



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 12:00 PM UTC

PDB ID : 1Q82 / pdb_00001q82
Title : Crystal Structure of CC-Puromycin bound to the A-site of the 50S ribosomal subunit
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-20
Resolution : 2.98 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

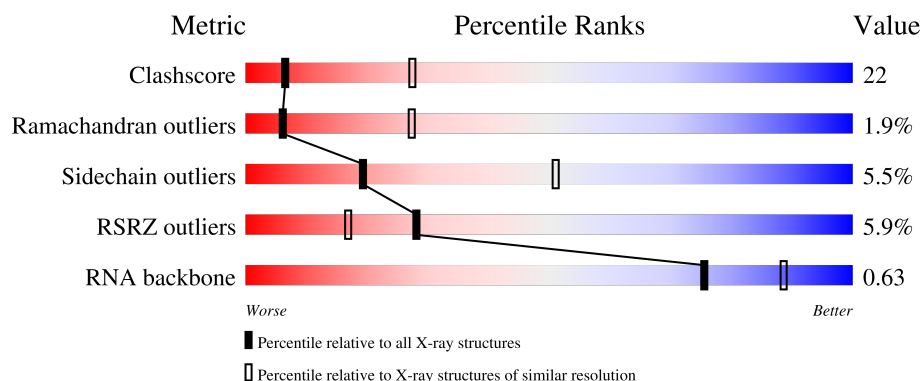
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)
RNA backbone	3983	1013 (3.18-2.78)

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	3% 50% 36% 8% 6%
2	B	122	6% 50% 36% 9% 5%
3	5	2	50% 50%
4	C	239	6% 51% 43% 6%
5	D	337	% 46% 46% 7%

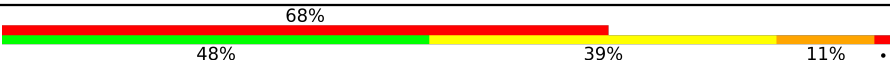
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Mol	Chain	Length	Quality of chain
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	

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Mol	Chain	Length	Quality of chain
31	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	8011	-	-	X	-
32	MG	A	8102	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	B	8383	-	-	-	X
35	CL	N	8518	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 98593 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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 RNA chain called CC-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	2	Total	C	N	O	P	0	0	0
			40	18	6	14	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	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 6 is a protein called 50S ribosomal protein L4E.

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

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	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 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called L37Ae 50S ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	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 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	109	Total Mg 109 109	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	D	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	1	1	Total Mg 1 1	0	0
32	4	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	71	Total Na 71 71	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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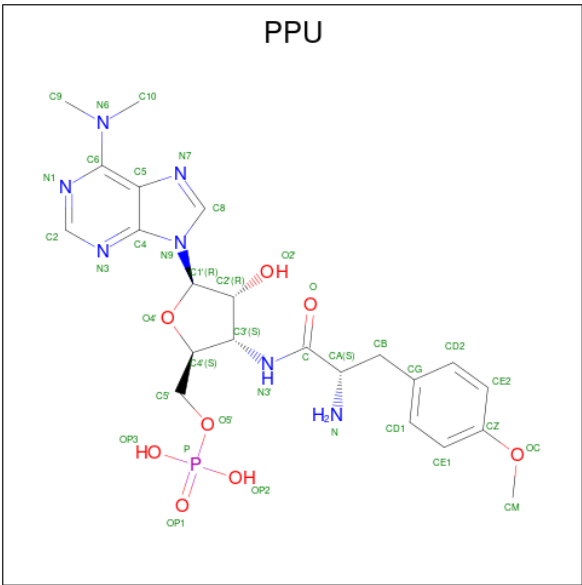
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Na 1	0	0
34	S	2	Total 2	Na 2	0	0
34	T	1	Total 1	Na 1	0	0
34	U	1	Total 1	Na 1	0	0
34	4	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	7	Total 7	Cl 7	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	4	Total 4	Cl 4	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	2	Total 2	Cl 2	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (CCD ID: PPU) (formula: C₂₂H₃₀N₇O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	5	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	P	1	Total	Cd	0	0
			1	1		
37	V	1	Total	Cd	0	0
			1	1		
37	1	1	Total	Cd	0	0
			1	1		
37	2	1	Total	Cd	0	0
			1	1		
37	4	1	Total	Cd	0	0
			1	1		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	5860	Total	O	0	0
			5860	5860		
38	B	146	Total	O	0	0
			146	146		
38	5	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	C	140	Total 140	O 140	0	0
38	D	146	Total 146	O 146	0	0
38	E	176	Total 176	O 176	0	0
38	F	52	Total 52	O 52	0	0
38	G	45	Total 45	O 45	0	0
38	H	32	Total 32	O 32	0	0
38	I	22	Total 22	O 22	0	0
38	J	78	Total 78	O 78	0	0
38	K	54	Total 54	O 54	0	0
38	L	64	Total 64	O 64	0	0
38	M	86	Total 86	O 86	0	0
38	N	138	Total 138	O 138	0	0
38	O	64	Total 64	O 64	0	0
38	P	44	Total 44	O 44	0	0
38	Q	70	Total 70	O 70	0	0
38	R	57	Total 57	O 57	0	0
38	S	83	Total 83	O 83	0	0
38	T	36	Total 36	O 36	0	0
38	U	38	Total 38	O 38	0	0
38	V	22	Total 22	O 22	0	0
38	W	16	Total 16	O 16	0	0

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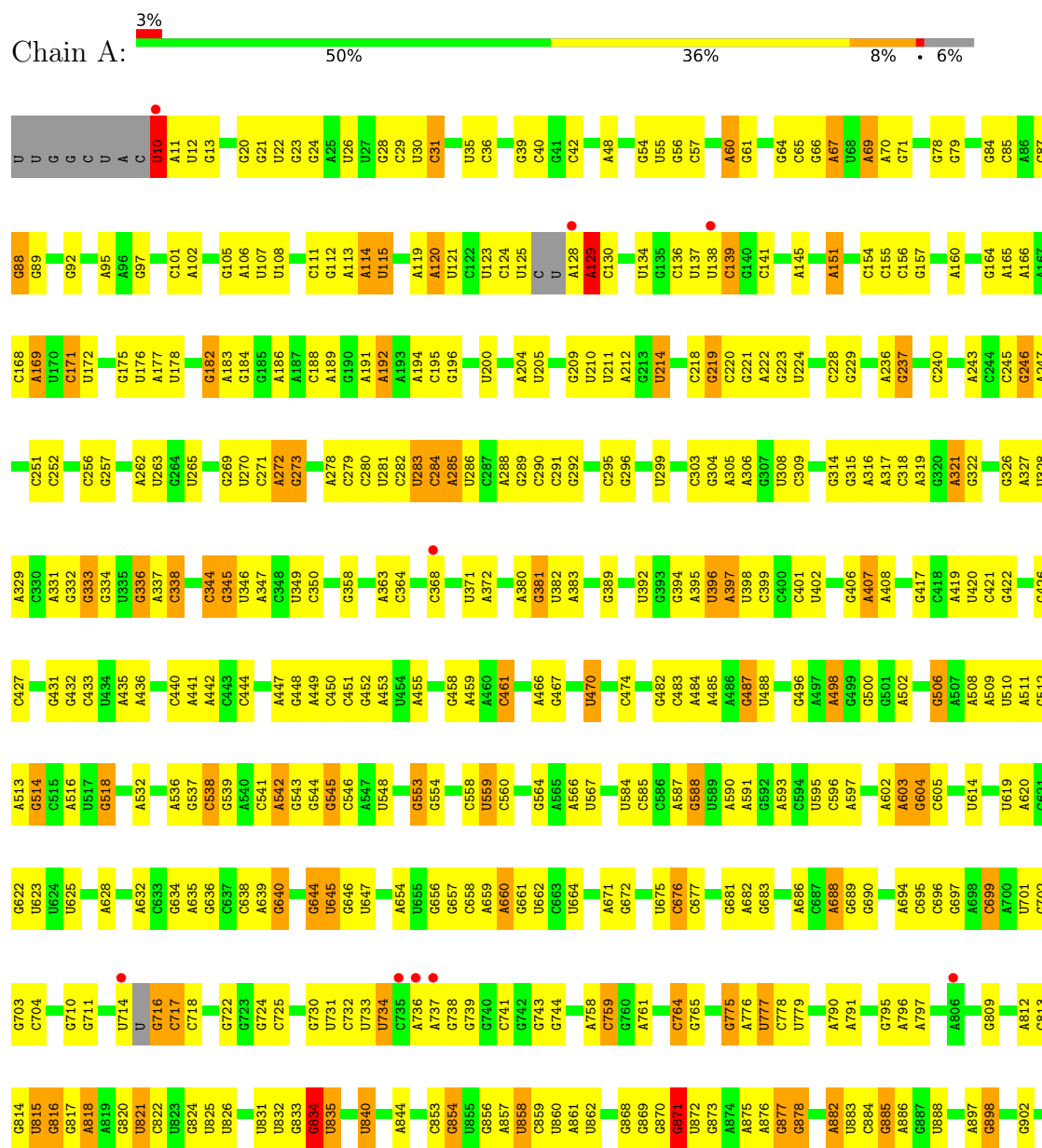
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	X	67	Total 67	O 67	0	0
38	Y	28	Total 28	O 28	0	0
38	Z	100	Total 100	O 100	0	0
38	1	36	Total 36	O 36	0	0
38	2	58	Total 58	O 58	0	0
38	3	37	Total 37	O 37	0	0
38	4	70	Total 70	O 70	0	0

3 Residue-property plots

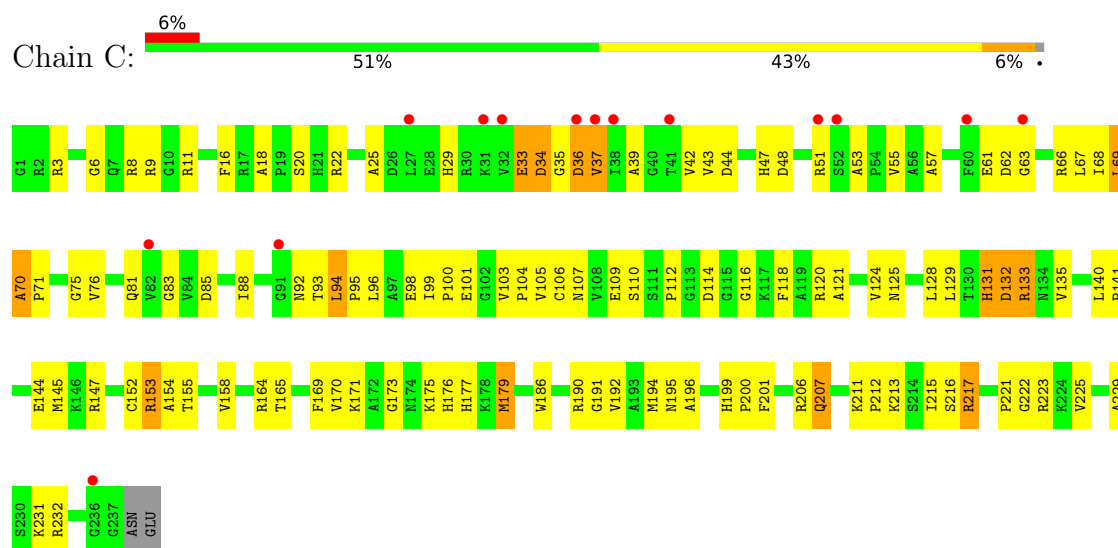
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

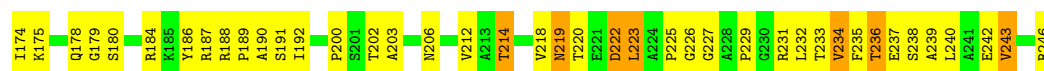
- Molecule 1: 23S ribosomal rna



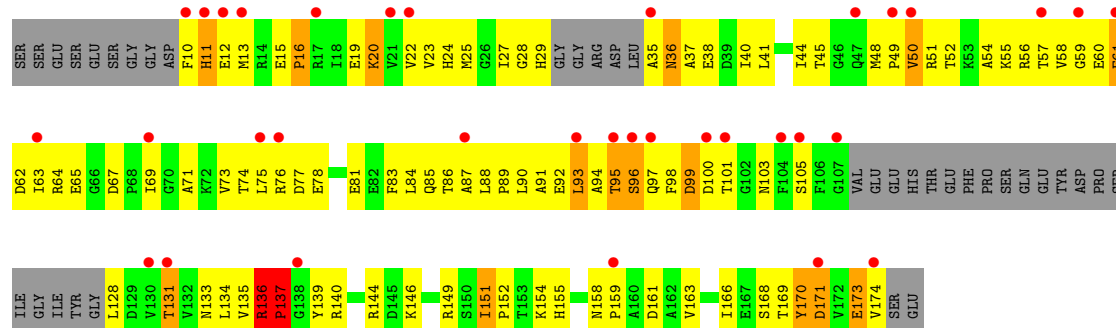
C2104	A2007	A1909	G1820	G1730	G1643	C1558	A1463	A1358	C1253	U185	A1086	G	C905
C2105	U2008	A1910	U1825	G1731	C1644	A1559	U1464	A1359	G1260	C1186	G1087	G	C906
C2106	G2009	U1915	U1826	A1732	U1645	U	C1467	C1360	A1261	U1187	A1088	A	G911
U2107	A2010	C1916	G1827	G1733	G1647	U1561	C1467	C1361	U1189	A1188	U	G	A912
A2108	A2011	C1917	G1828	C1734	C1651	G1562	A1471	U1362	G1265	A1189	A1097	C	A913
U2109	U2012	U1918	A1829	C1735	C1651	G1563	A1472	U1368	U1266	A1190	U1109	G	U917
G2111	G2013	A1919	A1830	A1736	U1654	C1564	U1473	U1368	U1267	A1191	G1110	G	G918
A2112	G2014	C1920	C1834	A1737	U1655	C1565	C1474	U1368	C1268	A1192	U	C	U919
G2113	U2016	A1921	U1835	C1738	A1656	C1566	C1474	U1368	U1269	A1193	G	C	C920
C2114	U2016	A1922	U1836	C1738	A1657	C1567	C1477	A1372	U1270	G1195	A	C	G921
U2115	A2019	G1923	A1839	U1741	A1657	U1569	U1478	G1376	U1270	C1196	A	A	G922
U2116	A2022	G1924	A1840	A1742	A1658	U1570	U1478	G1377	U1270	G1197	C999	A	A923
C2119	U2120	G1925	A1845	G1743	A1659	A1572	C1483	U1380	C1289	U1198	U1003	A	A924
U2120	C2026	G1926	U1846	U1749	G1660	A1573	A1484	U1380	C1289	U1199	U1003	A	G925
G2121	U2027	A1929	A1847	C1750	C1666	C1574	A1485	U1381	U1297	A1200	U1003	A	A926
C2122	U2028	G1930	G1848	G1751	A1667	A1580	U1488	U1382	U1297	A1201	A1006	A	A927
A2123	C2029	A1931	G1849	G1752	U1668	G1589	U1488	U1383	U1298	A1202	A1007	A	A928
G2124	U2033	G1932	U1850	C1753	A1669	U1590	A1494	G1385	G1299	G1203	C1008	A	A929
U2128	U2034	G1933	A1851	A1754	G1670	G1591	C1495	G1387	U1304	U1205	C1009	A	U932
G2134	A2039	C1940	A1852	A1755	U1677	G1592	C1496	U1388	C1305	U1206	A1013	A	G941
A2135	U2040	A1941	G1855	A1759	U1678	C1593	G1496	U1389	U1306	A1207	A1014	A	U942
G2136	G2044	C1943	A1856	C1762	G1680	U1596	U1498	G1390	A1307	U1208	A1015	A	A943
A	C2047	U1951	A1857	U1766	G1681	A1597	U1500	A1391	A1308	C1209	U1016	A	G948
C	U2050	U	U1858	A1767	A1682	A1598	A1501	A1392	U1309	G1210	C1023	A	U949
U	G2050	A	U1859	C1768	G1683	U1599	U1502	A1393	A1310	G1211	G1024	A	G950
G	U2051	C	U1860	C1769	A1684	G1600	A1504	A1394	C1311	C1212	C1024	A	A951
G	U2052	C	U1861	U1770	A1685	G1601	U1505	A1407	A1312	G1213	C1024	A	G952
U	U2053	U	U1862	C1772	G1686	C1602	U1506	U1408	A1313	G1214	C1024	A	G953
U	A2054	U	G1868	U1771	C1687	G1603	C1512	U1412	G1316	G1216	U1027	A	U954
C	U2055	U	A1869	C1772	G1688	G1605	C1513	U1417	G1324	G1217	U1029	A	A955
C	U2056	U	U1870	G1773	C1692	G1609	C1514	U1422	G1325	U1218	G1038	A	G958
C	U2057	U	U1871	A1776	U1696	G1610	A1515	C1423	A1328	U1219	U1041	A	G959
U	G2063	A	C1872	A1777	U1697	G1611	A1516	A1424	A1329	G1226	U1042	A	A961
U	U2064	C	G1873	A1778	C1699	A1612	U1517	U1427	A1330	C1229	C1043	A	C962
G	G2068	C	U1874	A1779	C1700	G1613	U1523	A1427	A1331	U1234	G1044	A	G968
C	C2071	U	U1875	C1787	A1701	G1614	U1524	A1430	C1332	G1235	G1045	A	U970
G	G2072	U	G1878	U1788	U1702	A1615	A1525	G1430	C1333	U1236	C1051	A	G
U	G2073	A	C1880	G1795	G1706	A1616	A1526	U1434	C1334	U1237	G1052	A	U
C	A2074	G	C1881	A1796	G1707	C1617	A1527	U1435	C1335	U1238	G1053	A	G
A	U2081	U	C1882	A1797	U1710	A1624	U1528	C1436	U1336	G1239	G1054	A	U
G	C2089	U	G1883	C1798	A1711	U1625	U1530	U1440	A1337	G1240	U1056	A	C
U	U2090	U	A1884	U1804	A1712	A1626	U1531	A1341	G1340	A1241	A1057	A	C
A	G2091	U	U1885	G1805	G1713	G1627	C1534	C1342	A1341	A1242	A1058	A	C
G	G2092	U	G1886	G1806	C1715	G1628	C1535	A1441	C1343	U1243	C1059	A	C
G	C2093	U	U1887	C1715	G1718	U1635	C1536	A1442	G1344	A1244	C1060	A	C
U	G2094	U	U1888	C1716	G1719	G1636	U1543	A1448	A1345	A1245	C1060	A	C
A	A2095	U	G1889	U1813	G1814	G1637	U1544	A1449	U1346	A1246	G1072	A	U
G	A2096	U	G1902	G1815	C1816	U1638	C1545	C1451	U1347	A1247	C1072	A	C
C	U2100	U	U1903	C1817	U1722	U1639	C1546	U1461	G1351	A1248	A1079	A	C
A	A2101	U	A1904	U1817	G1723	U1640	C1547	U1462	A1352	U1249	A1080	A	G
G	G2102	U	U1907	C1818	G1724	A1641	C1548	U1463	A1353	C1250	A1081	A	G
A	A2103	U	G1908	G1819	C1725	A1642	C1549	U1464	C1354	C1251	A1081	A	A

• Molecule 4: 50S ribosomal protein L2P

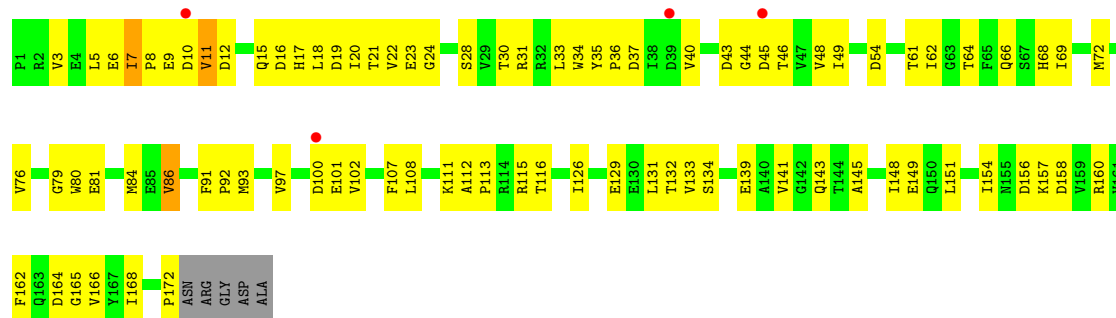




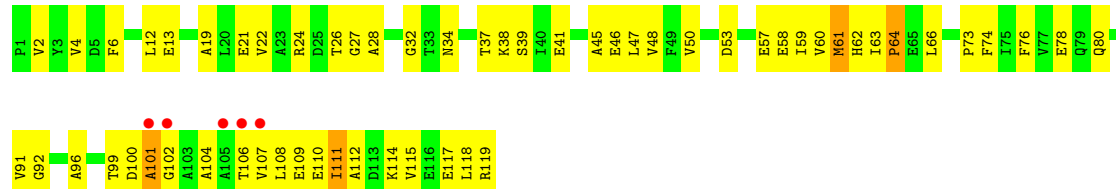
• Molecule 7: 50S ribosomal protein L5P



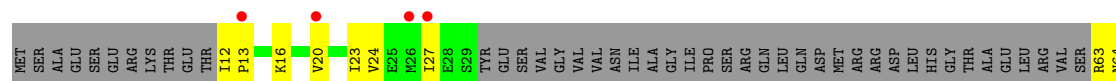
• Molecule 8: 50S ribosomal protein L6P

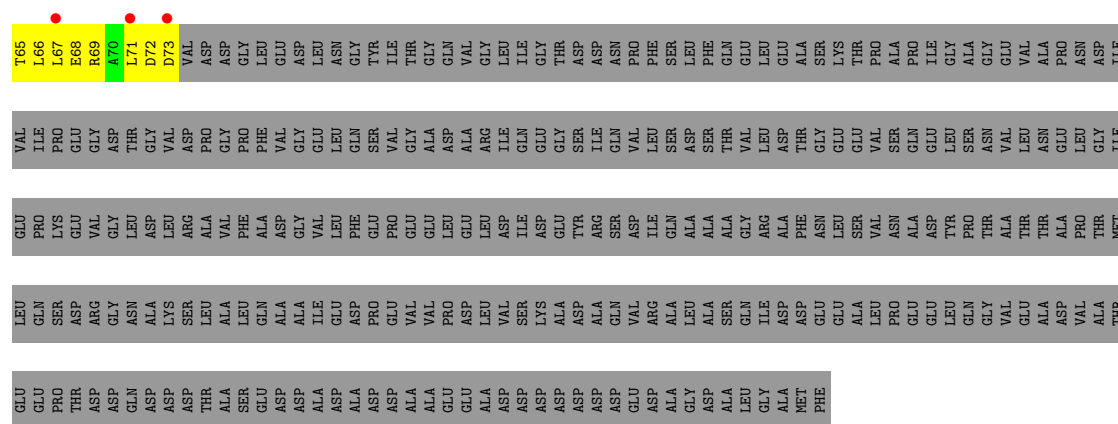


• Molecule 9: 50S ribosomal protein L7Ae

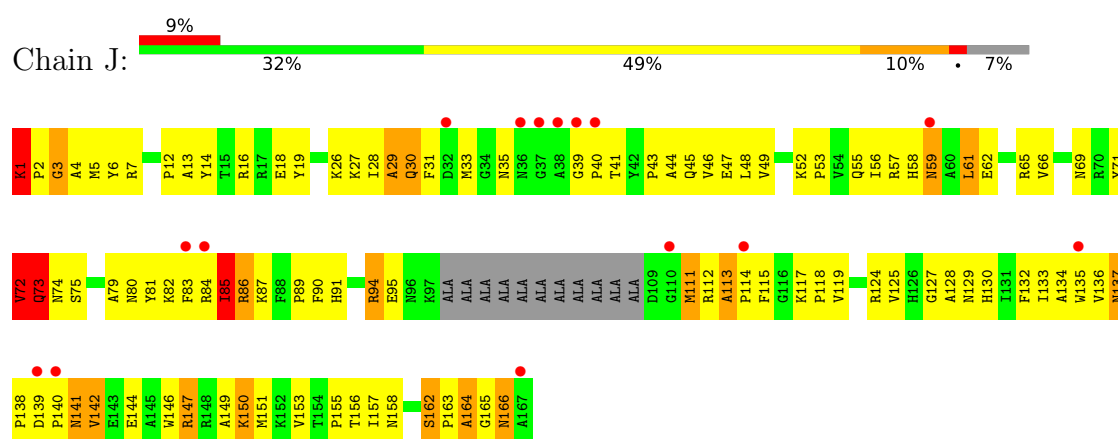


• Molecule 10: Acidic ribosomal protein P0 homolog

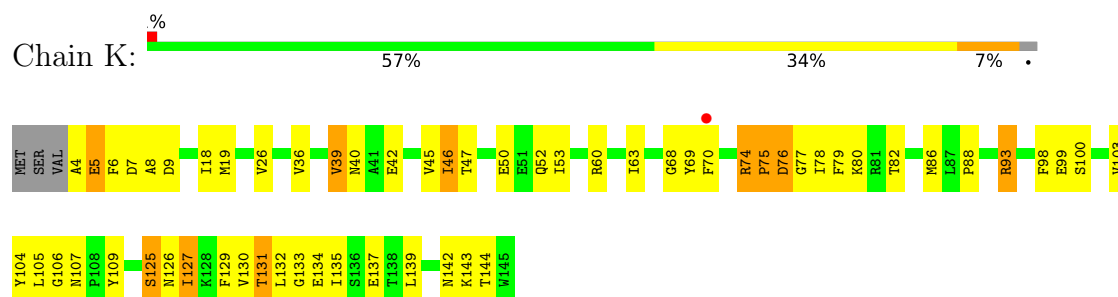




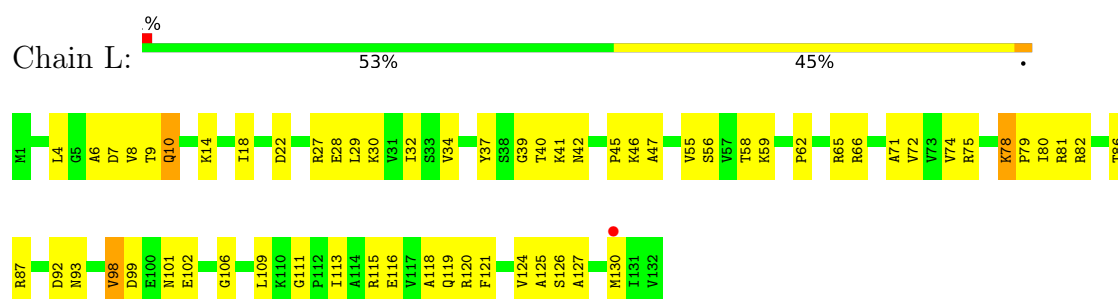
- Molecule 11: L10 Ribosomal Protein



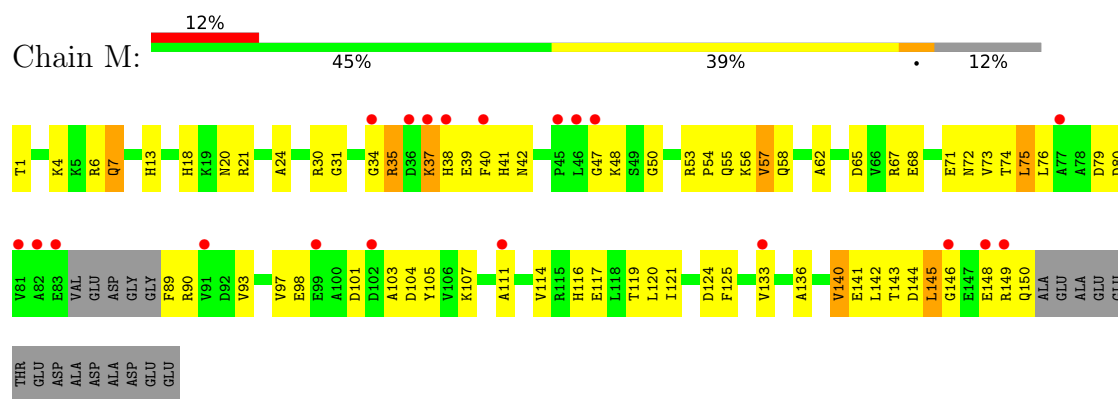
- Molecule 12: 50S ribosomal protein L13P



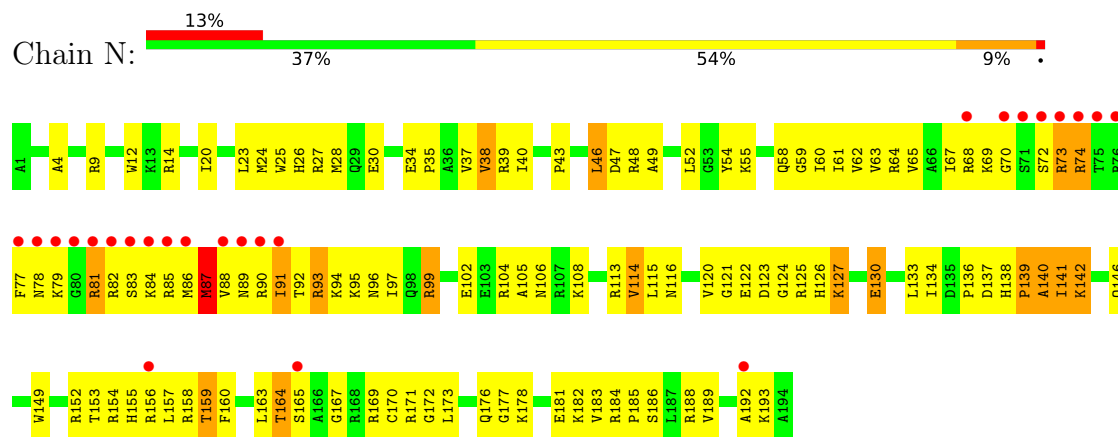
- Molecule 13: 50S ribosomal protein L14P



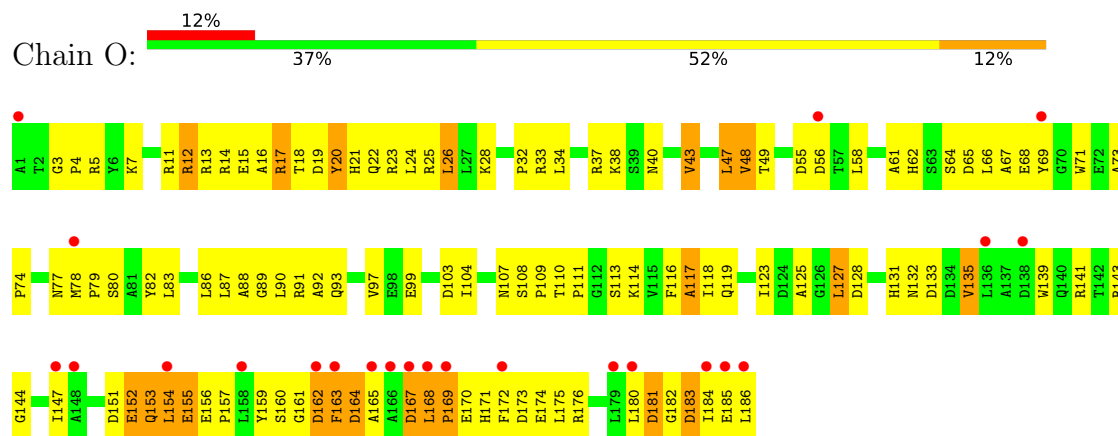
- Molecule 14: 50S ribosomal protein L15P



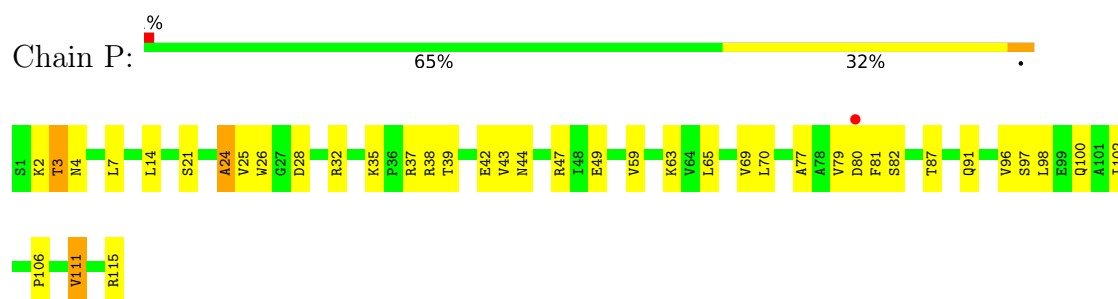
• Molecule 15: L15 Ribosomal Protein



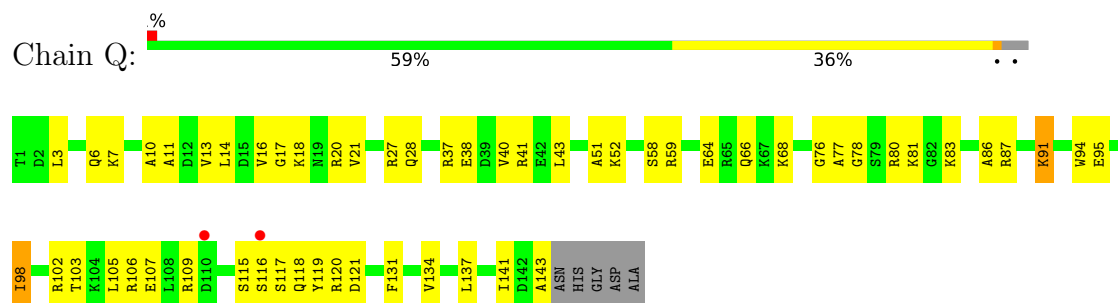
• Molecule 16: 50S ribosomal protein L18P



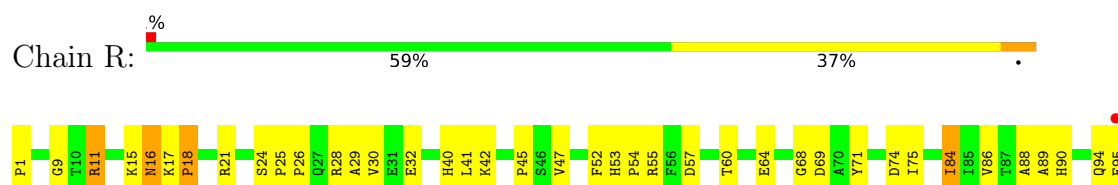
• Molecule 17: 50S ribosomal protein L18e



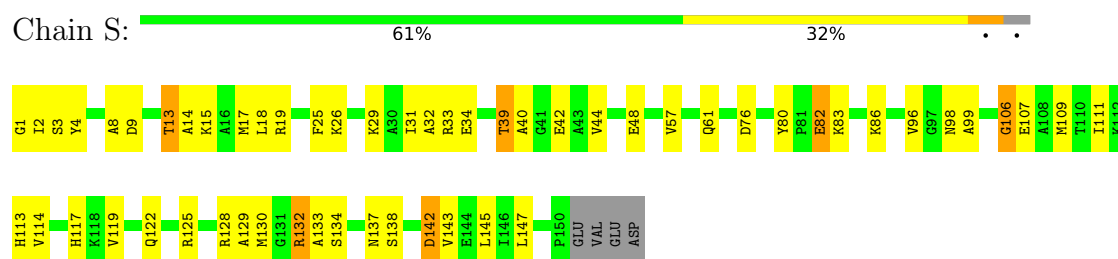
- Molecule 18: 50S ribosomal protein L19E



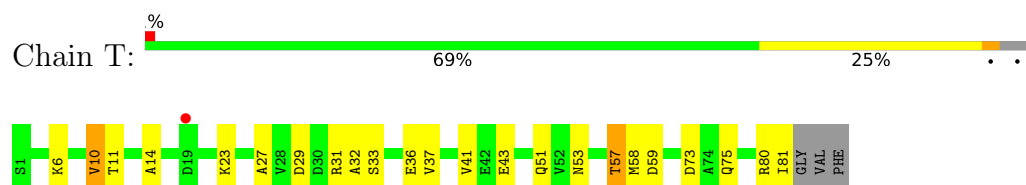
- Molecule 19: 50S ribosomal protein L21e



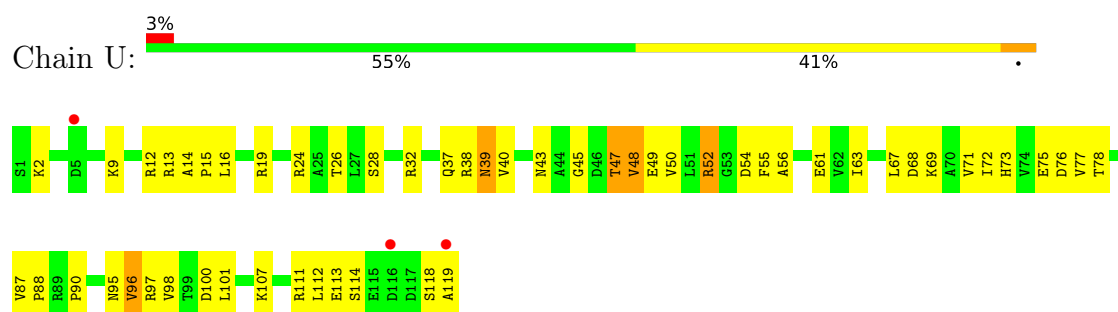
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P

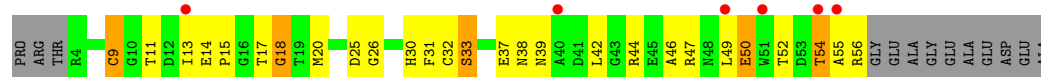


- Molecule 22: 50S ribosomal protein L24P

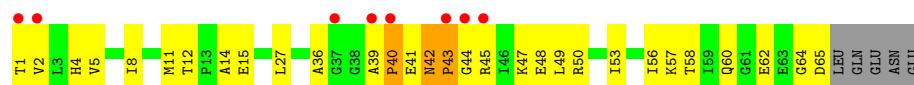


- Molecule 23: 50S ribosomal protein L24E

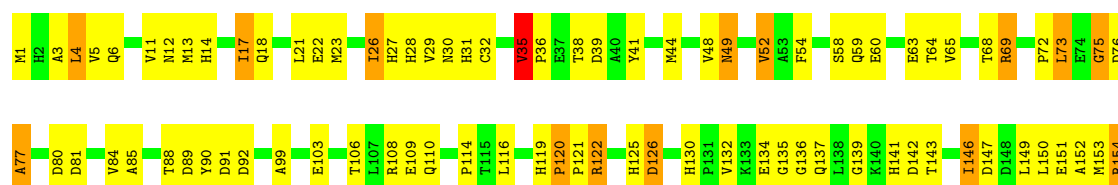




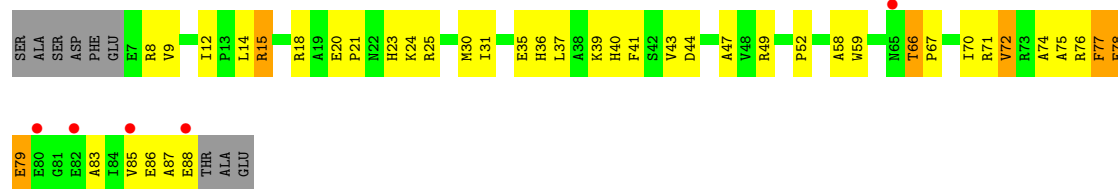
- Molecule 24: 50S ribosomal protein L29P



