:O5'	2.21	0.41
37:A:7107:HOH:O	5:E:107:ARG:NE	2.46	0.41
2:B:3011:A:O2'	2:B:3012:C:H3'	2.21	0.41
2:B:3042:C:N4	2:B:3044:A:N1	2.68	0.41
3:C:170:VAL:HG13	27:1:22:ILE:HG21	2.02	0.41
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.51	0.41
3:C:194:MET:HE1	37:C:8517:HOH:O	2.21	0.41
4:D:102:THR:HG23	4:D:182:VAL:HG12	2.03	0.41
4:D:240:GLY:HA3	37:D:8657:HOH:O	2.21	0.41
7:G:116:THR:HG22	7:G:151:LEU:HD22	2.03	0.41
7:G:172:PRO:HB3	37:G:6931:HOH:O	2.20	0.41
8:H:6:PHE:CD1	8:H:6:PHE:O	2.74	0.41
8:H:59:ILE:O	8:H:59:ILE:HG22	2.20	0.41
8:H:104:ALA:C	8:H:106:THR:N	2.78	0.41
10:J:65:ARG:HB3	37:J:8374:HOH:O	2.21	0.41
10:J:114:PRO:O	10:J:115:PHE:C	2.64	0.41
11:K:6:PHE:HB3	11:K:109:TYR:OH	2.21	0.41
13:M:64:ILE:O	13:M:64:ILE:HG23	2.20	0.41
13:M:98:GLU:O	13:M:99:GLU:HB2	2.21	0.41
14:N:69:LYS:HD3	14:N:125:ARG:HA	2.02	0.41
15:O:19:ASP:OD1	15:O:19:ASP:C	2.63	0.41
15:O:72:GLU:H	15:O:171:HIS:CE1	2.38	0.41
15:O:93:GLN:HG2	37:O:8557:HOH:O	2.21	0.41
16:P:35:LYS:HD3	37:P:3360:HOH:O	2.20	0.41
19:S:104:PHE:CB	19:S:109:MET:HE2	2.50	0.41
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:26:ALA:HB1	25:Y:59:TRP:CE2	2.56	0.41
25:Y:85:VAL:HG12	25:Y:86:GLU:N	2.36	0.41
26:Z:136:LYS:HG3	26:Z:138:ARG:HG2	2.02	0.41
26:Z:234:VAL:HG12	26:Z:235:GLU:N	2.36	0.41
27:1:13:ARG:NH1	37:1:8422:HOH:O	2.54	0.41
29:3:11:LEU:HD23	29:3:11:LEU:HA	1.78	0.41
30:4:35:TRP:HA	30:4:38:ARG:NH1	2.36	0.41
1:A:431:G:OP1	14:N:48:ARG:NH1	2.53	0.41
1:A:902:G:N7	13:M:18:HIS:CD2	2.87	0.41
1:A:1241:G:N3	11:K:86:MET:HE2	2.37	0.41
1:A:1299:G:N7	13:M:6:ARG:NH1	2.68	0.41
1:A:1421:C:O2'	1:A:1422:U:H5'	2.20	0.41
1:A:1440:U:P	37:A:4435:HOH:O	2.79	0.41
1:A:1679:C:O2'	1:A:1685:A:N1	2.44	0.41
1:A:1896:G:C6	1:A:1897:U:C4	3.08	0.41
1:A:1942:A:H3'	37:A:7324:HOH:O	2.21	0.41
1:A:1969:A:O2'	1:A:1970:G:H5'	2.21	0.41
1:A:2113:G:C6	1:A:2114:C:C4	3.09	0.41
1:A:2289:G:H21	1:A:2291:A:H2	1.65	0.41
1:A:2428:G:C4	1:A:2461:U:C5	3.09	0.41
1:A:2781:U:H2'	1:A:2782:G:C5'	2.51	0.41
1:A:2826:G:C6	1:A:2913:A:N6	2.89	0.41
1:A:2831:C:H2'	1:A:2832:C:H5'	2.03	0.41
3:C:190:ARG:NH2	37:C:8598:HOH:O	2.53	0.41
4:D:215:VAL:HA	4:D:220:VAL:HG22	2.02	0.41
7:G:137:ASP:O	7:G:141:VAL:HG23	2.21	0.41
8:H:21:GLU:O	8:H:24:ARG:CG	2.68	0.41
8:H:108:LEU:O	8:H:109:GLU:C	2.63	0.41
9:I:66:LEU:O	9:I:69:ARG:HB3	2.21	0.41
10:J:45:GLN:NE2	10:J:135:TRP:HE1	2.19	0.41
10:J:137:ASN:O	10:J:138:PRO:C	2.62	0.41
12:L:6:ALA:HB3	12:L:116:GLU:HG2	2.02	0.41
12:L:76:GLN:HB2	37:L:1433:HOH:O	2.21	0.41
14:N:108:LYS:N	14:N:108:LYS:HD3	2.36	0.41
15:O:139:TRP:HA	15:O:139:TRP:HE3	1.86	0.41
15:O:143:ARG:NH1	15:O:173:ASP:CG	2.79	0.41
16:P:45:LEU:HD12	16:P:88:LYS:HD2	2.02	0.41
19:S:104:PHE:HB2	19:S:109:MET:CE	2.51	0.41
19:S:119:VAL:CG2	19:S:142:ASP:HB2	2.51	0.41
24:X:41:TYR:O	24:X:45:VAL:HG13	2.21	0.41
25:Y:78:GLU:CG	25:Y:79:GLU:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:22:VAL:HG11	30:4:67:LEU:HD13	2.02	0.41
1:A:27:U:H2'	1:A:28:G:O4'	2.20	0.40
1:A:78:G:C6	1:A:79:G:C6	3.10	0.40
1:A:218:C:C5	1:A:220:C:C4	3.09	0.40
1:A:240:C:C5'	14:N:146:GLN:NE2	2.84	0.40
1:A:941:G:C2'	1:A:942:U:H5'	2.51	0.40
1:A:1044:C:H3'	1:A:1045:G:H5''	2.03	0.40
1:A:1132:A:N3	1:A:2521:A:O2'	2.51	0.40
1:A:1161:A:O5'	1:A:1161:A:C8	2.74	0.40
1:A:1790:C:H2'	1:A:1791:U:C6	2.55	0.40
1:A:1804:A:H2'	1:A:1805:G:H8	1.86	0.40
1:A:1827:G:C2	1:A:2023:G:C6	3.09	0.40
1:A:1992:U:C2	1:A:1994:A:OP2	2.75	0.40
1:A:2116:U:C4	1:A:2271:G:C6	3.09	0.40
1:A:2356:A:H2'	1:A:2357:G:O4'	2.20	0.40
1:A:2780:C:C4	1:A:2781:U:C4	3.10	0.40
1:A:2869:G:H2'	1:A:2870:C:C6	2.56	0.40
3:C:114:ASP:HB2	3:C:117:LYS:HE2	2.02	0.40
4:D:145:HIS:CD2	4:D:145:HIS:C	2.99	0.40
5:E:76:ARG:HD3	37:E:8365:HOH:O	2.21	0.40
7:G:118:ILE:HG23	7:G:144:THR:HG21	2.03	0.40
8:H:62:HIS:O	8:H:63:ILE:C	2.63	0.40
10:J:150:LYS:CG	37:J:8372:HOH:O	2.69	0.40
12:L:6:ALA:CB	12:L:116:GLU:HG2	2.51	0.40
14:N:12:TRP:CZ2	14:N:20:ILE:HD11	2.56	0.40
14:N:14:ARG:HB3	14:N:17:GLU:HG3	2.02	0.40
15:O:48:VAL:HG12	37:O:8555:HOH:O	2.21	0.40
15:O:141:ARG:CB	37:O:8571:HOH:O	2.66	0.40
15:O:175:LEU:HD12	15:O:175:LEU:HA	1.91	0.40
16:P:26:TRP:HA	16:P:26:TRP:CE3	2.55	0.40
22:V:9:CYS:O	22:V:52:THR:HG23	2.20	0.40
23:W:38:GLY:C	23:W:40:PRO:HD2	2.46	0.40
24:X:3:ALA:O	24:X:54:PHE:HA	2.22	0.40
1:A:380:A:OP2	14:N:9:ARG:HD2	2.22	0.40
1:A:2106:C:H2'	1:A:2107:U:C6	2.57	0.40
1:A:2407:G:O2'	1:A:2408:A:H5'	2.21	0.40
1:A:2415:A:H2'	1:A:2416:G:H5'	2.02	0.40
1:A:2690:U:H4'	7:G:111:LYS:CE	2.51	0.40
1:A:2750:G:H8	1:A:2750:G:O5'	2.05	0.40
2:B:3117:G:C2'	37:B:2118:HOH:O	2.69	0.40
3:C:36:ASP:HB2	3:C:83:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:159:PRO:O	6:F:163:VAL:HG23	2.20	0.40
7:G:24:GLY:HA3	7:G:76:VAL:HB	2.03	0.40
15:O:43:VAL:CG1	15:O:118:ILE:HD11	2.50	0.40
15:O:50:LEU:HD12	15:O:50:LEU:HA	1.87	0.40
23:W:4:HIS:O	23:W:8:ILE:HG13	2.21	0.40
23:W:42:ASN:N	23:W:43:PRO:HD3	2.36	0.40
24:X:13:MET:O	24:X:14:HIS:C	2.62	0.40
1:A:128:A:O2'	1:A:129:A:H5'	2.21	0.40
1:A:189:A:OP1	14:N:171:ARG:NH2	2.55	0.40
1:A:397:A:P	37:A:4317:HOH:O	2.79	0.40
1:A:1206:U:H2'	1:A:1207:A:O4'	2.22	0.40
1:A:1213:C:C2'	1:A:1214:G:H5'	2.51	0.40
1:A:2115:U:H2'	1:A:2116:U:C6	2.57	0.40
1:A:2123:A:P	14:N:89:ASN:ND2	2.94	0.40
1:A:2838:A:H2'	1:A:2839:C:O4'	2.21	0.40
1:A:2892:G:C6	1:A:2893:C:N3	2.90	0.40
2:B:3008:G:P	37:B:5071:HOH:O	2.79	0.40
3:C:173:GLY:O	3:C:176:HIS:HB3	2.20	0.40
3:C:215:ILE:HG13	3:C:216:SER:N	2.37	0.40
4:D:41:PHE:HB3	4:D:190:MET:CE	2.46	0.40
7:G:84:MET:HE1	7:G:148:ILE:HD13	2.02	0.40
8:H:22:VAL:HG21	8:H:104:ALA:HB2	2.02	0.40
9:I:20:VAL:O	9:I:24:VAL:HG23	2.21	0.40
11:K:79:PHE:HB3	11:K:103:VAL:HG11	2.02	0.40
13:M:61:ALA:HA	37:M:8564:HOH:O	2.21	0.40
22:V:9:CYS:HG	22:V:11:THR:HG23	1.85	0.40
23:W:8:ILE:HG21	23:W:59:ILE:HG13	2.03	0.40
26:Z:131:GLN:O	26:Z:132:ASP:HB2	2.21	0.40
30:4:65:THR:O	30:4:82:GLY:HA3	2.22	0.40
1:A:611:U:H2'	1:A:612:U:C6	2.57	0.40
1:A:1164:U:O5'	1:A:1164:U:H6	2.05	0.40
1:A:1494:A:C4	1:A:1495:C:C5	3.10	0.40
1:A:1562:C:O2	1:A:1562:C:C2'	2.69	0.40
1:A:1592:G:C5	1:A:1593:C:C4	3.09	0.40
1:A:2034:U:H2'	1:A:2035:C:H6	1.87	0.40
1:A:2038:A:O2'	1:A:2039:A:H5'	2.21	0.40
1:A:2502:C:H2'	1:A:2503:A:C5'	2.50	0.40
31:A:9001:SPR:O2A	31:A:9001:SPR:C8A	2.70	0.40
31:A:9001:SPR:H6	31:A:9001:SPR:H3	1.84	0.40
2:B:3004:G:O2'	15:O:44:ARG:NH2	2.55	0.40
3:C:36:ASP:HB2	3:C:85:ASP:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:36:ASN:C	37:F:7500:HOH:O	2.64	0.40
6:F:91:ALA:HB2	6:F:106:PHE:CD2	2.56	0.40
6:F:95:THR:CG2	6:F:174:VAL:HG22	2.51	0.40
7:G:11:VAL:HG11	7:G:22:VAL:HG13	2.04	0.40
7:G:91:PHE:HA	7:G:92:PRO:HD3	1.91	0.40
9:I:12:ILE:HG13	37:I:6833:HOH:O	2.21	0.40
10:J:26:LYS:CG	10:J:28:ILE:H	2.25	0.40
10:J:82:LYS:NZ	10:J:82:LYS:CB	2.84	0.40
10:J:167:ALA:HA	37:J:8362:HOH:O	2.20	0.40
15:O:38:LYS:HE2	15:O:107:ASN:ND2	2.36	0.40
15:O:42:HIS:CG	15:O:62:HIS:HE1	2.40	0.40
15:O:163:PHE:CZ	15:O:164:ASP:OD2	2.73	0.40
22:V:14:GLU:HA	22:V:15:PRO:HD2	1.93	0.40
29:3:18:ASN:HD22	29:3:18:ASN:HA	1.64	0.40
1:A:255:A:C5	1:A:256:C:C4	3.10	0.40
1:A:263:U:C2	8:H:59:ILE:HD12	2.57	0.40
1:A:840:U:H2'	19:S:128:ARG:NH1	2.37	0.40
1:A:2397:G:C5	1:A:2465:A:C6	3.10	0.40
1:A:2462:G:O6	30:4:61:PRO:HG3	2.21	0.40
1:A:2612:A:H2'	1:A:2649:A:N6	2.37	0.40
2:B:3065:A:C2'	2:B:3066:G:OP2	2.69	0.40
3:C:51:ARG:NH1	3:C:51:ARG:HB3	2.36	0.40
3:C:102:GLY:C	3:C:127:GLN:HE22	2.29	0.40
3:C:149:ASP:OD1	3:C:151:GLN:CB	2.69	0.40
4:D:156:LYS:HE3	37:D:8633:HOH:O	2.21	0.40
5:E:37:ALA:O	5:E:41:ASN:ND2	2.54	0.40
6:F:103:ASN:ND2	6:F:134:LEU:H	2.19	0.40
11:K:39:VAL:HG11	11:K:107:ASN:HB2	2.04	0.40
14:N:69:LYS:O	14:N:73:ARG:NH1	2.55	0.40
18:R:53:HIS:O	18:R:55:ARG:N	2.55	0.40
27:1:30:GLU:O	27:1:33:HIS:HB3	2.21	0.40
28:2:28:HIS:O	28:2:32:LYS:N	2.48	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	C	235/239 (98%)	205 (87%)	26 (11%)	4 (2%)	7	32
4	D	335/337 (99%)	307 (92%)	21 (6%)	7 (2%)	5	27
5	E	244/246 (99%)	225 (92%)	18 (7%)	1 (0%)	30	65
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	0	3
7	G	170/177 (96%)	158 (93%)	12 (7%)	0	100	100
8	H	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	7	32
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	129 (85%)	17 (11%)	6 (4%)	2	14
11	K	140/145 (97%)	131 (94%)	5 (4%)	4 (3%)	3	20
12	L	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	8	35
13	M	141/164 (86%)	118 (84%)	20 (14%)	3 (2%)	5	27
14	N	192/194 (99%)	172 (90%)	18 (9%)	2 (1%)	12	45
15	O	184/186 (99%)	165 (90%)	13 (7%)	6 (3%)	3	17
16	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
17	Q	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	18	53
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	43
19	S	148/154 (96%)	138 (93%)	10 (7%)	0	100	100
20	T	79/84 (94%)	72 (91%)	7 (9%)	0	100	100
21	U	117/119 (98%)	108 (92%)	9 (8%)	0	100	100
22	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	3	18
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	18	53
25	Y	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	4	23
26	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	9	36
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
29	3	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
30	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	5	26
All	All	3633/4235 (86%)	3299 (91%)	275 (8%)	59 (2%)	7	34