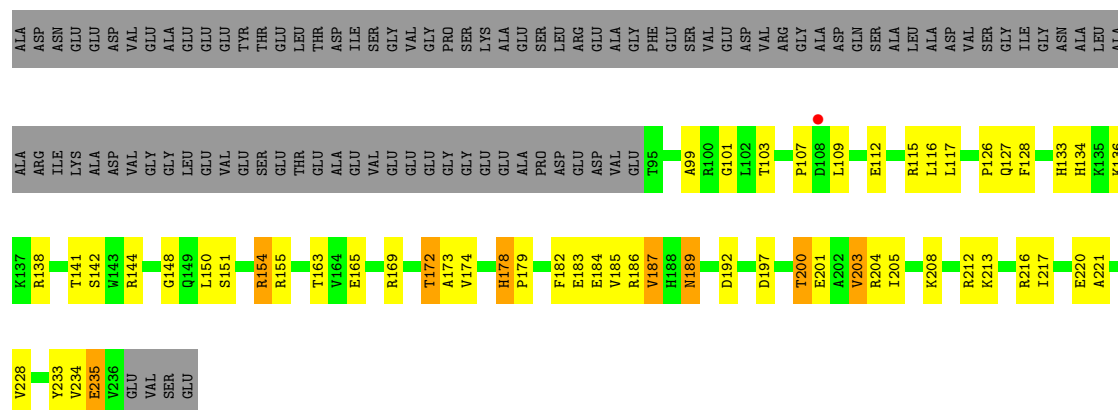
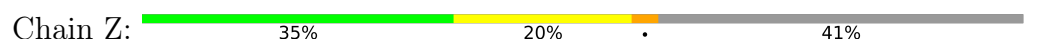
- Molecule 25: 50S ribosomal protein L30P



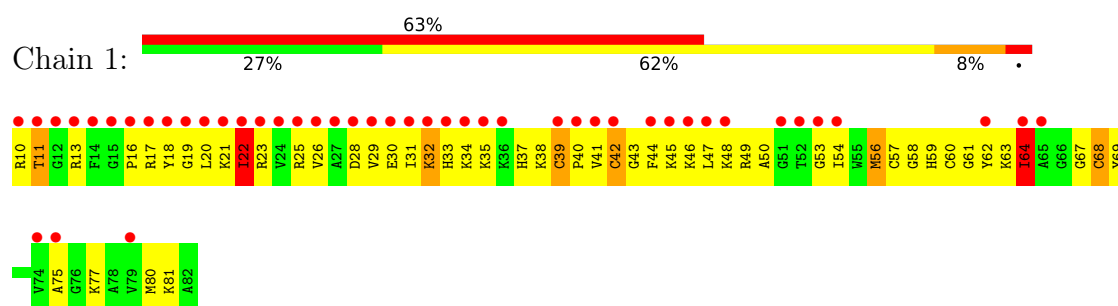
- Molecule 26: 50S ribosomal protein L31e



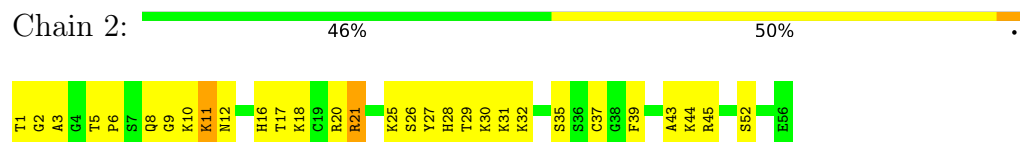
- Molecule 27: 50S ribosomal protein L32E



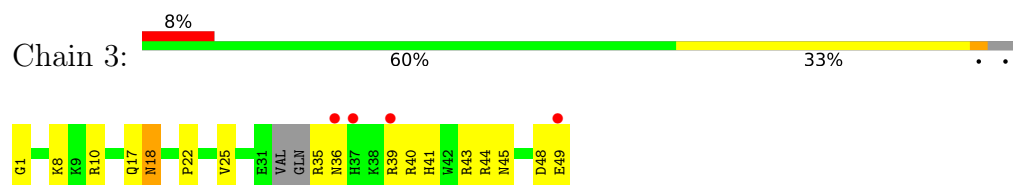
- Molecule 28: L37Ae 50S ribosomal protein



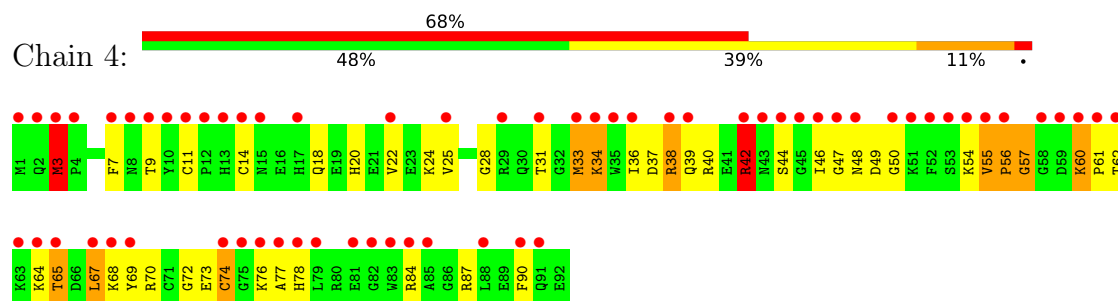
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S 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	213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.98 20.00 – 2.98	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.98) 91.5 (20.00-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.251 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: NA, CL, CD, PPU, MG, K

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	0.50	1/66076 (0.0%)	0.72	41/103052 (0.0%)
2	B	0.48	0/2905	0.79	7/4528 (0.2%)
3	5	1.66	0/43	2.37	2/64 (3.1%)
4	C	0.59	0/1787	1.13	8/2409 (0.3%)
5	D	0.58	0/2689	1.11	19/3652 (0.5%)
6	E	0.62	0/1883	1.11	10/2551 (0.4%)
7	F	0.46	0/1111	0.99	6/1498 (0.4%)
8	G	0.57	0/1382	0.96	2/1880 (0.1%)
9	H	0.47	0/896	0.95	2/1219 (0.2%)
10	I	0.49	0/241	0.89	0/324
11	J	0.62	0/1246	1.31	16/1686 (0.9%)
12	K	0.62	0/1135	1.04	6/1530 (0.4%)
13	L	0.60	0/1003	1.16	8/1351 (0.6%)
14	M	0.60	1/1126 (0.1%)	1.13	7/1504 (0.5%)
15	N	0.78	0/1633	1.23	15/2180 (0.7%)
16	O	0.50	0/1473	1.16	12/1999 (0.6%)
17	P	0.61	0/873	1.06	6/1181 (0.5%)
18	Q	0.55	0/1143	0.97	2/1521 (0.1%)
19	R	0.54	0/748	1.16	8/1005 (0.8%)
20	S	0.65	0/1172	1.08	8/1578 (0.5%)
21	T	0.50	0/648	0.99	1/875 (0.1%)
22	U	0.50	0/957	1.09	5/1289 (0.4%)
23	V	0.66	0/417	1.13	4/562 (0.7%)
24	W	0.50	0/502	1.01	2/675 (0.3%)
25	X	0.70	0/1218	1.07	8/1655 (0.5%)
26	Y	0.63	0/664	1.08	1/895 (0.1%)
27	Z	0.59	0/1146	1.05	5/1536 (0.3%)
28	1	0.97	1/575 (0.2%)	1.24	5/763 (0.7%)
29	2	0.65	0/437	1.12	4/578 (0.7%)
30	3	0.58	0/398	0.84	0/527
31	4	1.16	2/771 (0.3%)	1.18	6/1024 (0.6%)
All	All	0.54	5/98298 (0.0%)	0.84	226/147091 (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	143
2	B	1	4
All	All	2	147

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	22	ILE	CA-CB	6.87	1.61	1.54
31	4	33	MET	SD-CE	6.71	1.96	1.79
31	4	3	MET	SD-CE	6.48	1.95	1.79
1	A	2487	C	O5'-C5'	6.33	1.51	1.42
14	M	37	LYS	CA-C	5.20	1.55	1.52

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-14.52	64.43	108.00
1	A	1164	U	OP2-P-O3'	-14.52	64.44	108.00
2	B	3024	U	C2'-C3'-O3'	14.02	130.52	109.50
15	N	141	ILE	N-CA-C	-13.56	100.91	111.90
1	A	1563	G	C2'-C3'-O3'	13.34	129.51	109.50
1	A	1979	G	C2'-C3'-O3'	12.52	128.28	109.50
11	J	141	ASN	N-CA-C	-12.37	98.29	113.50
11	J	74	ASN	N-CA-C	-11.76	95.98	113.61
16	O	135	VAL	N-CA-C	-11.66	101.79	113.10
3	5	75	C	C1'-C2'-O2'	10.22	123.74	108.40
3	5	75	C	C3'-C2'-O2'	9.90	125.55	110.70
11	J	156	THR	N-CA-C	-9.46	96.49	110.48
15	N	74	ARG	N-CA-C	9.39	124.60	107.99
1	A	1563	G	C4'-C3'-O3'	9.04	122.97	109.40
2	B	3024	U	C4'-C3'-O3'	9.00	122.91	109.40
7	F	136	ARG	CA-C-N	8.87	130.93	119.84
7	F	136	ARG	C-N-CA	8.87	130.93	119.84
16	O	153	GLN	N-CA-C	-8.59	101.52	113.20
5	D	151	VAL	CA-C-N	8.58	127.89	118.97
5	D	151	VAL	C-N-CA	8.58	127.89	118.97
11	J	137	ASN	N-CA-C	-8.15	99.44	110.36
6	E	175	LYS	N-CA-C	8.11	120.78	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	2	21	ARG	N-CA-C	8.06	121.23	111.40
1	A	1942	A	C5'-C4'-C3'	8.05	128.07	116.00
16	O	169	PRO	N-CA-C	-8.00	104.19	114.03
8	G	11	VAL	N-CA-C	7.96	121.53	109.20
22	U	52	ARG	N-CA-C	7.93	123.73	113.18
16	O	13	ARG	N-CA-C	-7.90	103.25	113.12
31	4	55	VAL	CA-C-N	7.82	129.62	119.84
31	4	55	VAL	C-N-CA	7.82	129.62	119.84
4	C	48	ASP	CA-C-N	7.76	127.48	119.56
4	C	48	ASP	C-N-CA	7.76	127.48	119.56
7	F	151	ILE	CA-C-N	7.63	128.07	119.83
7	F	151	ILE	C-N-CA	7.63	128.07	119.83
5	D	157	LYS	N-CA-C	-7.58	104.64	114.04
11	J	147	ARG	N-CA-C	-7.58	103.03	111.82
14	M	47	GLY	N-CA-C	7.58	119.73	112.08
21	T	57	THR	N-CA-C	7.58	120.78	110.55
9	H	62	HIS	N-CA-C	7.46	120.48	111.82
1	A	834	G	C2'-C3'-O3'	-7.29	102.77	113.70
19	R	47	VAL	CA-C-N	7.25	126.51	118.97
19	R	47	VAL	C-N-CA	7.25	126.51	118.97
14	M	57	VAL	N-CA-C	-7.25	105.76	112.43
5	D	265	LEU	N-CA-C	7.23	121.19	110.48
7	F	100	ASP	N-CA-C	-7.11	104.61	113.28
15	N	87	MET	N-CA-C	7.09	120.51	110.23
13	L	111	GLY	CA-C-N	7.06	127.51	120.52
13	L	111	GLY	C-N-CA	7.06	127.51	120.52
9	H	111	ILE	N-CA-C	-6.95	103.70	110.72
15	N	73	ARG	N-CA-C	-6.90	96.55	108.56
19	R	84	ILE	N-CA-C	6.83	117.72	107.75
22	U	87	VAL	CA-C-N	6.72	126.48	119.76
22	U	87	VAL	C-N-CA	6.72	126.48	119.76
2	B	3039	U	N1-C1'-C2'	6.69	122.03	112.00
20	S	34	GLU	N-CA-C	6.68	118.64	111.36
15	N	70	GLY	N-CA-C	6.62	124.75	112.77
14	M	7	GLN	N-CA-C	6.58	119.46	111.82
6	E	78	ARG	N-CA-C	6.55	118.82	108.79
1	A	2419	U	N1-C1'-C2'	6.52	121.77	112.00
27	Z	183	GLU	N-CA-C	-6.51	99.08	109.76
29	2	3	ALA	N-CA-C	-6.48	105.36	113.20
1	A	1120	U	C5'-C4'-C3'	-6.47	106.29	116.00
11	J	113	ALA	CA-C-N	6.45	127.61	120.45
11	J	113	ALA	C-N-CA	6.45	127.61	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2012	U	N1-C1'-C2'	6.43	121.65	112.00
1	A	389	G	C5'-C4'-C3'	-6.42	106.38	116.00
25	X	143	THR	N-CA-C	-6.39	104.39	111.36
19	R	47	VAL	N-CA-C	6.38	113.87	107.55
5	D	213	GLY	CA-C-N	6.37	125.59	118.97
5	D	213	GLY	C-N-CA	6.37	125.59	118.97
12	K	75	PRO	N-CA-C	-6.34	105.94	113.86
15	N	139	PRO	N-CA-C	-6.32	101.55	111.34
20	S	122	GLN	N-CA-C	-6.28	98.93	108.67
1	A	2726	U	N1-C1'-C2'	6.24	121.35	112.00
24	W	42	ASN	CA-C-N	6.24	127.63	119.84
24	W	42	ASN	C-N-CA	6.24	127.63	119.84
15	N	127	LYS	N-CA-C	-6.23	98.10	108.75
31	4	60	LYS	N-CA-C	-6.18	102.28	110.07
17	P	2	LYS	N-CA-C	-6.18	102.21	110.55
5	D	111	ARG	N-CA-C	-6.17	105.75	113.28
31	4	42	ARG	N-CA-C	6.11	118.44	111.11
11	J	155	PRO	N-CA-C	6.11	120.58	111.41
28	1	39	CYS	N-CA-C	6.11	117.40	109.64
17	P	24	ALA	N-CA-C	-6.11	106.81	114.56
5	D	154	VAL	CA-C-N	6.07	127.43	119.84
5	D	154	VAL	C-N-CA	6.07	127.43	119.84
15	N	90	ARG	N-CA-C	6.05	120.50	113.18
13	L	8	VAL	N-CA-C	6.04	117.17	108.48
16	O	117	ALA	N-CA-C	-6.04	104.62	111.14
1	A	2096	A	N9-C1'-C2'	6.03	121.05	112.00
16	O	133	ASP	N-CA-C	6.03	118.62	111.33
6	E	219	ASN	N-CA-C	6.00	118.34	109.69
12	K	9	ASP	N-CA-C	-6.00	104.86	111.82
29	2	11	LYS	N-CA-C	5.96	118.87	109.39
15	N	91	ILE	N-CA-C	-5.96	101.88	109.80
25	X	126	ASP	N-CA-C	5.95	120.23	113.15
1	A	1450	C	C2'-C3'-O3'	-5.95	104.78	113.70
4	C	207	GLN	N-CA-C	5.94	118.36	108.20
14	M	145	LEU	N-CA-C	-5.94	104.88	111.71
13	L	71	ALA	N-CA-C	5.92	117.85	108.79
1	A	129	A	C2'-C3'-O3'	5.91	122.56	113.70
20	S	142	ASP	N-CA-C	-5.88	100.31	109.72
17	P	82	SER	N-CA-C	-5.86	102.76	110.43
1	A	2485	A	C3'-C2'-O2'	5.80	119.39	110.70
18	Q	95	GLU	N-CA-C	-5.79	105.05	111.36
1	A	921	G	N9-C1'-C2'	5.77	120.65	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	3	GLY	N-CA-C	-5.74	107.22	114.16
5	D	251	VAL	CA-C-N	5.72	126.99	119.84
5	D	251	VAL	C-N-CA	5.72	126.99	119.84
1	A	871	G	C5'-C4'-O4'	-5.71	101.23	109.80
11	J	1	LYS	CA-C-N	5.71	125.61	119.85
11	J	1	LYS	C-N-CA	5.71	125.61	119.85
14	M	20	ASN	N-CA-C	5.69	119.86	111.04
17	P	69	VAL	N-CA-C	5.69	116.68	108.48
15	N	92	THR	N-CA-C	-5.68	100.42	109.23
1	A	1723	G	C4'-C3'-O3'	-5.68	104.48	113.00
15	N	114	VAL	N-CA-C	5.67	116.33	108.84
4	C	133	ARG	N-CA-C	-5.67	106.20	113.23
25	X	69	ARG	N-CA-C	5.67	120.01	112.30
16	O	168	LEU	N-CA-C	5.66	120.98	108.64
29	2	43	ALA	N-CA-C	-5.63	105.22	111.36
6	E	186	TYR	N-CA-C	5.61	118.39	110.14
20	S	137	ASN	N-CA-C	5.61	118.84	110.14
1	A	1738	C	O4'-C4'-C3'	-5.61	98.39	104.00
15	N	121	GLY	N-CA-C	5.60	120.02	112.17
19	R	68	GLY	N-CA-C	-5.60	99.90	113.18
1	A	1651	C	N1-C1'-C2'	5.60	120.40	112.00
5	D	222	LYS	N-CA-C	-5.60	101.74	110.42
19	R	29	ALA	N-CA-C	-5.59	106.41	113.18
16	O	20	TYR	N-CA-C	5.59	118.30	111.82
25	X	35	VAL	CA-C-N	5.57	125.47	119.85
25	X	35	VAL	C-N-CA	5.57	125.47	119.85
17	P	43	VAL	N-CA-C	5.56	116.59	108.53
5	D	156	LYS	N-CA-C	5.55	117.90	110.35
11	J	7	ARG	N-CA-C	5.55	119.67	113.01
23	V	33	SER	N-CA-C	5.55	116.70	108.60
5	D	76	THR	CA-C-N	5.54	126.08	120.38
5	D	76	THR	C-N-CA	5.54	126.08	120.38
26	Y	79	GLU	N-CA-C	5.52	120.01	113.28
13	L	78	LYS	CA-C-N	5.51	125.82	119.92
13	L	78	LYS	C-N-CA	5.51	125.82	119.92
5	D	282	GLY	N-CA-C	-5.51	108.52	115.08
15	N	142	LYS	N-CA-C	-5.49	105.39	111.71
1	A	1359	U	N1-C1'-C2'	5.49	120.24	112.00
2	B	3039	U	C4'-C3'-O3'	-5.49	104.77	113.00
12	K	68	GLY	N-CA-C	5.49	119.53	112.18
23	V	18	GLY	N-CA-C	5.48	118.96	112.33
5	D	154	VAL	N-CA-C	5.46	112.95	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	88	PRO	N-CA-C	-5.45	102.13	112.33
20	S	76	ASP	N-CA-C	5.45	119.42	112.12
6	E	80	VAL	CA-C-N	5.45	126.65	119.84
6	E	80	VAL	C-N-CA	5.45	126.65	119.84
6	E	89	ALA	N-CA-C	5.43	116.88	111.07
5	D	217	ARG	N-CA-C	5.43	117.28	111.36
2	B	3003	A	C3'-C2'-O2'	-5.43	106.46	114.60
31	4	72	GLY	N-CA-C	5.42	120.41	114.40
4	C	118	PHE	N-CA-C	5.41	118.92	110.32
1	A	1839	A	C4'-C3'-O3'	-5.41	104.89	113.00
22	U	16	LEU	N-CA-C	5.41	117.60	111.11
1	A	470	U	N1-C1'-C2'	5.38	120.07	112.00
11	J	29	ALA	N-CA-C	5.37	116.82	111.07
1	A	1819	G	C5'-C4'-C3'	5.34	124.01	116.00
1	A	917	U	C5'-C4'-C3'	5.34	124.01	116.00
12	K	39	VAL	N-CA-C	5.33	117.00	108.89
16	O	48	VAL	N-CA-C	5.30	117.19	108.97
22	U	78	THR	N-CA-C	5.30	116.34	108.86
14	M	42	ASN	N-CA-C	5.29	119.02	112.24
1	A	1942	A	C5'-C4'-O4'	5.28	117.73	109.80
1	A	2121	G	C4'-C3'-O3'	-5.28	105.08	113.00
1	A	2071	C	N1-C1'-C2'	5.28	119.92	112.00
27	Z	221	ALA	N-CA-C	-5.28	105.44	111.14
20	S	3	SER	N-CA-C	-5.27	101.28	109.24
28	1	32	LYS	N-CA-C	-5.27	105.62	111.36
25	X	75	GLY	N-CA-C	5.27	117.41	112.04
4	C	70	ALA	N-CA-C	5.26	117.21	109.42
1	A	1940	C	C4'-C3'-O3'	-5.26	105.11	113.00
1	A	1592	G	N9-C1'-C2'	5.26	119.89	112.00
25	X	17	ILE	N-CA-C	-5.25	105.28	111.00
8	G	48	VAL	N-CA-C	5.24	115.44	108.11
23	V	50	GLU	N-CA-C	5.24	117.73	111.71
19	R	17	LYS	N-CA-C	-5.24	101.80	109.50
27	Z	101	GLY	N-CA-C	5.23	123.44	112.45
1	A	959	C	C4'-C3'-O3'	-5.23	105.16	113.00
11	J	73	GLN	N-CA-C	-5.22	104.39	111.55
7	F	137	PRO	N-CA-C	5.22	123.22	112.47
19	R	86	VAL	N-CA-C	5.21	116.16	108.45
28	1	64	ILE	N-CA-C	5.20	117.10	108.99
4	C	213	LYS	N-CA-C	5.19	118.88	112.54
13	L	46	LYS	N-CA-C	5.19	117.95	109.59
1	A	2090	G	N9-C1'-C2'	5.19	119.79	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3103	A	C5'-C4'-O4'	5.19	117.59	109.80
14	M	37	LYS	N-CA-C	5.19	116.37	108.12
1	A	1189	A	N9-C1'-C2'	5.18	119.76	112.00
1	A	2431	C	C3'-C2'-O2'	5.18	118.46	110.70
23	V	54	THR	N-CA-C	-5.16	104.73	111.02
13	L	124	VAL	N-CA-C	-5.15	105.52	110.72
1	A	1559	A	C2'-C3'-O3'	5.15	121.42	113.70
5	D	175	LEU	N-CA-C	-5.14	105.57	111.07
18	Q	43	LEU	N-CA-C	-5.14	106.27	112.54
27	Z	178	HIS	N-CA-C	-5.12	102.59	110.01
15	N	159	THR	N-CA-C	5.11	117.25	111.11
31	4	67	LEU	N-CA-C	5.10	117.62	109.81
15	N	176	GLN	N-CA-C	-5.10	107.11	113.38
1	A	1164	U	O3'-P-O5'	5.10	111.64	104.00
25	X	49	ASN	N-CA-C	5.10	121.66	110.80
20	S	57	VAL	CA-C-N	-5.08	114.34	119.83
20	S	57	VAL	C-N-CA	-5.08	114.34	119.83
6	E	64	GLY	N-CA-C	5.08	120.52	114.48
16	O	171	HIS	N-CA-C	-5.07	105.88	111.71
2	B	3002	U	C4'-C3'-O3'	5.06	117.00	109.40
17	P	79	VAL	N-CA-C	-5.06	105.61	110.72
11	J	85	ILE	N-CA-C	-5.06	99.88	107.37
1	A	2291	A	N9-C1'-C2'	5.05	119.58	112.00
16	O	131	HIS	N-CA-C	5.05	114.96	108.34
6	E	150	THR	N-CA-C	-5.05	105.66	111.07
4	C	222	GLY	N-CA-C	-5.04	107.89	113.79
1	A	1504	A	C1'-O4'-C4'	-5.04	104.86	109.90
12	K	100	SER	N-CA-C	-5.04	106.97	112.72
16	O	165	ALA	N-CA-C	-5.03	107.21	113.55
1	A	10	U	N1-C1'-C2'	5.03	119.54	112.00
1	A	2564	G	N9-C1'-C2'	5.03	119.54	112.00
11	J	111	MET	N-CA-C	-5.03	106.74	112.92
28	1	56	MET	CA-C-N	-5.01	116.03	123.05
28	1	56	MET	C-N-CA	-5.01	116.03	123.05
27	Z	187	VAL	N-CA-C	5.01	115.33	108.12
6	E	9	ASP	N-CA-C	-5.01	107.56	113.97

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

All (147) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	A	Sidechain
1	A	1027	G	Sidechain
1	A	1030	U	Sidechain
1	A	1038	G	Sidechain
1	A	1125	U	Sidechain
1	A	115	U	Sidechain
1	A	1191	A	Sidechain
1	A	1206	U	Sidechain
1	A	1226	G	Sidechain
1	A	1236	A	Sidechain
1	A	1244	U	Sidechain
1	A	1260	G	Sidechain
1	A	1261	A	Sidechain
1	A	1266	U	Sidechain
1	A	1297	U	Sidechain
1	A	1298	U	Sidechain
1	A	1309	U	Sidechain
1	A	1332	C	Sidechain
1	A	1347	U	Sidechain
1	A	1368	U	Sidechain
1	A	1376	G	Sidechain
1	A	1387	G	Sidechain
1	A	1412	U	Sidechain
1	A	1417	G	Sidechain
1	A	1430	G	Sidechain
1	A	1467	C	Sidechain
1	A	1478	U	Sidechain
1	A	1503	U	Sidechain
1	A	1531	U	Sidechain
1	A	1635	U	Sidechain
1	A	1645	U	Sidechain
1	A	1647	G	Sidechain
1	A	1681	G	Sidechain
1	A	1684	A	Sidechain
1	A	1688	G	Sidechain
1	A	1696	U	Sidechain
1	A	1701	A	Sidechain
1	A	1706	G	Sidechain
1	A	171	C	Sidechain
1	A	1736	A	Sidechain
1	A	1750	C	Sidechain
1	A	176	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1777	G	Sidechain
1	A	1818	C	Sidechain
1	A	182	G	Sidechain
1	A	1826	C	Sidechain
1	A	1828	G	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1846	U	Sidechain
1	A	1848	G	Sidechain
1	A	1878	G	Sidechain
1	A	1933	G	Sidechain
1	A	1972	U	Sidechain
1	A	1978	A	Sidechain
1	A	2022	A	Sidechain
1	A	2026	C	Sidechain
1	A	2063	U	Sidechain
1	A	2102	G	Sidechain
1	A	211	U	Sidechain
1	A	2110	G	Sidechain
1	A	2119	C	Sidechain
1	A	2124	G	Sidechain
1	A	214	U	Sidechain
1	A	22	U	Sidechain
1	A	224	U	Sidechain
1	A	2279	G	Sidechain
1	A	2306	U	Sidechain
1	A	2308	U	Sidechain
1	A	2313	C	Sidechain
1	A	2336	G	Sidechain
1	A	2390	U	Sidechain
1	A	2421	G	Sidechain
1	A	2429	A	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	246	G	Sidechain
1	A	2461	U	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain
1	A	2524	G	Sidechain
1	A	2526	C	Sidechain
1	A	2535	U	Sidechain
1	A	2590	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	26	U	Sidechain
1	A	2620	U	Sidechain
1	A	2621	U	Sidechain
1	A	2630	G	Sidechain
1	A	2634	G	Sidechain
1	A	265	U	Sidechain
1	A	2663	U	Sidechain
1	A	2673	U	Sidechain
1	A	2692	G	Sidechain
1	A	2736	U	Sidechain
1	A	2774	U	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	28	G	Sidechain
1	A	2800	A	Sidechain
1	A	2840	A	Sidechain
1	A	2842	G	Sidechain
1	A	315	G	Sidechain
1	A	321	A	Sidechain
1	A	333	G	Sidechain
1	A	344	C	Sidechain
1	A	395	A	Sidechain
1	A	396	U	Sidechain
1	A	407	A	Sidechain
1	A	435	A	Sidechain
1	A	436	A	Sidechain
1	A	458	G	Sidechain
1	A	459	A	Sidechain
1	A	48	A	Sidechain
1	A	483	C	Sidechain
1	A	502	A	Sidechain
1	A	506	G	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	55	U	Sidechain
1	A	614	U	Sidechain
1	A	619	U	Sidechain
1	A	640	G	Sidechain
1	A	664	U	Sidechain
1	A	676	C	Sidechain
1	A	722	G	Sidechain
1	A	734	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	743	G	Sidechain
1	A	761	A	Sidechain
1	A	764	C	Sidechain
1	A	775	G	Sidechain
1	A	815	U	Sidechain
1	A	816	G	Sidechain
1	A	818	A	Sidechain
1	A	854	G	Sidechain
1	A	873	G	Sidechain
1	A	888	U	Sidechain
1	A	897	A	Sidechain
1	A	898	G	Sidechain
1	A	906	C	Sidechain
1	A	919	U	Sidechain
1	A	932	U	Sidechain
1	A	950	G	Sidechain
1	A	954	U	Sidechain
2	B	3022	G	Sidechain
2	B	3024	U	Sidechain
2	B	3065	A	Sidechain
2	B	3099	U	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	29798	1225	0
2	B	2600	0	1326	83	0
3	5	40	0	22	5	0
4	C	1754	0	1763	131	0
5	D	2624	0	2533	194	0
6	E	1858	0	1816	140	0
7	F	1094	0	1085	142	0
8	G	1357	0	1266	91	0
9	H	885	0	854	64	0
10	I	240	0	231	26	0
11	J	1215	0	1215	160	0
12	K	1119	0	1098	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	993	0	1027	71	0
14	M	1114	0	1072	70	0
15	N	1605	0	1676	189	0
16	O	1444	0	1401	143	0
17	P	864	0	873	40	0
18	Q	1133	0	1127	64	0
19	R	734	0	728	29	0
20	S	1149	0	1122	59	0
21	T	641	0	605	28	0
22	U	949	0	923	51	0
23	V	410	0	368	36	0
24	W	499	0	511	27	0
25	X	1195	0	1137	106	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	65	0
28	1	563	0	601	77	0
29	2	430	0	426	40	0
30	3	393	0	406	30	0
31	4	755	0	732	63	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	2	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	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	2	0	0	0	0
34	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	4	1	0	0	1	0
35	A	7	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	1	0
36	5	37	0	28	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	36	0	0	12	0
38	2	58	0	0	5	0
38	3	37	0	0	4	0
38	4	70	0	0	11	0
38	5	1	0	0	0	0
38	A	5860	0	0	269	0
38	B	146	0	0	15	0
38	C	140	0	0	15	0
38	D	146	0	0	32	0
38	E	176	0	0	34	0
38	F	52	0	0	21	0
38	G	45	0	0	12	0
38	H	32	0	0	9	0
38	I	22	0	0	8	0
38	J	78	0	0	21	0
38	K	54	0	0	4	0
38	L	64	0	0	15	0
38	M	86	0	0	16	0
38	N	138	0	0	26	0
38	O	64	0	0	19	0
38	P	44	0	0	12	0
38	Q	70	0	0	11	0
38	R	57	0	0	5	0
38	S	83	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	T	36	0	0	5	0
38	U	38	0	0	2	0
38	V	22	0	0	5	0
38	W	16	0	0	3	0
38	X	67	0	0	10	0
38	Y	28	0	0	6	0
38	Z	100	0	0	16	0
All	All	98593	0	59556	3265	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 22.

All (3265) 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)
11:J:165:GLY:HA3	38:J:8398:HOH:O	1.43	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13
15:N:164:THR:HG22	15:N:167:GLY:H	1.10	1.12
1:A:1751:G:H2'	1:A:1752:G:H5''	1.30	1.10
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.30	1.10
6:E:236:THR:HG22	6:E:239:ALA:H	1.01	1.09
12:K:19:MET:HE3	12:K:132:LEU:HD11	1.22	1.09
6:E:5:ILE:HD11	6:E:16:VAL:HG23	1.34	1.08
7:F:134:LEU:HD11	7:F:166:ILE:HD11	1.34	1.08
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.26	1.08
28:1:39:CYS:SG	28:1:47:LEU:HD21	1.93	1.08
7:F:25:MET:HE2	7:F:41:LEU:HG	1.34	1.08
22:U:71:VAL:HG11	22:U:90:PRO:HB3	1.34	1.08
1:A:2121:G:OP2	38:A:3007:HOH:O	1.69	1.06
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.38	1.06
1:A:1160:G:H5'	1:A:1161:A:H5'	1.36	1.04
27:Z:200:THR:HG22	27:Z:201:GLU:HG3	1.39	1.04
25:X:149:LEU:HG	25:X:153:MET:HE2	1.39	1.03
1:A:156:C:H5''	15:N:171:ARG:HD3	1.39	1.03
28:1:40:PRO:HD3	28:1:47:LEU:HD11	1.39	1.03
1:A:870:G:H2'	1:A:871:G:H5''	1.40	1.02
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.40	1.02
1:A:2426:G:HI1'	38:A:5552:HOH:O	1.57	1.02
15:N:74:ARG:O	15:N:88:VAL:HG13	1.56	1.02
25:X:88:THR:HB	38:X:6679:HOH:O	1.60	1.01
15:N:24:MET:HE3	15:N:28:MET:HE3	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1835:U:H5	1:A:1840:A:N7	1.58	1.00
15:N:87:MET:HG2	31:4:46:ILE:HG21	1.39	1.00
1:A:1134:G:H4'	11:J:151:MET:HE1	1.42	1.00
7:F:105:SER:HB2	7:F:131:THR:HG23	1.43	1.00
6:E:127:ARG:NH2	6:E:225:PRO:HG2	1.77	0.99
1:A:2466:G:H5''	38:A:3142:HOH:O	1.61	0.99
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.42	0.98
5:D:86:ALA:HA	38:D:8583:HOH:O	1.64	0.98
15:N:35:PRO:HG2	15:N:38:VAL:HG23	1.42	0.98
1:A:1886:A:N3	38:A:4297:HOH:O	1.95	0.97
11:J:86:ARG:HH11	11:J:133:ILE:CG1	1.77	0.97
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.82	0.97
14:M:68:GLU:HA	38:M:8548:HOH:O	1.62	0.97
1:A:1474:C:H6	1:A:1474:C:H5'	1.30	0.97
2:B:3056:A:H2'	2:B:3057:A:H5''	1.45	0.96
21:T:57:THR:HG22	21:T:59:ASP:H	1.24	0.96
13:L:10:GLN:NE2	13:L:10:GLN:H	1.62	0.96
1:A:2717:C:H2'	1:A:2718:C:H5''	1.47	0.96
18:Q:115:SER:H	18:Q:118:GLN:HE21	0.99	0.96
1:A:2467:A:H2'	38:A:4927:HOH:O	1.64	0.95
5:D:321:PRO:HA	38:D:8657:HOH:O	1.66	0.95
1:A:962:C:H1'	16:O:5:ARG:NH1	1.82	0.94
1:A:871:G:H5'	1:A:871:G:H8	1.31	0.94
16:O:47:LEU:HD11	16:O:127:LEU:HD21	1.50	0.94
38:A:4337:HOH:O	15:N:14:ARG:HG2	1.65	0.93
21:T:57:THR:HG22	21:T:59:ASP:N	1.82	0.93
11:J:142:VAL:HG13	38:J:8381:HOH:O	1.68	0.93
26:Y:37:LEU:HD13	26:Y:85:VAL:HG21	1.47	0.93
2:B:3006:C:H5''	16:O:37:ARG:NH1	1.83	0.93
1:A:2533:C:H6	1:A:2533:C:H5'	1.32	0.93
2:B:3023:U:H4'	2:B:3024:U:OP2	1.69	0.93
6:E:104:ASP:HA	6:E:107:ARG:HH12	1.33	0.93
5:D:162:MET:HE2	5:D:310:ARG:HD3	1.51	0.92
13:L:29:LEU:HB3	13:L:55:VAL:HG11	1.49	0.92
1:A:856:G:H2'	38:A:4898:HOH:O	1.68	0.92
1:A:1116:U:HO2'	1:A:1118:A:H2	0.92	0.91
4:C:211:LYS:HB3	4:C:212:PRO:HD2	1.52	0.91
11:J:150:LYS:HB2	11:J:157:ILE:HD12	1.52	0.91
11:J:162:SER:HB2	11:J:163:PRO:HD3	1.53	0.91
13:L:10:GLN:H	13:L:10:GLN:HE21	1.10	0.91
6:E:2:GLN:HB3	38:E:8338:HOH:O	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:236:THR:HG22	6:E:239:ALA:N	1.85	0.90
15:N:35:PRO:CG	15:N:38:VAL:HG23	2.01	0.90
27:Z:212:ARG:HD2	38:Z:8605:HOH:O	1.70	0.90
1:A:1372:A:H3'	38:A:6651:HOH:O	1.68	0.90
5:D:162:MET:HE1	5:D:308:LEU:HD21	1.51	0.90
13:L:14:LYS:HB2	13:L:45:PRO:HG2	1.54	0.90
26:Y:78:GLU:HG2	26:Y:79:GLU:H	1.36	0.90
4:C:191:GLY:HA2	4:C:194:MET:HE2	1.52	0.90
15:N:69:LYS:O	15:N:73:ARG:NH2	2.04	0.90
1:A:871:G:H5'	1:A:871:G:C8	2.06	0.90
1:A:2122:C:OP2	38:A:6038:HOH:O	1.88	0.90
15:N:87:MET:CG	31:4:46:ILE:HG21	2.02	0.90
2:B:3076:G:H3'	2:B:3077:A:H5''	1.54	0.89
1:A:506:G:H22	1:A:509:A:H5'	1.35	0.89
11:J:27:LYS:H	11:J:58:HIS:HD2	1.14	0.89
5:D:264:GLU:HG2	5:D:267:LYS:HE2	1.51	0.89
16:O:49:THR:HG22	16:O:56:ASP:HB2	1.55	0.89
1:A:2780:C:H1'	8:G:143:GLN:HE21	1.38	0.89
11:J:29:ALA:HB3	11:J:65:ARG:HH12	1.38	0.89
26:Y:25:ARG:HD2	38:Y:3861:HOH:O	1.73	0.88
1:A:1679:C:H5'	38:A:8834:HOH:O	1.74	0.88
30:3:41:HIS:H	30:3:45:ASN:HD22	1.20	0.88
11:J:26:LYS:HD2	11:J:28:ILE:HD12	1.54	0.88
25:X:122:ARG:HH21	25:X:154:ARG:HD2	1.37	0.88
1:A:2717:C:C2'	1:A:2718:C:H5''	2.04	0.88
6:E:132:ASP:HB3	38:E:8364:HOH:O	1.74	0.88
10:I:23:ILE:HD13	10:I:67:LEU:HD23	1.56	0.88
15:N:164:THR:HG22	15:N:167:GLY:N	1.88	0.87
5:D:212:GLN:HB2	5:D:257:THR:HG21	1.56	0.87
16:O:144:GLY:O	16:O:147:ILE:HG22	1.73	0.87
1:A:1242:A:H5'	12:K:82:THR:HG23	1.53	0.87
4:C:223:ARG:HG3	38:C:8616:HOH:O	1.73	0.87
11:J:13:ALA:HA	11:J:91:HIS:HE1	1.38	0.87
25:X:88:THR:HG22	25:X:89:ASP:H	1.39	0.87
1:A:2123:A:OP2	38:A:4762:HOH:O	1.91	0.86
6:E:236:THR:HG21	38:E:8375:HOH:O	1.74	0.86
26:Y:15:ARG:HB3	26:Y:15:ARG:HH11	1.40	0.86
12:K:19:MET:CE	12:K:132:LEU:HD11	2.05	0.86
18:Q:115:SER:OG	18:Q:118:GLN:HG3	1.75	0.86
2:B:3025:G:H3'	2:B:3026:C:H5'	1.55	0.86
1:A:21:G:H5'	20:S:2:ILE:HA	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:A:H1'	1:A:1192:A:C2	2.10	0.86
1:A:542:A:H5'	1:A:542:A:H8	1.38	0.86
1:A:545:G:H5'	1:A:545:G:H8	1.40	0.86
1:A:870:G:C2'	1:A:871:G:H5''	2.06	0.86
1:A:1116:U:H3	1:A:1246:A:H62	1.23	0.86
20:S:9:ASP:O	20:S:13:THR:HB	1.76	0.86
28:1:39:CYS:HA	28:1:47:LEU:HD11	1.57	0.86
6:E:5:ILE:HD11	6:E:16:VAL:CG2	2.06	0.85
1:A:1244:U:OP1	12:K:18:ILE:HD13	1.76	0.85
5:D:140:LEU:HA	38:D:8583:HOH:O	1.75	0.85
1:A:2420:G:O2'	1:A:2421:G:H5'	1.75	0.85
15:N:74:ARG:HH11	15:N:74:ARG:HG3	1.41	0.85
18:Q:115:SER:H	18:Q:118:GLN:NE2	1.74	0.85
31:4:25:VAL:HG22	31:4:68:LYS:HG3	1.58	0.85
1:A:1474:C:H5'	1:A:1474:C:C6	2.12	0.85
15:N:164:THR:HG23	15:N:165:SER:N	1.90	0.85
16:O:87:LEU:HD12	16:O:186:LEU:HD21	1.57	0.85
6:E:246:ARG:HB3	6:E:246:ARG:NH1	1.91	0.85
11:J:162:SER:HB2	11:J:163:PRO:CD	2.07	0.85
1:A:506:G:H22	1:A:509:A:C5'	1.88	0.84
15:N:102:GLU:OE1	15:N:164:THR:HG21	1.77	0.84
1:A:645:U:OP2	14:M:4:LYS:HE2	1.77	0.84
1:A:1450:C:H4'	1:A:1451:C:OP2	1.76	0.84
6:E:140:VAL:HB	38:E:8457:HOH:O	1.77	0.84
2:B:3025:G:H3'	2:B:3026:C:C5'	2.07	0.84
5:D:41:PHE:CD1	5:D:79:MET:HE2	2.13	0.84
15:N:52:LEU:HD11	38:N:8616:HOH:O	1.76	0.84
16:O:83:LEU:HD13	16:O:175:LEU:HD23	1.60	0.84
25:X:122:ARG:NH2	25:X:154:ARG:HD2	1.92	0.84
29:2:8:GLN:HE22	29:2:11:LYS:NZ	1.74	0.84
38:B:8459:HOH:O	19:R:25:PRO:HB2	1.78	0.84
11:J:59:ASN:H	11:J:59:ASN:HD22	1.21	0.84
13:L:81:ARG:HB2	13:L:87:ARG:HH11	1.40	0.84
25:X:88:THR:HG23	25:X:110:GLN:NE2	1.93	0.83
29:2:8:GLN:HE22	29:2:11:LYS:HZ2	1.23	0.83
28:1:42:CYS:SG	28:1:44:PHE:HB2	2.17	0.83
1:A:2459:G:P	31:4:64:LYS:HB2	2.18	0.83
38:A:3219:HOH:O	15:N:157:LEU:HD11	1.77	0.83
11:J:13:ALA:HA	11:J:91:HIS:CE1	2.13	0.83
14:M:79:ASP:HB3	38:M:8564:HOH:O	1.78	0.83
1:A:960:G:H4'	38:A:6886:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:187:VAL:HG23	27:Z:192:ASP:HB2	1.61	0.83
5:D:201:ASP:HB2	5:D:312:ARG:HD2	1.59	0.83
31:4:70:ARG:HG2	31:4:77:ALA:HB2	1.60	0.83
25:X:6:GLN:HB2	25:X:26:ILE:HD12	1.59	0.83
7:F:27:ILE:HG22	7:F:28:GLY:H	1.43	0.83
13:L:10:GLN:HE21	13:L:10:GLN:N	1.77	0.83
1:A:1603:A:H5'	1:A:1605:G:O4'	1.78	0.82
15:N:74:ARG:NH2	38:N:8632:HOH:O	2.11	0.82
16:O:7:LYS:HE3	19:R:21:ARG:O	1.79	0.82
4:C:121:ALA:O	4:C:124:VAL:HG22	1.79	0.82
12:K:76:ASP:HA	38:K:5907:HOH:O	1.79	0.82
16:O:113:SER:HB2	38:O:8556:HOH:O	1.77	0.82
28:1:46:LYS:HB2	28:1:57:CYS:SG	2.19	0.82
7:F:154:LYS:H	7:F:154:LYS:HD2	1.44	0.82
16:O:86:LEU:HD12	16:O:125:ALA:HB2	1.60	0.82
38:A:7015:HOH:O	31:4:60:LYS:HG3	1.79	0.81
38:A:8631:HOH:O	15:N:82:ARG:HD2	1.80	0.81
29:2:25:LYS:HE2	38:3:7213:HOH:O	1.79	0.81
5:D:18:ARG:HG3	5:D:256:GLN:HG3	1.61	0.81
5:D:62:ARG:HA	5:D:65:MET:HE3	1.62	0.81
8:G:100:ASP:HB2	38:G:2789:HOH:O	1.79	0.81
11:J:26:LYS:HG2	11:J:28:ILE:H	1.44	0.81
1:A:2506:A:HO2'	1:A:2507:G:H8	0.81	0.81
1:A:1184:C:H1'	38:A:6922:HOH:O	1.81	0.81
1:A:1835:U:C5	1:A:1840:A:N7	2.48	0.81
38:A:4426:HOH:O	2:B:3103:A:H4'	1.81	0.81
11:J:55:GLN:HE21	11:J:124:ARG:HE	1.28	0.81
11:J:2:PRO:HB2	38:J:8365:HOH:O	1.81	0.80
4:C:192:VAL:HB	38:C:8606:HOH:O	1.81	0.80
7:F:20:LYS:HA	7:F:75:LEU:O	1.82	0.80
27:Z:187:VAL:HG23	27:Z:192:ASP:CB	2.12	0.80
28:1:38:LYS:HG2	28:1:45:LYS:HG2	1.62	0.80
1:A:1974:G:OP1	38:A:6321:HOH:O	1.99	0.80
1:A:2506:A:O2'	1:A:2507:G:H8	1.62	0.80
11:J:5:MET:HG3	38:J:8365:HOH:O	1.80	0.80
28:1:47:LEU:HD23	28:1:57:CYS:HB2	1.63	0.80
1:A:560:C:H42	1:A:597:A:H61	1.29	0.80
1:A:1205:U:H2'	1:A:1206:U:H5'	1.62	0.80
4:C:69:LEU:HD21	4:C:120:ARG:HB3	1.62	0.80
9:H:91:VAL:HG12	9:H:92:GLY:H	1.47	0.80
20:S:17:MET:HE1	20:S:19:ARG:NH2	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:9:CYS:SG	23:V:11:THR:HG23	2.21	0.79
1:A:289:G:H22	1:A:363:A:H2	1.30	0.79
1:A:1118:A:C8	1:A:1118:A:H3'	2.18	0.79
1:A:1684:A:H1'	30:3:43:ARG:HH22	1.47	0.79
1:A:2586:U:H3	1:A:2592:G:H22	1.30	0.79
1:A:1165:G:H4'	1:A:1174:A:O2'	1.81	0.79
1:A:2466:G:OP1	38:A:3142:HOH:O	2.00	0.79
14:M:133:VAL:HA	38:M:8577:HOH:O	1.80	0.79
1:A:346:U:H4'	38:A:6302:HOH:O	1.83	0.79
12:K:26:VAL:HG13	12:K:36:VAL:HG11	1.65	0.79
38:A:3278:HOH:O	15:N:189:VAL:HG21	1.83	0.78
1:A:31:C:H4'	38:A:6880:HOH:O	1.83	0.78
13:L:30:LYS:O	13:L:55:VAL:HG13	1.82	0.78
38:A:6460:HOH:O	19:R:9:GLY:HA2	1.82	0.78
6:E:246:ARG:HB3	6:E:246:ARG:HH11	1.45	0.78
12:K:99:GLU:HA	38:K:7377:HOH:O	1.84	0.78
26:Y:76:ARG:HH11	26:Y:76:ARG:HG3	1.49	0.78
1:A:381:G:H5''	38:A:3807:HOH:O	1.84	0.78
7:F:19:GLU:O	7:F:20:LYS:HG2	1.84	0.78
26:Y:30:MET:HE1	26:Y:58:ALA:HB3	1.63	0.78
6:E:47:GLY:HA2	6:E:92:PRO:HB2	1.65	0.78
13:L:74:VAL:HG13	13:L:113:ILE:HG23	1.65	0.78
27:Z:185:VAL:HA	38:Z:8566:HOH:O	1.84	0.78
5:D:145:HIS:HD2	5:D:146:THR:O	1.67	0.78
11:J:3:GLY:HA2	11:J:57:ARG:HH12	1.48	0.78
11:J:139:ASP:N	11:J:140:PRO:HD3	1.98	0.78
15:N:87:MET:HG2	31:4:46:ILE:CG2	2.14	0.78
27:Z:216:ARG:HD3	38:Z:8574:HOH:O	1.83	0.78
6:E:107:ARG:NH1	6:E:107:ARG:HB3	1.99	0.77
1:A:2468:A:H61	31:4:48:ASN:HD21	1.27	0.77
1:A:2812:A:H2	1:A:2814:A:H62	1.32	0.77
11:J:150:LYS:HE2	38:J:8383:HOH:O	1.84	0.77
12:K:74:ARG:HB3	12:K:74:ARG:HH11	1.48	0.77
25:X:4:LEU:HD22	25:X:52:VAL:HG21	1.66	0.77
1:A:288:A:H61	1:A:364:C:H42	1.32	0.77
1:A:1160:G:C5'	1:A:1161:A:H5'	2.14	0.77
9:H:91:VAL:HG12	9:H:92:GLY:N	2.00	0.77
38:A:5753:HOH:O	7:F:99:ASP:HA	1.84	0.77
9:H:96:ALA:HA	38:H:3111:HOH:O	1.84	0.77
12:K:103:VAL:HG12	38:K:5907:HOH:O	1.84	0.77
15:N:157:LEU:HA	35:N:8518:CL:CL	2.22	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:A:H3'	1:A:1118:A:H8	1.48	0.77
11:J:130:HIS:CD2	11:J:133:ILE:HD11	2.20	0.77
27:Z:220:GLU:HG2	38:Z:8553:HOH:O	1.85	0.77
28:1:77:LYS:HA	28:1:80:MET:HE2	1.67	0.77
1:A:338:C:H4'	6:E:174:ILE:CD1	2.15	0.76
12:K:133:GLY:O	12:K:137:GLU:HG3	1.85	0.76
8:G:97:VAL:HG12	38:G:4191:HOH:O	1.84	0.76
26:Y:71:ARG:HB3	26:Y:88:GLU:OE1	1.85	0.76
2:B:3014:G:H5'	2:B:3014:G:H8	1.50	0.76
2:B:3023:U:H6	2:B:3023:U:H5''	1.50	0.76
18:Q:59:ARG:NH2	18:Q:66:GLN:HE22	1.82	0.76
1:A:1058:A:H2'	1:A:1060:C:H5''	1.68	0.76
18:Q:115:SER:N	18:Q:118:GLN:HE21	1.80	0.76
1:A:450:C:OP1	6:E:184:ARG:NH2	2.17	0.76
1:A:559:U:H6	1:A:559:U:H5'	1.51	0.76
1:A:871:G:H8	1:A:871:G:C5'	1.98	0.76
1:A:962:C:H1'	16:O:5:ARG:HH12	1.50	0.76
1:A:2466:G:C5'	38:A:3142:HOH:O	2.23	0.76
2:B:3023:U:H3'	38:B:8482:HOH:O	1.85	0.76
28:1:29:VAL:O	28:1:33:HIS:HB2	1.86	0.76
11:J:59:ASN:HD22	11:J:59:ASN:N	1.83	0.76
1:A:2578:G:H5'	1:A:2578:G:H8	1.49	0.76
5:D:258:GLY:H	5:D:260:HIS:CE1	2.03	0.76
11:J:141:ASN:HA	38:J:8366:HOH:O	1.84	0.76
1:A:31:C:H2'	38:A:7147:HOH:O	1.86	0.76
25:X:68:THR:HG23	25:X:69:ARG:HG2	1.67	0.76
25:X:21:LEU:HD22	25:X:26:ILE:CD1	2.16	0.76
1:A:2271:G:OP2	38:A:8940:HOH:O	2.05	0.75
1:A:2467:A:H3'	38:A:4927:HOH:O	1.85	0.75
9:H:50:VAL:HG21	9:H:63:ILE:HG21	1.65	0.75
8:G:6:GLU:HA	8:G:46:THR:HG22	1.69	0.75
14:M:120:LEU:HD12	14:M:133:VAL:HG21	1.69	0.75
1:A:282:C:H1'	1:A:368:C:N4	2.00	0.75
1:A:1741:U:O2'	1:A:2723:G:H4'	1.87	0.75
4:C:88:ILE:HD13	4:C:100:PRO:HD3	1.68	0.75
11:J:27:LYS:N	11:J:58:HIS:HD2	1.84	0.75
1:A:711:G:H1'	38:A:6554:HOH:O	1.87	0.75
4:C:35:GLY:O	4:C:36:ASP:HB3	1.86	0.75
7:F:146:LYS:NZ	16:O:107:ASN:HD21	1.85	0.75
13:L:39:GLY:HA2	38:L:4183:HOH:O	1.86	0.75
25:X:72:PRO:HG2	25:X:77:ALA:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1771:U:H4'	28:1:20:LEU:HD21	1.67	0.75
24:W:1:THR:HG23	24:W:2:VAL:H	1.51	0.75
1:A:1134:G:C4'	11:J:151:MET:HE1	2.15	0.75
1:A:2094:G:H4'	5:D:245:SER:HB3	1.66	0.75
1:A:1191:A:H3'	1:A:1192:A:H5''	1.68	0.75
1:A:2508:C:H2'	38:A:6213:HOH:O	1.86	0.75
12:K:19:MET:HE2	12:K:79:PHE:HA	1.68	0.75
1:A:2433:A:H2'	1:A:2434:A:C8	2.22	0.75
2:B:3069:U:OP1	16:O:4:PRO:HG3	1.86	0.75
6:E:76:ARG:HD2	38:E:8439:HOH:O	1.85	0.75
8:G:107:PHE:CE2	8:G:108:LEU:HD13	2.22	0.75
11:J:28:ILE:HA	11:J:62:GLU:OE1	1.87	0.75
14:M:67:ARG:O	14:M:71:GLU:HG3	1.87	0.74
28:1:18:TYR:HB3	28:1:22:ILE:HG21	1.68	0.74
1:A:1751:G:C2'	1:A:1752:G:H5''	2.11	0.74
20:S:8:ALA:HB1	20:S:13:THR:HG21	1.69	0.74
5:D:190:MET:HE2	5:D:194:PHE:CD1	2.22	0.74
15:N:87:MET:CB	31:4:46:ILE:HG21	2.17	0.74
8:G:166:VAL:HG12	38:G:3134:HOH:O	1.87	0.74
28:1:38:LYS:HE2	28:1:45:LYS:HE2	1.68	0.74
31:4:65:THR:HG23	31:4:67:LEU:HG	1.69	0.74
1:A:2812:A:N7	38:A:6974:HOH:O	2.20	0.74
15:N:152:ARG:HG3	38:N:8559:HOH:O	1.87	0.74
23:V:13:ILE:HG12	23:V:32:CYS:CB	2.17	0.74
6:E:162:VAL:HG12	6:E:192:ILE:HD11	1.69	0.74
7:F:95:THR:O	7:F:97:GLN:N	2.18	0.74
16:O:164:ASP:CG	16:O:167:ASP:HA	2.13	0.74
38:B:8467:HOH:O	16:O:147:ILE:HD12	1.88	0.74
38:A:4067:HOH:O	15:N:87:MET:HE1	1.87	0.73
2:B:3056:A:C2'	2:B:3057:A:H5''	2.18	0.73
28:1:49:ARG:HD2	38:1:8426:HOH:O	1.87	0.73
1:A:2274:A:N3	15:N:86:MET:HE1	2.03	0.73
4:C:36:ASP:OD2	4:C:85:ASP:HB2	1.87	0.73
1:A:2755:G:H1'	38:A:4164:HOH:O	1.88	0.73
15:N:173:LEU:HD23	15:N:183:VAL:HG12	1.70	0.73
16:O:61:ALA:HB3	16:O:88:ALA:HB2	1.71	0.73
23:V:47:ARG:HG3	38:V:4381:HOH:O	1.88	0.73
1:A:2748:G:H2'	38:A:6999:HOH:O	1.88	0.73
25:X:137:GLN:HE21	25:X:141:HIS:HE1	1.36	0.73
1:A:820:G:OP1	28:1:17:ARG:NH2	2.20	0.73
1:A:1209:C:H4'	38:A:4753:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1701:A:H5'	38:A:5741:HOH:O	1.87	0.73
15:N:79:LYS:HD3	38:N:8563:HOH:O	1.88	0.73
1:A:1130:U:H2'	1:A:1131:G:O4'	1.89	0.73
1:A:1829:A:H61	28:1:18:TYR:HA	1.54	0.73
5:D:71:VAL:HG11	5:D:296:LEU:HB3	1.70	0.73
25:X:122:ARG:HG2	25:X:122:ARG:HH11	1.52	0.73
13:L:62:PRO:HG3	13:L:65:ARG:HH21	1.54	0.73
2:B:3024:U:O2'	2:B:3025:G:H4'	1.88	0.73
1:A:1160:G:H5'	1:A:1161:A:C5'	2.15	0.72
38:A:3951:HOH:O	15:N:146:GLN:HG2	1.89	0.72
7:F:35:ALA:N	38:F:5576:HOH:O	2.22	0.72
1:A:2404:G:O3'	38:A:6058:HOH:O	2.06	0.72
4:C:135:VAL:HG21	4:C:147:ARG:NH1	2.04	0.72
11:J:56:ILE:HG22	11:J:61:LEU:HD22	1.71	0.72
16:O:11:ARG:HG3	16:O:14:ARG:NH1	2.03	0.72
20:S:39:THR:HG23	20:S:107:GLU:O	1.89	0.72
31:4:74:CYS:SG	31:4:76:LYS:HB2	2.28	0.72
10:I:12:ILE:N	10:I:13:PRO:HD3	2.04	0.72
15:N:87:MET:CB	31:4:46:ILE:HD13	2.20	0.72
1:A:182:G:H5'	38:A:4632:HOH:O	1.87	0.72
38:A:4311:HOH:O	12:K:47:THR:HB	1.89	0.72
8:G:101:GLU:HB2	8:G:116:THR:O	1.90	0.72
5:D:179:LEU:O	5:D:183:GLU:HG2	1.90	0.72
15:N:72:SER:O	38:N:8655:HOH:O	2.06	0.72
1:A:1666:C:H2'	1:A:1667:A:H5'	1.70	0.72
1:A:2620:U:O2'	38:A:6629:HOH:O	2.06	0.72
11:J:137:ASN:O	11:J:139:ASP:N	2.22	0.72
20:S:39:THR:HG22	20:S:42:GLU:H	1.53	0.72
1:A:113:A:OP2	1:A:114:A:H2'	1.89	0.72
1:A:172:U:OP2	38:A:5669:HOH:O	2.07	0.72
5:D:141:ARG:HG2	5:D:165:ARG:HA	1.70	0.72
12:K:75:PRO:HG2	12:K:105:LEU:HD21	1.71	0.72
15:N:139:PRO:O	15:N:140:ALA:HB3	1.89	0.72
14:M:114:VAL:HG11	38:M:8577:HOH:O	1.89	0.72
15:N:59:GLY:HA3	15:N:141:ILE:CD1	2.19	0.72
38:A:6880:HOH:O	22:U:9:LYS:HB2	1.89	0.72
8:G:84:MET:HE1	8:G:148:ILE:CD1	2.20	0.72
19:R:64:GLU:HG3	19:R:74:ASP:OD2	1.89	0.72
1:A:272:A:H3'	38:A:6987:HOH:O	1.88	0.71
1:A:2346:C:O5'	1:A:2346:C:H6	1.73	0.71
10:I:12:ILE:HA	38:I:4499:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:106:GLY:HA3	38:L:5264:HOH:O	1.89	0.71
15:N:68:ARG:O	15:N:68:ARG:HD3	1.89	0.71
17:P:32:ARG:O	17:P:32:ARG:HD3	1.87	0.71
17:P:47:ARG:HH11	17:P:47:ARG:HG3	1.55	0.71
1:A:2467:A:C2'	38:A:4927:HOH:O	2.31	0.71
1:A:284:C:H4'	1:A:285:A:O5'	1.88	0.71
15:N:106:ASN:HD22	15:N:114:VAL:HG23	1.56	0.71
24:W:12:THR:HG22	24:W:15:GLU:CG	2.19	0.71
4:C:179:MET:HG2	4:C:186:TRP:CB	2.20	0.71
11:J:162:SER:CB	11:J:163:PRO:HD3	2.20	0.71
28:1:30:GLU:HA	28:1:33:HIS:HB3	1.73	0.71
4:C:76:VAL:HG23	28:1:63:LYS:HB3	1.73	0.71
11:J:139:ASP:HA	38:J:8370:HOH:O	1.88	0.71
1:A:2291:A:C8	1:A:2309:C:H5'	2.25	0.71
1:A:2310:G:OP2	11:J:114:PRO:HD2	1.89	0.71
1:A:2638:G:H1'	38:A:7218:HOH:O	1.90	0.71
2:B:3006:C:OP1	16:O:37:ARG:NH1	2.22	0.71
11:J:33:MET:HB2	11:J:83:PHE:HB3	1.72	0.71
1:A:1701:A:H4'	1:A:1702:U:H5''	1.72	0.71
6:E:12:THR:HB	38:E:8447:HOH:O	1.89	0.71
38:A:3555:HOH:O	5:D:27:ASN:HB2	1.90	0.71
23:V:13:ILE:HG12	23:V:32:CYS:HB3	1.70	0.71
1:A:877:G:H5'	1:A:878:G:OP1	1.91	0.71
1:A:1118:A:H62	1:A:1244:U:H3	1.39	0.71
14:M:34:GLY:HA3	14:M:38:HIS:CE1	2.25	0.71
25:X:81:ASP:OD1	25:X:92:ASP:HB2	1.91	0.71
1:A:113:A:H3'	1:A:114:A:H5''	1.71	0.71
13:L:81:ARG:HB2	13:L:87:ARG:NH1	2.04	0.71
1:A:1741:U:H5'	1:A:1742:A:OP1	1.90	0.70
1:A:2346:C:O2'	7:F:52:THR:HG21	1.91	0.70
1:A:2502:C:C2'	1:A:2503:A:H5'	2.21	0.70
6:E:46:TYR:CE2	6:E:98:ARG:NH1	2.59	0.70
16:O:48:VAL:CG1	16:O:55:ASP:HB3	2.20	0.70
1:A:1666:C:O2'	1:A:1667:A:H5''	1.91	0.70
1:A:2421:G:H4'	38:A:4257:HOH:O	1.91	0.70
38:A:5258:HOH:O	15:N:170:CYS:SG	2.48	0.70
15:N:122:GLU:OE2	15:N:127:LYS:HE2	1.91	0.70
6:E:104:ASP:HA	6:E:107:ARG:NH1	2.06	0.70
6:E:236:THR:H	6:E:239:ALA:HB3	1.55	0.70
7:F:91:ALA:HB1	38:F:5198:HOH:O	1.91	0.70
15:N:164:THR:CG2	15:N:167:GLY:H	1.95	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:10:ALA:HA	18:Q:13:VAL:HG12	1.73	0.70
20:S:18:LEU:HB2	20:S:143:VAL:HG12	1.72	0.70
1:A:1119:G:N2	1:A:1246:A:C2	2.59	0.70
1:A:1164:U:H3	1:A:1192:A:H2	1.38	0.70
1:A:2467:A:OP1	38:A:8560:HOH:O	2.09	0.70
11:J:14:TYR:H	11:J:91:HIS:CE1	2.09	0.70
23:V:9:CYS:HA	23:V:52:THR:HG23	1.72	0.70
25:X:4:LEU:HD22	25:X:52:VAL:CG2	2.21	0.70
1:A:1134:G:C5'	11:J:151:MET:HE1	2.21	0.70
1:A:2281:C:C2'	1:A:2282:U:H5'	2.20	0.70
2:B:3006:C:H5''	16:O:37:ARG:HH12	1.55	0.70
9:H:53:ASP:OD1	9:H:80:GLN:HB2	1.91	0.70
11:J:75:SER:O	11:J:79:ALA:HB2	1.92	0.70
38:A:9293:HOH:O	13:L:39:GLY:HA3	1.90	0.70
15:N:24:MET:HE3	15:N:28:MET:CE	2.20	0.70
6:E:25:PRO:HG2	38:E:8325:HOH:O	1.92	0.70
6:E:78:ARG:HG3	6:E:78:ARG:HH11	1.56	0.70
2:B:3023:U:H5''	2:B:3023:U:C6	2.27	0.70
11:J:26:LYS:HD3	11:J:89:PRO:HG3	1.73	0.70
26:Y:18:ARG:NH1	38:Y:4132:HOH:O	2.16	0.70
8:G:11:VAL:HG12	8:G:12:ASP:N	2.05	0.70
11:J:27:LYS:H	11:J:58:HIS:CD2	2.04	0.70
11:J:140:PRO:HB3	38:J:8381:HOH:O	1.92	0.70
12:K:107:ASN:ND2	12:K:109:TYR:H	1.90	0.70
15:N:12:TRP:CE2	15:N:20:ILE:HD11	2.27	0.70
15:N:74:ARG:HG3	15:N:74:ARG:NH1	2.02	0.70
25:X:149:LEU:CG	25:X:153:MET:HE2	2.20	0.70
1:A:299:U:H5'	38:A:6794:HOH:O	1.92	0.69
1:A:2837:U:H2'	38:A:6298:HOH:O	1.92	0.69
38:A:6913:HOH:O	6:E:188:ARG:HD3	1.92	0.69
9:H:63:ILE:HB	9:H:64:PRO:HD3	1.72	0.69
1:A:2526:C:O2'	1:A:2527:U:H5'	1.92	0.69
5:D:148:PRO:HD2	38:D:8584:HOH:O	1.91	0.69
20:S:39:THR:HB	20:S:42:GLU:HG3	1.73	0.69
1:A:461:C:H2'	38:A:3491:HOH:O	1.92	0.69
1:A:541:C:C2'	1:A:542:A:H5''	2.22	0.69
1:A:1080:C:H4'	1:A:1081:A:OP1	1.90	0.69
1:A:1377:C:H6	1:A:1377:C:H5'	1.57	0.69
1:A:2249:G:OP2	38:A:4912:HOH:O	2.10	0.69
27:Z:189:ASN:HD22	27:Z:189:ASN:C	2.00	0.69
1:A:1625:U:H4'	38:A:4149:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:139:VAL:HG13	38:E:8454:HOH:O	1.90	0.69
1:A:182:G:H4'	15:N:157:LEU:HD13	1.75	0.69
4:C:199:HIS:CD2	4:C:201:PHE:H	2.10	0.69
11:J:55:GLN:HE22	11:J:91:HIS:CD2	2.10	0.69
1:A:1380:U:OP1	38:A:7331:HOH:O	2.09	0.69
1:A:2433:A:H2'	1:A:2434:A:H8	1.56	0.69
14:M:143:THR:HG22	14:M:144:ASP:N	2.05	0.69
25:X:88:THR:HG22	25:X:89:ASP:N	2.08	0.69
1:A:541:C:H2'	1:A:542:A:C5'	2.22	0.69
4:C:33:GLU:O	4:C:34:ASP:HB2	1.92	0.69
1:A:2100:A:H5'	38:A:6844:HOH:O	1.92	0.69
2:B:3048:C:H4'	16:O:141:ARG:HH21	1.57	0.69
7:F:88:LEU:HB2	7:F:89:PRO:HD3	1.75	0.69
15:N:139:PRO:O	15:N:140:ALA:CB	2.41	0.69
16:O:159:TYR:HB3	16:O:162:ASP:HB2	1.74	0.69
24:W:39:ALA:N	24:W:40:PRO:HD2	2.08	0.69
25:X:13:MET:HE2	25:X:18:GLN:HA	1.75	0.69
1:A:69:A:H5'	1:A:69:A:C8	2.28	0.69
1:A:214:U:H5'	38:A:5600:HOH:O	1.91	0.69
2:B:3025:G:C3'	2:B:3026:C:H5'	2.22	0.69
17:P:47:ARG:NH1	38:P:4564:HOH:O	2.24	0.69
22:U:9:LYS:HE3	22:U:13:ARG:NH1	2.08	0.69
26:Y:72:VAL:HG22	26:Y:85:VAL:HG12	1.75	0.69
30:3:39:ARG:HG2	38:3:3143:HOH:O	1.93	0.69
1:A:447:A:OP1	22:U:2:LYS:HG2	1.92	0.69
9:H:110:GLU:HG2	38:H:6926:HOH:O	1.92	0.69
11:J:69:ASN:O	11:J:72:VAL:HG12	1.92	0.69
38:A:6913:HOH:O	6:E:188:ARG:CD	2.41	0.68
11:J:41:THR:HA	38:J:8396:HOH:O	1.91	0.68
15:N:60:ILE:C	15:N:61:ILE:HD12	2.17	0.68
1:A:1160:G:N3	38:A:5102:HOH:O	2.26	0.68
1:A:1743:G:N7	38:A:8768:HOH:O	2.25	0.68
4:C:93:THR:C	4:C:94:LEU:HD23	2.18	0.68
5:D:254:GLN:HG3	38:D:8530:HOH:O	1.92	0.68
28:1:47:LEU:CD2	28:1:57:CYS:HB2	2.23	0.68
30:3:41:HIS:N	30:3:45:ASN:HD22	1.89	0.68
1:A:371:U:H2'	1:A:372:A:H8	1.58	0.68
1:A:542:A:H5'	1:A:542:A:C8	2.27	0.68
1:A:2467:A:C3'	38:A:4927:HOH:O	2.42	0.68
2:B:3039:U:H1'	2:B:3044:A:H61	1.57	0.68
16:O:151:ASP:O	16:O:154:LEU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:51:GLN:HE21	21:T:53:ASN:HD21	1.41	0.68
1:A:1909:A:N1	1:A:2128:G:H1'	2.08	0.68
11:J:71:TYR:C	11:J:73:GLN:H	2.01	0.68
15:N:37:VAL:HG21	15:N:108:LYS:HG3	1.74	0.68