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU
8	H	101	ALA
10	J	162	SER
10	J	164	ALA
13	M	80	ASP
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
3	C	34	ASP
3	C	37	VAL
4	D	34	GLY
4	D	169	GLY
6	F	11	HIS
6	F	16	PRO
10	J	138	PRO
11	K	5	GLU
11	K	7	ASP
11	K	143	LYS
12	L	119	GLN
17	Q	116	SER
23	W	43	PRO
30	4	57	GLY
3	C	132	ASP
4	D	184	ASP
6	F	20	LYS
6	F	171	ASP
8	H	64	PRO
10	J	40	PRO
10	J	72	VAL
14	N	140	ALA
15	O	162	ASP
15	O	181	ASP
24	X	77	ALA
25	Y	77	PHE
30	4	56	PRO
6	F	36	ASN
6	F	147	ALA
12	L	126	SER

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Mol	Chain	Res	Type
13	M	21	ARG
15	O	167	ASP
27	1	81	LYS
4	D	2	GLN
4	D	185	GLY
5	E	232	LEU
6	F	61	PHE
14	N	18	GLY
18	R	54	PRO
6	F	82	GLU
10	J	140	PRO
13	M	147	GLU
23	W	40	PRO
4	D	5	ARG
11	K	78	ILE
25	Y	70	ILE
3	C	112	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	C	179/181 (99%)	167 (93%)	12 (7%)	15	46
4	D	282/282 (100%)	262 (93%)	20 (7%)	13	43
5	E	193/193 (100%)	178 (92%)	15 (8%)	11	39
6	F	117/147 (80%)	108 (92%)	9 (8%)	12	40
7	G	152/155 (98%)	148 (97%)	4 (3%)	40	72
8	H	92/92 (100%)	91 (99%)	1 (1%)	65	83
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	106 (87%)	16 (13%)	4	19
11	K	118/121 (98%)	109 (92%)	9 (8%)	12	41
12	L	106/106 (100%)	103 (97%)	3 (3%)	38	70
13	M	112/126 (89%)	109 (97%)	3 (3%)	39	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	166/166 (100%)	157 (95%)	9 (5%)	20	53
15	O	149/149 (100%)	142 (95%)	7 (5%)	23	58
16	P	93/93 (100%)	90 (97%)	3 (3%)	34	67
17	Q	113/116 (97%)	110 (97%)	3 (3%)	39	71
18	R	79/79 (100%)	75 (95%)	4 (5%)	21	55
19	S	117/121 (97%)	111 (95%)	6 (5%)	21	55
20	T	71/73 (97%)	70 (99%)	1 (1%)	59	80
21	U	105/105 (100%)	100 (95%)	5 (5%)	23	57
22	V	44/52 (85%)	42 (96%)	2 (4%)	24	59
23	W	51/56 (91%)	50 (98%)	1 (2%)	48	76
24	X	130/130 (100%)	122 (94%)	8 (6%)	16	49
25	Y	66/73 (90%)	62 (94%)	4 (6%)	17	49
26	Z	120/195 (62%)	112 (93%)	8 (7%)	15	46
27	1	56/56 (100%)	50 (89%)	6 (11%)	6	26
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	43	73
30	4	79/79 (100%)	73 (92%)	6 (8%)	12	41
All	All	3027/3441 (88%)	2861 (94%)	166 (6%)	19	53

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	C	36	ASP
3	C	55	VAL
3	C	68	ILE
3	C	69	LEU
3	C	94	LEU
3	C	131	HIS
3	C	153	ARG
3	C	175	LYS
3	C	179	MET
3	C	187	PRO
3	C	217	ARG
4	D	7	ARG
4	D	11	LEU

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Mol	Chain	Res	Type
4	D	27	ASN
4	D	33	ASP
4	D	63	GLU
4	D	84	LEU
4	D	97	LEU
4	D	98	THR
4	D	103	ASP
4	D	162	MET
4	D	190	MET
4	D	195	ARG
4	D	245	SER
4	D	251	VAL
4	D	254	GLN
4	D	256	GLN
4	D	264	GLU
4	D	304	PRO
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	67	GLN
5	E	78	ARG
5	E	81	PRO
5	E	94	THR
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
5	E	243	VAL
6	F	24	HIS
6	F	50	VAL
6	F	92	GLU
6	F	95	THR
6	F	99	ASP
6	F	131	THR
6	F	136	ARG
6	F	137	PRO
6	F	149	ARG

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Mol	Chain	Res	Type
7	G	7	ILE
7	G	36	PRO
7	G	86	VAL
7	G	102	VAL
8	H	12	LEU
10	J	1	LYS
10	J	18	GLU
10	J	30	GLN
10	J	59	ASN
10	J	61	LEU
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	85	ILE
10	J	86	ARG
10	J	93	ILE
10	J	94	ARG
10	J	142	VAL
10	J	150	LYS
10	J	155	PRO
10	J	166	ASN
11	K	46	ILE
11	K	52	GLN
11	K	74	ARG
11	K	76	ASP
11	K	93	ARG
11	K	120	SER
11	K	125	SER
11	K	127	ILE
11	K	131	THR
12	L	7	ASP
12	L	10	GLN
12	L	98	VAL
13	M	35	ARG
13	M	117	GLU
13	M	140	VAL
14	N	38	VAL
14	N	46	LEU
14	N	81	ARG
14	N	87	MET
14	N	93	ARG
14	N	99	ARG

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Mol	Chain	Res	Type
14	N	120	VAL
14	N	159	THR
14	N	164	THR
15	O	26	LEU
15	O	43	VAL
15	O	47	LEU
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU
15	O	163	PHE
16	P	3	THR
16	P	98	LEU
16	P	111	VAL
17	Q	52	LYS
17	Q	91	LYS
17	Q	98	ILE
18	R	11	ARG
18	R	16	ASN
18	R	57	ASP
18	R	95	GLU
19	S	13	THR
19	S	39	THR
19	S	64	SER
19	S	82	GLU
19	S	130	MET
19	S	132	ARG
20	T	10	VAL
21	U	26	THR
21	U	39	ASN
21	U	47	THR
21	U	48	VAL
21	U	96	VAL
22	V	9	CYS
22	V	28	THR
23	W	43	PRO
24	X	4	LEU
24	X	35	VAL
24	X	52	VAL
24	X	73	LEU
24	X	122	ARG
24	X	142	ASP
24	X	146	ILE

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Mol	Chain	Res	Type
24	X	154	ARG
25	Y	15	ARG
25	Y	27	ASP
25	Y	66	THR
25	Y	72	VAL
26	Z	103	THR
26	Z	154	ARG
26	Z	163	THR
26	Z	172	THR
26	Z	189	ASN
26	Z	200	THR
26	Z	203	VAL
26	Z	235	GLU
27	1	11	THR
27	1	22	ILE
27	1	32	LYS
27	1	42	CYS
27	1	60	CYS
27	1	64	ILE
29	3	18	ASN
30	4	14	CYS
30	4	38	ARG
30	4	42	ARG
30	4	56	PRO
30	4	65	THR
30	4	74	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	29	HIS
3	C	47	HIS
3	C	92	ASN
3	C	127	GLN
3	C	177	HIS
3	C	199	HIS
3	C	218	ASN
4	D	27	ASN
4	D	55	ASN
4	D	145	HIS
4	D	221	GLN
4	D	238	ASN

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Mol	Chain	Res	Type
4	D	260	HIS
4	D	318	ASN
5	E	2	GLN
5	E	39	GLN
5	E	67	GLN
5	E	129	HIS
5	E	163	HIS
6	F	103	ASN
6	F	133	ASN
7	G	106	ASN
7	G	143	GLN
9	I	17	GLN
9	I	64	ASN
10	J	8	ASN
10	J	45	GLN
10	J	55	GLN
10	J	58	HIS
10	J	59	ASN
10	J	69	ASN
10	J	74	ASN
10	J	80	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	137	ASN
10	J	166	ASN
11	K	29	GLN
11	K	52	GLN
11	K	89	HIS
11	K	107	ASN
12	L	10	GLN
12	L	42	ASN
13	M	18	HIS
13	M	41	HIS
13	M	42	ASN
13	M	43	HIS
13	M	58	GLN
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	106	ASN

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Mol	Chain	Res	Type
14	N	176	GLN
15	O	22	GLN
15	O	107	ASN
15	O	140	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN
18	R	16	ASN
18	R	40	HIS
18	R	67	GLN
19	S	22	GLN
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN
19	S	117	HIS
19	S	122	GLN
19	S	140	GLN
20	T	9	HIS
20	T	51	GLN
20	T	53	ASN
20	T	55	GLN
21	U	39	ASN
21	U	73	HIS
22	V	30	HIS
22	V	39	ASN
23	W	60	GLN
24	X	28	HIS
24	X	31	HIS
24	X	87	HIS
24	X	110	GLN
24	X	119	HIS
24	X	125	HIS
24	X	141	HIS
26	Z	133	HIS
26	Z	134	HIS
26	Z	149	GLN
26	Z	153	GLN
26	Z	189	ASN
27	1	33	HIS
27	1	70	GLN
28	2	8	GLN

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Mol	Chain	Res	Type
28	2	16	HIS
28	2	28	HIS
29	3	16	ASN
29	3	18	ASN
29	3	37	HIS
29	3	41	HIS
29	3	45	ASN
30	4	30	GLN
30	4	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	258 (9%)	40 (1%)
2	B	121/122 (99%)	15 (12%)	5 (4%)
All	All	2868/3044 (94%)	273 (9%)	45 (1%)

All (273) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A

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Mol	Chain	Res	Type
1	A	200	U
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	457	U
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	645	U
1	A	660	A
1	A	688	A
1	A	701	U
1	A	717	C

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Mol	Chain	Res	Type
1	A	759	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1083	C
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1127	C
1	A	1130	U
1	A	1137	G
1	A	1151	G
1	A	1162	G

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Mol	Chain	Res	Type
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1208	C
1	A	1216	G
1	A	1234	U
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1331	A
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1407	A
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1507	C
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1562	C
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C

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Mol	Chain	Res	Type
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1857	A
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1943	C
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1979	G
1	A	1980	U
1	A	1996	U
1	A	2004	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G

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Mol	Chain	Res	Type
1	A	2074	A
1	A	2096	A
1	A	2097	G
1	A	2101	A
1	A	2102	G
1	A	2103	A
1	A	2104	C
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2379	G
1	A	2422	U
1	A	2462	G
1	A	2465	A
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2510	C
1	A	2511	A
1	A	2526	C
1	A	2527	U
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G