20:S:106:GLY:HA2	20:S:109:MET:HE3	1.73	0.68
26:Y:78:GLU:CG	26:Y:79:GLU:H	2.06	0.68
1:A:2316:G:H8	38:A:5124:HOH:O	1.76	0.68
5:D:162:MET:HE2	5:D:310:ARG:CD	2.22	0.68
6:E:242:GLU:HG3	38:E:8383:HOH:O	1.92	0.68
1:A:516:A:OP2	38:A:5115:HOH:O	2.10	0.68
22:U:61:GLU:HG3	38:U:3851:HOH:O	1.93	0.68
25:X:6:GLN:HB2	25:X:26:ILE:CD1	2.23	0.68
25:X:21:LEU:HD22	25:X:26:ILE:HD11	1.76	0.68
1:A:541:C:H2'	1:A:542:A:H5''	1.75	0.68
16:O:164:ASP:OD2	16:O:167:ASP:HA	1.94	0.68
21:T:37:VAL:O	21:T:41:VAL:HG23	1.93	0.68
28:1:62:TYR:CE2	28:1:64:ILE:HG23	2.29	0.68
1:A:21:G:C5'	20:S:2:ILE:HA	2.23	0.68
1:A:2301:A:H5''	1:A:2302:A:H5'	1.75	0.68
1:A:2716:G:H5''	5:D:206:THR:HG21	1.76	0.68
1:A:485:A:N3	1:A:487:G:H5''	2.09	0.68
1:A:2830:U:H3'	38:A:4703:HOH:O	1.92	0.68
2:B:3013:A:O2'	2:B:3014:G:H5''	1.94	0.68
9:H:99:THR:HA	38:H:3461:HOH:O	1.94	0.68
25:X:22:GLU:HG2	25:X:27:HIS:CD2	2.28	0.68
1:A:739:G:C5	38:A:7001:HOH:O	2.47	0.67
12:K:107:ASN:HD21	12:K:109:TYR:HB2	1.59	0.67
1:A:545:G:H5'	1:A:545:G:C8	2.28	0.67
1:A:918:G:N7	38:A:9993:HOH:O	2.27	0.67
2:B:3092:G:H2'	2:B:3093:A:C8	2.29	0.67
5:D:175:LEU:HD23	5:D:175:LEU:C	2.19	0.67
15:N:78:ASN:ND2	38:N:8651:HOH:O	2.26	0.67
27:Z:155:ARG:NH1	38:Z:8562:HOH:O	2.26	0.67
1:A:69:A:H5'	1:A:69:A:H8	1.59	0.67
1:A:689:G:N3	38:A:8933:HOH:O	2.26	0.67
1:A:2748:G:H5'	38:A:6999:HOH:O	1.94	0.67
5:D:7:ARG:HG2	5:D:7:ARG:HH11	1.58	0.67
7:F:22:VAL:HG22	7:F:74:THR:HG22	1.76	0.67
1:A:281:U:H2'	1:A:282:C:O4'	1.95	0.67
1:A:1172:G:H1'	38:A:4448:HOH:O	1.93	0.67
1:A:2464:C:H5''	1:A:2465:A:OP1	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:84:MET:HE2	8:G:133:VAL:CG2	2.24	0.67
8:G:93:MET:HE1	8:G:165:GLY:N	2.09	0.67
16:O:73:ALA:N	38:O:8563:HOH:O	2.28	0.67
16:O:119:GLN:O	16:O:123:ILE:HG13	1.94	0.67
26:Y:41:PHE:O	26:Y:43:VAL:HG23	1.94	0.67
7:F:105:SER:CB	7:F:131:THR:HG23	2.21	0.67
15:N:89:ASN:HA	38:N:8557:HOH:O	1.94	0.67
17:P:42:GLU:HB2	38:P:2176:HOH:O	1.92	0.67
23:V:20:MET:HE2	23:V:30:HIS:NE2	2.10	0.67
27:Z:235:GLU:H	27:Z:235:GLU:CD	2.03	0.67
1:A:544:G:H2'	1:A:545:G:H5''	1.77	0.67
4:C:8:ARG:HG2	38:C:8558:HOH:O	1.94	0.67
17:P:38:ARG:NH1	38:P:7674:HOH:O	2.27	0.67
22:U:63:ILE:HD11	22:U:75:GLU:HB2	1.77	0.67
1:A:236:A:H4'	1:A:237:G:H5'	1.77	0.67
5:D:314:ALA:HB3	5:D:317:PRO:HG3	1.77	0.67
1:A:902:G:N7	14:M:18:HIS:HD2	1.92	0.67
1:A:1209:C:H2'	1:A:1210:G:H8	1.58	0.67
1:A:1874:U:H2'	4:C:120:ARG:HG3	1.75	0.67
23:V:14:GLU:O	23:V:17:THR:HB	1.95	0.67
13:L:55:VAL:HG12	13:L:56:SER:N	2.09	0.67
1:A:2851:G:O2'	1:A:2852:A:H5'	1.94	0.67
5:D:297:VAL:HB	38:D:8606:HOH:O	1.95	0.67
15:N:169:ARG:HD2	38:N:8591:HOH:O	1.95	0.67
1:A:2502:C:H2'	1:A:2503:A:H5'	1.77	0.66
1:A:2635:A:O2'	1:A:2636:C:H5'	1.94	0.66
11:J:127:GLY:O	11:J:128:ALA:HB3	1.95	0.66
25:X:88:THR:HG23	25:X:110:GLN:HE21	1.58	0.66
1:A:111:C:O2'	29:2:20:ARG:HG2	1.95	0.66
5:D:51:VAL:HG23	5:D:329:TYR:O	1.95	0.66
7:F:55:LYS:HA	38:F:6752:HOH:O	1.95	0.66
16:O:71:TRP:CE3	16:O:175:LEU:HD22	2.30	0.66
1:A:1667:A:H5'	1:A:1667:A:H8	1.60	0.66
1:A:2533:C:H5'	1:A:2533:C:C6	2.23	0.66
13:L:115:ARG:HG3	13:L:116:GLU:N	2.08	0.66
15:N:164:THR:CG2	15:N:165:SER:N	2.58	0.66
1:A:2459:G:OP2	31:4:64:LYS:HD2	1.94	0.66
1:A:2780:C:H1'	8:G:143:GLN:NE2	2.09	0.66
5:D:329:TYR:CE2	23:V:15:PRO:HG2	2.30	0.66
13:L:34:VAL:HG22	13:L:47:ALA:HB2	1.76	0.66
1:A:1829:A:N6	28:1:18:TYR:HA	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:94:LEU:HD23	4:C:94:LEU:N	2.10	0.66
9:H:2:VAL:HG22	9:H:57:GLU:OE1	1.94	0.66
7:F:97:GLN:HG2	7:F:97:GLN:O	1.95	0.66
13:L:74:VAL:HG11	13:L:113:ILE:HG12	1.76	0.66
15:N:172:GLY:O	15:N:183:VAL:HG11	1.96	0.66
7:F:64:ARG:HG2	7:F:67:ASP:HB3	1.77	0.66
5:D:141:ARG:HD2	5:D:163:GLU:OE2	1.95	0.66
7:F:51:ARG:HD3	38:F:7636:HOH:O	1.96	0.66
18:Q:38:GLU:HA	18:Q:41:ARG:HH11	1.60	0.66
1:A:1119:G:H22	1:A:1246:A:H2	1.42	0.66
1:A:1874:U:OP1	38:A:3810:HOH:O	2.14	0.66
1:A:2502:C:H4'	11:J:151:MET:HG2	1.78	0.66
1:A:2505:G:O2'	1:A:2506:A:H5'	1.95	0.66
1:A:2768:A:H2'	1:A:2769:C:O4'	1.94	0.66
20:S:44:VAL:O	20:S:48:GLU:HG3	1.96	0.66
28:1:53:GLY:HA2	28:1:67:GLY:O	1.96	0.66
1:A:282:C:O2'	1:A:283:U:H5'	1.96	0.65
1:A:2271:G:P	38:A:8940:HOH:O	2.54	0.65
8:G:7:ILE:HD11	8:G:11:VAL:C	2.21	0.65
13:L:28:GLU:OE2	13:L:58:THR:HG21	1.96	0.65
1:A:814:G:H4'	38:A:9628:HOH:O	1.96	0.65
2:B:3001:U:O3'	2:B:3003:A:H5''	1.96	0.65
4:C:153:ARG:HB2	4:C:153:ARG:HH11	1.61	0.65
6:E:1:MET:HG2	6:E:2:GLN:H	1.61	0.65
11:J:3:GLY:HA2	11:J:57:ARG:NH1	2.10	0.65
11:J:47:GLU:HB3	11:J:133:ILE:HD13	1.78	0.65
28:1:30:GLU:HA	28:1:33:HIS:CB	2.26	0.65
1:A:1130:U:H5'	38:A:7130:HOH:O	1.95	0.65
1:A:1681:G:H5''	1:A:1682:A:H5'	1.79	0.65
2:B:3014:G:H5'	2:B:3014:G:C8	2.31	0.65
5:D:238:ASN:HD22	5:D:240:GLY:H	1.44	0.65
15:N:30:GLU:O	15:N:34:GLU:HG3	1.97	0.65
18:Q:98:ILE:HD12	18:Q:102:ARG:NE	2.12	0.65
27:Z:142:SER:OG	38:Z:8616:HOH:O	2.15	0.65
4:C:191:GLY:HA2	4:C:194:MET:CE	2.27	0.65
7:F:136:ARG:HD2	7:F:155:HIS:O	1.95	0.65
1:A:1477:C:O2'	1:A:1478:U:H5'	1.96	0.65
1:A:2363:G:O3'	19:R:11:ARG:NH1	2.28	0.65
13:L:27:ARG:HD2	38:L:4747:HOH:O	1.97	0.65
15:N:37:VAL:HG21	15:N:108:LYS:CG	2.26	0.65
16:O:91:ARG:HG3	16:O:186:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:87:ARG:HG2	38:Q:190:HOH:O	1.96	0.65
22:U:50:VAL:HG12	22:U:56:ALA:HA	1.78	0.65
1:A:2414:A:H2'	1:A:2415:A:C8	2.31	0.65
4:C:94:LEU:HG	4:C:99:ILE:HD11	1.77	0.65
5:D:140:LEU:HD23	38:D:8583:HOH:O	1.96	0.65
6:E:127:ARG:HG2	6:E:127:ARG:HH11	1.61	0.65
13:L:62:PRO:HG3	13:L:65:ARG:NH2	2.11	0.65
15:N:87:MET:HB2	15:N:91:ILE:HD11	1.78	0.65
20:S:99:ALA:HB1	20:S:109:MET:CE	2.15	0.65
1:A:1886:A:H4'	38:1:8405:HOH:O	1.97	0.65
1:A:2618:G:N7	38:A:3140:HOH:O	2.30	0.65
7:F:41:LEU:HA	7:F:44:ILE:HG22	1.78	0.65
31:4:11:CYS:SG	38:4:8534:HOH:O	2.54	0.65
1:A:2432:C:O2'	1:A:2433:A:H5'	1.96	0.65
11:J:118:PRO:HD2	38:J:8340:HOH:O	1.97	0.65
15:N:84:LYS:HA	31:4:46:ILE:O	1.96	0.65
1:A:2064:U:H5'	1:A:2652:U:O3'	1.97	0.65
1:A:733:U:OP2	38:A:5671:HOH:O	2.14	0.64
2:B:3029:C:H2'	2:B:3030:C:H5'	1.77	0.64
20:S:18:LEU:HB2	20:S:143:VAL:CG1	2.27	0.64
25:X:4:LEU:HD23	25:X:54:PHE:HB3	1.79	0.64
26:Y:78:GLU:HG2	26:Y:79:GLU:N	2.11	0.64
1:A:2054:A:N3	20:S:128:ARG:NH2	2.45	0.64
1:A:2276:U:H2'	1:A:2277:U:C6	2.33	0.64
8:G:11:VAL:HG13	8:G:23:GLU:O	1.97	0.64
18:Q:38:GLU:HA	18:Q:41:ARG:NH1	2.12	0.64
27:Z:141:THR:HG23	38:Z:8594:HOH:O	1.96	0.64
1:A:2064:U:H4'	1:A:2653:A:OP1	1.97	0.64
28:1:42:CYS:SG	28:1:43:GLY:N	2.70	0.64
1:A:2428:G:C5	38:A:3276:HOH:O	2.50	0.64
12:K:74:ARG:HH11	12:K:74:ARG:CB	2.10	0.64
28:1:30:GLU:HB2	38:1:8413:HOH:O	1.98	0.64
1:A:777:U:OP1	38:A:6954:HOH:O	2.14	0.64
1:A:1187:U:H2'	38:A:6356:HOH:O	1.98	0.64
1:A:1773:G:C8	28:1:16:PRO:HA	2.32	0.64
15:N:87:MET:HB3	31:4:46:ILE:HG21	1.80	0.64
25:X:13:MET:HE2	25:X:18:GLN:CA	2.28	0.64
25:X:65:VAL:HA	25:X:68:THR:HG22	1.80	0.64
28:1:31:ILE:O	28:1:35:LYS:HG3	1.98	0.64
1:A:558:C:O2'	1:A:559:U:H5''	1.97	0.64
1:A:2769:C:H2'	1:A:2770:G:O4'	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3023:U:H3'	2:B:3024:U:H5''	1.78	0.64
5:D:248:ARG:NH2	38:D:8524:HOH:O	2.31	0.64
13:L:22:ASP:HB2	38:L:5264:HOH:O	1.96	0.64
13:L:34:VAL:CG2	13:L:47:ALA:HB2	2.27	0.64
24:W:39:ALA:C	24:W:41:GLU:H	2.06	0.64
1:A:1441:G:O2'	1:A:1442:A:H5'	1.98	0.64
1:A:2119:C:O2'	1:A:2120:U:H5'	1.97	0.64
29:2:21:ARG:HD2	29:2:37:CYS:SG	2.38	0.64
1:A:1942:A:H3'	38:A:6804:HOH:O	1.98	0.64
1:A:2314:G:C2'	1:A:2315:C:H5'	2.28	0.64
6:E:115:LEU:O	6:E:118:THR:HB	1.97	0.64
15:N:59:GLY:HA3	15:N:141:ILE:HD11	1.78	0.64
4:C:131:HIS:O	4:C:132:ASP:HB2	1.96	0.63
5:D:36:PRO:HA	5:D:168:GLY:HA3	1.80	0.63
7:F:101:THR:HG22	38:F:7400:HOH:O	1.97	0.63
13:L:58:THR:HG22	13:L:59:LYS:HG3	1.80	0.63
14:M:89:PHE:N	38:M:8575:HOH:O	2.32	0.63
15:N:84:LYS:HE2	38:N:8580:HOH:O	1.97	0.63
20:S:18:LEU:HD12	20:S:143:VAL:HG11	1.79	0.63
25:X:38:THR:HG22	38:X:3580:HOH:O	1.97	0.63
2:B:3049:G:H5''	38:B:8467:HOH:O	1.99	0.63
7:F:23:VAL:HG22	7:F:73:VAL:HB	1.78	0.63
11:J:58:HIS:HA	11:J:61:LEU:HD23	1.80	0.63
13:L:92:ASP:OD1	38:L:5638:HOH:O	2.15	0.63
27:Z:200:THR:HG22	27:Z:201:GLU:CG	2.20	0.63
1:A:544:G:C2'	1:A:545:G:H5''	2.28	0.63
1:A:1923:G:H4'	31:4:31:THR:O	1.98	0.63
1:A:2465:A:H3'	38:A:3142:HOH:O	1.97	0.63
8:G:79:GLY:HA3	38:G:7046:HOH:O	1.98	0.63
26:Y:31:ILE:O	26:Y:35:GLU:HG3	1.98	0.63
30:3:22:PRO:HG2	30:3:25:VAL:HG23	1.80	0.63
31:4:55:VAL:HG22	38:4:8510:HOH:O	1.99	0.63
1:A:157:G:H4'	15:N:95:LYS:HE3	1.80	0.63
1:A:1329:A:H2	38:A:4165:HOH:O	1.80	0.63
32:A:8011:MG:MG	38:A:3800:HOH:O	1.40	0.63
4:C:101:GLU:OE2	4:C:131:HIS:HB2	1.99	0.63
6:E:168:ARG:NH2	6:E:190:ALA:O	2.31	0.63
7:F:69:ILE:HG22	7:F:69:ILE:O	1.97	0.63
12:K:45:VAL:HG21	12:K:129:PHE:CD1	2.34	0.63
15:N:37:VAL:HG13	15:N:63:VAL:HG11	1.79	0.63
28:1:37:HIS:HB2	28:1:47:LEU:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2467:A:P	38:A:8560:HOH:O	2.57	0.63
5:D:280:VAL:CG1	5:D:334:SER:HA	2.29	0.63
8:G:7:ILE:HG22	8:G:45:ASP:O	1.98	0.63
9:H:107:VAL:O	9:H:111:ILE:HG13	1.98	0.63
11:J:53:PRO:HG3	11:J:127:GLY:H	1.63	0.63
11:J:151:MET:HA	11:J:151:MET:HE3	1.79	0.63
16:O:152:GLU:C	16:O:154:LEU:H	2.05	0.63
17:P:87:THR:O	17:P:91:GLN:HG3	1.99	0.63
1:A:1595:G:O2'	1:A:1596:U:H5'	1.98	0.63
2:B:3028:U:H5''	16:O:40:ASN:ND2	2.14	0.63
7:F:95:THR:C	7:F:97:GLN:H	2.07	0.63
15:N:34:GLU:HB3	15:N:35:PRO:HD2	1.80	0.63
1:A:396:U:OP2	31:4:38:ARG:NH1	2.32	0.63
8:G:20:ILE:CD1	8:G:33:LEU:HD12	2.29	0.63
14:M:143:THR:HG22	14:M:145:LEU:H	1.63	0.63
1:A:2890:A:H1'	23:V:56:ARG:NH2	2.14	0.63
8:G:23:GLU:HG2	8:G:28:SER:HB3	1.81	0.63
11:J:47:GLU:HB3	11:J:133:ILE:CD1	2.28	0.63
15:N:185:PRO:HG2	15:N:189:VAL:HG11	1.81	0.63
21:T:23:LYS:HE2	38:T:8330:HOH:O	1.99	0.63
1:A:2105:C:H2'	1:A:2106:C:C6	2.33	0.63
5:D:138:GLY:O	5:D:139:ASP:O	2.16	0.63
18:Q:103:THR:HA	18:Q:106:ARG:NH1	2.14	0.63
22:U:71:VAL:HG11	22:U:90:PRO:CB	2.22	0.63
30:3:35:ARG:HB2	38:3:2691:HOH:O	1.98	0.63
11:J:75:SER:C	11:J:79:ALA:HB2	2.24	0.62
12:K:131:THR:HG22	12:K:134:GLU:H	1.63	0.62
1:A:2548:C:OP2	5:D:5:ARG:NH2	2.32	0.62
4:C:88:ILE:HG22	4:C:88:ILE:O	1.97	0.62
11:J:166:ASN:N	11:J:166:ASN:HD22	1.96	0.62
12:K:45:VAL:HG23	12:K:130:VAL:O	1.98	0.62
15:N:114:VAL:HG21	15:N:159:THR:HG21	1.80	0.62
27:Z:187:VAL:CG2	27:Z:192:ASP:HB2	2.29	0.62
1:A:240:C:H4'	15:N:146:GLN:NE2	2.15	0.62
1:A:1116:U:O2'	1:A:1118:A:H2	1.72	0.62
1:A:2004:U:H4'	38:A:4780:HOH:O	1.98	0.62
10:I:12:ILE:N	10:I:13:PRO:CD	2.63	0.62
38:C:8627:HOH:O	28:1:75:ALA:HB3	1.98	0.62
6:E:78:ARG:HG3	6:E:78:ARG:NH1	2.13	0.62
7:F:23:VAL:HG23	7:F:23:VAL:O	1.99	0.62
9:H:46:GLU:N	38:H:3461:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:4556:HOH:O	5:D:216:LYS:HA	2.00	0.62
6:E:107:ARG:HB3	6:E:107:ARG:HH11	1.64	0.62
6:E:233:THR:HG22	6:E:234:VAL:N	2.13	0.62
15:N:91:ILE:HG23	38:N:8649:HOH:O	1.99	0.62
1:A:56:G:H5''	24:W:50:ARG:NH1	2.13	0.62
1:A:189:A:OP1	15:N:171:ARG:NH2	2.32	0.62
1:A:714:U:H3'	38:A:6403:HOH:O	2.00	0.62
7:F:37:ALA:O	7:F:40:ILE:HG12	1.99	0.62
15:N:64:ARG:HD2	38:N:8587:HOH:O	1.98	0.62
24:W:64:GLY:O	24:W:65:ASP:HB2	1.99	0.62
1:A:1594:C:OP2	18:Q:120:ARG:HD2	2.00	0.62
15:N:104:ARG:O	15:N:108:LYS:HE2	2.00	0.62
16:O:183:ASP:OD2	16:O:186:LEU:HD12	1.99	0.62
26:Y:37:LEU:CD1	26:Y:85:VAL:HG21	2.28	0.62
1:A:280:C:H2'	1:A:281:U:O4'	2.00	0.62
1:A:488:U:H2'	38:A:3497:HOH:O	1.99	0.62
22:U:48:VAL:HG22	22:U:97:ARG:O	2.00	0.62
29:2:28:HIS:HD2	29:2:30:LYS:H	1.48	0.62
32:A:8011:MG:MG	38:A:3470:HOH:O	1.42	0.62
5:D:145:HIS:CD2	5:D:146:THR:O	2.52	0.62
15:N:52:LEU:HD13	15:N:116:ASN:HB3	1.82	0.62
16:O:61:ALA:CB	16:O:88:ALA:HB2	2.30	0.62
25:X:26:ILE:HG13	25:X:26:ILE:O	1.97	0.62
1:A:558:C:H5'	38:A:4732:HOH:O	1.99	0.62
1:A:1213:C:O2'	1:A:1214:G:H5'	2.00	0.62
1:A:1713:G:H1'	38:A:4547:HOH:O	2.00	0.62
28:1:23:ARG:NH1	38:1:8404:HOH:O	2.32	0.62
1:A:603:A:H5''	1:A:604:G:OP1	1.99	0.61
1:A:1534:C:N3	38:A:8988:HOH:O	2.31	0.61
1:A:2421:G:H3'	1:A:2422:U:H5''	1.82	0.61
1:A:2506:A:O2'	1:A:2507:G:O5'	2.18	0.61
23:V:44:ARG:HB3	38:V:3805:HOH:O	1.99	0.61
1:A:56:G:H5''	24:W:50:ARG:HH12	1.63	0.61
1:A:671:A:O2'	1:A:672:G:H2'	2.00	0.61
1:A:1669:A:H2'	1:A:1670:G:C8	2.35	0.61
1:A:2281:C:H2'	1:A:2282:U:H5'	1.80	0.61
9:H:50:VAL:CG2	9:H:63:ILE:HG21	2.30	0.61
24:W:42:ASN:HB3	38:W:7247:HOH:O	2.00	0.61
1:A:1120:U:C6	1:A:1120:U:H5''	2.36	0.61
5:D:36:PRO:HA	5:D:168:GLY:CA	2.31	0.61
15:N:85:ARG:HA	15:N:87:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:30:GLU:HB3	28:1:34:LYS:HE3	1.81	0.61
1:A:183:A:H5'	15:N:157:LEU:HD12	1.82	0.61
1:A:948:G:N7	38:A:5313:HOH:O	2.30	0.61
1:A:1886:A:O2'	28:1:20:LEU:HB2	1.99	0.61
8:G:20:ILE:HD11	8:G:40:VAL:HG11	1.81	0.61
11:J:84:ARG:NH2	11:J:135:TRP:HH2	1.98	0.61
18:Q:94:TRP:CZ2	18:Q:98:ILE:HG13	2.35	0.61
27:Z:117:LEU:HD12	27:Z:174:VAL:HG11	1.83	0.61
1:A:1086:A:C6	25:X:11:VAL:HG11	2.34	0.61
1:A:1234:U:N3	5:D:244:PRO:HB3	2.16	0.61
1:A:1884:G:O6	4:C:190:ARG:HD2	2.00	0.61
7:F:25:MET:CE	7:F:37:ALA:HB1	2.31	0.61
11:J:62:GLU:O	11:J:66:VAL:HG23	2.00	0.61
14:M:21:ARG:N	38:M:8534:HOH:O	2.34	0.61
15:N:155:HIS:CE1	15:N:158:ARG:HE	2.18	0.61
5:D:217:ARG:HG3	5:D:257:THR:HG22	1.81	0.61
10:I:12:ILE:HD12	38:I:692:HOH:O	2.00	0.61
11:J:141:ASN:CA	38:J:8366:HOH:O	2.46	0.61
16:O:80:SER:HB2	38:O:8536:HOH:O	2.01	0.61
18:Q:143:ALA:HA	38:Q:170:HOH:O	2.00	0.61
21:T:80:ARG:HG2	38:T:8337:HOH:O	2.01	0.61
9:H:50:VAL:HG13	9:H:60:VAL:HG11	1.82	0.61
15:N:81:ARG:O	15:N:86:MET:HE2	2.01	0.61
16:O:89:GLY:O	16:O:92:ALA:HB3	2.00	0.61
26:Y:15:ARG:HB3	26:Y:15:ARG:NH1	2.15	0.61
28:1:39:CYS:CB	28:1:47:LEU:HD21	2.30	0.61
1:A:338:C:H4'	6:E:174:ILE:HD11	1.83	0.61
1:A:1862:C:H1'	38:A:6681:HOH:O	2.00	0.61
1:A:1878:G:H1'	38:A:5581:HOH:O	2.01	0.61
2:B:3039:U:H1'	2:B:3044:A:N6	2.15	0.61
5:D:204:GLY:HA3	38:D:8653:HOH:O	2.00	0.61
6:E:118:THR:O	6:E:136:VAL:HG13	2.01	0.61
7:F:25:MET:HE1	7:F:37:ALA:O	2.01	0.61
11:J:55:GLN:NE2	11:J:124:ARG:HE	1.98	0.61
28:1:19:GLY:O	28:1:23:ARG:HG2	2.01	0.61
1:A:1972:U:H2'	1:A:1973:A:H5'	1.82	0.61
5:D:154:VAL:HG12	5:D:156:LYS:HG2	1.83	0.61
5:D:312:ARG:HD3	5:D:315:VAL:HG13	1.83	0.61
6:E:219:ASN:O	6:E:222:ASP:OD1	2.18	0.61
7:F:146:LYS:HZ3	16:O:107:ASN:HD21	1.45	0.61
8:G:7:ILE:HD11	8:G:11:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:15:GLN:HG3	8:G:20:ILE:HG12	1.83	0.61
8:G:84:MET:HE1	8:G:148:ILE:HD13	1.82	0.61
13:L:32:ILE:HD11	13:L:56:SER:HB3	1.83	0.61
22:U:55:PHE:CD2	22:U:77:VAL:HG13	2.36	0.61
1:A:1919:A:H4'	38:A:4324:HOH:O	1.99	0.61
2:B:3002:U:OP2	2:B:3002:U:H4'	2.01	0.61
12:K:74:ARG:O	12:K:78:ILE:HG12	2.00	0.61
20:S:132:ARG:HG2	20:S:133:ALA:N	2.16	0.61
8:G:93:MET:HE1	8:G:165:GLY:H	1.65	0.60
11:J:136:VAL:HG22	11:J:137:ASN:O	2.00	0.60
11:J:150:LYS:CB	11:J:157:ILE:HD12	2.27	0.60
15:N:149:TRP:O	15:N:152:ARG:HG2	1.99	0.60
25:X:84:VAL:HG12	38:X:6679:HOH:O	2.01	0.60
1:A:2717:C:H2'	1:A:2718:C:C5'	2.27	0.60
1:A:2827:A:H2'	1:A:2828:G:O4'	2.00	0.60
11:J:26:LYS:HD2	11:J:28:ILE:CD1	2.30	0.60
22:U:49:GLU:OE2	22:U:97:ARG:HD2	2.01	0.60
1:A:871:G:C8	1:A:871:G:C5'	2.77	0.60
1:A:2405:C:P	38:A:6058:HOH:O	2.58	0.60
2:B:3007:G:H4'	16:O:55:ASP:OD2	2.00	0.60
5:D:305:ASP:O	5:D:306:LYS:HB2	2.01	0.60
15:N:55:LYS:HB2	15:N:60:ILE:CD1	2.31	0.60
22:U:48:VAL:HG22	22:U:97:ARG:C	2.27	0.60
31:4:48:ASN:ND2	31:4:50:GLY:H	1.99	0.60
1:A:558:C:C2'	1:A:559:U:H5''	2.31	0.60
1:A:2710:U:H1'	38:A:7082:HOH:O	2.01	0.60
4:C:105:VAL:HG13	4:C:155:THR:O	2.02	0.60
5:D:81:ALA:O	5:D:186:GLY:HA3	2.01	0.60
5:D:221:GLN:HE22	13:L:42:ASN:HD22	1.49	0.60
12:K:75:PRO:HG2	12:K:105:LEU:CD2	2.31	0.60
1:A:553:G:P	27:Z:204:ARG:HH22	2.24	0.60
38:B:8477:HOH:O	16:O:23:ARG:HD3	2.00	0.60
5:D:85:ARG:NH1	38:D:8634:HOH:O	2.34	0.60
7:F:38:GLU:HB3	7:F:49:PRO:HG2	1.83	0.60
22:U:69:LYS:O	22:U:71:VAL:HG23	2.02	0.60
25:X:26:ILE:O	25:X:26:ILE:CG1	2.49	0.60
28:1:39:CYS:HA	28:1:47:LEU:CD1	2.29	0.60
1:A:659:A:H5''	38:A:6557:HOH:O	2.00	0.60
18:Q:78:GLY:O	38:Q:157:HOH:O	2.17	0.60
1:A:285:A:H2'	1:A:286:U:O4'	2.01	0.60
1:A:2089:A:O2'	1:A:2090:G:H5'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2419:U:H5'	1:A:2420:G:H5'	1.84	0.60
1:A:2908:A:H2'	1:A:2909:G:O4'	2.01	0.60
7:F:23:VAL:HG21	7:F:45:THR:HG21	1.81	0.60
8:G:23:GLU:HG2	8:G:28:SER:CB	2.32	0.60
1:A:1182:C:H1'	1:A:1192:A:H8	1.67	0.60
1:A:1185:U:H2'	1:A:1186:C:C6	2.36	0.60
1:A:1730:G:H5'	1:A:1731:C:C5	2.36	0.60
15:N:138:HIS:ND1	15:N:139:PRO:O	2.32	0.60
25:X:21:LEU:HD21	25:X:48:VAL:HG11	1.84	0.60
1:A:134:U:C2	1:A:145:A:C2	2.90	0.60
1:A:282:C:H1'	1:A:368:C:H42	1.65	0.60
1:A:2019:A:H5'	38:A:4024:HOH:O	2.01	0.60
1:A:2690:U:O2'	8:G:111:LYS:HE3	2.00	0.60
6:E:104:ASP:O	6:E:108:GLN:HG3	2.02	0.60
7:F:50:VAL:O	7:F:71:ALA:HA	2.02	0.60
9:H:58:GLU:HA	9:H:61:MET:HG3	1.82	0.60
15:N:52:LEU:HD21	38:N:8616:HOH:O	2.01	0.60
15:N:74:ARG:O	15:N:88:VAL:CG1	2.43	0.60
1:A:281:U:H3'	38:A:6668:HOH:O	2.02	0.60
1:A:821:U:H2'	1:A:822:C:H6	1.67	0.60
7:F:57:THR:HG23	7:F:63:ILE:HG22	1.83	0.60
12:K:39:VAL:HG13	12:K:106:GLY:O	2.01	0.60
22:U:48:VAL:HG23	22:U:98:VAL:HA	1.84	0.60
24:W:4:HIS:HB3	38:W:6622:HOH:O	2.02	0.60
1:A:349:U:O2'	1:A:350:C:H5'	2.02	0.59
38:A:9444:HOH:O	26:Y:23:HIS:HD2	1.84	0.59
13:L:109:LEU:HD13	13:L:113:ILE:HD11	1.84	0.59
1:A:263:U:O4'	9:H:59:ILE:HD13	2.03	0.59
1:A:639:A:H2'	1:A:640:G:C8	2.37	0.59
6:E:236:THR:O	6:E:237:GLU:C	2.45	0.59
16:O:12:ARG:HD3	16:O:18:THR:OG1	2.01	0.59
23:V:9:CYS:CA	23:V:52:THR:HG23	2.32	0.59
25:X:4:LEU:O	25:X:32:CYS:HA	2.02	0.59
1:A:2408:A:H2	38:A:9595:HOH:O	1.84	0.59
5:D:1:PRO:O	5:D:2:GLN:HB2	2.01	0.59
6:E:115:LEU:HD21	6:E:243:VAL:HG13	1.83	0.59
6:E:180:SER:HB2	38:E:8451:HOH:O	2.02	0.59
8:G:81:GLU:HG2	8:G:134:SER:HB3	1.83	0.59
13:L:28:GLU:HG2	13:L:58:THR:HB	1.84	0.59
15:N:87:MET:HB3	31:4:46:ILE:HD13	1.83	0.59
1:A:824:G:C8	38:A:3800:HOH:O	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:2:GLN:HA	38:D:8622:HOH:O	2.02	0.59
5:D:43:GLY:O	5:D:308:LEU:HD12	2.02	0.59
9:H:46:GLU:O	9:H:73:PRO:HD2	2.02	0.59
16:O:48:VAL:HG11	16:O:55:ASP:HB3	1.84	0.59
22:U:47:THR:HB	22:U:100:ASP:HB3	1.83	0.59
1:A:289:G:N2	1:A:363:A:H2	1.98	0.59
1:A:2428:G:O6	1:A:2464:C:H1'	2.03	0.59
4:C:109:GLU:HG2	4:C:116:GLY:N	2.17	0.59
7:F:135:VAL:HG22	7:F:136:ARG:H	1.66	0.59
12:K:80:LYS:HE2	12:K:98:PHE:CZ	2.38	0.59
16:O:37:ARG:NE	38:O:8534:HOH:O	2.34	0.59
25:X:141:HIS:HB2	25:X:146:ILE:HG12	1.84	0.59
26:Y:66:THR:HG23	26:Y:67:PRO:HD2	1.84	0.59
1:A:182:G:O3'	15:N:157:LEU:CD1	2.51	0.59
1:A:738:G:H3'	38:A:6507:HOH:O	2.03	0.59
11:J:35:ASN:ND2	11:J:80:ASN:HA	2.18	0.59
16:O:182:GLY:N	38:O:8567:HOH:O	2.32	0.59
25:X:106:THR:OG1	25:X:109:GLU:HG3	2.02	0.59
1:A:1170:U:O2'	1:A:1172:G:N7	2.27	0.59
14:M:37:LYS:O	38:M:8525:HOH:O	2.17	0.59
14:M:54:PRO:HG2	14:M:57:VAL:CG2	2.33	0.59
28:1:28:ASP:O	28:1:31:ILE:HG22	2.02	0.59
1:A:20:G:H21	20:S:117:HIS:HD2	1.51	0.59
1:A:2429:A:O2'	1:A:2430:A:H5'	2.03	0.59
38:A:4990:HOH:O	5:D:298:LYS:HD3	2.02	0.59
5:D:75:GLU:C	5:D:77:PRO:HD3	2.28	0.59
7:F:11:HIS:O	7:F:12:GLU:HB3	2.02	0.59
14:M:136:ALA:HB3	38:M:8577:HOH:O	2.03	0.59
16:O:154:LEU:O	16:O:155:GLU:HB3	2.03	0.59
22:U:24:ARG:HH21	22:U:39:ASN:HD22	1.50	0.59
1:A:449:A:N7	6:E:43:LYS:HG2	2.18	0.59
1:A:775:G:OP1	29:2:16:HIS:HE1	1.85	0.59
2:B:3040:C:N4	7:F:51:ARG:HB2	2.18	0.59
7:F:170:TYR:O	7:F:171:ASP:HB3	2.01	0.59
22:U:52:ARG:HB2	22:U:95:ASN:HB3	1.85	0.59
1:A:1666:C:C2'	1:A:1667:A:H5'	2.32	0.59
1:A:1918:U:OP2	38:A:3513:HOH:O	2.17	0.59
1:A:2896:A:H5''	38:A:5559:HOH:O	2.02	0.59
38:A:6333:HOH:O	15:N:178:LYS:HB2	2.02	0.59
4:C:100:PRO:HG2	4:C:103:VAL:HG21	1.83	0.59
10:I:64:ASN:HD22	10:I:64:ASN:N	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:59:GLY:HA3	15:N:141:ILE:HD12	1.85	0.59
27:Z:144:ARG:CZ	38:Z:8616:HOH:O	2.51	0.59
1:A:157:G:H4'	15:N:95:LYS:CE	2.33	0.58
1:A:2413:A:N7	16:O:109:PRO:HB3	2.18	0.58
5:D:195:ARG:HG2	5:D:323:LEU:HD22	1.85	0.58
1:A:1183:C:N4	38:A:3888:HOH:O	2.32	0.58
7:F:64:ARG:CG	7:F:67:ASP:HB3	2.33	0.58
11:J:56:ILE:HG22	11:J:61:LEU:CD2	2.32	0.58
14:M:125:PHE:CZ	14:M:140:VAL:HG13	2.37	0.58
16:O:163:PHE:HA	38:O:8520:HOH:O	2.02	0.58
20:S:132:ARG:NH2	38:S:8582:HOH:O	2.35	0.58
24:W:49:LEU:O	24:W:53:ILE:HG13	2.03	0.58
29:2:10:LYS:HG3	38:2:2979:HOH:O	2.02	0.58
1:A:120:A:H2'	1:A:120:A:N3	2.18	0.58
1:A:371:U:H2'	1:A:372:A:C8	2.37	0.58
15:N:72:SER:OG	15:N:74:ARG:HB2	2.02	0.58
1:A:1759:A:N3	1:A:1818:C:H2'	2.17	0.58
38:A:3680:HOH:O	27:Z:186:ARG:HD2	2.03	0.58
2:B:3044:A:O4'	7:F:76:ARG:NE	2.36	0.58
2:B:3057:A:N6	38:B:8444:HOH:O	2.36	0.58
5:D:264:GLU:HG2	5:D:267:LYS:CE	2.28	0.58
6:E:107:ARG:HH11	6:E:107:ARG:CB	2.16	0.58
13:L:37:TYR:CD2	38:L:7169:HOH:O	2.52	0.58
15:N:48:ARG:NH2	38:N:8567:HOH:O	2.35	0.58
27:Z:187:VAL:HB	38:Z:8575:HOH:O	2.03	0.58
1:A:567:U:H5''	38:A:5862:HOH:O	2.03	0.58
4:C:25:ALA:HA	38:C:8573:HOH:O	2.03	0.58
6:E:237:GLU:HB2	38:E:8436:HOH:O	2.01	0.58
27:Z:187:VAL:HG23	27:Z:192:ASP:HB3	1.85	0.58
1:A:184:G:H5''	15:N:153:THR:HG22	1.86	0.58
1:A:739:G:N7	38:A:7001:HOH:O	2.36	0.58
1:A:1168:C:H2'	1:A:1169:U:O4'	2.03	0.58
2:B:3047:A:C2	2:B:3048:C:C2	2.91	0.58
5:D:62:ARG:HA	5:D:65:MET:CE	2.33	0.58
6:E:103:ASN:HB3	38:E:8308:HOH:O	2.02	0.58
7:F:38:GLU:OE2	7:F:51:ARG:CZ	2.52	0.58
15:N:172:GLY:C	15:N:183:VAL:HG11	2.29	0.58
20:S:14:ALA:HB3	20:S:147:LEU:HB2	1.86	0.58
20:S:99:ALA:CB	20:S:109:MET:HE1	2.16	0.58
1:A:29:C:O2'	1:A:30:U:H5'	2.04	0.58
1:A:661:G:C5	1:A:686:A:C2	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2462:G:N7	31:4:60:LYS:NZ	2.45	0.58
1:A:2578:G:H5'	1:A:2578:G:C8	2.36	0.58
7:F:99:ASP:HB2	7:F:103:ASN:HB2	1.84	0.58
16:O:169:PRO:O	16:O:172:PHE:HB3	2.04	0.58
1:A:646:G:H2'	1:A:647:U:C6	2.38	0.58
2:B:3006:C:C5'	16:O:37:ARG:NH1	2.61	0.58
2:B:3051:A:H5'	16:O:160:SER:HB3	1.86	0.58
5:D:307:ARG:HH11	5:D:307:ARG:HB2	1.68	0.58
12:K:130:VAL:HG12	12:K:131:THR:N	2.18	0.58
18:Q:10:ALA:HA	18:Q:13:VAL:CG1	2.32	0.58
1:A:820:G:C6	4:C:171:LYS:HB2	2.39	0.58
1:A:1053:G:OP1	11:J:12:PRO:HG3	2.02	0.58
1:A:1123:A:C6	1:A:1238:C:H5'	2.39	0.58
1:A:1351:G:O2'	38:A:4032:HOH:O	2.17	0.58
1:A:2073:G:OP2	1:A:2490:A:H5'	2.02	0.58
1:A:2274:A:H1'	15:N:86:MET:SD	2.43	0.58
1:A:2316:G:H2'	38:A:4385:HOH:O	2.02	0.58
8:G:3:VAL:HG22	8:G:49:ILE:HB	1.86	0.58
18:Q:64:GLU:HG2	38:Q:171:HOH:O	2.04	0.58
24:W:8:ILE:HA	24:W:11:MET:HE3	1.86	0.58
27:Z:184:GLU:OE1	27:Z:204:ARG:NH1	2.36	0.58
1:A:542:A:H1'	38:A:4158:HOH:O	2.04	0.58
1:A:2427:C:OP2	31:4:84:ARG:HD2	2.03	0.58
1:A:2676:C:H4'	12:K:70:PHE:CE1	2.39	0.58
1:A:2878:U:H2'	1:A:2879:A:O4'	2.04	0.58
11:J:44:ALA:HA	11:J:163:PRO:O	2.03	0.58
16:O:184:ILE:HG22	16:O:185:GLU:HG3	1.84	0.58
18:Q:59:ARG:HH22	18:Q:66:GLN:HE22	1.51	0.58
1:A:1942:A:O2'	1:A:1943:C:H5'	2.04	0.57
5:D:205:VAL:O	5:D:307:ARG:NE	2.37	0.57
9:H:47:LEU:HB2	9:H:108:LEU:HD11	1.86	0.57
11:J:26:LYS:HD3	11:J:89:PRO:CG	2.33	0.57
15:N:35:PRO:O	38:N:8539:HOH:O	2.17	0.57
1:A:1819:G:H2'	1:A:1820:G:H4'	1.85	0.57
38:B:8477:HOH:O	16:O:20:TYR:CE2	2.53	0.57
4:C:109:GLU:HG2	4:C:116:GLY:H	1.69	0.57
6:E:162:VAL:HG13	6:E:232:LEU:HD21	1.85	0.57
15:N:61:ILE:HG13	38:N:8624:HOH:O	2.03	0.57
7:F:166:ILE:HD12	38:F:6326:HOH:O	2.04	0.57
1:A:1162:G:H2'	38:A:6045:HOH:O	2.04	0.57
4:C:192:VAL:HG12	4:C:207:GLN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:11:HIS:C	7:F:13:MET:H	2.12	0.57
14:M:104:ASP:O	14:M:105:TYR:HB3	2.04	0.57
15:N:186:SER:O	15:N:189:VAL:HG12	2.03	0.57
16:O:141:ARG:HB3	38:O:8566:HOH:O	2.05	0.57
1:A:128:A:H3'	1:A:128:A:C8	2.38	0.57
1:A:820:G:C5	4:C:171:LYS:HB2	2.40	0.57
1:A:2324:G:H4'	1:A:2418:G:O2'	2.04	0.57
1:A:2421:G:H3'	1:A:2422:U:C5'	2.35	0.57
1:A:2866:U:C2	38:A:6955:HOH:O	2.53	0.57
4:C:179:MET:HG2	4:C:186:TRP:HB2	1.86	0.57
14:M:143:THR:CG2	14:M:144:ASP:N	2.67	0.57
21:T:43:GLU:HB3	38:T:8345:HOH:O	2.04	0.57
1:A:1528:A:H2'	1:A:1529:G:O4'	2.04	0.57
1:A:1753:C:O2	5:D:229:ARG:NH2	2.38	0.57
1:A:2011:A:P	38:A:5418:HOH:O	2.63	0.57
1:A:2783:A:H3'	38:A:4707:HOH:O	2.02	0.57
9:H:57:GLU:O	9:H:61:MET:HG3	2.05	0.57
25:X:21:LEU:HD22	25:X:26:ILE:HD13	1.86	0.57
25:X:137:GLN:HE21	25:X:141:HIS:CE1	2.21	0.57
1:A:1119:G:H2'	12:K:52:GLN:NE2	2.19	0.57
1:A:1474:C:H6	1:A:1474:C:C5'	2.11	0.57
1:A:1497:G:H4'	1:A:1627:G:O2'	2.04	0.57
1:A:1500:U:P	18:Q:41:ARG:HH22	2.27	0.57
1:A:2365:G:H4'	19:R:45:PRO:O	2.04	0.57
4:C:29:HIS:CE1	4:C:107:ASN:ND2	2.73	0.57
5:D:320:GLN:HG3	5:D:321:PRO:HD2	1.87	0.57
17:P:59:VAL:HG23	17:P:111:VAL:HG23	1.86	0.57
1:A:1299:G:O6	14:M:6:ARG:HD3	2.05	0.57
1:A:1669:A:H2'	1:A:1670:G:H8	1.69	0.57
10:I:12:ILE:HG13	38:I:6833:HOH:O	2.04	0.57
15:N:106:ASN:ND2	35:N:8518:CL:CL	2.74	0.57
16:O:49:THR:CG2	16:O:56:ASP:HB2	2.33	0.57
16:O:90:LEU:HB2	16:O:186:LEU:HD22	1.86	0.57
28:1:47:LEU:HD23	28:1:57:CYS:CB	2.34	0.57
1:A:138:U:H5''	1:A:139:C:OP2	2.05	0.57
11:J:85:ILE:HB	11:J:132:PHE:CE2	2.40	0.57
1:A:105:G:O2'	1:A:106:A:H5'	2.04	0.57
1:A:638:C:H2'	1:A:639:A:C8	2.40	0.57
1:A:1134:G:H4'	11:J:151:MET:CE	2.29	0.57
38:A:4879:HOH:O	4:C:164:ARG:NE	2.36	0.57
5:D:62:ARG:CA	5:D:65:MET:HE3	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:190:MET:HE2	5:D:194:PHE:HD1	1.69	0.57
11:J:45:GLN:HE21	11:J:135:TRP:NE1	2.03	0.57
25:X:4:LEU:HD21	25:X:52:VAL:HG11	1.87	0.57
27:Z:115:ARG:NE	38:Z:8560:HOH:O	2.37	0.57
29:2:52:SER:HA	38:2:4248:HOH:O	2.04	0.57
1:A:396:U:H1'	38:A:7089:HOH:O	2.03	0.56
1:A:825:U:H5''	1:A:826:U:OP1	2.05	0.56
1:A:1086:A:N6	25:X:11:VAL:HG11	2.20	0.56
1:A:1118:A:C8	1:A:1118:A:C3'	2.85	0.56
1:A:1766:U:O2	1:A:1778:A:H5'	2.05	0.56
1:A:2359:G:N7	38:A:3196:HOH:O	2.32	0.56
1:A:2793:A:N3	38:A:3982:HOH:O	2.33	0.56
5:D:82:VAL:O	5:D:82:VAL:HG12	2.04	0.56
9:H:21:GLU:O	9:H:24:ARG:HG3	2.05	0.56
9:H:110:GLU:O	9:H:114:LYS:HG3	2.04	0.56
15:N:186:SER:OG	15:N:189:VAL:HG12	2.05	0.56
16:O:33:ARG:NH1	16:O:103:ASP:OD2	2.30	0.56
30:3:18:ASN:HD21	30:3:40:ARG:H	1.52	0.56
4:C:211:LYS:HB3	4:C:212:PRO:CD	2.30	0.56
5:D:30:PRO:HB2	5:D:39:GLN:NE2	2.18	0.56
6:E:27:ARG:HG3	6:E:29:ASP:OD1	2.05	0.56
8:G:69:ILE:HA	8:G:72:MET:CE	2.35	0.56
12:K:39:VAL:HG11	12:K:107:ASN:HB2	1.85	0.56
16:O:64:SER:C	16:O:66:LEU:H	2.12	0.56
16:O:139:TRP:HA	16:O:139:TRP:CE3	2.39	0.56
24:W:12:THR:CG2	24:W:15:GLU:HG3	2.25	0.56
28:1:11:THR:CG2	28:1:23:ARG:HB2	2.35	0.56
1:A:595:U:O2'	1:A:596:C:H5'	2.05	0.56
1:A:2314:G:H2'	1:A:2315:C:H5'	1.87	0.56
1:A:2694:A:H4'	8:G:91:PHE:CE1	2.40	0.56
4:C:88:ILE:HD13	4:C:100:PRO:CD	2.35	0.56
5:D:55:ASN:HB3	5:D:64:GLY:H	1.70	0.56
11:J:13:ALA:CA	11:J:91:HIS:HE1	2.15	0.56
11:J:130:HIS:CG	11:J:133:ILE:HD11	2.40	0.56
14:M:104:ASP:HB3	38:M:8570:HOH:O	2.05	0.56
21:T:51:GLN:NE2	21:T:53:ASN:HD21	2.03	0.56
24:W:39:ALA:N	24:W:40:PRO:CD	2.69	0.56
25:X:38:THR:HB	38:X:5390:HOH:O	2.06	0.56
25:X:60:GLU:O	25:X:63:GLU:HB2	2.05	0.56
30:3:41:HIS:H	30:3:45:ASN:ND2	1.96	0.56
1:A:383:A:H4'	38:A:4801:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:84:MET:HE1	8:G:148:ILE:HD12	1.86	0.56
21:T:51:GLN:HE21	21:T:53:ASN:ND2	2.03	0.56
27:Z:186:ARG:HG2	27:Z:186:ARG:HH11	1.71	0.56
31:4:38:ARG:O	31:4:42:ARG:HB2	2.06	0.56
1:A:272:A:H5'	1:A:273:G:OP2	2.05	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.56
1:A:2241:C:O2'	1:A:2242:U:H5'	2.05	0.56
1:A:2529:G:O2'	1:A:2530:C:H5'	2.05	0.56
1:A:2620:U:O4	36:5:76:PPU:C	2.54	0.56
1:A:2718:C:H6	1:A:2718:C:H5'	1.70	0.56
1:A:2814:A:OP2	38:A:4548:HOH:O	2.17	0.56
6:E:133:ARG:HD2	38:E:8414:HOH:O	2.05	0.56
6:E:162:VAL:HG12	6:E:162:VAL:O	2.04	0.56
6:E:178:GLN:O	6:E:179:GLY:C	2.48	0.56
16:O:154:LEU:HG	16:O:155:GLU:H	1.70	0.56
18:Q:103:THR:O	18:Q:107:GLU:HG3	2.06	0.56
20:S:29:LYS:HB3	38:S:8531:HOH:O	2.05	0.56
24:W:58:THR:O	24:W:62:GLU:HG3	2.05	0.56
1:A:168:C:O2'	1:A:169:A:H5'	2.06	0.56
1:A:283:U:H5''	1:A:284:C:P	2.45	0.56
1:A:316:A:H5'	22:U:54:ASP:OD2	2.05	0.56
6:E:214:THR:HG21	38:E:8407:HOH:O	2.05	0.56
7:F:44:ILE:HG12	7:F:83:PHE:HE1	1.69	0.56
9:H:19:ALA:O	9:H:22:VAL:HG22	2.06	0.56
14:M:148:GLU:HA	38:M:8576:HOH:O	2.05	0.56
18:Q:58:SER:HB3	38:Q:186:HOH:O	2.04	0.56
18:Q:105:LEU:CD2	18:Q:137:LEU:HD21	2.36	0.56
2:B:3049:G:O2'	2:B:3050:G:H5'	2.06	0.56
5:D:207:LYS:HG2	5:D:304:PRO:HB3	1.88	0.56
16:O:58:LEU:HD12	16:O:58:LEU:N	2.21	0.56
16:O:80:SER:CB	38:O:8536:HOH:O	2.53	0.56
31:4:74:CYS:SG	31:4:76:LYS:CB	2.94	0.56
1:A:2502:C:C4'	11:J:151:MET:HG2	2.35	0.56
5:D:280:VAL:HG13	5:D:334:SER:HA	1.88	0.56
7:F:44:ILE:HG23	7:F:45:THR:HG23	1.88	0.56
13:L:125:ALA:C	13:L:127:ALA:H	2.12	0.56
25:X:154:ARG:C	38:X:4276:HOH:O	2.47	0.56
1:A:154:C:H2'	1:A:155:C:H6	1.70	0.56
1:A:2093:G:H5''	38:D:8526:HOH:O	2.06	0.56
1:A:2664:A:H8	1:A:2664:A:OP1	1.89	0.56
8:G:31:ARG:NH1	38:G:5919:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:87:MET:CG	31:4:46:ILE:HD13	2.36	0.56
29:2:8:GLN:NE2	29:2:11:LYS:NZ	2.52	0.56
1:A:2507:G:H2'	1:A:2510:C:H42	1.71	0.56
1:A:2721:U:H4'	13:L:87:ARG:HG3	1.88	0.56
7:F:144:ARG:NH2	38:F:3839:HOH:O	2.39	0.56
11:J:39:GLY:O	11:J:41:THR:N	2.39	0.56
11:J:59:ASN:H	11:J:59:ASN:ND2	1.97	0.56
12:K:126:ASN:O	12:K:129:PHE:HE2	1.89	0.56
16:O:34:LEU:HA	16:O:47:LEU:HD23	1.87	0.56
17:P:7:LEU:HD22	38:P:5650:HOH:O	2.05	0.56
22:U:9:LYS:HE3	22:U:13:ARG:HH11	1.71	0.56
1:A:121:U:OP2	30:3:10:ARG:NH2	2.39	0.55
1:A:2672:C:H1'	38:D:8634:HOH:O	2.06	0.55
9:H:107:VAL:HG23	38:H:6617:HOH:O	2.05	0.55
21:T:32:ALA:HA	21:T:36:GLU:OE1	2.06	0.55
1:A:113:A:H3'	1:A:114:A:C5'	2.36	0.55
8:G:21:THR:HG23	8:G:30:THR:OG1	2.06	0.55
8:G:133:VAL:HG12	8:G:141:VAL:HG13	1.88	0.55
15:N:104:ARG:O	15:N:108:LYS:HG2	2.06	0.55
18:Q:109:ARG:NH1	18:Q:119:TYR:CE2	2.74	0.55
26:Y:43:VAL:HG12	26:Y:44:ASP:N	2.21	0.55
1:A:558:C:H2'	1:A:559:U:C5'	2.36	0.55
1:A:1682:A:H5''	38:A:8961:HOH:O	2.06	0.55
2:B:3028:U:H2'	2:B:3029:C:C6	2.42	0.55
4:C:215:ILE:HG13	4:C:216:SER:N	2.22	0.55
6:E:236:THR:CG2	6:E:239:ALA:H	1.95	0.55
14:M:1:THR:HA	38:M:8526:HOH:O	2.06	0.55
16:O:71:TRP:HE3	16:O:175:LEU:HD22	1.72	0.55
16:O:143:ARG:HA	16:O:172:PHE:CD2	2.41	0.55
31:4:44:SER:HA	31:4:49:ASP:OD1	2.06	0.55
1:A:1209:C:H2'	1:A:1210:G:C8	2.41	0.55
1:A:1393:A:H2'	1:A:1394:C:C6	2.41	0.55
14:M:90:ARG:NH2	14:M:121:ILE:HD11	2.20	0.55
25:X:108:ARG:HE	25:X:114:PRO:HG3	1.71	0.55
1:A:338:C:H5''	38:E:8426:HOH:O	2.06	0.55
1:A:2904:U:H4'	26:Y:8:ARG:NH1	2.20	0.55
4:C:95:PRO:HG2	4:C:98:GLU:HG2	1.88	0.55
23:V:33:SER:O	23:V:37:GLU:HG3	2.07	0.55
26:Y:20:GLU:CD	26:Y:21:PRO:HD2	2.31	0.55
27:Z:133:HIS:HD2	38:Z:8588:HOH:O	1.88	0.55
27:Z:216:ARG:CD	38:Z:8574:HOH:O	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:G:N2	1:A:509:A:H5'	2.16	0.55
1:A:635:A:H2'	1:A:636:G:H5''	1.87	0.55
5:D:195:ARG:HD2	5:D:324:ASP:OD1	2.06	0.55
5:D:204:GLY:C	38:D:8653:HOH:O	2.49	0.55
15:N:114:VAL:HB	15:N:159:THR:HG23	1.87	0.55
21:T:57:THR:C	21:T:59:ASP:H	2.15	0.55
24:W:64:GLY:O	24:W:65:ASP:CB	2.55	0.55
29:2:2:GLY:O	29:2:6:PRO:HG2	2.07	0.55
1:A:57:C:H5''	38:A:6218:HOH:O	2.06	0.55
1:A:182:G:O3'	15:N:157:LEU:HD13	2.07	0.55
1:A:1659:A:H2'	1:A:1660:G:O4'	2.07	0.55
1:A:2361:A:H5''	38:A:8523:HOH:O	2.06	0.55
5:D:119:HIS:O	5:D:121:PRO:HD3	2.06	0.55
9:H:100:ASP:HB3	38:H:5691:HOH:O	2.07	0.55
14:M:145:LEU:O	14:M:148:GLU:HG3	2.07	0.55
15:N:52:LEU:HD13	15:N:116:ASN:CG	2.31	0.55
19:R:11:ARG:HD3	38:R:5620:HOH:O	2.07	0.55
30:3:22:PRO:HG2	30:3:25:VAL:CG2	2.35	0.55
31:4:34:LYS:HB2	31:4:37:ASP:OD2	2.06	0.55
1:A:1166:A:H1'	1:A:1192:A:N1	2.21	0.55
1:A:1191:A:C3'	1:A:1192:A:H5''	2.37	0.55
1:A:2326:U:H4'	1:A:2412:G:C4'	2.37	0.55
4:C:140:LEU:HB3	4:C:141:PRO:HD2	1.88	0.55
7:F:140:ARG:O	7:F:144:ARG:HG2	2.06	0.55
11:J:71:TYR:C	11:J:73:GLN:N	2.63	0.55
1:A:777:U:O2'	29:2:11:LYS:HG2	2.06	0.55
2:B:3029:C:C2'	2:B:3030:C:H5'	2.36	0.55
4:C:211:LYS:NZ	38:C:8582:HOH:O	2.39	0.55
7:F:23:VAL:CG2	7:F:73:VAL:HB	2.36	0.55
8:G:34:TRP:O	12:K:127:ILE:HD11	2.06	0.55
16:O:73:ALA:HB2	16:O:163:PHE:CZ	2.42	0.55
20:S:26:LYS:NZ	38:S:8517:HOH:O	2.34	0.55
20:S:82:GLU:O	20:S:86:LYS:HG3	2.07	0.55
1:A:970:U:H2'	38:A:5786:HOH:O	2.06	0.55
1:A:2478:U:H2'	1:A:2479:A:C8	2.41	0.55
11:J:48:LEU:HG	11:J:157:ILE:HG21	1.89	0.55
16:O:62:HIS:HB3	16:O:65:ASP:OD1	2.07	0.55
21:T:6:LYS:HB2	21:T:27:ALA:O	2.06	0.55
22:U:37:GLN:OE1	22:U:118:SER:HA	2.06	0.55
26:Y:21:PRO:HG2	26:Y:24:LYS:HD3	1.88	0.55
1:A:125:U:H2'	38:A:3261:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:G:P	38:A:3782:HOH:O	2.65	0.54
1:A:1165:G:OP1	1:A:1165:G:H3'	2.08	0.54
2:B:3023:U:H6	2:B:3023:U:C5'	2.20	0.54
8:G:11:VAL:CG1	8:G:12:ASP:N	2.70	0.54
18:Q:105:LEU:HD21	18:Q:137:LEU:HD21	1.88	0.54
31:4:3:MET:O	31:4:90:PHE:HA	2.07	0.54
1:A:514:G:H8	1:A:514:G:O5'	1.90	0.54
1:A:962:C:C1'	16:O:5:ARG:NH1	2.64	0.54
1:A:1187:U:O2'	1:A:1189:A:H2	1.91	0.54
1:A:1512:G:O2'	1:A:1513:C:H5'	2.06	0.54
1:A:2415:A:N3	16:O:26:LEU:HD13	2.22	0.54
4:C:192:VAL:HG12	4:C:192:VAL:O	2.07	0.54
4:C:192:VAL:CG1	4:C:207:GLN:HB3	2.38	0.54
9:H:117:GLU:C	9:H:119:ARG:H	2.15	0.54
11:J:46:VAL:HG12	11:J:146:TRP:HZ3	1.72	0.54
11:J:147:ARG:HA	11:J:150:LYS:NZ	2.23	0.54
13:L:4:LEU:HD22	13:L:116:GLU:HB3	1.89	0.54
16:O:132:ASN:O	16:O:135:VAL:HG12	2.06	0.54
20:S:132:ARG:CZ	38:S:8582:HOH:O	2.55	0.54
26:Y:15:ARG:HH11	26:Y:15:ARG:CB	2.15	0.54
5:D:51:VAL:CG2	5:D:327:VAL:HG13	2.36	0.54
5:D:314:ALA:CB	5:D:317:PRO:HG3	2.37	0.54
12:K:42:GLU:O	12:K:131:THR:HG23	2.07	0.54
15:N:46:LEU:HG	38:N:8622:HOH:O	2.07	0.54
15:N:61:ILE:HD12	15:N:61:ILE:N	2.21	0.54
22:U:32:ARG:NH1	22:U:38:ARG:HH12	2.05	0.54
1:A:21:G:H4'	20:S:2:ILE:HG22	1.88	0.54
1:A:204:A:H2'	1:A:205:U:H5'	1.88	0.54
1:A:711:G:C2	1:A:718:C:C2	2.96	0.54
1:A:1422:U:H2'	1:A:1423:C:C6	2.42	0.54
1:A:1500:U:OP2	18:Q:41:ARG:NH2	2.40	0.54
1:A:2320:U:H4'	1:A:2321:A:O4'	2.08	0.54
2:B:3023:U:C3'	2:B:3024:U:H5''	2.38	0.54
2:B:3042:C:H2'	38:B:8505:HOH:O	2.07	0.54
4:C:199:HIS:HD2	4:C:201:PHE:H	1.52	0.54
7:F:27:ILE:HG22	7:F:28:GLY:N	2.15	0.54
7:F:41:LEU:HA	7:F:44:ILE:CG2	2.36	0.54
9:H:101:ALA:HA	38:H:5413:HOH:O	2.07	0.54
19:R:40:HIS:HD2	19:R:60:THR:OG1	1.90	0.54
25:X:149:LEU:HG	25:X:153:MET:CE	2.27	0.54
1:A:1120:U:H5''	1:A:1120:U:H6	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:G:N3	12:K:86:MET:HE2	2.22	0.54
1:A:2547:C:OP2	5:D:5:ARG:NH1	2.40	0.54
2:B:3020:G:O2'	2:B:3021:G:H5'	2.07	0.54
8:G:126:ILE:HB	8:G:131:LEU:CD2	2.37	0.54
11:J:136:VAL:HG23	38:J:8344:HOH:O	2.07	0.54
14:M:149:ARG:O	14:M:150:GLN:HB2	2.07	0.54
17:P:14:LEU:HD23	17:P:102:ILE:HD11	1.88	0.54
1:A:541:C:H2'	1:A:542:A:H5'	1.88	0.54
1:A:824:G:N7	38:A:3800:HOH:O	2.39	0.54
1:A:1951:G:N2	38:A:5718:HOH:O	2.40	0.54
1:A:2429:A:H2'	1:A:2430:A:C8	2.42	0.54
38:A:6231:HOH:O	16:O:4:PRO:HD2	2.07	0.54
4:C:164:ARG:HA	28:1:69:TYR:CE1	2.43	0.54
20:S:119:VAL:HG21	20:S:142:ASP:CG	2.32	0.54
22:U:9:LYS:CE	22:U:13:ARG:NH1	2.71	0.54
25:X:35:VAL:HG23	25:X:41:TYR:CD2	2.42	0.54
28:1:42:CYS:SG	28:1:44:PHE:N	2.61	0.54
1:A:951:A:C2'	1:A:952:G:H5'	2.38	0.54
1:A:2349:G:OP1	7:F:20:LYS:NZ	2.36	0.54
1:A:2761:A:C4	1:A:2763:G:C8	2.95	0.54
4:C:173:GLY:O	4:C:176:HIS:HB3	2.07	0.54
6:E:16:VAL:HG12	6:E:17:ASP:N	2.22	0.54
10:I:64:ASN:O	10:I:68:GLU:HG3	2.08	0.54
31:4:87:ARG:HG3	38:4:8570:HOH:O	2.06	0.54
1:A:2437:A:H2'	1:A:2438:G:C8	2.43	0.54
1:A:2758:G:H2'	1:A:2759:C:C6	2.43	0.54
5:D:66:GLU:OE1	5:D:328:ARG:HD2	2.08	0.54
8:G:126:ILE:HB	8:G:131:LEU:HD23	1.89	0.54
1:A:2015:A:H2'	1:A:2016:U:O4'	2.07	0.54
1:A:2329:C:O2'	1:A:2330:U:H5'	2.08	0.54
1:A:2717:C:O2'	1:A:2718:C:H5''	2.06	0.54
5:D:2:GLN:CD	38:D:8622:HOH:O	2.50	0.54
5:D:55:ASN:HB3	5:D:63:GLU:HA	1.89	0.54
5:D:168:GLY:N	5:D:174:ARG:HD3	2.22	0.54
11:J:166:ASN:N	11:J:166:ASN:ND2	2.56	0.54
12:K:131:THR:HG22	12:K:133:GLY:N	2.23	0.54
15:N:164:THR:HB	38:N:8520:HOH:O	2.08	0.54
23:V:44:ARG:CB	38:V:3805:HOH:O	2.54	0.54
1:A:506:G:H22	1:A:509:A:H5''	1.70	0.54
1:A:1527:A:H1'	1:A:1528:A:C8	2.43	0.54
1:A:1713:G:C2'	38:A:4547:HOH:O	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1829:A:H5''	38:A:9578:HOH:O	2.07	0.54
1:A:1887:U:OP1	28:1:21:LYS:HG3	2.08	0.54
38:A:5970:HOH:O	30:3:1:GLY:HA3	2.07	0.54
38:A:7138:HOH:O	15:N:154:ARG:HB2	2.07	0.54
2:B:3035:C:H5''	38:B:8456:HOH:O	2.08	0.54
6:E:236:THR:HA	38:E:8457:HOH:O	2.08	0.54
7:F:65:GLU:HG3	38:F:6752:HOH:O	2.06	0.54
11:J:45:GLN:HE21	11:J:135:TRP:HE1	1.56	0.54
13:L:34:VAL:HB	38:L:7169:HOH:O	2.08	0.54
25:X:5:VAL:HG22	25:X:32:CYS:HB2	1.90	0.54
26:Y:76:ARG:HG3	26:Y:76:ARG:NH1	2.21	0.54
1:A:329:A:OP2	6:E:206:ASN:HB2	2.08	0.53
1:A:447:A:O2'	1:A:448:G:H5'	2.08	0.53
1:A:778:C:C4	1:A:779:U:C4	2.96	0.53
1:A:1174:A:C5	1:A:1201:C:H4'	2.43	0.53
1:A:1641:A:H2'	1:A:1642:A:H5'	1.89	0.53
1:A:2265:U:H2'	1:A:2266:A:C8	2.43	0.53
7:F:64:ARG:CD	7:F:67:ASP:HB3	2.38	0.53
13:L:75:ARG:CZ	38:L:4172:HOH:O	2.56	0.53
14:M:65:ASP:CG	14:M:111:ALA:HB3	2.33	0.53
15:N:87:MET:SD	31:4:46:ILE:HD13	2.48	0.53
17:P:39:THR:O	17:P:115:ARG:NH2	2.41	0.53
25:X:5:VAL:HG11	25:X:153:MET:HE1	1.90	0.53
25:X:110:GLN:NE2	25:X:110:GLN:HA	2.24	0.53
1:A:558:C:H2'	1:A:559:U:H5'	1.91	0.53
1:A:816:G:H5'	1:A:1598:A:H4'	1.90	0.53
1:A:1250:C:O2'	1:A:1251:C:H5'	2.08	0.53
4:C:164:ARG:HB2	28:1:68:CYS:SG	2.48	0.53
6:E:200:PRO:HB3	6:E:212:VAL:HG23	1.90	0.53
10:I:12:ILE:N	38:I:4714:HOH:O	2.41	0.53
11:J:81:TYR:CD1	11:J:81:TYR:C	2.86	0.53
17:P:4:ASN:HB3	17:P:7:LEU:HB3	1.90	0.53
21:T:57:THR:CG2	21:T:58:MET:N	2.71	0.53
23:V:9:CYS:HA	23:V:52:THR:CG2	2.38	0.53
1:A:113:A:OP1	38:A:9242:HOH:O	2.19	0.53
1:A:644:G:N3	1:A:644:G:H5'	2.24	0.53
1:A:1097:A:H5''	25:X:125:HIS:NE2	2.24	0.53
1:A:1909:A:H2'	1:A:1910:A:C8	2.42	0.53
5:D:72:THR:HB	38:D:8606:HOH:O	2.09	0.53
5:D:248:ARG:O	5:D:251:VAL:CG1	2.56	0.53
22:U:24:ARG:HH21	22:U:39:ASN:ND2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:1:MET:HB2	25:X:103:GLU:HG2	1.90	0.53
27:Z:126:PRO:HG2	27:Z:128:PHE:CE1	2.43	0.53
29:2:25:LYS:HD2	30:3:49:GLU:H	1.72	0.53
1:A:1666:C:O2'	1:A:1667:A:C5'	2.56	0.53
1:A:1730:G:H5'	1:A:1731:C:C6	2.44	0.53
1:A:2028:U:H2'	1:A:2029:C:C6	2.43	0.53
1:A:2791:U:H1'	1:A:2792:A:H5''	1.90	0.53
4:C:105:VAL:HG11	4:C:154:ALA:HB1	1.89	0.53
7:F:99:ASP:CB	7:F:103:ASN:H	2.22	0.53
8:G:86:VAL:CG1	8:G:129:GLU:HA	2.38	0.53
9:H:28:ALA:HB3	9:H:99:THR:O	2.08	0.53
38:L:408:HOH:O	23:V:37:GLU:HB3	2.08	0.53
14:M:54:PRO:HG2	14:M:57:VAL:HG21	1.89	0.53
16:O:43:VAL:HG13	16:O:118:ILE:HD11	1.89	0.53
20:S:18:LEU:HD12	20:S:143:VAL:CG1	2.39	0.53
1:A:42:C:H1'	38:A:4157:HOH:O	2.08	0.53
1:A:681:G:H5'	1:A:681:G:N3	2.24	0.53
1:A:1617:C:C4	1:A:1643:C:H4'	2.43	0.53
4:C:95:PRO:HA	4:C:153:ARG:HA	1.91	0.53
4:C:105:VAL:CG1	4:C:154:ALA:HB1	2.39	0.53
9:H:91:VAL:CG1	9:H:92:GLY:H	2.18	0.53
23:V:46:ALA:HB1	23:V:52:THR:HG21	1.90	0.53
1:A:344:C:H2'	1:A:345:G:O4'	2.08	0.53
1:A:1192:A:H3'	1:A:1193:A:H5'	1.90	0.53
1:A:1268:C:O2'	1:A:1269:G:H5'	2.09	0.53
1:A:1362:U:H5'	38:A:9762:HOH:O	2.09	0.53
1:A:2326:U:H4'	1:A:2412:G:H4'	1.90	0.53
4:C:37:VAL:HG22	38:C:8610:HOH:O	2.08	0.53
7:F:54:ALA:HB2	7:F:69:ILE:HD12	1.90	0.53
9:H:91:VAL:CG1	9:H:92:GLY:N	2.70	0.53
11:J:147:ARG:HA	11:J:150:LYS:HZ2	1.73	0.53
15:N:61:ILE:HA	38:N:8624:HOH:O	2.09	0.53
15:N:108:LYS:HE3	38:N:8614:HOH:O	2.08	0.53
24:W:44:GLY:O	24:W:48:GLU:HG2	2.08	0.53
1:A:538:C:OP2	27:Z:134:HIS:HE1	1.92	0.53
1:A:902:G:N7	14:M:18:HIS:CD2	2.75	0.53
1:A:1200:A:H4'	38:A:6798:HOH:O	2.09	0.53
1:A:1242:A:OP2	12:K:60:ARG:NH2	2.38	0.53
4:C:217:ARG:HG2	4:C:229:ALA:HB2	1.91	0.53
5:D:74:ILE:HD13	5:D:309:VAL:HG21	1.91	0.53
7:F:86:THR:C	7:F:89:PRO:HD2	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:12:ILE:HB	38:I:4714:HOH:O	2.07	0.53
1:A:1185:U:H5'	38:A:6922:HOH:O	2.09	0.53
38:A:5778:HOH:O	7:F:55:LYS:HB2	2.07	0.53
13:L:55:VAL:HG12	13:L:56:SER:H	1.73	0.53
15:N:38:VAL:C	15:N:63:VAL:HG13	2.34	0.53
18:Q:10:ALA:CA	18:Q:13:VAL:HG12	2.39	0.53
24:W:39:ALA:O	24:W:41:GLU:N	2.41	0.53
1:A:212:A:O4'	1:A:214:U:C6	2.62	0.53
1:A:703:G:O2'	1:A:704:C:H5'	2.09	0.53
1:A:1151:G:OP1	10:I:16:LYS:NZ	2.40	0.53
1:A:1180:U:H2'	1:A:1181:A:O4'	2.09	0.53
1:A:2256:G:H2'	1:A:2257:G:H5'	1.91	0.53
1:A:2459:G:OP1	31:4:64:LYS:N	2.21	0.53
38:A:4311:HOH:O	12:K:47:THR:CB	2.51	0.53
6:E:77:ALA:O	6:E:78:ARG:HG3	2.08	0.53
9:H:99:THR:O	9:H:100:ASP:HB2	2.08	0.53
15:N:87:MET:HB2	15:N:91:ILE:CD1	2.39	0.53
18:Q:16:VAL:HG12	18:Q:17:GLY:N	2.24	0.53
20:S:39:THR:O	20:S:40:ALA:C	2.50	0.53
1:A:776:A:OP1	29:2:28:HIS:HE1	1.92	0.53
1:A:1328:A:OP1	27:Z:169:ARG:HD2	2.08	0.53
1:A:2594:C:O2'	1:A:2595:U:H5'	2.09	0.53
38:A:9566:HOH:O	20:S:83:LYS:HB3	2.08	0.53
38:A:9733:HOH:O	4:C:221:PRO:HA	2.07	0.53
4:C:211:LYS:NZ	38:C:8635:HOH:O	2.38	0.53
5:D:315:VAL:HG23	5:D:316:ARG:HG2	1.91	0.53
9:H:100:ASP:O	9:H:101:ALA:O	2.27	0.53
12:K:131:THR:HB	12:K:134:GLU:HG3	1.91	0.53
14:M:101:ASP:C	14:M:103:ALA:H	2.15	0.53
16:O:157:PRO:HA	38:O:8526:HOH:O	2.09	0.53
18:Q:115:SER:O	18:Q:117:SER:N	2.42	0.53
25:X:90:TYR:CE2	25:X:99:ALA:HB2	2.44	0.53
27:Z:178:HIS:CG	27:Z:179:PRO:HD2	2.44	0.53
1:A:1014:A:H5''	2:B:3101:G:O2'	2.09	0.52
1:A:1060:C:H6	1:A:1060:C:H5'	1.73	0.52
1:A:2107:U:O2'	1:A:2108:A:H5'	2.09	0.52
5:D:27:ASN:HD22	5:D:27:ASN:H	1.57	0.52
5:D:42:ALA:HB1	5:D:308:LEU:HD11	1.90	0.52
6:E:95:GLU:OE1	6:E:95:GLU:N	2.39	0.52
7:F:174:VAL:HG13	38:F:6555:HOH:O	2.08	0.52
8:G:31:ARG:NH1	8:G:68:HIS:CG	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:65:VAL:HG21	15:N:105:ALA:HB2	1.91	0.52
28:1:10:ARG:HG3	28:1:11:THR:N	2.25	0.52
31:4:40:ARG:HD2	38:4:8547:HOH:O	2.07	0.52
1:A:1701:A:H4'	1:A:1702:U:C5'	2.39	0.52
1:A:1819:G:H2'	1:A:1820:G:C5'	2.39	0.52
1:A:2478:U:H2'	1:A:2479:A:H8	1.74	0.52
8:G:20:ILE:HD12	8:G:33:LEU:CD1	2.40	0.52
11:J:4:ALA:HB3	38:J:8365:HOH:O	2.08	0.52
20:S:82:GLU:HG3	20:S:83:LYS:N	2.24	0.52
25:X:125:HIS:HE1	38:X:3071:HOH:O	1.92	0.52
1:A:88:G:H5'	1:A:88:G:H8	1.75	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.09	0.52
1:A:559:U:H2'	1:A:560:C:O4'	2.10	0.52
1:A:1333:U:H2'	1:A:1334:C:C6	2.44	0.52
1:A:1505:U:H6	1:A:1505:U:H5'	1.73	0.52
1:A:1834:C:H2'	1:A:1840:A:N6	2.24	0.52
1:A:2123:A:H5'	15:N:89:ASN:HD21	1.74	0.52
1:A:2435:U:H1'	38:A:4900:HOH:O	2.08	0.52
2:B:3041:C:H4'	7:F:48:MET:HB2	1.90	0.52
4:C:18:ALA:O	4:C:20:SER:N	2.39	0.52
10:I:12:ILE:HG22	10:I:12:ILE:O	2.08	0.52
11:J:117:LYS:O	11:J:119:VAL:HG13	2.09	0.52
12:K:107:ASN:C	12:K:107:ASN:HD22	2.17	0.52
28:1:26:VAL:O	28:1:30:GLU:HG3	2.09	0.52
1:A:1015:C:H2'	1:A:1016:U:C6	2.44	0.52
1:A:1159:G:H21	1:A:1189:A:H8	1.56	0.52
1:A:1205:U:H2'	1:A:1206:U:C5'	2.38	0.52
2:B:3025:G:H5''	2:B:3026:C:C6	2.45	0.52
10:I:69:ARG:NH1	38:I:3513:HOH:O	2.42	0.52
11:J:150:LYS:NZ	38:J:8379:HOH:O	2.40	0.52
13:L:9:THR:O	13:L:10:GLN:C	2.52	0.52
15:N:184:ARG:HG3	15:N:185:PRO:HA	1.92	0.52
16:O:159:TYR:HE2	16:O:163:PHE:HE2	1.57	0.52
17:P:96:VAL:HA	38:P:4258:HOH:O	2.08	0.52
20:S:61:GLN:NE2	38:S:8539:HOH:O	2.42	0.52
28:1:50:ALA:HB3	28:1:54:ILE:HG22	1.91	0.52
1:A:380:A:OP2	15:N:9:ARG:HD2	2.09	0.52
1:A:401:C:H2'	1:A:402:U:C6	2.45	0.52
1:A:622:G:O2'	1:A:623:U:H5'	2.09	0.52
1:A:657:G:OP1	6:E:27:ARG:NH2	2.40	0.52
1:A:1008:C:O2'	1:A:1009:U:H5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:A:O2'	1:A:1208:C:H2'	2.09	0.52