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Mol	Chain	Res	Type
1	A	2649	A
1	A	2650	U
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2718	C
1	A	2719	A
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2812	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3007	G
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	407	A
1	A	603	A
1	A	644	G
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	898	G
1	A	1080	C
1	A	1164	U
1	A	1232	A
1	A	1237	U
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1506	U
1	A	1563	G
1	A	1667	A
1	A	1692	C
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2103	A
1	A	2313	C
1	A	2379	G
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2761	A
1	A	2791	U
2	B	3002	U
2	B	3023	U

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Mol	Chain	Res	Type
2	B	3025	G
2	B	3065	A
2	B	3103	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 235 ligands modelled in this entry, 234 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	SPR	A	9001	1	62,62,62	2.86	29 (46%)	78,89,89	2.96	32 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SPR	A	9001	1	-	12/61/113/113	0/3/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9001	SPR	C3C-C4C	7.13	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9001	SPR	C4C-N4C	6.68	1.63	1.47
31	A	9001	SPR	C4A-C5A	6.45	1.64	1.52
31	A	9001	SPR	C7-C6	5.72	1.65	1.53
31	A	9001	SPR	O1A-C5	5.59	1.58	1.43
31	A	9001	SPR	C6-C5	-5.50	1.42	1.52
31	A	9001	SPR	O5A-C5A	-4.90	1.33	1.44
31	A	9001	SPR	C2A-C3A	4.80	1.61	1.53
31	A	9001	SPR	O15-C1	-4.59	1.21	1.34
31	A	9001	SPR	O1C-C9	4.20	1.52	1.44
31	A	9001	SPR	C2C-C1C	4.05	1.63	1.50
31	A	9001	SPR	O4A-C1B	-3.89	1.31	1.41
31	A	9001	SPR	O1C-C1C	-3.69	1.31	1.41
31	A	9001	SPR	C14-C15	3.69	1.60	1.52
31	A	9001	SPR	C6B-C5B	3.38	1.59	1.51
31	A	9001	SPR	C5C-C4C	3.17	1.64	1.52
31	A	9001	SPR	C12-C13	2.94	1.43	1.33
31	A	9001	SPR	O19-C19	2.83	1.36	1.20
31	A	9001	SPR	C14-C13	2.64	1.57	1.50
31	A	9001	SPR	O3B-C3B	-2.53	1.40	1.44
31	A	9001	SPR	C2B-C3B	2.51	1.58	1.53
31	A	9001	SPR	C3-C4	2.42	1.57	1.52
31	A	9001	SPR	O5B-C5B	2.34	1.50	1.44
31	A	9001	SPR	O15-C15	2.27	1.51	1.47
31	A	9001	SPR	C9-C10	2.27	1.57	1.50
31	A	9001	SPR	C2B-C1B	2.26	1.56	1.51
31	A	9001	SPR	C3C-C2C	-2.23	1.47	1.52
31	A	9001	SPR	C7C-N4C	2.13	1.53	1.46
31	A	9001	SPR	C5B-C4B	2.09	1.57	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9001	SPR	C8A-N3A-C7A	-9.56	82.41	110.49
31	A	9001	SPR	O19-C19-C18	-7.97	102.19	125.38
31	A	9001	SPR	O1C-C9-C8	7.70	124.98	108.08
31	A	9001	SPR	C7C-N4C-C4C	7.60	135.04	113.15
31	A	9001	SPR	O1C-C1C-O5C	-6.05	90.45	109.97
31	A	9001	SPR	C16-C15-C14	5.72	123.58	113.26
31	A	9001	SPR	C15-C14-C13	-5.70	102.86	114.11
31	A	9001	SPR	C4A-C3A-N3A	-5.49	98.69	111.68
31	A	9001	SPR	C6A-C5A-C4A	-4.49	106.71	113.39
31	A	9001	SPR	O5A-C5A-C4A	4.22	117.00	109.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9001	SPR	O4A-C4A-C5A	4.09	117.19	106.77
31	A	9001	SPR	C14-C13-C12	-4.06	120.26	125.44
31	A	9001	SPR	C3C-C4C-C5C	3.94	117.89	110.14
31	A	9001	SPR	C17-O4-C4	-3.93	104.40	114.47
31	A	9001	SPR	C7A-N3A-C3A	-3.51	102.98	113.25
31	A	9001	SPR	O4A-C1B-C2B	3.03	114.06	108.99
31	A	9001	SPR	C1C-O5C-C5C	-2.92	105.82	113.82
31	A	9001	SPR	O2A-C2A-C1A	-2.91	103.15	110.08
31	A	9001	SPR	O5B-C1B-C2B	2.75	117.21	112.08
31	A	9001	SPR	C15-O15-C1	2.64	121.59	117.78
31	A	9001	SPR	C1A-O1A-C5	2.62	124.20	117.98
31	A	9001	SPR	O15-C15-C14	2.60	113.83	107.09
31	A	9001	SPR	O5C-C1C-C2C	2.59	116.75	111.23
31	A	9001	SPR	C1A-C2A-C3A	-2.58	105.06	109.20
31	A	9001	SPR	O15-C15-C16	-2.50	102.36	107.96
31	A	9001	SPR	C1C-O1C-C9	-2.39	109.86	113.84
31	A	9001	SPR	C3C-C4C-N4C	2.38	121.20	115.55
31	A	9001	SPR	O1-C1-C2	-2.23	119.46	124.65
31	A	9001	SPR	C3C-C2C-C1C	-2.20	105.90	110.88
31	A	9001	SPR	O15-C1-C2	2.11	115.21	111.43
31	A	9001	SPR	C20-C8-C9	-2.09	107.46	110.94
31	A	9001	SPR	C1B-O4A-C4A	-2.01	110.71	114.72

There are no chirality outliers.

All (12) torsion outliers are listed below:

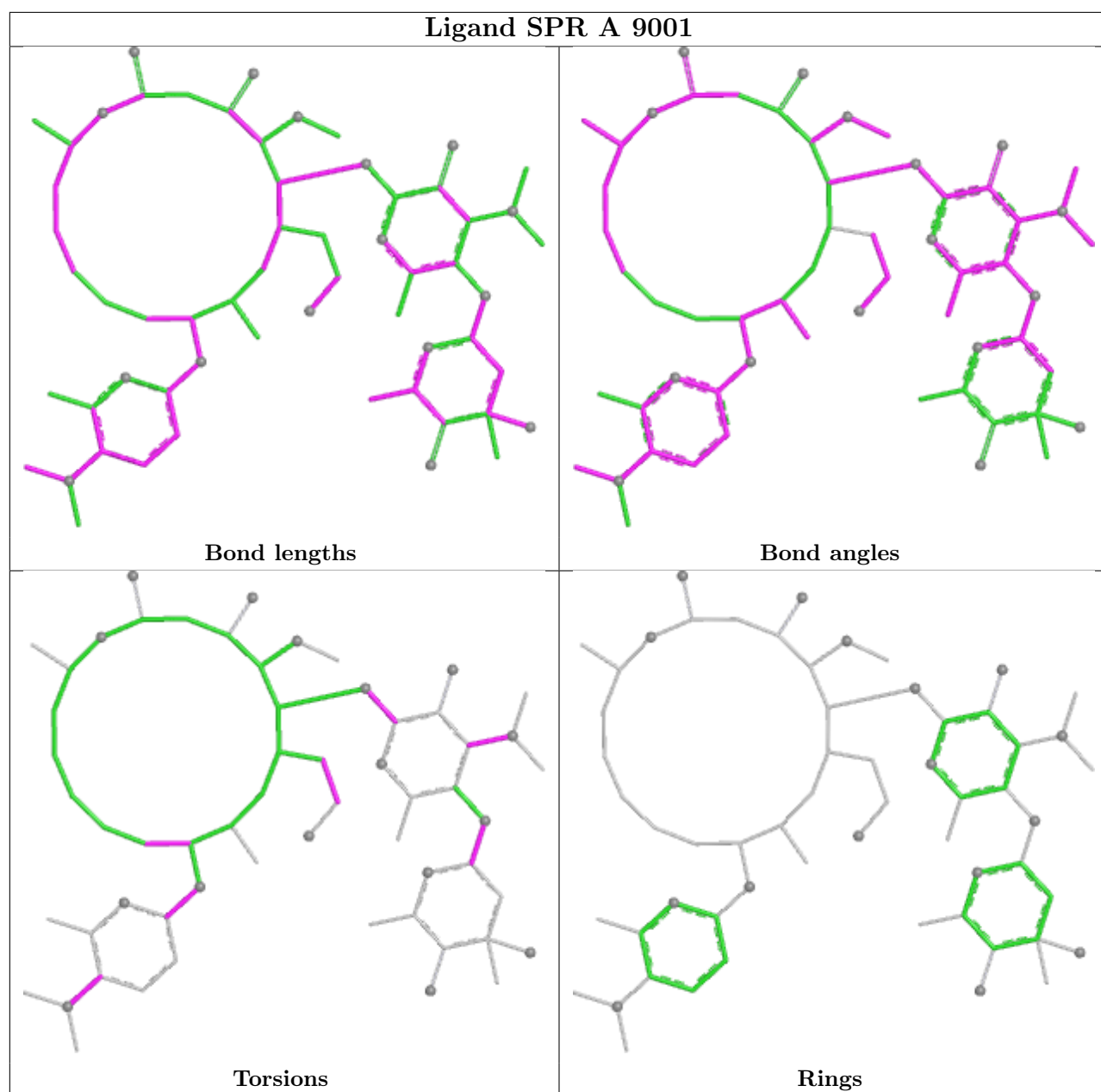
Mol	Chain	Res	Type	Atoms
31	A	9001	SPR	C4A-C3A-N3A-C7A
31	A	9001	SPR	O5B-C1B-O4A-C4A
31	A	9001	SPR	C5C-C4C-N4C-C7C
31	A	9001	SPR	C5C-C4C-N4C-C8C
31	A	9001	SPR	O5C-C1C-O1C-C9
31	A	9001	SPR	C2B-C1B-O4A-C4A
31	A	9001	SPR	C2C-C1C-O1C-C9
31	A	9001	SPR	C3C-C4C-N4C-C8C
31	A	9001	SPR	C2A-C3A-N3A-C7A
31	A	9001	SPR	C6-C18-C19-O19
31	A	9001	SPR	C11-C10-C9-O1C
31	A	9001	SPR	C2A-C1A-O1A-C5