1:A:2276:U:H2'	1:A:2277:U:H6	1.74	0.52
1:A:2467:A:O2'	1:A:2468:A:H2'	2.08	0.52
1:A:2587:U:H2'	1:A:2589:U:H5''	1.91	0.52
6:E:127:ARG:HG2	6:E:127:ARG:NH1	2.24	0.52
6:E:150:THR:HA	6:E:203:ALA:O	2.09	0.52
7:F:58:VAL:HG12	7:F:59:GLY:N	2.24	0.52
7:F:146:LYS:NZ	16:O:107:ASN:ND2	2.57	0.52
25:X:122:ARG:HH22	25:X:154:ARG:C	2.17	0.52
27:Z:99:ALA:HB2	27:Z:233:TYR:CZ	2.44	0.52
27:Z:172:THR:HG22	27:Z:173:ALA:N	2.24	0.52
1:A:566:A:H2'	1:A:567:U:O4'	2.09	0.52
1:A:1176:C:H1'	38:A:3422:HOH:O	2.10	0.52
1:A:2064:U:H5'	1:A:2652:U:H4'	1.90	0.52
1:A:2694:A:H4'	8:G:91:PHE:HE1	1.74	0.52
1:A:2769:C:C2'	1:A:2770:G:H5'	2.40	0.52
5:D:305:ASP:O	5:D:306:LYS:CB	2.56	0.52
5:D:307:ARG:HH11	5:D:307:ARG:CG	2.22	0.52
8:G:11:VAL:HG12	8:G:12:ASP:H	1.74	0.52
13:L:74:VAL:CG1	13:L:113:ILE:HG12	2.40	0.52
18:Q:115:SER:C	18:Q:117:SER:H	2.18	0.52
28:1:38:LYS:HE2	28:1:45:LYS:CE	2.38	0.52
1:A:513:A:N3	38:A:3157:HOH:O	2.33	0.52
1:A:797:A:O4'	28:1:10:ARG:N	2.42	0.52
5:D:217:ARG:HG3	5:D:257:THR:CG2	2.39	0.52
6:E:37:ALA:HB2	38:E:8382:HOH:O	2.09	0.52
6:E:142:ASP:OD1	6:E:236:THR:HG23	2.09	0.52
9:H:58:GLU:OE1	15:N:27:ARG:NH2	2.39	0.52
12:K:93:ARG:HB3	12:K:93:ARG:HH11	1.74	0.52
14:M:73:VAL:HG23	14:M:74:THR:H	1.73	0.52
1:A:401:C:P	38:A:5258:HOH:O	2.68	0.52
1:A:1450:C:C4'	1:A:1451:C:OP2	2.54	0.52
1:A:1718:G:OP2	18:Q:20:ARG:HD2	2.09	0.52
1:A:2505:G:H8	38:A:5108:HOH:O	1.93	0.52
1:A:2630:G:O6	4:C:206:ARG:NH2	2.43	0.52
4:C:199:HIS:HD2	4:C:201:PHE:HB2	1.75	0.52
5:D:144:THR:HG22	5:D:145:HIS:N	2.25	0.52
7:F:54:ALA:CB	7:F:69:ILE:HD12	2.40	0.52
11:J:46:VAL:O	11:J:146:TRP:HH2	1.93	0.52
11:J:86:ARG:HD3	11:J:130:HIS:HD2	1.74	0.52
25:X:41:TYR:HA	25:X:44:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:G:P	15:N:48:ARG:HH12	2.33	0.52
1:A:625:U:H5''	1:A:1044:C:N4	2.25	0.52
1:A:1188:A:C5	1:A:1189:A:C2	2.98	0.52
1:A:1654:U:H2'	4:C:47:HIS:CD2	2.45	0.52
1:A:2715:G:N2	5:D:264:GLU:OE1	2.43	0.52
4:C:81:GLN:HB2	4:C:92:ASN:ND2	2.24	0.52
4:C:99:ILE:O	4:C:131:HIS:CE1	2.63	0.52
6:E:236:THR:C	38:E:8454:HOH:O	2.52	0.52
11:J:144:GLU:OE1	11:J:144:GLU:HA	2.10	0.52
17:P:25:VAL:HG23	17:P:26:TRP:N	2.25	0.52
25:X:88:THR:CG2	25:X:89:ASP:H	2.19	0.52
28:1:37:HIS:O	28:1:45:LYS:HA	2.10	0.52
30:3:40:ARG:HG2	30:3:40:ARG:HH11	1.74	0.52
1:A:218:C:OP2	1:A:220:C:N4	2.42	0.52
1:A:832:U:H2'	1:A:833:G:C8	2.45	0.52
9:H:60:VAL:O	9:H:61:MET:C	2.52	0.52
11:J:48:LEU:CD1	11:J:157:ILE:HG21	2.39	0.52
11:J:139:ASP:N	11:J:140:PRO:CD	2.72	0.52
13:L:118:ALA:C	13:L:120:ARG:H	2.18	0.52
14:M:35:ARG:O	14:M:40:PHE:HA	2.10	0.52
14:M:53:ARG:NH2	14:M:57:VAL:HG12	2.25	0.52
16:O:154:LEU:HG	16:O:155:GLU:N	2.24	0.52
1:A:1055:G:OP2	11:J:94:ARG:NH1	2.43	0.51
1:A:1654:U:H2'	4:C:47:HIS:HD2	1.74	0.51
1:A:2724:U:H2'	1:A:2725:G:O4'	2.10	0.51
1:A:2781:U:H2'	1:A:2782:G:H5'	1.91	0.51
1:A:2896:A:H2'	1:A:2896:A:N3	2.25	0.51
7:F:92:GLU:O	7:F:93:LEU:O	2.28	0.51
10:I:23:ILE:O	10:I:27:ILE:HG13	2.10	0.51
1:A:920:C:H5''	1:A:921:G:O5'	2.10	0.51
1:A:2115:U:H2'	1:A:2116:U:C6	2.45	0.51
1:A:2307:A:C2	1:A:2308:U:N3	2.78	0.51
1:A:2524:G:H21	1:A:2526:C:N4	2.08	0.51
1:A:2756:U:H3	1:A:2896:A:H2	1.56	0.51
11:J:127:GLY:O	11:J:128:ALA:CB	2.58	0.51
14:M:57:VAL:HG12	14:M:57:VAL:O	2.10	0.51
23:V:14:GLU:OE1	23:V:15:PRO:HD2	2.10	0.51
25:X:90:TYR:N	25:X:90:TYR:CD1	2.78	0.51
25:X:122:ARG:HG2	25:X:152:ALA:O	2.09	0.51
1:A:542:A:H2'	1:A:543:G:O4'	2.10	0.51
1:A:2533:C:H6	1:A:2533:C:C5'	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:125:ASN:ND2	38:C:8542:HOH:O	2.39	0.51
9:H:48:VAL:HG23	9:H:74:PHE:CB	2.41	0.51
22:U:111:ARG:HB3	22:U:119:ALA:HB2	1.93	0.51
25:X:21:LEU:HD21	25:X:48:VAL:CG1	2.40	0.51
1:A:136:C:H2'	1:A:137:U:O4'	2.10	0.51
1:A:911:G:H5'	1:A:932:U:OP1	2.10	0.51
1:A:926:A:O2'	14:M:41:HIS:CD2	2.63	0.51
1:A:1056:U:H2'	1:A:1057:A:O4'	2.11	0.51
1:A:1874:U:P	4:C:51:ARG:HD2	2.50	0.51
1:A:2121:G:O2'	31:4:47:GLY:HA2	2.11	0.51
1:A:2432:C:H2'	1:A:2433:A:H8	1.75	0.51
1:A:2749:U:O2'	1:A:2751:C:OP2	2.17	0.51
7:F:169:THR:O	7:F:170:TYR:HB2	2.11	0.51
15:N:47:ASP:CG	15:N:48:ARG:N	2.68	0.51
31:4:39:GLN:HA	31:4:42:ARG:NH2	2.26	0.51
1:A:797:A:C4'	28:1:10:ARG:N	2.73	0.51
1:A:1568:G:O2'	1:A:1569:U:H5'	2.09	0.51
1:A:2039:A:H4'	1:A:2760:C:O2'	2.11	0.51
1:A:2270:G:H4'	4:C:223:ARG:HH12	1.75	0.51
38:A:6167:HOH:O	27:Z:165:GLU:HB3	2.10	0.51
2:B:3030:C:OP1	7:F:137:PRO:O	2.28	0.51
4:C:192:VAL:O	4:C:207:GLN:HG2	2.10	0.51
7:F:29:HIS:C	38:F:5858:HOH:O	2.53	0.51
11:J:150:LYS:HA	11:J:153:VAL:HG22	1.92	0.51
16:O:162:ASP:O	38:O:8520:HOH:O	2.18	0.51
16:O:180:LEU:O	16:O:181:ASP:HB3	2.10	0.51
20:S:25:PHE:CE2	20:S:29:LYS:HE2	2.46	0.51
23:V:52:THR:HG22	23:V:54:THR:N	2.26	0.51
26:Y:43:VAL:CG1	26:Y:47:ALA:HB3	2.41	0.51
1:A:111:C:H2'	1:A:112:G:O4'	2.11	0.51
1:A:245:C:H2'	1:A:246:G:H5'	1.92	0.51
1:A:289:G:O2'	1:A:290:C:H5'	2.11	0.51
1:A:711:G:N2	1:A:718:C:C2	2.79	0.51
1:A:2081:A:H4'	12:K:69:TYR:CE1	2.46	0.51
1:A:2256:G:C2'	1:A:2257:G:H5'	2.41	0.51
1:A:2787:C:H5	38:A:4115:HOH:O	1.93	0.51
6:E:39:GLN:O	6:E:43:LYS:HD3	2.11	0.51
7:F:135:VAL:HG22	7:F:136:ARG:N	2.25	0.51
8:G:5:LEU:HD21	8:G:66:GLN:HG3	1.91	0.51
8:G:7:ILE:CG2	8:G:45:ASP:O	2.58	0.51
10:I:66:LEU:O	10:I:69:ARG:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:59:GLY:CA	15:N:141:ILE:HD11	2.41	0.51
23:V:52:THR:HG22	23:V:54:THR:H	1.76	0.51
25:X:14:HIS:HB2	25:X:17:ILE:HG13	1.93	0.51
26:Y:72:VAL:HG22	26:Y:85:VAL:CG1	2.38	0.51
28:1:25:ARG:O	28:1:29:VAL:HG23	2.10	0.51
1:A:306:A:P	22:U:38:ARG:HH21	2.33	0.51
1:A:470:U:O2'	29:2:16:HIS:HD2	1.93	0.51
1:A:1052:G:N3	1:A:1052:G:H2'	2.24	0.51
1:A:1589:G:N2	1:A:1605:G:H1'	2.26	0.51
1:A:1882:C:O2'	1:A:2012:U:OP2	2.26	0.51
1:A:2055:A:H4'	20:S:132:ARG:NH2	2.25	0.51
1:A:2363:G:O2'	19:R:11:ARG:HG3	2.11	0.51
7:F:10:PHE:CG	7:F:11:HIS:N	2.79	0.51
8:G:84:MET:HE2	8:G:133:VAL:HG23	1.93	0.51
8:G:92:PRO:HB2	38:G:4917:HOH:O	2.11	0.51
9:H:99:THR:O	9:H:99:THR:HG23	2.10	0.51
15:N:113:ARG:NH2	15:N:156:ARG:HG2	2.26	0.51
28:1:57:CYS:O	28:1:61:GLY:N	2.41	0.51
29:2:25:LYS:HD2	30:3:49:GLU:N	2.25	0.51
29:2:25:LYS:HG3	30:3:49:GLU:H	1.76	0.51
1:A:1787:C:H4'	1:A:2883:A:O4'	2.10	0.51
1:A:2897:C:H2'	1:A:2898:G:H8	1.75	0.51
5:D:211:THR:HA	5:D:255:GLY:O	2.11	0.51
7:F:86:THR:O	7:F:90:LEU:HG	2.11	0.51
11:J:56:ILE:HG21	11:J:61:LEU:HD13	1.93	0.51
25:X:31:HIS:HB3	38:X:5420:HOH:O	2.11	0.51
1:A:305:A:C5	1:A:329:A:C2	2.99	0.51
1:A:960:G:H2'	1:A:960:G:N3	2.26	0.51
1:A:1008:C:OP1	11:J:16:ARG:NH2	2.40	0.51
38:A:4879:HOH:O	4:C:164:ARG:CZ	2.59	0.51
5:D:125:GLU:O	5:D:129:ARG:HG3	2.10	0.51
5:D:329:TYR:HE2	23:V:15:PRO:HG2	1.74	0.51
6:E:140:VAL:HG12	6:E:141:SER:N	2.26	0.51
7:F:169:THR:C	7:F:170:TYR:HD1	2.18	0.51
8:G:69:ILE:HA	8:G:72:MET:HE2	1.92	0.51
9:H:101:ALA:HB2	9:H:108:LEU:HD22	1.93	0.51
16:O:82:TYR:OH	16:O:176:ARG:NH1	2.44	0.51
19:R:30:VAL:O	19:R:30:VAL:HG12	2.11	0.51
20:S:29:LYS:HD3	38:S:8531:HOH:O	2.11	0.51
21:T:58:MET:SD	30:3:8:LYS:HE3	2.50	0.51
1:A:737:A:H2'	1:A:738:G:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1741:U:HO2'	1:A:2723:G:H4'	1.73	0.51
1:A:2779:G:H21	8:G:143:GLN:NE2	2.09	0.51
5:D:32:ASP:HA	38:D:8575:HOH:O	2.10	0.51
11:J:83:PHE:HZ	11:J:146:TRP:HE1	1.55	0.51
16:O:3:GLY:HA3	38:O:8512:HOH:O	2.10	0.51
16:O:139:TRP:HA	16:O:139:TRP:HE3	1.76	0.51
31:4:24:LYS:HG2	35:4:8504:CL:CL	2.48	0.51
1:A:204:A:C2'	1:A:205:U:H5'	2.40	0.50
1:A:1197:G:N2	38:A:5692:HOH:O	2.43	0.50
1:A:1592:G:O2'	1:A:1593:C:O4'	2.22	0.50
1:A:1699:C:H4'	38:A:5901:HOH:O	2.10	0.50
1:A:2094:G:C4'	5:D:245:SER:HB3	2.39	0.50
1:A:2112:A:H2'	1:A:2113:G:C8	2.46	0.50
1:A:2795:C:O2'	1:A:2796:U:H5'	2.11	0.50
5:D:235:ARG:HA	38:D:8596:HOH:O	2.10	0.50
6:E:33:LYS:HE2	38:E:8361:HOH:O	2.10	0.50
21:T:57:THR:CG2	21:T:59:ASP:HB2	2.40	0.50
28:1:58:GLY:HA3	38:1:8437:HOH:O	2.10	0.50
1:A:2897:C:O2'	1:A:2898:G:H5'	2.11	0.50
5:D:189:ALA:HB1	38:D:8566:HOH:O	2.10	0.50
10:I:12:ILE:O	10:I:13:PRO:C	2.53	0.50
15:N:49:ALA:C	15:N:54:TYR:HB3	2.36	0.50
31:4:69:TYR:HB2	31:4:78:HIS:CE1	2.46	0.50
1:A:192:A:N6	1:A:194:A:C2	2.80	0.50
1:A:821:U:O2'	1:A:822:C:H5'	2.12	0.50
1:A:1119:G:H8	12:K:52:GLN:HE22	1.59	0.50
1:A:1559:A:H1'	38:A:5328:HOH:O	2.11	0.50
1:A:2004:U:H1'	38:A:9690:HOH:O	2.10	0.50
1:A:2266:A:H2'	1:A:2267:G:H8	1.76	0.50
38:A:4057:HOH:O	15:N:83:SER:HA	2.10	0.50
38:A:5651:HOH:O	30:3:44:ARG:HG2	2.11	0.50
6:E:5:ILE:CD1	6:E:16:VAL:HG23	2.24	0.50
6:E:127:ARG:HD2	6:E:229:PRO:O	2.11	0.50
7:F:95:THR:C	7:F:97:GLN:N	2.67	0.50
8:G:15:GLN:HG2	8:G:19:ASP:O	2.11	0.50
26:Y:8:ARG:NH1	38:Y:2479:HOH:O	2.23	0.50
27:Z:235:GLU:CD	27:Z:235:GLU:N	2.68	0.50
1:A:220:C:OP2	1:A:2431:C:H1'	2.12	0.50
1:A:564:G:H1'	38:A:5768:HOH:O	2.12	0.50
1:A:1015:C:H6	1:A:1015:C:O5'	1.93	0.50
1:A:1205:U:C2'	1:A:1206:U:H5'	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2266:A:H2'	1:A:2267:G:C8	2.46	0.50
4:C:194:MET:HE3	4:C:199:HIS:HB2	1.93	0.50
7:F:49:PRO:HG3	38:F:5828:HOH:O	2.10	0.50
7:F:64:ARG:O	7:F:67:ASP:OD2	2.29	0.50
8:G:20:ILE:CD1	8:G:40:VAL:HG11	2.41	0.50
11:J:47:GLU:CB	11:J:133:ILE:HD13	2.41	0.50
14:M:72:ASN:O	14:M:76:LEU:HG	2.11	0.50
15:N:173:LEU:HD23	15:N:183:VAL:CG1	2.41	0.50
23:V:52:THR:CG2	23:V:54:THR:HB	2.42	0.50
25:X:11:VAL:O	25:X:12:ASN:HB2	2.11	0.50
1:A:858:U:H2'	1:A:859:C:C6	2.47	0.50
1:A:1768:C:H2'	1:A:1769:C:O4'	2.10	0.50
1:A:1829:A:C8	1:A:1885:A:C8	2.99	0.50
4:C:94:LEU:HG	4:C:99:ILE:CD1	2.42	0.50
6:E:79:ARG:O	6:E:87:ARG:HG2	2.11	0.50
7:F:41:LEU:CA	7:F:44:ILE:HG22	2.40	0.50
14:M:73:VAL:HG23	14:M:74:THR:N	2.26	0.50
31:4:18:GLN:OE1	31:4:73:GLU:HB3	2.12	0.50
1:A:646:G:H2'	1:A:647:U:H6	1.77	0.50
1:A:1523:G:H2'	1:A:1524:U:C6	2.47	0.50
1:A:1787:C:OP1	18:Q:68:LYS:HE2	2.11	0.50
2:B:3076:G:C3'	2:B:3077:A:H5''	2.35	0.50
6:E:178:GLN:C	6:E:180:SER:N	2.67	0.50
7:F:84:LEU:C	7:F:86:THR:H	2.19	0.50
8:G:37:ASP:OD1	12:K:125:SER:HB3	2.11	0.50
9:H:48:VAL:CG2	9:H:74:PHE:HB3	2.40	0.50
1:A:128:A:H3'	1:A:128:A:H8	1.77	0.50
1:A:419:A:C2	1:A:2449:G:C2	3.00	0.50
1:A:1804:A:H2'	1:A:1805:G:C8	2.46	0.50
4:C:51:ARG:HB2	38:C:8620:HOH:O	2.11	0.50
5:D:103:ASP:HB2	38:D:8594:HOH:O	2.11	0.50
7:F:173:GLU:O	7:F:174:VAL:C	2.54	0.50
9:H:32:GLY:N	38:H:3111:HOH:O	2.44	0.50
15:N:59:GLY:C	15:N:141:ILE:HD11	2.37	0.50
18:Q:80:ARG:HG2	18:Q:87:ARG:CZ	2.41	0.50
20:S:96:VAL:HG13	20:S:106:GLY:HA3	1.93	0.50
1:A:702:G:O2'	1:A:703:G:H5'	2.12	0.50
1:A:858:U:H2'	1:A:859:C:H6	1.77	0.50
1:A:1557:G:O2'	1:A:1558:C:H5'	2.12	0.50
1:A:1636:G:O2'	1:A:1637:A:H5'	2.11	0.50
1:A:2256:G:H2'	1:A:2257:G:C5'	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2382:A:H5'	38:4:8531:HOH:O	2.11	0.50
1:A:2404:G:OP1	19:R:69:ASP:N	2.38	0.50
1:A:2531:U:O2'	1:A:2532:A:H5'	2.12	0.50
4:C:75:GLY:HA2	28:1:63:LYS:O	2.12	0.50
5:D:4:SER:O	5:D:5:ARG:HB2	2.12	0.50
7:F:65:GLU:HA	38:F:6752:HOH:O	2.12	0.50
10:I:73:ASP:C	38:I:2994:HOH:O	2.54	0.50
11:J:65:ARG:NH1	38:J:8385:HOH:O	2.44	0.50
15:N:85:ARG:NE	38:N:8519:HOH:O	2.34	0.50
20:S:119:VAL:O	20:S:119:VAL:HG12	2.11	0.50
22:U:19:ARG:HD3	22:U:67:LEU:O	2.11	0.50
29:2:25:LYS:HG2	29:2:25:LYS:O	2.12	0.50
31:4:7:PHE:HE2	31:4:22:VAL:HG21	1.76	0.50
1:A:303:C:O2'	1:A:304:G:H5'	2.12	0.50
1:A:832:U:H2'	1:A:833:G:H8	1.76	0.50
1:A:2304:G:H5'	38:R:1719:HOH:O	2.10	0.50
1:A:2911:C:H2'	1:A:2912:C:C6	2.47	0.50
7:F:23:VAL:HG21	7:F:45:THR:CG2	2.42	0.50
9:H:27:GLY:HA3	38:H:5413:HOH:O	2.12	0.50
21:T:53:ASN:ND2	38:T:8321:HOH:O	2.44	0.50
21:T:81:ILE:HG23	38:T:8337:HOH:O	2.11	0.50
24:W:11:MET:HB3	24:W:15:GLU:HB2	1.93	0.50
25:X:122:ARG:CG	25:X:152:ALA:O	2.60	0.50
1:A:119:A:H2'	1:A:120:A:H5''	1.94	0.49
1:A:656:G:OP2	17:P:37:ARG:HD2	2.11	0.49
1:A:1079:A:N1	1:A:2068:G:O2'	2.42	0.49
1:A:2278:U:H2'	38:A:7060:HOH:O	2.11	0.49
1:A:2361:A:H2'	1:A:2362:A:C8	2.47	0.49
4:C:53:ALA:HB3	38:C:8620:HOH:O	2.11	0.49
4:C:105:VAL:HG12	4:C:106:CYS:N	2.27	0.49
5:D:56:ASP:OD1	5:D:322:ARG:HB3	2.10	0.49
5:D:132:HIS:CE1	5:D:171:VAL:HG21	2.46	0.49
5:D:223:ARG:HG3	5:D:232:TRP:O	2.12	0.49
8:G:18:LEU:HD13	8:G:34:TRP:CD1	2.47	0.49
9:H:34:ASN:HA	15:N:4:ALA:HB2	1.94	0.49
13:L:72:VAL:HG11	13:L:121:PHE:CD1	2.47	0.49
14:M:140:VAL:HG23	38:M:8562:HOH:O	2.11	0.49
18:Q:7:LYS:HD3	18:Q:21:VAL:HG21	1.94	0.49
20:S:39:THR:HB	20:S:42:GLU:CG	2.41	0.49
1:A:734:U:O2'	1:A:737:A:N6	2.45	0.49
1:A:820:G:O2'	1:A:856:G:H4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:U:H2'	1:A:822:C:C6	2.47	0.49
1:A:883:U:O2	1:A:883:U:C2'	2.60	0.49
1:A:922:A:N7	1:A:2281:C:H5'	2.27	0.49
1:A:1127:C:H2'	1:A:1128:U:H5'	1.93	0.49
1:A:1887:U:OP1	28:1:21:LYS:HE3	2.12	0.49
6:E:246:ARG:HH11	6:E:246:ARG:CB	2.18	0.49
14:M:48:LYS:NZ	38:M:8531:HOH:O	2.45	0.49
19:R:24:SER:O	38:R:2847:HOH:O	2.19	0.49
23:V:39:ASN:ND2	23:V:44:ARG:HH11	2.10	0.49
1:A:1495:C:H1'	1:A:1573:A:H1'	1.94	0.49
1:A:2453:G:H5'	38:A:4173:HOH:O	2.11	0.49
2:B:3031:C:H1'	38:B:8392:HOH:O	2.11	0.49
8:G:116:THR:HG22	8:G:151:LEU:HD22	1.93	0.49
10:I:63:ARG:N	38:I:2569:HOH:O	2.45	0.49
11:J:59:ASN:N	11:J:59:ASN:ND2	2.56	0.49
15:N:122:GLU:HB2	15:N:126:HIS:O	2.12	0.49
1:A:61:G:OP1	30:3:17:GLN:HG2	2.12	0.49
1:A:484:A:N1	1:A:506:G:H4'	2.28	0.49
1:A:920:C:H4'	1:A:921:G:C2	2.47	0.49
1:A:1015:C:H2'	1:A:1016:U:H6	1.75	0.49
6:E:162:VAL:CG1	6:E:192:ILE:HD11	2.42	0.49
12:K:39:VAL:HG12	12:K:40:ASN:ND2	2.26	0.49
12:K:52:GLN:HG3	12:K:53:ILE:N	2.28	0.49
14:M:143:THR:HG22	14:M:144:ASP:H	1.77	0.49
26:Y:36:HIS:CE1	26:Y:40:HIS:CD2	3.01	0.49
27:Z:189:ASN:C	27:Z:189:ASN:ND2	2.70	0.49
1:A:251:C:H1'	15:N:58:GLN:HE22	1.76	0.49
1:A:921:G:H4'	1:A:924:G:C6	2.47	0.49
1:A:1116:U:H3	1:A:1246:A:N6	2.00	0.49
1:A:1762:C:H4'	38:A:4138:HOH:O	2.11	0.49
1:A:1778:A:H2'	1:A:1779:A:H5'	1.94	0.49
1:A:1819:G:H5'	38:A:5281:HOH:O	2.12	0.49
1:A:2004:U:O2	1:A:2004:U:H2'	2.11	0.49
1:A:2123:A:H3'	1:A:2124:G:H8	1.77	0.49
1:A:2419:U:H5''	1:A:2420:G:C5'	2.41	0.49
1:A:2505:G:C2'	1:A:2506:A:H5'	2.42	0.49
4:C:57:ALA:HA	4:C:67:LEU:HD23	1.94	0.49
4:C:129:LEU:CD1	4:C:145:MET:HE1	2.42	0.49
15:N:52:LEU:HD13	15:N:116:ASN:CB	2.42	0.49
21:T:29:ASP:OD2	21:T:31:ARG:NH1	2.46	0.49
1:A:283:U:H5''	1:A:284:C:OP2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:A:N6	1:A:1229:C:H2'	2.28	0.49
38:A:9103:HOH:O	15:N:165:SER:HB3	2.12	0.49
6:E:118:THR:HG23	38:E:8305:HOH:O	2.12	0.49
9:H:6:PHE:CD1	9:H:6:PHE:O	2.66	0.49
9:H:13:GLU:OE2	9:H:78:GLU:HG2	2.12	0.49
11:J:165:GLY:C	11:J:166:ASN:HD22	2.21	0.49
12:K:74:ARG:NH1	12:K:76:ASP:HB2	2.27	0.49
12:K:142:ASN:O	12:K:144:THR:N	2.45	0.49
15:N:95:LYS:HG2	15:N:99:ARG:HB3	1.94	0.49
17:P:77:ALA:HA	17:P:96:VAL:O	2.13	0.49
29:2:21:ARG:HD2	29:2:39:PHE:HB2	1.94	0.49
31:4:62:THR:HB	38:4:8549:HOH:O	2.11	0.49
31:4:84:ARG:HB3	38:4:8549:HOH:O	2.11	0.49
1:A:219:G:O5'	1:A:220:C:H5''	2.13	0.49
1:A:228:C:H2'	1:A:229:G:H5'	1.95	0.49
1:A:500:G:H21	20:S:98:ASN:HD21	1.60	0.49
1:A:1125:U:H2'	1:A:1126:C:H5'	1.95	0.49
1:A:1189:A:H1'	1:A:1209:C:C1'	2.43	0.49
1:A:1883:U:O2'	1:A:1884:G:H5'	2.13	0.49
1:A:2712:G:H5'	38:L:4183:HOH:O	2.13	0.49
6:E:141:SER:HB3	38:E:8421:HOH:O	2.13	0.49
8:G:43:ASP:HA	38:G:5864:HOH:O	2.12	0.49
8:G:84:MET:HE2	8:G:133:VAL:HG21	1.94	0.49
12:K:19:MET:HE1	12:K:78:ILE:HG22	1.95	0.49
12:K:79:PHE:HB3	12:K:103:VAL:HG11	1.94	0.49
16:O:34:LEU:HD13	16:O:47:LEU:HD21	1.94	0.49
16:O:67:ALA:C	16:O:69:TYR:N	2.70	0.49
23:V:52:THR:HG22	23:V:54:THR:HB	1.95	0.49
25:X:6:GLN:CB	25:X:26:ILE:HD12	2.38	0.49
1:A:541:C:C2'	1:A:542:A:C5'	2.88	0.49
1:A:553:G:O4'	1:A:1325:G:H5'	2.13	0.49
5:D:304:PRO:HD2	5:D:307:ARG:HD2	1.95	0.49
7:F:35:ALA:HB1	38:F:3279:HOH:O	2.12	0.49
16:O:143:ARG:HH12	16:O:173:ASP:CG	2.21	0.49
16:O:170:GLU:O	16:O:174:GLU:HG3	2.13	0.49
20:S:111:ILE:HG23	20:S:145:LEU:HD11	1.95	0.49
25:X:3:ALA:O	25:X:54:PHE:HA	2.12	0.49
25:X:139:GLY:O	25:X:141:HIS:HD2	1.95	0.49
29:2:17:THR:N	29:2:27:TYR:O	2.38	0.49
1:A:834:G:H4'	1:A:835:U:OP2	2.13	0.49
1:A:1164:U:C4'	1:A:1165:G:OP1	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1535:G:H2'	1:A:1536:C:C6	2.48	0.49
1:A:1651:C:OP1	38:A:4986:HOH:O	2.20	0.49
1:A:1813:U:O2'	18:Q:81:LYS:HE3	2.13	0.49
1:A:2262:C:O5'	1:A:2262:C:H6	1.95	0.49
1:A:2815:G:N7	12:K:80:LYS:NZ	2.61	0.49
6:E:129:HIS:CE1	6:E:231:ARG:HA	2.48	0.49
10:I:71:LEU:C	10:I:73:ASP:H	2.21	0.49
15:N:157:LEU:HB3	15:N:160:PHE:HD1	1.76	0.49
28:1:11:THR:OG1	28:1:23:ARG:HB2	2.13	0.49
1:A:314:G:N2	1:A:316:A:H3'	2.27	0.49
1:A:558:C:C2'	1:A:559:U:C5'	2.91	0.49
1:A:1218:U:H2'	1:A:1219:U:C6	2.48	0.49
1:A:1299:G:N2	38:A:4165:HOH:O	2.46	0.49
38:A:6913:HOH:O	6:E:188:ARG:HD2	2.11	0.49
4:C:36:ASP:HA	4:C:83:GLY:HA3	1.95	0.49
8:G:80:TRP:O	8:G:134:SER:HA	2.12	0.49
10:I:20:VAL:O	10:I:24:VAL:HG23	2.13	0.49
16:O:161:GLY:O	16:O:162:ASP:C	2.55	0.49
20:S:114:VAL:O	20:S:114:VAL:HG13	2.13	0.49
27:Z:144:ARG:NH2	38:Z:8616:HOH:O	2.45	0.49
29:2:26:SER:HB3	29:2:35:SER:OG	2.11	0.49
29:2:44:LYS:NZ	38:2:7145:HOH:O	2.45	0.49
31:4:73:GLU:HB3	38:4:8559:HOH:O	2.12	0.49
1:A:65:C:O2'	1:A:66:G:H5'	2.13	0.48
1:A:401:C:C5'	38:A:5258:HOH:O	2.61	0.48
1:A:1735:C:O2'	1:A:1736:A:H5'	2.13	0.48
5:D:44:TYR:OH	5:D:148:PRO:HG3	2.13	0.48
5:D:108:GLU:HB3	5:D:111:ARG:HD2	1.94	0.48
8:G:20:ILE:HD11	8:G:33:LEU:HD12	1.93	0.48
11:J:149:ALA:C	11:J:151:MET:H	2.20	0.48
15:N:77:PHE:HD2	38:N:8526:HOH:O	1.96	0.48
16:O:18:THR:HA	38:O:8525:HOH:O	2.12	0.48
16:O:152:GLU:C	16:O:154:LEU:N	2.71	0.48
16:O:154:LEU:O	16:O:155:GLU:CB	2.61	0.48
23:V:31:PHE:CG	23:V:37:GLU:HG2	2.48	0.48
25:X:6:GLN:HA	25:X:52:VAL:HG23	1.93	0.48
1:A:278:A:H2'	1:A:279:C:O4'	2.14	0.48
1:A:926:A:O2'	14:M:41:HIS:HD2	1.96	0.48
1:A:1733:A:H4'	5:D:212:GLN:HA	1.94	0.48
1:A:2010:A:H2'	38:A:5418:HOH:O	2.12	0.48
1:A:2053:G:OP1	20:S:138:SER:OG	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2251:G:H2'	1:A:2252:A:C8	2.49	0.48
1:A:2559:C:H4'	38:A:6714:HOH:O	2.13	0.48
2:B:3025:G:N2	38:B:8512:HOH:O	2.45	0.48
5:D:177:HIS:O	5:D:181:ILE:HG13	2.13	0.48
8:G:132:THR:O	8:G:132:THR:HG23	2.12	0.48
9:H:47:LEU:HD22	9:H:108:LEU:CD1	2.44	0.48
14:M:143:THR:CG2	14:M:144:ASP:H	2.26	0.48
31:4:42:ARG:HH11	31:4:42:ARG:HG3	1.78	0.48
1:A:1164:U:O4'	1:A:1165:G:OP1	2.31	0.48
1:A:1166:A:H61	1:A:1180:U:H3	1.60	0.48
1:A:1494:A:H1'	1:A:1495:C:C6	2.48	0.48
1:A:2542:C:H5''	1:A:2608:C:N4	2.27	0.48
5:D:148:PRO:HB2	5:D:156:LYS:O	2.13	0.48
7:F:35:ALA:O	7:F:37:ALA:N	2.46	0.48
7:F:49:PRO:HA	7:F:73:VAL:HG22	1.95	0.48
7:F:62:ASP:HA	38:F:4233:HOH:O	2.13	0.48
7:F:154:LYS:H	7:F:154:LYS:CD	2.19	0.48
11:J:48:LEU:HD13	11:J:146:TRP:HB3	1.95	0.48
11:J:75:SER:HB3	11:J:79:ALA:HB1	1.95	0.48
27:Z:197:ASP:C	27:Z:197:ASP:OD1	2.55	0.48
1:A:338:C:H4'	6:E:174:ILE:HD12	1.95	0.48
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.77	0.48
1:A:1706:G:C5	1:A:1707:G:C6	3.02	0.48
1:A:2620:U:H1'	38:A:6629:HOH:O	2.13	0.48
1:A:2906:A:H5'	1:A:2907:C:O4'	2.13	0.48
5:D:251:VAL:HG23	5:D:252:PRO:HD2	1.95	0.48
7:F:36:ASN:HA	38:F:7500:HOH:O	2.12	0.48
15:N:154:ARG:HD3	38:N:8646:HOH:O	2.12	0.48
16:O:32:PRO:HD2	16:O:99:GLU:O	2.14	0.48
16:O:155:GLU:O	16:O:156:GLU:HG3	2.14	0.48
19:R:32:GLU:HA	19:R:71:TYR:OH	2.13	0.48
27:Z:189:ASN:HA	27:Z:217:ILE:HD11	1.95	0.48
28:1:56:MET:HA	28:1:62:TYR:O	2.14	0.48
31:4:11:CYS:HB2	31:4:20:HIS:CE1	2.48	0.48
1:A:107:U:H2'	1:A:108:U:H5'	1.96	0.48
1:A:870:G:C3'	1:A:871:G:H5''	2.43	0.48
38:A:9264:HOH:O	14:M:41:HIS:HE1	1.96	0.48
2:B:3054:A:O2'	2:B:3055:U:H5'	2.13	0.48
6:E:7:ASP:C	6:E:9:ASP:H	2.22	0.48
12:K:77:GLY:O	12:K:78:ILE:C	2.57	0.48
13:L:98:VAL:HG22	13:L:102:GLU:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:24:ARG:NH2	22:U:39:ASN:HD22	2.10	0.48
23:V:13:ILE:HG12	23:V:32:CYS:HB2	1.95	0.48
26:Y:76:ARG:O	26:Y:77:PHE:HB3	2.12	0.48
1:A:488:U:C2'	38:A:3497:HOH:O	2.57	0.48
1:A:1116:U:O2'	1:A:1118:A:C2	2.57	0.48
1:A:1120:U:H5'	1:A:1121:G:OP2	2.13	0.48
1:A:1503:U:H2'	1:A:1504:A:O4'	2.14	0.48
1:A:1574:C:H6	1:A:1574:C:O5'	1.96	0.48
1:A:2679:G:H2'	1:A:2681:A:OP2	2.13	0.48
38:A:7167:HOH:O	6:E:94:THR:HG21	2.14	0.48
6:E:54:LEU:HD21	6:E:87:ARG:HD2	1.95	0.48
13:L:55:VAL:CG1	13:L:56:SER:N	2.77	0.48
16:O:82:TYR:C	16:O:82:TYR:CD2	2.91	0.48
16:O:182:GLY:O	16:O:183:ASP:O	2.31	0.48
18:Q:3:LEU:HA	18:Q:6:GLN:OE1	2.13	0.48
22:U:75:GLU:O	22:U:76:ASP:HB2	2.13	0.48
30:3:40:ARG:HG3	30:3:45:ASN:CB	2.44	0.48
1:A:221:G:H2'	1:A:222:A:C8	2.48	0.48
1:A:1687:C:O2	29:2:9:GLY:HA2	2.14	0.48
1:A:2720:C:O2	13:L:87:ARG:NH2	2.46	0.48
38:A:6603:HOH:O	29:2:1:THR:HB	2.12	0.48
38:A:6862:HOH:O	22:U:2:LYS:HE2	2.13	0.48
4:C:195:ASN:O	4:C:196:ALA:C	2.56	0.48
5:D:156:LYS:HE3	38:D:8630:HOH:O	2.13	0.48
5:D:320:GLN:HG3	5:D:321:PRO:CD	2.43	0.48
6:E:19:PRO:HG2	6:E:22:PHE:CD1	2.49	0.48
11:J:112:ARG:O	11:J:113:ALA:C	2.57	0.48
12:K:39:VAL:CG1	12:K:107:ASN:HB2	2.42	0.48
13:L:82:ARG:NH2	13:L:115:ARG:HG2	2.29	0.48
15:N:115:LEU:HD13	15:N:116:ASN:HB2	1.96	0.48
25:X:126:ASP:HB3	25:X:135:GLY:O	2.14	0.48
27:Z:107:PRO:HB3	27:Z:182:PHE:CE2	2.49	0.48
1:A:420:U:H2'	1:A:421:C:C6	2.48	0.48
1:A:1211:G:O2'	1:A:1212:C:H5'	2.13	0.48
1:A:1269:G:H2'	1:A:1270:U:C6	2.49	0.48
1:A:1434:A:H2'	1:A:1436:C:C5	2.49	0.48
1:A:1562:C:O2	1:A:1562:C:H2'	2.14	0.48
1:A:1788:U:C2	1:A:1805:G:N2	2.81	0.48
1:A:2256:G:O2'	1:A:2257:G:H5'	2.13	0.48
1:A:2428:G:C6	1:A:2464:C:H1'	2.48	0.48
1:A:2472:C:O2'	1:A:2634:G:H4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:75:C:N4	36:5:76:PPU:H102	2.28	0.48
5:D:24:PRO:CG	5:D:204:GLY:HA2	2.44	0.48
5:D:27:ASN:HB3	38:D:8628:HOH:O	2.12	0.48
11:J:139:ASP:H	11:J:140:PRO:HD3	1.73	0.48
12:K:107:ASN:HD22	12:K:109:TYR:H	1.59	0.48
16:O:67:ALA:HA	16:O:71:TRP:HB3	1.96	0.48
18:Q:7:LYS:CD	18:Q:21:VAL:CG2	2.92	0.48
24:W:56:ILE:O	24:W:60:GLN:HG3	2.12	0.48
30:3:48:ASP:O	30:3:49:GLU:HB2	2.13	0.48
1:A:60:A:C2	1:A:61:G:C8	3.02	0.48
1:A:283:U:H5	1:A:284:C:N4	2.11	0.48
1:A:1006:A:N1	1:A:2311:A:H1'	2.29	0.48
1:A:1543:G:N1	1:A:1641:A:OP2	2.36	0.48
1:A:1819:G:H2'	1:A:1820:G:C4'	2.44	0.48
1:A:2089:A:C2'	1:A:2090:G:H5'	2.44	0.48
5:D:55:ASN:HB3	5:D:64:GLY:N	2.28	0.48
5:D:307:ARG:HH11	5:D:307:ARG:CB	2.26	0.48
7:F:159:PRO:O	7:F:163:VAL:HG23	2.14	0.48
8:G:11:VAL:CG1	8:G:12:ASP:H	2.27	0.48
13:L:18:ILE:HG22	13:L:93:ASN:HB2	1.96	0.48
13:L:40:THR:O	13:L:41:LYS:C	2.57	0.48
15:N:67:ILE:HG21	15:N:97:ILE:HG23	1.96	0.48
16:O:22:GLN:HG2	16:O:26:LEU:HD22	1.94	0.48
1:A:128:A:C8	1:A:128:A:C3'	2.97	0.48
1:A:422:G:C6	1:A:2446:G:C6	3.02	0.48
1:A:1308:A:O4'	6:E:226:GLY:HA3	2.14	0.48
1:A:1525:G:H5'	1:A:1526:A:OP2	2.14	0.48
1:A:2729:C:O2'	1:A:2730:G:H5'	2.14	0.48
1:A:2768:A:O2'	1:A:2769:C:H5'	2.14	0.48
4:C:69:LEU:CD2	4:C:120:ARG:HB3	2.38	0.48
4:C:88:ILE:CD1	4:C:100:PRO:HD3	2.43	0.48
5:D:76:THR:N	5:D:77:PRO:HD3	2.28	0.48
15:N:81:ARG:HB3	15:N:86:MET:HG2	1.96	0.48
17:P:25:VAL:HG23	17:P:26:TRP:H	1.79	0.48
25:X:21:LEU:HB3	25:X:26:ILE:HG12	1.95	0.48
1:A:282:C:H2'	1:A:283:U:O4'	2.13	0.47
1:A:1878:G:O2'	1:A:1879:U:C6	2.66	0.47
1:A:2281:C:O2'	1:A:2282:U:H5'	2.14	0.47
1:A:2456:A:H5'	38:A:5164:HOH:O	2.13	0.47
38:A:8728:HOH:O	4:C:11:ARG:HD3	2.13	0.47
4:C:36:ASP:O	4:C:37:VAL:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:133:ARG:NH2	38:E:8431:HOH:O	2.46	0.47
8:G:18:LEU:HD13	8:G:34:TRP:CG	2.48	0.47
18:Q:18:LYS:O	18:Q:21:VAL:HG22	2.13	0.47
18:Q:27:ARG:HA	38:Q:177:HOH:O	2.13	0.47
26:Y:25:ARG:HG2	38:Y:5356:HOH:O	2.12	0.47
29:2:25:LYS:HD2	30:3:48:ASP:HA	1.95	0.47
1:A:195:C:H2'	1:A:196:G:H5'	1.96	0.47
1:A:639:A:H2'	1:A:640:G:H8	1.77	0.47
1:A:1666:C:C2'	1:A:1667:A:C5'	2.92	0.47
1:A:2120:U:H2'	1:A:2121:G:O4'	2.14	0.47
1:A:2900:G:H2'	1:A:2901:C:O4'	2.14	0.47
38:A:9041:HOH:O	18:Q:81:LYS:HG2	2.13	0.47
5:D:54:VAL:HB	38:D:8613:HOH:O	2.14	0.47
5:D:221:GLN:HE22	13:L:42:ASN:ND2	2.11	0.47
6:E:61:PHE:HB3	38:E:8450:HOH:O	2.13	0.47
20:S:113:HIS:O	20:S:145:LEU:HD12	2.13	0.47
25:X:64:THR:O	25:X:68:THR:HG22	2.14	0.47
1:A:1205:U:C2'	1:A:1206:U:C5'	2.92	0.47
1:A:1377:C:H5'	1:A:1377:C:C6	2.44	0.47
1:A:2300:A:H4'	1:A:2301:A:O5'	2.14	0.47
1:A:2445:U:H2'	1:A:2446:G:C8	2.49	0.47
38:A:4446:HOH:O	11:J:57:ARG:HG3	2.14	0.47
4:C:192:VAL:CG1	4:C:192:VAL:O	2.62	0.47
5:D:85:ARG:NH2	5:D:99:GLU:OE2	2.40	0.47
6:E:162:VAL:O	6:E:162:VAL:CG1	2.61	0.47
16:O:24:LEU:O	16:O:28:LYS:HG2	2.14	0.47
16:O:67:ALA:C	16:O:69:TYR:H	2.22	0.47
23:V:17:THR:HG22	23:V:18:GLY:N	2.28	0.47
1:A:240:C:O2	1:A:240:C:H2'	2.15	0.47
1:A:694:A:H2'	1:A:695:C:H5'	1.96	0.47
1:A:943:A:C5	25:X:23:MET:HE2	2.50	0.47
4:C:132:ASP:OD1	4:C:133:ARG:N	2.47	0.47
5:D:11:LEU:C	38:D:8617:HOH:O	2.57	0.47
5:D:16:ARG:NE	38:D:8553:HOH:O	2.25	0.47
8:G:107:PHE:CZ	8:G:108:LEU:HD13	2.49	0.47
11:J:57:ARG:C	11:J:59:ASN:N	2.70	0.47
13:L:86:THR:HG22	13:L:87:ARG:N	2.29	0.47
14:M:146:GLY:C	14:M:148:GLU:H	2.22	0.47
15:N:123:ASP:C	15:N:123:ASP:OD1	2.55	0.47
1:A:39:G:N2	1:A:444:C:C2	2.83	0.47
1:A:432:G:O2'	1:A:433:C:H5'	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:A:H2'	1:A:1516:C:C6	2.49	0.47
1:A:2676:C:H4'	12:K:70:PHE:HE1	1.76	0.47
1:A:2715:G:O2'	5:D:262:ARG:HD2	2.14	0.47
1:A:2748:G:C5'	38:A:6999:HOH:O	2.58	0.47
38:A:9067:HOH:O	5:D:267:LYS:HD3	2.14	0.47
4:C:165:THR:O	4:C:165:THR:HG22	2.13	0.47
6:E:20:ASP:O	6:E:23:GLU:HB2	2.15	0.47
6:E:142:ASP:OD2	6:E:238:SER:OG	2.29	0.47
18:Q:10:ALA:O	18:Q:13:VAL:HG12	2.14	0.47
26:Y:74:ALA:CB	26:Y:85:VAL:HG22	2.45	0.47
27:Z:203:VAL:HG12	27:Z:228:VAL:HG22	1.96	0.47
1:A:398:U:H2'	1:A:399:C:C6	2.50	0.47
1:A:816:G:C6	1:A:817:G:N1	2.82	0.47
1:A:1494:A:C4	1:A:1495:C:C5	3.03	0.47
1:A:2010:A:C2'	38:A:5418:HOH:O	2.63	0.47
1:A:2781:U:H2'	1:A:2782:G:C5'	2.45	0.47
1:A:2894:C:O2'	1:A:2895:C:H5'	2.14	0.47
2:B:3042:C:O2	7:F:76:ARG:NH1	2.47	0.47
4:C:96:LEU:HD22	4:C:128:LEU:HD13	1.95	0.47
18:Q:115:SER:C	18:Q:117:SER:N	2.71	0.47
23:V:38:ASN:O	23:V:42:LEU:HG	2.15	0.47
27:Z:154:ARG:NH1	27:Z:155:ARG:HG3	2.30	0.47
1:A:154:C:H2'	1:A:155:C:C6	2.49	0.47
1:A:654:A:OP2	17:P:38:ARG:HD3	2.15	0.47
1:A:1072:G:OP2	27:Z:154:ARG:NH2	2.41	0.47
1:A:1268:C:H2'	1:A:1269:G:H8	1.79	0.47
1:A:1565:C:O4'	1:A:2738:G:H1'	2.15	0.47
1:A:2407:G:O2'	1:A:2408:A:H5'	2.14	0.47
1:A:2697:A:H2'	1:A:2698:G:O4'	2.14	0.47
4:C:39:ALA:HB3	4:C:61:GLU:OE2	2.15	0.47
5:D:41:PHE:CZ	5:D:79:MET:HG3	2.49	0.47
6:E:1:MET:HG2	6:E:2:GLN:NE2	2.30	0.47
6:E:25:PRO:HD2	38:E:8434:HOH:O	2.14	0.47
6:E:233:THR:CG2	6:E:234:VAL:N	2.78	0.47
14:M:97:VAL:HG12	14:M:98:GLU:O	2.14	0.47
15:N:69:LYS:O	15:N:73:ARG:CZ	2.62	0.47
18:Q:11:ALA:HB2	18:Q:18:LYS:HA	1.97	0.47
21:T:29:ASP:CG	21:T:31:ARG:NH1	2.73	0.47
25:X:88:THR:HG23	25:X:110:GLN:HB3	1.97	0.47
26:Y:85:VAL:HG12	26:Y:86:GLU:N	2.29	0.47
28:1:47:LEU:HD13	28:1:64:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:U:H2'	1:A:13:G:H5'	1.97	0.47
1:A:474:C:O3'	6:E:73:LEU:HD21	2.14	0.47
1:A:926:A:H1'	14:M:38:HIS:O	2.14	0.47
1:A:1189:A:H1'	1:A:1209:C:H1'	1.97	0.47
1:A:2271:G:H2'	1:A:2271:G:N3	2.29	0.47
1:A:2866:U:H4'	1:A:2867:G:H5'	1.97	0.47
5:D:63:GLU:O	5:D:63:GLU:HG3	2.14	0.47
5:D:322:ARG:HB2	38:D:8608:HOH:O	2.14	0.47
9:H:21:GLU:HA	9:H:24:ARG:HE	1.79	0.47
12:K:45:VAL:HG22	12:K:46:ILE:N	2.29	0.47
15:N:46:LEU:HB2	38:N:8607:HOH:O	2.15	0.47
15:N:184:ARG:HB2	15:N:184:ARG:CZ	2.45	0.47
16:O:73:ALA:HB1	16:O:74:PRO:HD2	1.96	0.47
21:T:29:ASP:OD1	21:T:31:ARG:NH1	2.47	0.47
23:V:47:ARG:CG	38:V:4381:HOH:O	2.56	0.47
25:X:21:LEU:HD13	25:X:26:ILE:HD11	1.97	0.47
25:X:122:ARG:HH11	25:X:122:ARG:CG	2.24	0.47
29:2:18:LYS:HB2	30:3:49:GLU:HG2	1.97	0.47
1:A:331:A:C6	1:A:332:G:C4	3.02	0.47
1:A:383:A:C6	1:A:407:A:C8	3.03	0.47
1:A:929:A:H8	1:A:929:A:O5'	1.98	0.47
1:A:1189:A:H1'	1:A:1209:C:O4'	2.15	0.47
1:A:1342:C:O2'	1:A:1343:C:H5'	2.15	0.47
1:A:2016:U:O5'	1:A:2016:U:H6	1.97	0.47
7:F:59:GLY:C	7:F:61:PHE:H	2.23	0.47
20:S:119:VAL:CG2	20:S:142:ASP:HB2	2.44	0.47
26:Y:75:ALA:O	26:Y:83:ALA:HA	2.15	0.47
29:2:21:ARG:HD3	29:2:45:ARG:NE	2.30	0.47
1:A:84:G:O2'	1:A:85:C:H5'	2.15	0.47
1:A:392:U:O2'	15:N:182:LYS:HE2	2.14	0.47
1:A:731:U:H2'	1:A:732:C:C6	2.50	0.47
1:A:1119:G:N2	1:A:1246:A:H2	2.08	0.47
1:A:2104:C:O2	1:A:2486:A:C2	2.68	0.47
1:A:2346:C:H4'	7:F:52:THR:HG22	1.97	0.47
1:A:2781:U:C2'	1:A:2782:G:H5'	2.45	0.47
1:A:2834:G:OP1	26:Y:39:LYS:HE2	2.15	0.47
4:C:135:VAL:HG21	4:C:147:ARG:CZ	2.45	0.47
6:E:7:ASP:OD1	6:E:11:ASN:O	2.33	0.47
6:E:35:VAL:HG21	6:E:227:GLY:HA2	1.95	0.47
11:J:162:SER:CB	11:J:163:PRO:CD	2.80	0.47
1:A:544:G:H2'	1:A:545:G:C5'	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:A:H4'	28:1:10:ARG:N	2.30	0.46
1:A:1845:A:OP2	4:C:190:ARG:NH1	2.45	0.46
4:C:9:ARG:HG2	4:C:16:PHE:CD2	2.50	0.46
5:D:7:ARG:HH11	5:D:7:ARG:CG	2.25	0.46
5:D:87:TYR:O	5:D:138:GLY:N	2.42	0.46
6:E:65:ARG:HG3	6:E:67:GLN:HB2	1.98	0.46
9:H:37:THR:O	9:H:41:GLU:HG3	2.15	0.46
10:I:16:LYS:O	10:I:20:VAL:HG23	2.15	0.46
17:P:96:VAL:HG13	17:P:100:GLN:HB2	1.97	0.46
18:Q:37:ARG:O	18:Q:40:VAL:HB	2.15	0.46
18:Q:143:ALA:HA	38:Q:197:HOH:O	2.15	0.46
25:X:76:ASP:O	25:X:77:ALA:C	2.59	0.46
25:X:88:THR:CG2	25:X:110:GLN:NE2	2.72	0.46
31:4:31:THR:HB	31:4:33:MET:HE3	1.97	0.46
1:A:171:C:C2'	1:A:172:U:H5'	2.45	0.46
1:A:175:G:H2'	15:N:192:ALA:HB3	1.96	0.46
1:A:188:C:H5''	15:N:163:LEU:HD21	1.97	0.46
1:A:288:A:H2'	1:A:289:G:C8	2.50	0.46
1:A:383:A:C2	1:A:407:A:C4	3.03	0.46
1:A:1007:A:H2'	11:J:19:TYR:CZ	2.50	0.46
1:A:1249:U:H2'	1:A:1250:C:C6	2.51	0.46
1:A:1331:A:OP2	27:Z:142:SER:OG	2.25	0.46
1:A:1730:G:H4'	1:A:1731:C:O5'	2.15	0.46
1:A:2247:C:H5''	38:A:6802:HOH:O	2.15	0.46
1:A:2279:G:OP1	38:A:4571:HOH:O	2.21	0.46
2:B:3041:C:O4'	7:F:50:VAL:HG23	2.16	0.46
2:B:3049:G:H2'	2:B:3050:G:O4'	2.15	0.46
4:C:179:MET:HA	4:C:179:MET:HE3	1.96	0.46
4:C:211:LYS:HD3	38:C:8625:HOH:O	2.14	0.46
5:D:175:LEU:C	5:D:175:LEU:CD2	2.88	0.46
7:F:103:ASN:ND2	7:F:134:LEU:H	2.12	0.46
8:G:22:VAL:O	8:G:28:SER:HA	2.15	0.46
9:H:50:VAL:CG1	9:H:60:VAL:HG11	2.45	0.46
16:O:5:ARG:HG3	19:R:18:PRO:CB	2.45	0.46
22:U:71:VAL:HG12	22:U:72:ILE:N	2.30	0.46
31:4:74:CYS:SG	31:4:76:LYS:CG	3.03	0.46
1:A:177:A:H2'	1:A:178:U:O4'	2.16	0.46
1:A:407:A:H2'	1:A:408:A:C8	2.51	0.46
1:A:1304:U:H2'	1:A:1305:C:C6	2.51	0.46
1:A:1684:A:O2'	1:A:1685:A:H5''	2.15	0.46
1:A:2451:G:O6	38:A:9891:HOH:O	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3092:G:C6	2:B:3093:A:C6	3.04	0.46
5:D:41:PHE:HB3	5:D:190:MET:HE1	1.97	0.46
11:J:95:GLU:HB3	11:J:119:VAL:HG11	1.96	0.46
11:J:140:PRO:HA	11:J:142:VAL:HG12	1.98	0.46
16:O:93:GLN:HG2	38:O:8554:HOH:O	2.13	0.46
1:A:281:U:O2'	1:A:282:C:H5'	2.16	0.46
1:A:2428:G:N7	38:A:3276:HOH:O	2.46	0.46
2:B:3064:C:H2'	2:B:3065:A:H5'	1.98	0.46
5:D:24:PRO:HG2	5:D:204:GLY:HA2	1.96	0.46
7:F:25:MET:HE3	7:F:37:ALA:HB1	1.98	0.46
8:G:10:ASP:HA	38:G:3707:HOH:O	2.15	0.46
11:J:14:TYR:N	11:J:91:HIS:CE1	2.81	0.46
17:P:47:ARG:HG3	17:P:47:ARG:NH1	2.27	0.46
31:4:11:CYS:HB2	31:4:20:HIS:HE1	1.80	0.46
1:A:317:A:H5''	22:U:52:ARG:HD2	1.97	0.46
1:A:952:G:OP1	19:R:42:LYS:HE2	2.15	0.46
1:A:1342:C:C2'	1:A:1343:C:H5'	2.46	0.46
1:A:1504:A:O2'	1:A:1506:U:OP2	2.31	0.46
1:A:1713:G:C1'	38:A:4547:HOH:O	2.60	0.46
1:A:1776:A:C8	1:A:1778:A:O4'	2.68	0.46
1:A:2265:U:H2'	1:A:2266:A:H8	1.81	0.46
5:D:310:ARG:HD2	38:D:8648:HOH:O	2.15	0.46
11:J:113:ALA:N	11:J:114:PRO:HD3	2.31	0.46
11:J:157:ILE:CG2	11:J:158:ASN:N	2.78	0.46
25:X:35:VAL:HA	25:X:36:PRO:HD3	1.78	0.46
29:2:29:THR:O	29:2:32:LYS:CE	2.64	0.46
1:A:816:G:OP1	18:Q:91:LYS:NZ	2.44	0.46
1:A:1161:A:H8	1:A:1161:A:O5'	1.99	0.46
1:A:1850:U:H2'	1:A:1851:G:H8	1.80	0.46
1:A:2121:G:C2'	1:A:2122:C:H5'	2.44	0.46
1:A:2840:A:OP1	5:D:211:THR:HG23	2.16	0.46
7:F:99:ASP:HB3	7:F:103:ASN:H	1.80	0.46
16:O:58:LEU:N	16:O:58:LEU:CD1	2.78	0.46
17:P:32:ARG:NE	38:P:3360:HOH:O	2.48	0.46
1:A:95:A:H5''	1:A:97:G:O4'	2.16	0.46
1:A:1930:A:H2'	1:A:1931:A:C8	2.51	0.46
1:A:2769:C:O2'	1:A:2770:G:H5'	2.16	0.46
5:D:60:SER:C	5:D:62:ARG:H	2.23	0.46
7:F:57:THR:HG23	7:F:63:ILE:CB	2.45	0.46
15:N:153:THR:O	15:N:156:ARG:HG3	2.15	0.46
20:S:39:THR:CB	20:S:42:GLU:HG3	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:3:18:ASN:ND2	30:3:40:ARG:H	2.14	0.46
1:A:169:A:C6	1:A:2469:A:C6	3.04	0.46
1:A:660:A:H4'	1:A:661:G:O5'	2.16	0.46
1:A:815:U:C4	1:A:816:G:C6	3.03	0.46
1:A:1754:A:H2'	1:A:1755:A:O4'	2.15	0.46
1:A:2028:U:H2'	1:A:2029:C:H6	1.79	0.46
1:A:2432:C:H4'	31:4:36:ILE:HG12	1.97	0.46
1:A:2443:C:H3'	38:A:9970:HOH:O	2.16	0.46
38:A:5155:HOH:O	16:O:21:HIS:HE1	1.99	0.46
7:F:23:VAL:O	7:F:23:VAL:CG2	2.63	0.46
11:J:43:PRO:HD2	11:J:137:ASN:HA	1.97	0.46
11:J:72:VAL:HG11	11:J:81:TYR:CZ	2.51	0.46
11:J:157:ILE:HG22	11:J:158:ASN:N	2.30	0.46
15:N:114:VAL:HG21	15:N:159:THR:CG2	2.46	0.46
16:O:164:ASP:C	16:O:164:ASP:OD1	2.58	0.46
1:A:1306:U:OP1	6:E:184:ARG:HD2	2.16	0.46
1:A:2362:A:H2'	1:A:2363:G:C8	2.51	0.46
1:A:2672:C:O2'	1:A:2673:U:H5'	2.16	0.46
1:A:2777:G:O2'	1:A:2778:A:H5'	2.15	0.46
1:A:2781:U:H1'	8:G:139:GLU:OE2	2.15	0.46
3:5:74:C:H2'	3:5:75:C:C5'	2.46	0.46
5:D:42:ALA:HB3	5:D:79:MET:SD	2.56	0.46
5:D:185:GLY:HA2	38:D:8633:HOH:O	2.16	0.46
6:E:34:ALA:HB3	6:E:220:THR:HG21	1.98	0.46
7:F:86:THR:HG23	38:F:7477:HOH:O	2.15	0.46
22:U:12:ARG:O	22:U:19:ARG:NH2	2.48	0.46
27:Z:117:LEU:HD12	27:Z:174:VAL:CG1	2.45	0.46
28:1:10:ARG:HA	38:1:8413:HOH:O	2.16	0.46
30:3:40:ARG:HA	30:3:45:ASN:ND2	2.30	0.46
1:A:392:U:H4'	15:N:193:LYS:HB3	1.98	0.46
1:A:941:G:O2'	1:A:942:U:H5'	2.16	0.46
38:A:5700:HOH:O	4:C:22:ARG:HG2	2.16	0.46
9:H:39:SER:HB3	9:H:45:ALA:HB2	1.97	0.46
17:P:32:ARG:HE	17:P:35:LYS:HD2	1.81	0.46
27:Z:112:GLU:OE1	27:Z:112:GLU:HA	2.16	0.46
27:Z:189:ASN:ND2	27:Z:192:ASP:H	2.13	0.46
1:A:407:A:H5'	38:A:5485:HOH:O	2.16	0.45
1:A:419:A:C2	1:A:2449:G:N3	2.84	0.45
1:A:1592:G:O2'	1:A:1593:C:O5'	2.34	0.45
1:A:1634:G:H3'	38:A:3386:HOH:O	2.14	0.45
1:A:1644:C:H2'	1:A:1645:U:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3041:C:C6	7:F:50:VAL:HG21	2.51	0.45
6:E:118:THR:CG2	6:E:137:PRO:HB3	2.45	0.45
6:E:218:VAL:HG12	38:E:8429:HOH:O	2.16	0.45
7:F:135:VAL:HG21	7:F:139:TYR:CD1	2.51	0.45
8:G:20:ILE:HD12	8:G:33:LEU:HD12	1.95	0.45
13:L:6:ALA:HB3	13:L:116:GLU:HG2	1.98	0.45
13:L:130:MET:SD	23:V:25:ASP:O	2.73	0.45
15:N:68:ARG:O	15:N:68:ARG:CD	2.63	0.45
21:T:73:ASP:OD1	21:T:75:GLN:HB2	2.16	0.45
25:X:121:PRO:HA	25:X:153:MET:HG2	1.98	0.45
30:3:40:ARG:HG2	30:3:40:ARG:NH1	2.30	0.45
1:A:541:C:O2'	1:A:542:A:H5''	2.16	0.45
1:A:677:C:H4'	6:E:246:ARG:NH2	2.32	0.45
1:A:1200:A:C4'	38:A:6798:HOH:O	2.64	0.45
1:A:1246:A:O2'	1:A:1247:A:H3'	2.16	0.45
1:A:1667:A:H5'	1:A:1667:A:C8	2.48	0.45
1:A:1902:G:H2'	1:A:1903:U:O4'	2.16	0.45
1:A:2266:A:P	38:A:5323:HOH:O	2.73	0.45
1:A:2763:G:OP1	13:L:9:THR:OG1	2.20	0.45
1:A:2785:C:H4'	1:A:2786:G:OP2	2.17	0.45
4:C:101:GLU:HG2	4:C:131:HIS:ND1	2.31	0.45
4:C:112:PRO:HD3	4:C:152:CYS:SG	2.56	0.45
4:C:217:ARG:HH11	4:C:217:ARG:CG	2.29	0.45
5:D:254:GLN:HG2	5:D:255:GLY:N	2.31	0.45
7:F:35:ALA:C	7:F:37:ALA:N	2.74	0.45
13:L:74:VAL:HG12	13:L:75:ARG:HG3	1.97	0.45
13:L:99:ASP:OD1	13:L:101:ASN:N	2.49	0.45
14:M:104:ASP:HB2	38:M:8580:HOH:O	2.16	0.45
19:R:28:ARG:NH1	38:R:6206:HOH:O	2.43	0.45
25:X:75:GLY:HA3	38:X:5763:HOH:O	2.17	0.45
26:Y:25:ARG:NH1	38:Y:3861:HOH:O	2.49	0.45
27:Z:115:ARG:HG3	35:Z:8517:CL:CL	2.53	0.45
38:A:4393:HOH:O	15:N:14:ARG:HB3	2.16	0.45
5:D:7:ARG:CD	5:D:9:GLY:O	2.65	0.45
7:F:25:MET:HE1	7:F:40:ILE:CG1	2.46	0.45
9:H:26:THR:HB	9:H:102:GLY:C	2.41	0.45
12:K:70:PHE:CD2	12:K:70:PHE:O	2.69	0.45
18:Q:28:GLN:N	38:Q:203:HOH:O	2.50	0.45
27:Z:136:LYS:HE2	27:Z:138:ARG:NH1	2.31	0.45
30:3:49:GLU:CD	38:3:719:HOH:O	2.58	0.45
1:A:380:A:H5''	15:N:48:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:C:O2'	1:A:452:G:H5'	2.16	0.45
1:A:466:A:H2'	1:A:467:G:O4'	2.16	0.45
1:A:590:A:H2'	1:A:591:A:H5'	1.99	0.45
1:A:603:A:H4'	1:A:604:G:O5'	2.16	0.45
1:A:790:A:H2'	1:A:791:A:O4'	2.16	0.45
1:A:1336:U:C2	1:A:1337:A:C8	3.04	0.45
1:A:1351:G:OP1	6:E:96:LYS:NZ	2.39	0.45
1:A:1384:C:H5'	26:Y:30:MET:HG2	1.99	0.45
1:A:1440:U:P	38:A:3954:HOH:O	2.73	0.45
1:A:1609:C:H2'	1:A:1610:G:H8	1.81	0.45
7:F:58:VAL:CG1	7:F:59:GLY:N	2.78	0.45
15:N:37:VAL:CG2	15:N:108:LYS:HG3	2.45	0.45
16:O:184:ILE:HG22	16:O:185:GLU:N	2.30	0.45
22:U:55:PHE:O	22:U:56:ALA:C	2.59	0.45
23:V:9:CYS:SG	23:V:11:THR:N	2.83	0.45
1:A:291:C:H2'	1:A:292:G:O4'	2.16	0.45
1:A:382:U:C5	1:A:406:G:N2	2.84	0.45
1:A:628:A:C8	1:A:2071:C:N4	2.85	0.45
1:A:818:A:O2'	28:1:13:ARG:HD3	2.16	0.45
1:A:1057:A:C6	1:A:1058:A:C6	3.05	0.45
1:A:1279:U:H5''	38:A:9093:HOH:O	2.16	0.45
1:A:2044:G:OP1	26:Y:23:HIS:HE1	2.00	0.45
1:A:2314:G:O2'	1:A:2315:C:H5'	2.16	0.45
1:A:2353:A:H4'	1:A:2354:A:O5'	2.16	0.45
1:A:2819:C:O4'	5:D:96:PRO:HB2	2.16	0.45
4:C:153:ARG:HH11	4:C:153:ARG:CB	2.29	0.45
5:D:14:GLY:HA2	5:D:15:PRO:C	2.41	0.45
6:E:235:PHE:HE2	6:E:243:VAL:HG21	1.80	0.45
7:F:25:MET:SD	7:F:40:ILE:HD11	2.56	0.45
7:F:67:ASP:O	7:F:69:ILE:HG13	2.16	0.45
8:G:157:LYS:NZ	38:G:2401:HOH:O	2.49	0.45
11:J:26:LYS:NZ	11:J:31:PHE:CZ	2.84	0.45
15:N:184:ARG:HB2	15:N:184:ARG:NH1	2.32	0.45
24:W:45:ARG:C	24:W:47:LYS:N	2.73	0.45
25:X:146:ILE:HG23	25:X:150:LEU:CD1	2.47	0.45
27:Z:186:ARG:HG2	27:Z:186:ARG:NH1	2.31	0.45
28:1:59:HIS:HA	38:1:8439:HOH:O	2.15	0.45
1:A:1225:C:H4'	38:A:8903:HOH:O	2.16	0.45
1:A:1805:G:H2'	1:A:1806:G:H8	1.81	0.45
4:C:8:ARG:NH1	38:C:8558:HOH:O	2.42	0.45
5:D:248:ARG:O	5:D:251:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:117:GLU:C	9:H:119:ARG:N	2.74	0.45
10:I:64:ASN:N	10:I:64:ASN:ND2	2.64	0.45
12:K:130:VAL:CG1	12:K:131:THR:N	2.79	0.45
13:L:27:ARG:CD	38:L:4747:HOH:O	2.61	0.45
14:M:121:ILE:HG12	14:M:141:GLU:HB2	1.97	0.45
1:A:247:A:C8	1:A:262:A:N6	2.85	0.45
1:A:2050:G:H5''	20:S:80:TYR:O	2.17	0.45
1:A:2385:G:H2'	1:A:2386:U:C6	2.51	0.45
1:A:2670:G:O2'	1:A:2671:U:H5'	2.16	0.45
16:O:25:ARG:HA	16:O:28:LYS:HG3	1.97	0.45
29:2:25:LYS:CG	30:3:49:GLU:H	2.29	0.45
1:A:222:A:H2'	1:A:223:G:O4'	2.16	0.45
1:A:1677:U:OP2	30:3:8:LYS:NZ	2.50	0.45
1:A:1878:G:C1'	38:A:5581:HOH:O	2.63	0.45
1:A:2116:U:C4	1:A:2271:G:C6	3.05	0.45
1:A:2299:G:O6	19:R:1:PRO:HA	2.16	0.45
1:A:2434:A:O3'	31:4:28:GLY:HA3	2.16	0.45
2:B:3055:U:H4'	2:B:3056:A:C8	2.52	0.45
38:E:8358:HOH:O	17:P:3:THR:HG21	2.17	0.45
7:F:60:GLU:C	7:F:62:ASP:N	2.72	0.45
9:H:28:ALA:CB	9:H:99:THR:HG23	2.46	0.45
11:J:6:TYR:HE2	11:J:94:ARG:O	2.00	0.45
11:J:86:ARG:NH1	11:J:130:HIS:CD2	2.85	0.45
14:M:38:HIS:CD2	14:M:39:GLU:HG3	2.51	0.45
15:N:83:SER:HA	15:N:86:MET:HE3	1.99	0.45
16:O:19:ASP:N	38:O:8525:HOH:O	2.15	0.45
17:P:26:TRP:HA	17:P:26:TRP:CE3	2.52	0.45
25:X:38:THR:HG22	25:X:39:ASP:N	2.32	0.45
1:A:758:A:H2'	1:A:759:C:O4'	2.17	0.45
1:A:2432:C:H2'	1:A:2433:A:C8	2.51	0.45
1:A:2468:A:C8	31:4:54:LYS:HE2	2.51	0.45
1:A:2591:C:H2'	1:A:2592:G:O4'	2.17	0.45
1:A:2656:G:O2'	1:A:2657:G:H5'	2.17	0.45
2:B:3008:G:O6	16:O:11:ARG:NH1	2.48	0.45
2:B:3034:A:H1'	16:O:153:GLN:HE22	1.82	0.45
8:G:16:ASP:O	8:G:17:HIS:HB2	2.17	0.45
11:J:163:PRO:HG2	38:J:8339:HOH:O	2.16	0.45
12:K:6:PHE:HB3	12:K:109:TYR:OH	2.17	0.45
13:L:87:ARG:CZ	38:L:4854:HOH:O	2.65	0.45
14:M:140:VAL:CG2	38:M:8562:HOH:O	2.64	0.45
15:N:49:ALA:HB1	15:N:54:TYR:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:73:ALA:HB1	16:O:74:PRO:CD	2.47	0.45
17:P:39:THR:HB	38:P:3360:HOH:O	2.16	0.45
28:1:22:ILE:HG22	28:1:23:ARG:N	2.32	0.45
1:A:92:G:H4'	24:W:44:GLY:HA3	1.98	0.45
1:A:101:C:H2'	1:A:102:A:H8	1.82	0.45
1:A:392:U:C5'	15:N:193:LYS:HB3	2.47	0.45
1:A:496:G:C6	1:A:498:A:C6	3.05	0.45
1:A:553:G:H5'	38:A:9994:HOH:O	2.15	0.45
1:A:831:U:O2	38:A:3936:HOH:O	2.21	0.45
1:A:1014:A:H2'	1:A:1015:C:H5'	1.99	0.45
1:A:1427:A:N6	38:A:6184:HOH:O	2.40	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.17	0.45
4:C:199:HIS:CE1	4:C:225:VAL:HG11	2.52	0.45
5:D:8:LYS:HG3	5:D:220:VAL:HG12	1.98	0.45
5:D:101:TRP:HB2	5:D:119:HIS:CD2	2.52	0.45
6:E:192:ILE:CG2	6:E:234:VAL:HG12	2.48	0.45
8:G:69:ILE:HA	8:G:72:MET:HE3	1.99	0.45
8:G:116:THR:CG2	8:G:151:LEU:HD22	2.47	0.45
13:L:29:LEU:HB3	13:L:55:VAL:CG1	2.35	0.45
14:M:7:GLN:HB3	14:M:13:HIS:CE1	2.52	0.45
15:N:69:LYS:HD3	15:N:125:ARG:HA	1.98	0.45
16:O:15:GLU:HB2	16:O:17:ARG:HG3	1.99	0.45
16:O:141:ARG:N	38:O:8566:HOH:O	2.50	0.45
17:P:21:SER:OG	17:P:106:PRO:HB2	2.17	0.45
18:Q:14:LEU:HD13	18:Q:51:ALA:HB2	1.98	0.45
19:R:41:LEU:HB3	19:R:52:PHE:CZ	2.51	0.45
21:T:11:THR:H	21:T:14:ALA:HB3	1.81	0.45
25:X:139:GLY:O	25:X:141:HIS:CD2	2.70	0.45
27:Z:154:ARG:HH12	27:Z:155:ARG:HG3	1.82	0.45
1:A:696:C:C2'	1:A:697:G:H5'	2.48	0.44
1:A:821:U:H5''	38:A:9546:HOH:O	2.16	0.44
1:A:1886:A:C2'	38:A:4297:HOH:O	2.65	0.44
1:A:2356:A:H2'	1:A:2357:G:O4'	2.16	0.44
1:A:2435:U:OP1	31:4:28:GLY:HA3	2.16	0.44
38:A:6880:HOH:O	22:U:9:LYS:HD2	2.17	0.44
5:D:52:VAL:O	5:D:53:LEU:HD12	2.16	0.44
5:D:238:ASN:ND2	5:D:240:GLY:H	2.14	0.44
7:F:173:GLU:HG3	7:F:174:VAL:N	2.32	0.44
15:N:35:PRO:CG	15:N:38:VAL:CG2	2.87	0.44
16:O:163:PHE:O	16:O:164:ASP:O	2.34	0.44
25:X:13:MET:HE2	25:X:18:GLN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:57:CYS:O	28:1:61:GLY:HA2	2.17	0.44
1:A:553:G:H2'	1:A:554:G:H5'	1.98	0.44
1:A:876:A:N3	1:A:876:A:H2'	2.32	0.44
1:A:2122:C:H3'	38:A:4762:HOH:O	2.17	0.44
1:A:2467:A:HO2'	1:A:2468:A:H2'	1.81	0.44
1:A:2547:C:H2'	1:A:2548:C:H6	1.81	0.44
4:C:66:ARG:HB2	4:C:66:ARG:HH11	1.80	0.44
6:E:237:GLU:N	38:E:8454:HOH:O	2.50	0.44
11:J:150:LYS:HE2	38:J:8379:HOH:O	2.16	0.44
16:O:38:LYS:HE3	16:O:38:LYS:HB2	1.76	0.44
17:P:14:LEU:CD2	17:P:102:ILE:HD11	2.46	0.44
20:S:39:THR:CG2	20:S:42:GLU:HG3	2.48	0.44
27:Z:144:ARG:NE	38:Z:8616:HOH:O	2.49	0.44
1:A:584:U:H3'	38:A:5555:HOH:O	2.17	0.44
1:A:1461:U:H2'	1:A:1462:C:C6	2.51	0.44
1:A:1523:G:C6	1:A:1524:U:O4	2.70	0.44
1:A:1827:G:H2'	1:A:1828:G:C8	2.52	0.44
1:A:1921:A:C6	1:A:1922:A:C2	3.06	0.44
1:A:1970:G:C5'	38:A:6529:HOH:O	2.65	0.44
5:D:258:GLY:N	5:D:260:HIS:CE1	2.78	0.44
5:D:280:VAL:CG1	5:D:281:ASP:N	2.80	0.44
9:H:6:PHE:CD1	9:H:6:PHE:C	2.96	0.44
11:J:45:GLN:NE2	11:J:135:TRP:HE1	2.16	0.44
13:L:125:ALA:C	13:L:127:ALA:N	2.75	0.44
16:O:108:SER:HA	16:O:109:PRO:HD3	1.81	0.44
20:S:125:ARG:HG2	38:S:8541:HOH:O	2.16	0.44
22:U:73:HIS:CD2	22:U:88:PRO:HG3	2.52	0.44
23:V:49:LEU:O	23:V:55:ALA:CB	2.65	0.44
25:X:121:PRO:CA	25:X:153:MET:HG2	2.48	0.44
29:2:29:THR:O	29:2:32:LYS:HE2	2.18	0.44
31:4:7:PHE:HE2	31:4:22:VAL:CG2	2.30	0.44
31:4:7:PHE:CE1	31:4:9:THR:HB	2.52	0.44
1:A:407:A:C2	1:A:408:A:C4	3.05	0.44
1:A:602:A:O2'	1:A:605:C:H4'	2.17	0.44
1:A:661:G:C4	1:A:686:A:C2	3.06	0.44
1:A:1189:A:N3	38:A:7139:HOH:O	2.50	0.44
1:A:2055:A:H5'	20:S:134:SER:HB2	2.00	0.44
1:A:2503:A:OP1	11:J:147:ARG:NH2	2.38	0.44
1:A:2766:A:O2'	5:D:265:LEU:O	2.30	0.44
4:C:194:MET:HE3	4:C:199:HIS:CB	2.48	0.44
5:D:154:VAL:CG1	5:D:156:LYS:HG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:27:ILE:HD11	7:F:37:ALA:CB	2.47	0.44
7:F:81:GLU:O	7:F:85:GLN:HG3	2.17	0.44
8:G:9:GLU:HG3	8:G:10:ASP:N	2.33	0.44
20:S:31:ILE:O	20:S:32:ALA:C	2.59	0.44
20:S:129:ALA:O	20:S:130:MET:HB2	2.17	0.44
22:U:38:ARG:HH11	22:U:38:ARG:HG3	1.81	0.44
25:X:58:SER:O	25:X:59:GLN:C	2.60	0.44
1:A:1423:C:O2'	1:A:1424:A:H5'	2.18	0.44
1:A:2453:G:H4'	14:M:50:GLY:C	2.42	0.44
5:D:17:LYS:O	5:D:260:HIS:HD2	2.01	0.44
7:F:57:THR:HG23	7:F:63:ILE:CG2	2.46	0.44