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9001	SPR	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2754/2922 (94%)	-0.04	72 (2%) 57 34	23, 51, 96, 143	0
2	B	122/122 (100%)	0.57	7 (5%) 29 15	37, 70, 100, 150	0
3	C	237/239 (99%)	0.17	5 (2%) 63 40	32, 63, 96, 110	0
4	D	337/337 (100%)	0.10	2 (0%) 85 69	28, 57, 84, 95	0
5	E	246/246 (100%)	-0.04	2 (0%) 82 64	24, 50, 74, 85	0
6	F	140/176 (79%)	1.08	18 (12%) 7 5	60, 103, 122, 127	0
7	G	172/177 (97%)	0.33	5 (2%) 53 31	43, 68, 92, 98	0
8	H	119/119 (100%)	0.47	2 (1%) 69 45	59, 79, 102, 107	0
9	I	29/348 (8%)	1.52	9 (31%) 1 1	76, 94, 102, 104	0
10	J	156/167 (93%)	0.26	5 (3%) 50 29	35, 58, 85, 93	0
11	K	142/145 (97%)	-0.07	0 100 100	36, 50, 76, 84	0
12	L	132/132 (100%)	0.13	0 100 100	35, 56, 78, 82	0
13	M	145/164 (88%)	0.32	2 (1%) 73 51	31, 74, 108, 117	0
14	N	194/194 (100%)	0.40	19 (9%) 13 7	37, 55, 91, 98	0
15	O	186/186 (100%)	0.88	15 (8%) 18 9	48, 74, 112, 122	0
16	P	115/115 (100%)	0.16	0 100 100	39, 59, 75, 79	0
17	Q	143/148 (96%)	0.23	3 (2%) 63 40	38, 60, 76, 84	0
18	R	95/95 (100%)	0.06	1 (1%) 78 57	38, 51, 64, 79	0
19	S	150/154 (97%)	-0.23	0 100 100	32, 45, 66, 75	0
20	T	81/84 (96%)	0.17	0 100 100	47, 65, 84, 89	0
21	U	119/119 (100%)	0.27	3 (2%) 58 35	44, 62, 86, 97	0
22	V	53/66 (80%)	1.60	14 (26%) 1 1	85, 94, 102, 110	0
23	W	65/70 (92%)	0.49	4 (6%) 26 14	55, 81, 112, 118	0
24	X	154/154 (100%)	-0.07	0 100 100	32, 49, 66, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	82/91 (90%)	0.32	3 (3%) 45 25	42, 58, 84, 99	0
26	Z	142/240 (59%)	-0.11	2 (1%) 73 51	25, 46, 70, 85	0
27	1	73/73 (100%)	1.90	28 (38%) 1 1	79, 98, 103, 104	0
28	2	56/56 (100%)	-0.38	0 100 100	30, 39, 45, 49	0
29	3	46/48 (95%)	0.27	0 100 100	40, 66, 90, 102	0
30	4	92/92 (100%)	2.51	60 (65%) 0 0	91, 103, 108, 111	0
All	All	6577/7279 (90%)	0.18	281 (4%) 40 21	23, 57, 102, 150	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	N	80	GLY	8.1
1	A	1173	A	7.4
14	N	89	ASN	7.3
14	N	70	GLY	6.9
30	4	12	PRO	6.8
1	A	1176	C	5.8
1	A	2433	A	5.8
27	1	16	PRO	5.7
23	W	1	THR	5.7
1	A	1175	G	5.5
14	N	71	SER	5.5
30	4	79	LEU	5.4
30	4	33	MET	5.1
27	1	22	ILE	5.1
27	1	40	PRO	4.9
14	N	81	ARG	4.9
30	4	48	ASN	4.9
1	A	1168	C	4.8
14	N	83	SER	4.8
30	4	60	LYS	4.8
14	N	82	ARG	4.7
30	4	85	ALA	4.6
30	4	1	MET	4.6
1	A	735	C	4.4
4	D	1	PRO	4.4
1	A	2432	C	4.3
30	4	43	ASN	4.2
30	4	84	ARG	4.2
1	A	1160	G	4.2

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Mol	Chain	Res	Type	RSRZ
27	1	18	TYR	4.1
27	1	26	VAL	4.0
6	F	10	PHE	4.0
1	A	1184	C	4.0
27	1	12	GLY	4.0
27	1	13	ARG	3.9
30	4	51	LYS	3.9
1	A	1190	G	3.9
1	A	2436	U	3.9
1	A	1171	A	3.8
1	A	1188	A	3.8
2	B	3022	G	3.7
1	A	736	A	3.7
30	4	83	TRP	3.7
14	N	90	ARG	3.7
2	B	3001	U	3.6
1	A	1193	A	3.6
30	4	10	TYR	3.6
30	4	52	PHE	3.6
1	A	1165	G	3.5
1	A	1167	G	3.5
6	F	102	GLY	3.5
27	1	20	LEU	3.5
30	4	65	THR	3.5
1	A	1169	U	3.5
30	4	76	LYS	3.4
30	4	78	HIS	3.4
1	A	1172	G	3.4
1	A	1198	U	3.4
14	N	88	VAL	3.4
1	A	1925	G	3.4
30	4	42	ARG	3.4
9	I	27	ILE	3.4
15	O	148	ALA	3.3
22	V	49	LEU	3.3
30	4	88	LEU	3.3
9	I	26	MET	3.3
14	N	72	SER	3.3
27	1	31	ILE	3.3
27	1	44	PHE	3.3
30	4	7	PHE	3.3
30	4	22	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1161	A	3.2
30	4	11	CYS	3.2
15	O	147	ILE	3.2
14	N	77	PHE	3.2
30	4	17	HIS	3.2
30	4	61	PRO	3.2
30	4	54	LYS	3.1
1	A	1181	A	3.1
27	1	17	ARG	3.1
15	O	179	LEU	3.1
27	1	41	VAL	3.1
1	A	2345	A	3.1
9	I	71	LEU	3.1
30	4	2	GLN	3.1
2	B	3025	G	3.1
25	Y	88	GLU	3.1
1	A	1177	A	3.1
3	C	36	ASP	3.1
30	4	69	TYR	3.1
27	1	35	LYS	3.0
22	V	51	TRP	3.0
30	4	36	ILE	3.0
1	A	2257	G	3.0
30	4	13	HIS	3.0
27	1	29	VAL	3.0
1	A	1180	U	3.0
27	1	34	LYS	3.0
30	4	4	PRO	3.0
17	Q	116	SER	2.9
1	A	737	A	2.9
1	A	1964	U	2.9
14	N	68	ARG	2.9
1	A	1199	A	2.9
18	R	95	GLU	2.9
1	A	1205	U	2.9
7	G	45	ASP	2.9
1	A	1174	A	2.9
30	4	55	VAL	2.9
1	A	10	U	2.9
2	B	3002	U	2.9
27	1	14	PHE	2.9
30	4	56	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
14	N	79	LYS	2.8
1	A	2434	A	2.8
2	B	3024	U	2.8
6	F	63	ILE	2.8
22	V	31	PHE	2.8
25	Y	80	GLU	2.8
26	Z	108	ASP	2.8
6	F	171	ASP	2.8
1	A	138	U	2.8
1	A	734	U	2.8
23	W	39	ALA	2.8
27	1	32	LYS	2.8
1	A	1162	G	2.8
1	A	1197	G	2.8
9	I	23	ILE	2.8
30	4	82	GLY	2.7
15	O	166	ALA	2.7
30	4	34	LYS	2.7
6	F	131	THR	2.7
22	V	55	ALA	2.7
14	N	73	ARG	2.7
30	4	39	GLN	2.7
30	4	31	THR	2.7
15	O	169	PRO	2.7
27	1	42	CYS	2.7
27	1	11	THR	2.7
1	A	1159	G	2.7
1	A	2249	G	2.7
1	A	2250	G	2.7
1	A	1194	A	2.6
30	4	53	SER	2.6
30	4	77	ALA	2.6
6	F	69	ILE	2.6
10	J	32	ASP	2.6
27	1	15	GLY	2.6
30	4	67	LEU	2.6
22	V	13	ILE	2.6
30	4	59	ASP	2.6
6	F	21	VAL	2.6
1	A	2511	A	2.6
30	4	46	ILE	2.6
25	Y	82	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
27	1	30	GLU	2.6
1	A	1170	U	2.6
1	A	1206	U	2.6
30	4	9	THR	2.6
30	4	35	TRP	2.6
30	4	68	LYS	2.6
14	N	74	ARG	2.6
30	4	63	LYS	2.6
30	4	64	LYS	2.6
27	1	64	ILE	2.5
1	A	1166	A	2.5
5	E	135	GLU	2.5
1	A	1204	C	2.5
30	4	74	CYS	2.5
21	U	1	SER	2.5
14	N	78	ASN	2.5
22	V	40	ALA	2.5
1	A	1186	C	2.5
9	I	29	SER	2.5
15	O	154	LEU	2.5
30	4	47	GLY	2.5
22	V	46	ALA	2.5
6	F	62	ASP	2.5
9	I	63	ARG	2.5
7	G	10	ASP	2.4
10	J	135	TRP	2.4
14	N	76	ARG	2.4
1	A	1187	U	2.4
30	4	3	MET	2.4
3	C	31	LYS	2.4
1	A	1203	G	2.4
22	V	50	GLU	2.4
30	4	16	GLU	2.4
17	Q	1	THR	2.4
9	I	24	VAL	2.4
14	N	192	ALA	2.4
1	A	1195	G	2.4
1	A	2344	G	2.4
30	4	62	THR	2.4
30	4	15	ASN	2.4
27	1	48	LYS	2.4
1	A	1192	A	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1924	A	2.4
30	4	25	VAL	2.4
1	A	2507	G	2.3
3	C	237	GLY	2.3
27	1	33	HIS	2.3
30	4	14	CYS	2.3
2	B	3023	U	2.3
27	1	47	LEU	2.3
27	1	24	VAL	2.3
8	H	105	ALA	2.3
22	V	52	THR	2.3
22	V	8	TYR	2.3
27	1	39	CYS	2.3
15	O	66	LEU	2.3
15	O	158	LEU	2.3
1	A	1207	A	2.3
13	M	148	GLU	2.3
1	A	1916	C	2.3
6	F	172	VAL	2.3
23	W	2	VAL	2.3
9	I	13	PRO	2.3
27	1	19	GLY	2.3
15	O	1	ALA	2.3
1	A	999	C	2.3
1	A	1183	C	2.3
15	O	168	LEU	2.3
7	G	81	GLU	2.2
13	M	83	GLU	2.2
1	A	1185	U	2.2
1	A	1917	G	2.2
1	A	2410	G	2.2
6	F	95	THR	2.2
1	A	1189	A	2.2
1	A	1202	A	2.2
30	4	8	ASN	2.2
7	G	100	ASP	2.2
30	4	58	GLY	2.2
8	H	106	THR	2.2
14	N	75	THR	2.2
6	F	23	VAL	2.2
17	Q	58	SER	2.2
1	A	2378	U	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1191	A	2.2
23	W	40	PRO	2.2
10	J	164	ALA	2.2
21	U	119	ALA	2.2
3	C	85	ASP	2.2
1	A	2321	A	2.2
22	V	23	HIS	2.2
6	F	50	VAL	2.1
21	U	82	THR	2.1
30	4	91	GLN	2.1
30	4	44	SER	2.1
6	F	138	GLY	2.1
15	O	162	ASP	2.1
22	V	9	CYS	2.1
30	4	75	GLY	2.1
15	O	172	PHE	2.1
9	I	20	VAL	2.1
1	A	1915	U	2.1
10	J	40	PRO	2.1
15	O	79	PRO	2.1
4	D	191	ASN	2.1
1	A	1163	G	2.1
1	A	2324	G	2.1
6	F	44	ILE	2.1
7	G	39	ASP	2.1
6	F	104	PHE	2.1
30	4	71	CYS	2.1
10	J	167	ALA	2.1
26	Z	235	GLU	2.1
1	A	1524	U	2.0
6	F	58	VAL	2.0
6	F	174	VAL	2.0
22	V	34	SER	2.0
30	4	49	ASP	2.0
15	O	157	PRO	2.0
3	C	32	VAL	2.0
5	E	16	VAL	2.0
1	A	2379	G	2.0
22	V	42	LEU	2.0
2	B	3055	U	2.0
6	F	100	ASP	2.0
15	O	186	LEU	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 oligosaccharides 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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	CL	4	8504	1/1	0.41	0.13	95,95,95,95	0
33	NA	B	8383	1/1	0.43	0.34	63,63,63,63	0
33	NA	T	8312	1/1	0.49	0.37	124,124,124,124	0
36	CD	4	8404	1/1	0.51	0.36	156,156,156,156	0
33	NA	A	8366	1/1	0.52	0.14	49,49,49,49	0
32	MG	A	8050	1/1	0.60	0.15	85,85,85,85	0
32	MG	A	8092	1/1	0.63	0.20	91,91,91,91	0
33	NA	A	8384	1/1	0.64	0.30	114,114,114,114	0
32	MG	A	8049	1/1	0.65	0.14	89,89,89,89	0
33	NA	A	8382	1/1	0.66	0.26	62,62,62,62	0
36	CD	P	8405	1/1	0.66	0.28	169,169,169,169	0
33	NA	A	8371	1/1	0.66	0.36	54,54,54,54	0
32	MG	A	8090	1/1	0.72	0.13	36,36,36,36	0
33	NA	A	8331	1/1	0.73	0.23	61,61,61,61	0
33	NA	B	8351	1/1	0.73	0.12	69,69,69,69	0
33	NA	A	8318	1/1	0.73	0.15	34,34,34,34	0
33	NA	S	8337	1/1	0.73	0.08	49,49,49,49	0
32	MG	A	8104	1/1	0.74	0.10	40,40,40,40	0
33	NA	A	8385	1/1	0.75	0.17	41,41,41,41	0
32	MG	A	8067	1/1	0.76	0.14	50,50,50,50	0
33	NA	A	8365	1/1	0.76	0.18	49,49,49,49	0
33	NA	A	8313	1/1	0.77	0.13	63,63,63,63	0
33	NA	A	8373	1/1	0.77	0.14	59,59,59,59	0
33	NA	A	8329	1/1	0.78	0.15	70,70,70,70	0
33	NA	A	8332	1/1	0.79	0.11	58,58,58,58	0
33	NA	A	8377	1/1	0.79	0.28	60,60,60,60	0
32	MG	A	8070	1/1	0.79	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	A	8367	1/1	0.80	0.14	52,52,52,52	0
31	SPR	A	9001	59/59	0.80	0.18	78,88,95,95	0
33	NA	A	8360	1/1	0.82	0.33	55,55,55,55	0
33	NA	A	8369	1/1	0.82	0.24	52,52,52,52	0
36	CD	1	8403	1/1	0.82	0.21	138,138,138,138	0
34	CL	R	8511	1/1	0.82	0.22	63,63,63,63	0
34	CL	O	8507	1/1	0.83	0.12	62,62,62,62	0
33	NA	A	8362	1/1	0.83	0.25	69,69,69,69	0
33	NA	A	8356	1/1	0.83	0.20	58,58,58,58	0
32	MG	A	8103	1/1	0.83	0.17	55,55,55,55	0
34	CL	A	8512	1/1	0.83	0.12	32,32,32,32	0
34	CL	N	8518	1/1	0.83	0.14	56,56,56,56	0
32	MG	A	8114	1/1	0.84	0.12	92,92,92,92	0
32	MG	A	8040	1/1	0.84	0.18	78,78,78,78	0
32	MG	A	8046	1/1	0.84	0.09	79,79,79,79	0
33	NA	A	8363	1/1	0.84	0.34	66,66,66,66	0
33	NA	J	8309	1/1	0.84	0.09	21,21,21,21	0
34	CL	A	8515	1/1	0.85	0.33	100,100,100,100	0
35	K	A	8602	1/1	0.85	0.28	68,68,68,68	0
33	NA	A	8352	1/1	0.85	0.14	52,52,52,52	0
32	MG	A	8116	1/1	0.85	0.09	67,67,67,67	0
32	MG	A	8082	1/1	0.85	0.09	52,52,52,52	0
34	CL	M	8510	1/1	0.86	0.11	87,87,87,87	0
33	NA	A	8328	1/1	0.86	0.07	45,45,45,45	0
33	NA	A	8372	1/1	0.86	0.26	55,55,55,55	0
33	NA	A	8364	1/1	0.86	0.11	40,40,40,40	0
33	NA	A	8355	1/1	0.86	0.24	55,55,55,55	0
32	MG	A	8024	1/1	0.86	0.65	116,116,116,116	0
33	NA	A	8305	1/1	0.86	0.12	34,34,34,34	0
33	NA	A	8326	1/1	0.86	0.10	46,46,46,46	0
34	CL	C	8509	1/1	0.86	0.17	86,86,86,86	0
33	NA	S	8386	1/1	0.87	0.11	53,53,53,53	0
34	CL	P	8508	1/1	0.87	0.12	93,93,93,93	0
32	MG	A	8102	1/1	0.87	0.46	87,87,87,87	0
32	MG	1	8105	1/1	0.87	0.09	44,44,44,44	0
32	MG	A	8094	1/1	0.87	0.19	85,85,85,85	0
33	NA	A	8374	1/1	0.87	0.30	63,63,63,63	0
33	NA	A	8341	1/1	0.87	0.12	43,43,43,43	0
33	NA	A	8308	1/1	0.87	0.18	69,69,69,69	0
35	K	A	8601	1/1	0.88	0.10	73,73,73,73	0
33	NA	A	8379	1/1	0.88	0.13	41,41,41,41	0
34	CL	K	8521	1/1	0.88	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CD	V	8401	1/1	0.88	0.28	142,142,142,142	0
32	MG	A	8117	1/1	0.88	0.08	31,31,31,31	0
33	NA	A	8324	1/1	0.88	0.33	51,51,51,51	0
34	CL	D	8519	1/1	0.89	0.18	65,65,65,65	0
32	MG	A	8062	1/1	0.89	0.07	72,72,72,72	0
32	MG	A	8101	1/1	0.89	0.14	55,55,55,55	0
32	MG	A	8088	1/1	0.89	0.10	45,45,45,45	0
32	MG	A	8093	1/1	0.89	0.13	56,56,56,56	0
32	MG	A	8118	1/1	0.89	0.14	62,62,62,62	0
33	NA	A	8320	1/1	0.89	0.08	33,33,33,33	0
32	MG	A	8085	1/1	0.90	0.13	72,72,72,72	0
33	NA	A	8323	1/1	0.90	0.16	50,50,50,50	0
32	MG	A	8089	1/1	0.90	0.11	84,84,84,84	0
33	NA	A	8368	1/1	0.90	0.14	47,47,47,47	0
32	MG	A	8096	1/1	0.90	0.07	53,53,53,53	0
33	NA	A	8350	1/1	0.90	0.09	34,34,34,34	0
34	CL	A	8505	1/1	0.90	0.13	88,88,88,88	0
33	NA	A	8301	1/1	0.90	0.16	43,43,43,43	0
33	NA	A	8330	1/1	0.91	0.09	43,43,43,43	0
34	CL	A	8503	1/1	0.91	0.10	50,50,50,50	0
33	NA	A	8321	1/1	0.91	0.16	39,39,39,39	0
33	NA	A	8306	1/1	0.91	0.20	56,56,56,56	0
32	MG	U	8073	1/1	0.91	0.04	42,42,42,42	0
34	CL	A	8517	1/1	0.91	0.09	55,55,55,55	0
34	CL	A	8522	1/1	0.91	0.39	75,75,75,75	0
35	K	A	8603	1/1	0.91	0.07	88,88,88,88	0
32	MG	A	8081	1/1	0.91	0.11	58,58,58,58	0
32	MG	A	8106	1/1	0.91	0.08	47,47,47,47	0
33	NA	A	8353	1/1	0.91	0.09	38,38,38,38	0
32	MG	B	8095	1/1	0.91	0.09	67,67,67,67	0
32	MG	A	8042	1/1	0.92	0.07	44,44,44,44	0
32	MG	A	8113	1/1	0.92	0.11	45,45,45,45	0
34	CL	A	8516	1/1	0.92	0.14	44,44,44,44	0
32	MG	Z	8109	1/1	0.92	0.10	53,53,53,53	0
32	MG	A	8045	1/1	0.92	0.08	54,54,54,54	0
32	MG	A	8119	1/1	0.92	0.15	71,71,71,71	0
33	NA	A	8378	1/1	0.92	0.14	37,37,37,37	0
32	MG	A	8111	1/1	0.93	0.07	69,69,69,69	0
33	NA	A	8381	1/1	0.93	0.07	51,51,51,51	0
32	MG	4	8078	1/1	0.93	0.10	74,74,74,74	0
32	MG	A	8047	1/1	0.93	0.11	62,62,62,62	0
33	NA	A	8302	1/1	0.93	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	A	8333	1/1	0.93	0.10	33,33,33,33	0
33	NA	A	8322	1/1	0.93	0.14	46,46,46,46	0
33	NA	A	8342	1/1	0.93	0.12	47,47,47,47	0
33	NA	A	8344	1/1	0.93	0.06	30,30,30,30	0
33	NA	A	8303	1/1	0.93	0.12	51,51,51,51	0
32	MG	A	8041	1/1	0.93	0.06	46,46,46,46	0
32	MG	A	8076	1/1	0.93	0.06	71,71,71,71	0
33	NA	A	8327	1/1	0.93	0.09	32,32,32,32	0
32	MG	A	8087	1/1	0.93	0.05	48,48,48,48	0
33	NA	A	8375	1/1	0.93	0.13	53,53,53,53	0
33	NA	A	8357	1/1	0.93	0.10	67,67,67,67	0
33	NA	A	8359	1/1	0.93	0.13	61,61,61,61	0
32	MG	A	8097	1/1	0.94	0.12	44,44,44,44	0
32	MG	A	8064	1/1	0.94	0.13	24,24,24,24	0
32	MG	A	8066	1/1	0.94	0.08	83,83,83,83	0
34	CL	A	8513	1/1	0.94	0.07	56,56,56,56	0
34	CL	A	8514	1/1	0.94	0.10	61,61,61,61	0
34	CL	S	8506	1/1	0.94	0.07	46,46,46,46	0
32	MG	A	8001	1/1	0.94	0.07	39,39,39,39	0
33	NA	A	8340	1/1	0.94	0.06	31,31,31,31	0
33	NA	A	8319	1/1	0.94	0.11	52,52,52,52	0
33	NA	R	8348	1/1	0.94	0.06	37,37,37,37	0
32	MG	A	8115	1/1	0.94	0.07	59,59,59,59	0
32	MG	A	8091	1/1	0.94	0.05	48,48,48,48	0
34	CL	K	8502	1/1	0.94	0.04	52,52,52,52	0
33	NA	A	8370	1/1	0.94	0.14	49,49,49,49	0
33	NA	A	8349	1/1	0.95	0.12	53,53,53,53	0
32	MG	A	8110	1/1	0.95	0.08	47,47,47,47	0
33	NA	A	8317	1/1	0.95	0.04	27,27,27,27	0
33	NA	E	8304	1/1	0.95	0.09	35,35,35,35	0
34	CL	Z	8520	1/1	0.95	0.11	35,35,35,35	0
32	MG	A	8022	1/1	0.95	0.07	41,41,41,41	0
33	NA	A	8376	1/1	0.95	0.16	78,78,78,78	0
33	NA	A	8354	1/1	0.95	0.08	40,40,40,40	0
32	MG	A	8055	1/1	0.95	0.05	71,71,71,71	0
32	MG	A	8057	1/1	0.95	0.05	49,49,49,49	0
33	NA	A	8310	1/1	0.95	0.06	29,29,29,29	0
33	NA	A	8343	1/1	0.95	0.05	16,16,16,16	0
33	NA	A	8311	1/1	0.95	0.06	42,42,42,42	0
33	NA	A	8314	1/1	0.96	0.09	33,33,33,33	0
33	NA	A	8315	1/1	0.96	0.09	30,30,30,30	0
33	NA	A	8316	1/1	0.96	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8075	1/1	0.96	0.04	57,57,57,57	0
32	MG	A	8029	1/1	0.96	0.04	51,51,51,51	0
32	MG	A	8079	1/1	0.96	0.08	39,39,39,39	0
32	MG	A	8099	1/1	0.96	0.10	38,38,38,38	0
33	NA	A	8338	1/1	0.96	0.06	67,67,67,67	0
33	NA	C	8345	1/1	0.96	0.05	42,42,42,42	0
33	NA	A	8307	1/1	0.96	0.07	39,39,39,39	0
32	MG	A	8023	1/1	0.96	0.06	42,42,42,42	0
32	MG	A	8061	1/1	0.96	0.04	44,44,44,44	0
34	CL	K	8501	1/1	0.96	0.05	56,56,56,56	0
32	MG	A	8084	1/1	0.96	0.12	48,48,48,48	0
32	MG	A	8018	1/1	0.96	0.05	61,61,61,61	0
33	NA	A	8339	1/1	0.97	0.05	16,16,16,16	0
32	MG	A	8015	1/1	0.97	0.06	57,57,57,57	0
32	MG	A	8008	1/1	0.97	0.05	49,49,49,49	0
32	MG	A	8012	1/1	0.97	0.06	52,52,52,52	0
33	NA	A	8361	1/1	0.97	0.10	53,53,53,53	0
32	MG	A	8039	1/1	0.97	0.05	50,50,50,50	0
32	MG	A	8071	1/1	0.97	0.06	91,91,91,91	0
32	MG	A	8098	1/1	0.97	0.14	50,50,50,50	0
32	MG	A	8072	1/1	0.97	0.07	80,80,80,80	0
32	MG	A	8100	1/1	0.97	0.07	69,69,69,69	0
33	NA	A	8335	1/1	0.97	0.11	52,52,52,52	0
33	NA	A	8336	1/1	0.97	0.04	49,49,49,49	0
33	NA	A	8325	1/1	0.97	0.09	52,52,52,52	0
32	MG	A	8031	1/1	0.98	0.05	31,31,31,31	0
32	MG	A	8063	1/1	0.98	0.06	78,78,78,78	0
33	NA	K	8346	1/1	0.98	0.02	27,27,27,27	0
33	NA	M	8380	1/1	0.98	0.05	55,55,55,55	0
33	NA	N	8347	1/1	0.98	0.04	21,21,21,21	0
33	NA	A	8334	1/1	0.98	0.10	36,36,36,36	0
32	MG	A	8112	1/1	0.98	0.10	44,44,44,44	0
32	MG	A	8033	1/1	0.98	0.04	30,30,30,30	0
32	MG	A	8083	1/1	0.98	0.07	47,47,47,47	0
32	MG	A	8034	1/1	0.98	0.04	39,39,39,39	0
32	MG	A	8053	1/1	0.98	0.04	52,52,52,52	0
32	MG	A	8044	1/1	0.98	0.07	52,52,52,52	0
32	MG	A	8056	1/1	0.98	0.04	53,53,53,53	0
32	MG	A	8035	1/1	0.98	0.04	54,54,54,54	0
32	MG	A	8074	1/1	0.98	0.07	31,31,31,31	0
32	MG	C	8065	1/1	0.98	0.04	57,57,57,57	0
32	MG	L	8069	1/1	0.98	0.04	50,50,50,50	0

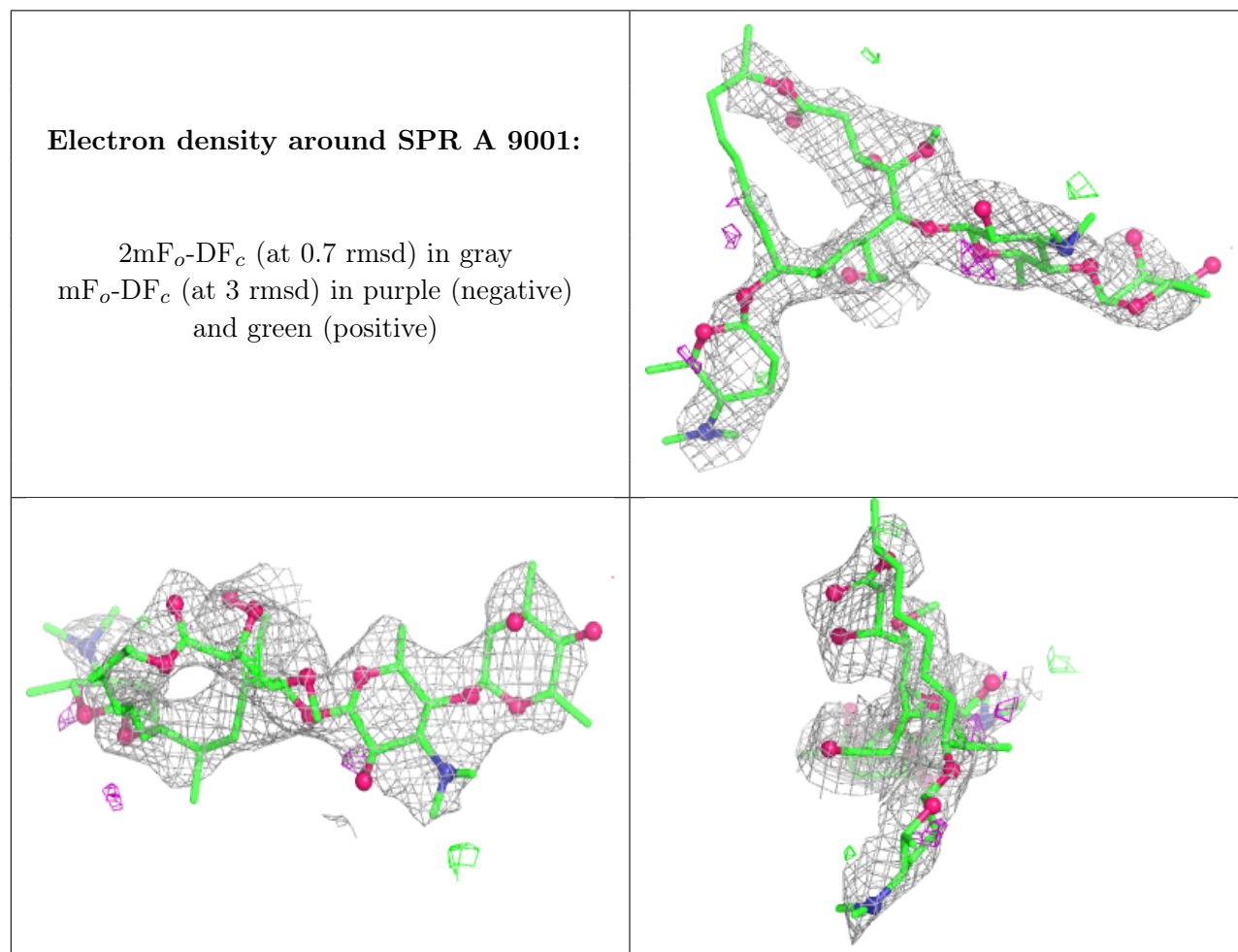
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8060	1/1	0.98	0.05	45,45,45,45	0
36	CD	2	8402	1/1	0.98	0.03	59,59,59,59	0
32	MG	A	8014	1/1	0.98	0.04	30,30,30,30	0
32	MG	A	8025	1/1	0.99	0.02	60,60,60,60	0
32	MG	A	8027	1/1	0.99	0.04	63,63,63,63	0
32	MG	A	8028	1/1	0.99	0.06	44,44,44,44	0
32	MG	A	8006	1/1	0.99	0.04	48,48,48,48	0
32	MG	A	8048	1/1	0.99	0.03	45,45,45,45	0
32	MG	A	8030	1/1	0.99	0.02	26,26,26,26	0
32	MG	A	8107	1/1	0.99	0.02	47,47,47,47	0
32	MG	A	8108	1/1	0.99	0.08	88,88,88,88	0
32	MG	A	8016	1/1	0.99	0.03	41,41,41,41	0
32	MG	A	8080	1/1	0.99	0.03	50,50,50,50	0
32	MG	A	8051	1/1	0.99	0.07	56,56,56,56	0
32	MG	A	8052	1/1	0.99	0.04	45,45,45,45	0
32	MG	A	8032	1/1	0.99	0.08	34,34,34,34	0
32	MG	A	8054	1/1	0.99	0.05	48,48,48,48	0
32	MG	A	8017	1/1	0.99	0.04	27,27,27,27	0
32	MG	A	8086	1/1	0.99	0.05	50,50,50,50	0
32	MG	A	8003	1/1	0.99	0.02	24,24,24,24	0
32	MG	A	8019	1/1	0.99	0.04	35,35,35,35	0
32	MG	A	8058	1/1	0.99	0.04	43,43,43,43	0
32	MG	A	8059	1/1	0.99	0.04	31,31,31,31	0
32	MG	A	8037	1/1	0.99	0.04	48,48,48,48	0
32	MG	A	8038	1/1	0.99	0.03	35,35,35,35	0
32	MG	A	8021	1/1	0.99	0.04	27,27,27,27	0
32	MG	A	8010	1/1	0.99	0.06	40,40,40,40	0
32	MG	A	8004	1/1	0.99	0.04	48,48,48,48	0
32	MG	A	8005	1/1	0.99	0.03	44,44,44,44	0
32	MG	A	8043	1/1	0.99	0.03	39,39,39,39	0
32	MG	A	8068	1/1	0.99	0.04	58,58,58,58	0
32	MG	A	8026	1/1	1.00	0.06	11,11,11,11	0
32	MG	A	8077	1/1	1.00	0.03	31,31,31,31	0
32	MG	A	8020	1/1	1.00	0.04	51,51,51,51	0
32	MG	A	8007	1/1	1.00	0.04	23,23,23,23	0
32	MG	A	8036	1/1	1.00	0.03	45,45,45,45	0
32	MG	A	8011	1/1	1.00	0.03	52,52,52,52	0
32	MG	A	8002	1/1	1.00	0.01	31,31,31,31	0
32	MG	A	8013	1/1	1.00	0.03	46,46,46,46	0
32	MG	A	8009	1/1	1.00	0.06	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.