14:M:142:LEU:HG	14:M:146:GLY:HA3	2.00	0.44
16:O:67:ALA:HA	16:O:71:TRP:H	1.81	0.44
16:O:104:ILE:O	16:O:107:ASN:HB2	2.17	0.44
19:R:75:ILE:CD1	19:R:84:ILE:HD11	2.48	0.44
25:X:4:LEU:HD23	25:X:4:LEU:HA	1.82	0.44
1:A:716:G:H2'	1:A:717:C:O5'	2.18	0.44
1:A:764:C:H2'	1:A:765:G:O4'	2.18	0.44
1:A:1041:U:H2'	1:A:1042:U:H5'	2.00	0.44
1:A:1313:A:H5'	27:Z:208:LYS:O	2.17	0.44
1:A:1462:C:H2'	1:A:1463:A:C8	2.53	0.44
1:A:1829:A:H61	28:1:18:TYR:CA	2.26	0.44
1:A:1859:A:H8	1:A:1859:A:O5'	2.01	0.44
1:A:2466:G:P	38:A:3142:HOH:O	2.73	0.44
1:A:2635:A:C2'	1:A:2636:C:H5'	2.46	0.44
38:A:3472:HOH:O	31:4:57:GLY:HA2	2.17	0.44
38:A:4009:HOH:O	15:N:94:LYS:HE3	2.18	0.44
2:B:3092:G:H22	11:J:52:LYS:NZ	2.15	0.44
4:C:199:HIS:CD2	4:C:201:PHE:HB2	2.52	0.44
6:E:120:ASP:OD1	6:E:120:ASP:C	2.60	0.44
26:Y:9:VAL:HG13	26:Y:88:GLU:OE2	2.18	0.44
27:Z:213:LYS:O	27:Z:217:ILE:HG13	2.18	0.44
1:A:40:C:H4'	38:A:6462:HOH:O	2.17	0.44
1:A:1189:A:C4	38:A:7139:HOH:O	2.56	0.44
1:A:1299:G:N7	14:M:6:ARG:NH1	2.65	0.44
1:A:1644:C:O2'	1:A:1645:U:H5'	2.17	0.44
1:A:2387:U:H2'	1:A:2388:C:C6	2.53	0.44
1:A:2873:C:N4	1:A:2874:G:C6	2.86	0.44
4:C:94:LEU:N	4:C:94:LEU:CD2	2.81	0.44
6:E:126:ASP:C	6:E:128:GLY:N	2.75	0.44
7:F:81:GLU:C	7:F:83:PHE:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:39:VAL:HG11	12:K:107:ASN:CB	2.48	0.44
12:K:46:ILE:HG12	12:K:53:ILE:HD13	1.99	0.44
15:N:24:MET:HE1	15:N:120:VAL:O	2.18	0.44
16:O:71:TRP:N	38:O:8539:HOH:O	2.50	0.44
19:R:88:ALA:O	19:R:90:HIS:N	2.51	0.44
28:1:48:LYS:HG2	38:1:8429:HOH:O	2.18	0.44
1:A:1008:C:H2'	1:A:1009:U:C6	2.53	0.44
1:A:1135:G:H5'	38:A:5388:HOH:O	2.17	0.44
1:A:2620:U:O4	36:5:76:PPU:O	2.36	0.44
1:A:2909:G:H2'	1:A:2910:A:H8	1.83	0.44
38:A:6955:HOH:O	23:V:50:GLU:CD	2.60	0.44
6:E:7:ASP:OD2	6:E:9:ASP:HB2	2.18	0.44
8:G:162:PHE:CD1	8:G:162:PHE:N	2.85	0.44
9:H:58:GLU:HG3	9:H:61:MET:HE2	1.99	0.44
13:L:80:ILE:O	13:L:80:ILE:HG13	2.17	0.44
17:P:44:ASN:HA	17:P:65:LEU:O	2.18	0.44
22:U:113:GLU:O	22:U:114:SER:C	2.60	0.44
31:4:60:LYS:HD2	31:4:61:PRO:HD2	1.99	0.44
1:A:716:G:C2'	1:A:717:C:O5'	2.66	0.44
1:A:1637:A:H2'	1:A:1638:U:C6	2.53	0.44
1:A:1874:U:OP1	4:C:51:ARG:HD2	2.18	0.44
1:A:2123:A:OP1	15:N:89:ASN:ND2	2.51	0.44
11:J:26:LYS:HG3	11:J:58:HIS:HB2	2.00	0.44
11:J:47:GLU:HG2	11:J:133:ILE:HD12	1.99	0.44
13:L:30:LYS:C	13:L:55:VAL:HG13	2.40	0.44
13:L:45:PRO:HB2	38:L:7169:HOH:O	2.17	0.44
21:T:29:ASP:OD1	21:T:31:ARG:HG3	2.17	0.44
27:Z:126:PRO:HG2	27:Z:128:PHE:CZ	2.53	0.44
28:1:33:HIS:HE1	28:1:49:ARG:NE	2.16	0.44
28:1:40:PRO:CD	28:1:47:LEU:HD11	2.29	0.44
29:2:8:GLN:NE2	29:2:11:LYS:HZ2	2.02	0.44
1:A:634:G:O2'	1:A:1358:A:OP1	2.36	0.43
1:A:656:G:H2'	1:A:657:G:H8	1.83	0.43
1:A:883:U:O2	1:A:883:U:H2'	2.17	0.43
1:A:1391:G:H2'	1:A:1392:A:H5'	2.00	0.43
1:A:1711:A:O2'	1:A:1712:A:H5'	2.18	0.43
1:A:1825:U:O2'	1:A:1826:C:H5'	2.18	0.43
2:B:3057:A:H2'	2:B:3058:G:H5'	2.00	0.43
5:D:248:ARG:O	5:D:251:VAL:HG12	2.18	0.43
5:D:274:GLU:HA	5:D:292:GLY:O	2.18	0.43
6:E:218:VAL:CG1	38:E:8429:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:36:PRO:HD3	12:K:127:ILE:HD12	2.00	0.43
16:O:78:MET:HB2	16:O:79:PRO:HD3	1.99	0.43
16:O:86:LEU:HD12	16:O:125:ALA:CB	2.40	0.43
17:P:26:TRP:N	38:P:3062:HOH:O	2.49	0.43
17:P:26:TRP:HA	17:P:26:TRP:HE3	1.82	0.43
22:U:96:VAL:HG13	22:U:97:ARG:N	2.32	0.43
28:1:10:ARG:CG	28:1:11:THR:N	2.81	0.43
28:1:38:LYS:HD3	38:1:8423:HOH:O	2.17	0.43
28:1:57:CYS:O	28:1:61:GLY:CA	2.65	0.43
1:A:24:G:N2	1:A:518:G:H1'	2.33	0.43
1:A:860:U:H2'	1:A:861:A:C8	2.53	0.43
1:A:1265:G:H1'	38:A:4475:HOH:O	2.17	0.43
1:A:1385:G:O3'	26:Y:49:ARG:NH1	2.52	0.43
1:A:1471:A:H2'	1:A:1472:C:C6	2.53	0.43
1:A:1730:G:C5'	1:A:1731:C:H6	2.31	0.43
1:A:2255:A:C6	1:A:2256:G:C5	3.06	0.43
1:A:2438:G:H2'	1:A:2439:C:O4'	2.18	0.43
1:A:2779:G:O2'	1:A:2780:C:H5'	2.18	0.43
38:A:6486:HOH:O	4:C:211:LYS:HG2	2.17	0.43
2:B:3107:C:H5	38:B:8437:HOH:O	2.00	0.43
3:5:74:C:H2'	3:5:75:C:H5'	2.01	0.43
5:D:88:GLU:O	5:D:88:GLU:HG3	2.18	0.43
6:E:84:VAL:O	6:E:85:LYS:HB2	2.18	0.43
7:F:19:GLU:HG3	38:F:6165:HOH:O	2.18	0.43
7:F:128:LEU:HD23	7:F:128:LEU:C	2.43	0.43
9:H:26:THR:HB	9:H:102:GLY:HA3	1.99	0.43
14:M:62:ALA:HB2	14:M:103:ALA:CB	2.48	0.43
16:O:34:LEU:HA	16:O:47:LEU:CD2	2.48	0.43
16:O:116:PHE:CB	38:O:8556:HOH:O	2.66	0.43
23:V:9:CYS:HG	23:V:11:THR:HG23	1.83	0.43
24:W:5:VAL:HG23	38:W:2271:HOH:O	2.18	0.43
26:Y:76:ARG:NH1	26:Y:76:ARG:CG	2.80	0.43
1:A:295:C:H2'	1:A:296:G:O4'	2.18	0.43
1:A:567:U:C5'	38:A:5862:HOH:O	2.65	0.43
1:A:886:A:OP2	1:A:2113:G:H5'	2.19	0.43
1:A:1119:G:H8	12:K:52:GLN:NE2	2.15	0.43
1:A:1329:A:C2	38:A:4165:HOH:O	2.57	0.43
1:A:1624:A:H4'	1:A:1626:A:H5''	2.01	0.43
1:A:1925:G:O2'	1:A:1926:G:H5'	2.19	0.43
1:A:2123:A:H5'	15:N:89:ASN:ND2	2.34	0.43
1:A:2621:U:H5	38:A:9479:HOH:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:223:ARG:CG	38:C:8616:HOH:O	2.48	0.43
5:D:60:SER:C	5:D:62:ARG:N	2.75	0.43
7:F:170:TYR:N	7:F:170:TYR:CD1	2.87	0.43
8:G:112:ALA:HA	8:G:113:PRO:HD3	1.88	0.43
18:Q:83:LYS:O	18:Q:86:ALA:HB3	2.18	0.43
20:S:33:ARG:NH1	38:S:8542:HOH:O	2.51	0.43
21:T:10:VAL:O	21:T:10:VAL:HG22	2.19	0.43
25:X:85:ALA:HB2	25:X:91:ASP:O	2.18	0.43
25:X:122:ARG:NH1	25:X:152:ALA:O	2.51	0.43
26:Y:9:VAL:HG22	26:Y:88:GLU:OE2	2.18	0.43
27:Z:234:VAL:HG12	27:Z:235:GLU:N	2.33	0.43
31:4:73:GLU:HB2	38:4:8525:HOH:O	2.18	0.43
1:A:171:C:OP2	15:N:84:LYS:HG3	2.18	0.43
1:A:401:C:H2'	1:A:402:U:H6	1.81	0.43
1:A:2461:U:O2	1:A:2466:G:H1'	2.18	0.43
7:F:99:ASP:O	7:F:159:PRO:HG3	2.18	0.43
7:F:151:ILE:HA	7:F:152:PRO:HD3	1.80	0.43
9:H:61:MET:SD	15:N:23:LEU:HD11	2.58	0.43
13:L:37:TYR:HD2	38:L:7169:HOH:O	1.92	0.43
15:N:47:ASP:CG	15:N:48:ARG:H	2.26	0.43
18:Q:16:VAL:HG13	18:Q:20:ARG:NH1	2.33	0.43
22:U:48:VAL:CG2	22:U:98:VAL:HA	2.48	0.43
26:Y:70:ILE:O	26:Y:70:ILE:HG23	2.17	0.43
27:Z:127:GLN:O	27:Z:128:PHE:C	2.61	0.43
27:Z:150:LEU:O	27:Z:151:SER:C	2.60	0.43
31:4:22:VAL:HG12	31:4:90:PHE:HE2	1.83	0.43
1:A:101:C:H2'	1:A:102:A:C8	2.53	0.43
1:A:160:A:C4	1:A:177:A:C2	3.06	0.43
1:A:482:G:H4'	1:A:508:A:N1	2.34	0.43
1:A:536:A:H3'	38:A:4525:HOH:O	2.17	0.43
1:A:1624:A:H5'	1:A:1626:A:O4'	2.19	0.43
1:A:2321:A:O2'	1:A:2322:U:H3'	2.18	0.43
1:A:2780:C:C1'	8:G:143:GLN:NE2	2.81	0.43
38:A:9957:HOH:O	12:K:46:ILE:HD12	2.18	0.43
2:B:3045:A:C8	2:B:3046:C:C5	3.07	0.43
3:5:74:C:H2'	3:5:75:C:O4'	2.17	0.43
6:E:5:ILE:HG12	38:E:8436:HOH:O	2.19	0.43
7:F:15:GLU:HA	7:F:16:PRO:HD3	1.85	0.43
11:J:163:PRO:O	11:J:164:ALA:HB2	2.18	0.43
16:O:77:ASN:OD1	16:O:80:SER:HB2	2.18	0.43
28:1:13:ARG:NH1	38:1:8419:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1:40:PRO:HG2	28:1:64:ILE:HD13	2.01	0.43
29:2:45:ARG:HB3	38:2:988:HOH:O	2.18	0.43
1:A:97:G:C2	22:U:107:LYS:HD2	2.53	0.43
1:A:812:A:H2'	1:A:813:C:O4'	2.19	0.43
1:A:844:A:C6	1:A:882:A:C5	3.06	0.43
1:A:913:A:N3	1:A:1042:U:O2'	2.44	0.43
1:A:962:C:H5'	38:A:6424:HOH:O	2.19	0.43
1:A:1058:A:H2'	1:A:1060:C:C5'	2.42	0.43
1:A:1159:G:H1	1:A:1208:C:H42	1.67	0.43
1:A:1311:G:C2	1:A:1312:G:C8	3.07	0.43
1:A:1572:A:H2'	1:A:1573:A:C8	2.53	0.43
1:A:2450:C:O5'	1:A:2450:C:H6	2.02	0.43
38:A:3911:HOH:O	31:4:34:LYS:HD3	2.18	0.43
4:C:33:GLU:H	4:C:33:GLU:CD	2.20	0.43
6:E:95:GLU:H	6:E:95:GLU:CD	2.27	0.43
15:N:37:VAL:CG1	15:N:63:VAL:HG11	2.47	0.43
15:N:96:ASN:ND2	38:N:8541:HOH:O	2.49	0.43
16:O:90:LEU:CB	16:O:186:LEU:HD22	2.49	0.43
20:S:15:LYS:HE3	38:S:8577:HOH:O	2.18	0.43
21:T:57:THR:HG21	21:T:59:ASP:HB2	2.01	0.43
27:Z:187:VAL:HG12	27:Z:205:ILE:HA	2.00	0.43
1:A:559:U:H5'	1:A:559:U:C6	2.42	0.43
1:A:675:U:H2'	1:A:676:C:H5'	2.00	0.43
1:A:860:U:H2'	38:A:5151:HOH:O	2.19	0.43
1:A:1164:U:C1'	1:A:1165:G:OP1	2.67	0.43
1:A:1592:G:H2'	1:A:1593:C:C6	2.54	0.43
1:A:1644:C:C2	1:A:1645:U:C6	3.07	0.43
1:A:2106:C:H2'	1:A:2107:U:C6	2.53	0.43
1:A:2247:C:C5'	38:A:6802:HOH:O	2.67	0.43
1:A:2851:G:C2'	1:A:2852:A:H5'	2.49	0.43
2:B:3003:A:N6	2:B:3022:G:H1'	2.33	0.43
2:B:3065:A:O2'	2:B:3066:G:P	2.75	0.43
8:G:7:ILE:HA	8:G:8:PRO:HD3	1.92	0.43
9:H:58:GLU:CD	15:N:27:ARG:HH22	2.27	0.43
15:N:39:ARG:NH2	38:N:8624:HOH:O	2.51	0.43
16:O:47:LEU:HD13	16:O:97:VAL:HG11	2.01	0.43
17:P:39:THR:CB	38:P:3360:HOH:O	2.66	0.43
20:S:40:ALA:O	20:S:44:VAL:HG23	2.18	0.43
22:U:38:ARG:HG3	22:U:38:ARG:NH1	2.33	0.43
27:Z:187:VAL:O	27:Z:187:VAL:HG13	2.17	0.43
1:A:290:C:O2'	1:A:291:C:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:G:O2'	1:A:327:A:H5'	2.18	0.43
1:A:661:G:C6	1:A:686:A:C2	3.06	0.43
1:A:731:U:O2'	1:A:732:C:H5'	2.18	0.43
1:A:885:G:H5''	1:A:886:A:H5'	1.99	0.43
1:A:955:A:C2	1:A:1013:A:C4	3.06	0.43
1:A:1167:G:O2'	1:A:1168:C:H5'	2.19	0.43
1:A:1422:U:H2'	1:A:1423:C:H6	1.80	0.43
1:A:2563:U:H2'	1:A:2565:C:O5'	2.19	0.43
2:B:3039:U:H3'	2:B:3040:C:H5''	1.99	0.43
4:C:61:GLU:C	4:C:63:GLY:H	2.27	0.43
5:D:71:VAL:CG1	5:D:296:LEU:HB3	2.46	0.43
5:D:204:GLY:CA	38:D:8653:HOH:O	2.61	0.43
7:F:19:GLU:O	7:F:133:ASN:HB3	2.19	0.43
11:J:83:PHE:CD1	11:J:134:ALA:HB2	2.54	0.43
13:L:10:GLN:NE2	13:L:10:GLN:N	2.43	0.43
16:O:47:LEU:HD12	16:O:92:ALA:HB1	2.00	0.43
22:U:43:ASN:C	22:U:45:GLY:H	2.27	0.43
25:X:26:ILE:HB	38:X:5420:HOH:O	2.17	0.43
25:X:38:THR:CB	38:X:5390:HOH:O	2.66	0.43
1:A:54:G:O2'	1:A:69:A:N1	2.51	0.43
1:A:696:C:O2'	1:A:697:G:H5'	2.19	0.43
1:A:1269:G:H2'	1:A:1270:U:H6	1.84	0.43
1:A:1714:C:O2'	1:A:1715:C:H5'	2.18	0.43
1:A:2113:G:C6	1:A:2114:C:C4	3.06	0.43
1:A:2577:A:H5'	38:A:7211:HOH:O	2.19	0.43
9:H:104:ALA:C	9:H:106:THR:N	2.76	0.43
11:J:31:PHE:HA	11:J:85:ILE:CG2	2.49	0.43
11:J:62:GLU:HA	38:J:8385:HOH:O	2.18	0.43
20:S:17:MET:HE1	20:S:19:ARG:CZ	2.48	0.43
21:T:33:SER:O	21:T:37:VAL:HG23	2.18	0.43
21:T:57:THR:HG22	21:T:59:ASP:HB2	2.01	0.43
25:X:106:THR:HG1	25:X:109:GLU:HG3	1.84	0.43
1:A:319:A:H4'	1:A:338:C:C5	2.53	0.43
1:A:440:C:H2'	1:A:441:A:C8	2.54	0.43
1:A:588:G:O6	25:X:154:ARG:NH1	2.52	0.43
1:A:818:A:H5''	38:A:6050:HOH:O	2.19	0.43
1:A:952:G:N3	1:A:2302:A:H2'	2.33	0.43
1:A:1051:C:H2'	1:A:1052:G:O4'	2.19	0.43
1:A:2515:C:H2'	1:A:2516:G:O4'	2.18	0.43
1:A:2604:A:H5'	38:A:5256:HOH:O	2.18	0.43
38:A:6363:HOH:O	8:G:157:LYS:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3003:A:H2'	38:B:8421:HOH:O	2.19	0.43
2:B:3031:C:H2'	2:B:3032:G:O4'	2.19	0.43
4:C:135:VAL:HG11	4:C:147:ARG:NH2	2.34	0.43
6:E:1:MET:HG2	6:E:2:GLN:N	2.32	0.43
6:E:200:PRO:HB3	6:E:212:VAL:CG2	2.49	0.43
7:F:76:ARG:O	7:F:77:ASP:HB2	2.19	0.43
17:P:96:VAL:CG1	17:P:100:GLN:HB2	2.48	0.43
18:Q:59:ARG:HH22	18:Q:66:GLN:NE2	2.17	0.43
25:X:65:VAL:HA	25:X:68:THR:CG2	2.49	0.43
1:A:622:G:P	27:Z:148:GLY:HA3	2.59	0.42
1:A:854:G:N7	38:A:3800:HOH:O	2.36	0.42
1:A:968:G:O2'	1:A:969:G:H5'	2.19	0.42
1:A:1236:A:H2'	1:A:1237:U:O4'	2.19	0.42
1:A:2359:G:H3'	38:A:5160:HOH:O	2.19	0.42
1:A:2502:C:H2'	1:A:2503:A:C5'	2.46	0.42
4:C:70:ALA:HA	4:C:71:PRO:HD3	1.91	0.42
5:D:215:VAL:O	5:D:219:GLY:HA2	2.18	0.42
6:E:246:ARG:NE	38:E:8429:HOH:O	2.51	0.42
12:K:104:TYR:HA	38:K:2238:HOH:O	2.19	0.42
14:M:105:TYR:CD1	14:M:105:TYR:C	2.97	0.42
17:P:24:ALA:N	38:P:3062:HOH:O	2.52	0.42
18:Q:13:VAL:HG21	18:Q:41:ARG:HG2	2.01	0.42
25:X:110:GLN:HE21	25:X:110:GLN:HA	1.83	0.42
1:A:128:A:O2'	1:A:129:A:H5'	2.18	0.42
1:A:426:G:H2'	1:A:427:C:O4'	2.18	0.42
1:A:1182:C:H1'	1:A:1192:A:C8	2.51	0.42
1:A:1667:A:H2'	1:A:1668:U:C6	2.54	0.42
1:A:1771:U:O2'	28:1:23:ARG:NH2	2.50	0.42
1:A:2673:U:C2'	1:A:2674:G:H5'	2.49	0.42
1:A:2735:U:H2'	1:A:2736:U:C6	2.54	0.42
38:A:3159:HOH:O	15:N:79:LYS:HD2	2.18	0.42
5:D:132:HIS:CE1	5:D:171:VAL:CG2	3.02	0.42
5:D:212:GLN:HB2	5:D:257:THR:CG2	2.38	0.42
6:E:107:ARG:NH1	6:E:107:ARG:CB	2.73	0.42
6:E:129:HIS:HD2	6:E:165:ASP:OD2	2.01	0.42
7:F:77:ASP:HB3	7:F:78:GLU:H	1.57	0.42
7:F:99:ASP:CB	7:F:103:ASN:HB2	2.49	0.42
13:L:99:ASP:OD1	13:L:99:ASP:C	2.61	0.42
14:M:24:ALA:HB2	14:M:30:ARG:HD2	2.00	0.42
15:N:38:VAL:O	15:N:38:VAL:HG12	2.17	0.42
15:N:133:LEU:HD12	15:N:133:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:110:THR:HA	16:O:111:PRO:HD3	1.90	0.42
18:Q:58:SER:CB	38:Q:186:HOH:O	2.66	0.42
18:Q:134:VAL:O	18:Q:137:LEU:HB3	2.19	0.42
26:Y:74:ALA:HB2	26:Y:85:VAL:HG13	2.00	0.42
29:2:28:HIS:CE1	29:2:31:LYS:HE2	2.54	0.42
1:A:1298:U:H2'	1:A:1299:G:C8	2.54	0.42
1:A:1389:G:H1'	1:A:1435:U:O2	2.19	0.42
1:A:1681:G:H5''	1:A:1682:A:OP1	2.19	0.42
1:A:1730:G:C5'	1:A:1731:C:C6	3.03	0.42
1:A:1907:U:C4	1:A:1908:G:C5	3.07	0.42
1:A:2247:C:O2'	1:A:2248:C:H5'	2.20	0.42
1:A:2453:G:H3'	38:A:5380:HOH:O	2.18	0.42
2:B:3025:G:C8	2:B:3026:C:H5'	2.55	0.42
4:C:36:ASP:HB2	4:C:85:ASP:H	1.84	0.42
5:D:7:ARG:NH1	5:D:11:LEU:HD22	2.34	0.42
5:D:53:LEU:HD21	5:D:270:ILE:HD12	2.00	0.42
13:L:130:MET:SD	23:V:26:GLY:HA3	2.59	0.42
17:P:96:VAL:HG12	17:P:97:SER:O	2.18	0.42
25:X:119:HIS:HD2	25:X:120:PRO:O	2.02	0.42
26:Y:43:VAL:CG1	26:Y:44:ASP:N	2.81	0.42
1:A:35:U:O2'	1:A:36:C:H5'	2.20	0.42
1:A:321:A:O2'	1:A:322:G:H5'	2.19	0.42
1:A:332:G:H4'	22:U:2:LYS:O	2.19	0.42
1:A:553:G:C2'	1:A:554:G:H5'	2.49	0.42
1:A:951:A:H2'	1:A:952:G:H5'	2.01	0.42
1:A:1494:A:C2	1:A:1495:C:C4	3.07	0.42
1:A:1657:A:H2'	1:A:1658:A:C8	2.54	0.42
1:A:1871:U:O4'	1:A:1873:G:C8	2.73	0.42
1:A:1896:G:C6	1:A:1897:U:C4	3.07	0.42
1:A:2122:C:P	38:A:6038:HOH:O	2.67	0.42
1:A:2573:G:N3	38:A:6756:HOH:O	2.36	0.42
1:A:2911:C:H2'	1:A:2912:C:H6	1.84	0.42
2:B:3045:A:C5	2:B:3046:C:C4	3.07	0.42
2:B:3045:A:C5	2:B:3046:C:C5	3.07	0.42
5:D:79:MET:HE3	5:D:144:THR:HG21	2.00	0.42
5:D:277:GLU:N	5:D:278:PRO:CD	2.82	0.42
7:F:94:ALA:HB3	7:F:174:VAL:HA	2.01	0.42
8:G:31:ARG:HH12	8:G:68:HIS:CG	2.37	0.42
9:H:34:ASN:O	9:H:38:LYS:HG3	2.19	0.42
13:L:28:GLU:HB3	13:L:59:LYS:HB2	2.01	0.42
15:N:25:TRP:HE3	15:N:26:HIS:HD2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:38:VAL:O	15:N:63:VAL:HG13	2.20	0.42
22:U:19:ARG:NH1	22:U:68:ASP:O	2.52	0.42
25:X:80:ASP:O	25:X:84:VAL:HG23	2.18	0.42
26:Y:71:ARG:HD3	38:Y:2171:HOH:O	2.18	0.42
1:A:394:G:H1	15:N:181:GLU:CD	2.28	0.42
1:A:1314:U:H5''	1:A:1316:G:O4'	2.18	0.42
1:A:1324:G:C2	1:A:1334:C:O2	2.73	0.42
1:A:1566:C:H2'	1:A:1567:A:H8	1.85	0.42
1:A:1701:A:H5''	1:A:1702:U:H3'	2.02	0.42
1:A:1869:A:H2'	1:A:1870:C:O4'	2.20	0.42
1:A:2112:A:H2'	1:A:2113:G:H8	1.84	0.42
1:A:2530:C:O2'	1:A:2531:U:H5'	2.20	0.42
1:A:2634:G:O2'	1:A:2635:A:H5'	2.19	0.42
1:A:2637:A:H5'	38:A:8784:HOH:O	2.20	0.42
1:A:2883:A:H2'	1:A:2884:G:O4'	2.20	0.42
2:B:3003:A:H2	2:B:3021:G:N3	2.17	0.42
4:C:200:PRO:HG2	4:C:225:VAL:HG21	2.01	0.42
5:D:7:ARG:NH2	5:D:250:THR:O	2.53	0.42
5:D:275:GLY:O	5:D:291:ASP:HA	2.19	0.42
6:E:76:ARG:HG2	6:E:78:ARG:NH1	2.34	0.42
6:E:212:VAL:HG23	6:E:212:VAL:O	2.20	0.42
9:H:22:VAL:HG21	9:H:104:ALA:HB2	2.01	0.42
11:J:49:VAL:O	11:J:157:ILE:HG23	2.20	0.42
11:J:84:ARG:CZ	11:J:135:TRP:HH2	2.32	0.42
15:N:84:LYS:O	15:N:87:MET:HG2	2.20	0.42
16:O:86:LEU:O	16:O:90:LEU:HG	2.19	0.42
18:Q:7:LYS:HD3	18:Q:21:VAL:CG2	2.49	0.42
18:Q:16:VAL:HG12	18:Q:20:ARG:HB2	2.00	0.42
18:Q:141:ILE:C	18:Q:143:ALA:H	2.26	0.42
22:U:55:PHE:HB2	38:U:6384:HOH:O	2.20	0.42
1:A:23:G:O2'	1:A:24:G:H5'	2.19	0.42
1:A:877:G:C5'	1:A:878:G:OP1	2.64	0.42
1:A:950:G:O2'	1:A:951:A:H5'	2.18	0.42
1:A:960:G:N3	1:A:960:G:C2'	2.82	0.42
1:A:1010:C:H4'	16:O:4:PRO:HB2	2.02	0.42
1:A:1044:C:H5''	38:A:8542:HOH:O	2.19	0.42
1:A:1943:C:O4'	4:C:212:PRO:HA	2.19	0.42
1:A:2252:A:C5	1:A:2253:G:H1'	2.54	0.42
1:A:2443:C:O3'	14:M:56:LYS:HE3	2.19	0.42
4:C:110:SER:N	4:C:114:ASP:OD2	2.52	0.42
4:C:173:GLY:O	4:C:177:HIS:CD2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:7:ARG:HD3	5:D:9:GLY:O	2.20	0.42
6:E:184:ARG:NE	38:E:8415:HOH:O	2.43	0.42
6:E:236:THR:O	6:E:239:ALA:N	2.53	0.42
8:G:15:GLN:NE2	8:G:40:VAL:O	2.53	0.42
11:J:53:PRO:HA	11:J:125:VAL:O	2.20	0.42
11:J:84:ARG:CZ	11:J:135:TRP:CH2	3.02	0.42
12:K:79:PHE:O	12:K:79:PHE:HD2	2.01	0.42
14:M:53:ARG:HH22	14:M:57:VAL:HG12	1.83	0.42
14:M:55:GLN:HA	14:M:58:GLN:NE2	2.33	0.42
15:N:63:VAL:O	15:N:130:GLU:HA	2.19	0.42
16:O:47:LEU:HD23	16:O:47:LEU:HA	1.72	0.42
19:R:53:HIS:O	19:R:55:ARG:N	2.53	0.42
25:X:65:VAL:HG12	25:X:116:LEU:HD13	2.01	0.42
28:1:38:LYS:HG2	38:1:8408:HOH:O	2.20	0.42
1:A:171:C:O2'	1:A:172:U:H5'	2.20	0.42
1:A:2004:U:H5''	1:A:2005:G:C8	2.54	0.42
1:A:2335:C:C2	1:A:2350:G:C2	3.07	0.42
2:B:3055:U:H4'	2:B:3056:A:H8	1.83	0.42
2:B:3078:G:O2'	2:B:3079:U:P	2.78	0.42
4:C:125:ASN:HB3	4:C:158:VAL:HG12	2.02	0.42
4:C:169:PHE:O	4:C:170:VAL:HB	2.20	0.42
5:D:82:VAL:HG12	5:D:101:TRP:CE3	2.54	0.42
8:G:101:GLU:OE2	8:G:115:ARG:HD3	2.19	0.42
13:L:118:ALA:C	13:L:120:ARG:N	2.78	0.42
15:N:115:LEU:HD13	15:N:115:LEU:C	2.44	0.42
15:N:185:PRO:CG	15:N:189:VAL:HG11	2.48	0.42
16:O:107:ASN:OD1	35:O:8507:CL:CL	2.75	0.42
20:S:4:TYR:N	38:S:8546:HOH:O	2.52	0.42
22:U:28:SER:O	22:U:32:ARG:HG3	2.18	0.42
22:U:96:VAL:CG1	22:U:97:ARG:N	2.79	0.42
23:V:9:CYS:SG	38:V:6796:HOH:O	2.62	0.42
25:X:73:LEU:HD12	25:X:73:LEU:HA	1.88	0.42
1:A:67:A:H5''	1:A:69:A:C8	2.55	0.42
1:A:251:C:O2'	1:A:252:C:H5'	2.19	0.42
1:A:419:A:H1'	1:A:1921:A:C2	2.55	0.42
1:A:553:G:P	27:Z:204:ARG:NH2	2.92	0.42
1:A:949:U:O2'	19:R:40:HIS:HE1	2.03	0.42
1:A:1268:C:H2'	1:A:1269:G:C8	2.54	0.42
1:A:1483:C:O2'	1:A:1484:G:H5'	2.20	0.42
1:A:1603:A:H4'	1:A:1605:G:C8	2.55	0.42
1:A:1743:G:H1'	38:A:4365:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1855:G:H8	4:C:144:GLU:OE2	2.03	0.42
1:A:2346:C:H4'	7:F:52:THR:CG2	2.48	0.42
38:A:3626:HOH:O	26:Y:59:TRP:HB2	2.19	0.42
38:A:5000:HOH:O	15:N:58:GLN:HG3	2.19	0.42
2:B:3048:C:H4'	16:O:141:ARG:NH2	2.27	0.42
8:G:61:THR:O	8:G:62:ILE:C	2.62	0.42
9:H:4:VAL:HG13	9:H:76:PHE:CE1	2.54	0.42
17:P:26:TRP:HB2	38:P:3062:HOH:O	2.20	0.42
26:Y:85:VAL:HG12	26:Y:86:GLU:H	1.85	0.42
29:2:12:ASN:HB3	38:2:5389:HOH:O	2.19	0.42
1:A:303:C:H2'	1:A:304:G:O4'	2.20	0.42
1:A:1501:A:C6	1:A:1502:A:C6	3.07	0.42
1:A:2311:A:H5''	11:J:115:PHE:CD2	2.54	0.42
1:A:2452:G:OP2	38:A:6202:HOH:O	2.21	0.42
1:A:2456:A:H2'	1:A:2457:U:C6	2.55	0.42
1:A:2607:U:C4	5:D:242:TRP:CZ2	3.07	0.42
1:A:2896:A:OP1	26:Y:15:ARG:NH1	2.52	0.42
1:A:2909:G:O2'	1:A:2910:A:H5'	2.20	0.42
4:C:128:LEU:HG	38:C:8583:HOH:O	2.19	0.42
5:D:132:HIS:HB2	5:D:137:LEU:HD22	2.02	0.42
5:D:277:GLU:N	5:D:278:PRO:HD2	2.34	0.42
8:G:24:GLY:HA3	8:G:76:VAL:HB	2.02	0.42
8:G:64:THR:HG22	8:G:68:HIS:CD2	2.55	0.42
8:G:145:ALA:HB1	8:G:168:ILE:CD1	2.50	0.42
12:K:4:ALA:O	12:K:5:GLU:O	2.38	0.42
12:K:19:MET:HE3	12:K:132:LEU:CD1	2.17	0.42
13:L:121:PHE:HB3	38:L:2659:HOH:O	2.19	0.42
15:N:40:ILE:HG13	15:N:40:ILE:O	2.20	0.42
16:O:116:PHE:HB2	38:O:8556:HOH:O	2.18	0.42
16:O:162:ASP:HB3	16:O:163:PHE:H	1.61	0.42
18:Q:76:GLY:O	18:Q:77:ALA:C	2.63	0.42
19:R:16:ASN:HD22	19:R:16:ASN:HA	1.59	0.42
25:X:28:HIS:HD2	25:X:31:HIS:CE1	2.38	0.42
1:A:111:C:O2'	1:A:112:G:H5'	2.20	0.42
1:A:221:G:C6	1:A:222:A:C6	3.08	0.42
1:A:319:A:H4'	1:A:338:C:C4	2.55	0.42
1:A:449:A:C8	6:E:43:LYS:HG2	2.54	0.42
1:A:1242:A:H5'	12:K:82:THR:CG2	2.39	0.42
1:A:2655:U:C4	1:A:2656:G:N7	2.88	0.42
38:A:8592:HOH:O	5:D:214:PRO:HD2	2.20	0.42
2:B:3012:C:H5'	2:B:3070:U:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:115:LEU:HD12	6:E:115:LEU:HA	1.90	0.42
7:F:55:LYS:O	7:F:56:ARG:HB2	2.20	0.42
11:J:71:TYR:O	11:J:73:GLN:N	2.53	0.42
12:K:39:VAL:CG1	12:K:40:ASN:N	2.81	0.42
14:M:90:ARG:NH1	14:M:119:THR:HG21	2.35	0.42
1:A:155:C:OP2	15:N:188:ARG:HD3	2.20	0.41
1:A:512:G:O3'	1:A:513:A:H8	2.03	0.41
1:A:758:A:OP1	14:M:31:GLY:N	2.50	0.41
1:A:795:G:HO2'	1:A:796:A:P	2.43	0.41
1:A:876:A:N3	1:A:876:A:C2'	2.83	0.41
1:A:1241:G:C2	12:K:86:MET:HE2	2.54	0.41
1:A:1384:C:H6	1:A:1384:C:O5'	2.03	0.41
1:A:2430:A:H2'	1:A:2431:C:C6	2.54	0.41
4:C:43:VAL:O	4:C:44:ASP:HB2	2.20	0.41
4:C:103:VAL:HA	4:C:104:PRO:HD3	1.80	0.41
5:D:146:THR:O	5:D:159:PRO:HB3	2.19	0.41
5:D:224:LYS:HD3	5:D:224:LYS:HA	1.75	0.41
8:G:35:TYR:HA	12:K:127:ILE:HD12	2.02	0.41
9:H:63:ILE:O	9:H:64:PRO:C	2.61	0.41
9:H:109:GLU:O	9:H:112:ALA:HB3	2.21	0.41
11:J:45:GLN:HG3	11:J:135:TRP:NE1	2.35	0.41
13:L:115:ARG:CG	13:L:116:GLU:N	2.79	0.41
14:M:73:VAL:HG21	14:M:116:HIS:CD2	2.55	0.41
16:O:91:ARG:HG3	16:O:186:LEU:CD2	2.48	0.41
18:Q:11:ALA:HB1	18:Q:16:VAL:O	2.20	0.41
18:Q:121:ASP:HB2	38:Q:201:HOH:O	2.19	0.41
20:S:25:PHE:N	38:S:8508:HOH:O	2.51	0.41
1:A:699:C:C2	1:A:744:G:C2	3.08	0.41
1:A:1192:A:O2'	1:A:1193:A:OP1	2.29	0.41
1:A:1562:C:H42	1:A:2738:G:H1	1.67	0.41
1:A:1930:A:H1'	1:A:2128:G:H5'	2.02	0.41
1:A:1973:A:H5'	1:A:1973:A:H8	1.84	0.41
1:A:2385:G:H2'	1:A:2386:U:H6	1.85	0.41
1:A:2506:A:O2'	1:A:2507:G:P	2.78	0.41
3:5:74:C:C4	3:5:75:C:C2	3.08	0.41
5:D:205:VAL:O	5:D:307:ARG:CD	2.68	0.41
6:E:36:ARG:NH1	38:E:8400:HOH:O	2.53	0.41
7:F:158:ASN:HB2	7:F:161:ASP:OD2	2.20	0.41
8:G:139:GLU:CD	38:G:5919:HOH:O	2.63	0.41
12:K:135:ILE:O	12:K:139:LEU:HG	2.20	0.41
15:N:133:LEU:O	15:N:134:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:177:GLY:O	15:N:178:LYS:C	2.63	0.41
16:O:69:TYR:HE2	16:O:183:ASP:OD2	2.03	0.41
25:X:146:ILE:HG23	25:X:150:LEU:HD12	2.02	0.41
26:Y:43:VAL:HG12	26:Y:47:ALA:HB3	2.01	0.41
1:A:182:G:C4'	15:N:157:LEU:HD13	2.47	0.41
1:A:183:A:C5'	15:N:157:LEU:HD12	2.50	0.41
1:A:209:G:C6	1:A:210:U:N3	2.89	0.41
1:A:245:C:C2'	1:A:246:G:H5'	2.50	0.41
1:A:1448:A:C6	1:A:1451:C:C2	3.09	0.41
1:A:1545:C:H2'	1:A:1546:G:O4'	2.20	0.41
1:A:1851:G:O2'	1:A:1852:A:H5'	2.20	0.41
1:A:2108:A:C2	1:A:2110:G:C8	3.08	0.41
1:A:2388:C:O2'	1:A:2389:U:H5'	2.20	0.41
1:A:2769:C:H2'	1:A:2770:G:C5'	2.50	0.41
5:D:69:VAL:HA	5:D:70:PRO:HD3	1.95	0.41
5:D:279:THR:HG22	5:D:280:VAL:O	2.21	0.41
6:E:191:SER:OG	6:E:192:ILE:N	2.53	0.41
8:G:172:PRO:HB3	38:G:6931:HOH:O	2.20	0.41
11:J:65:ARG:CZ	38:J:8385:HOH:O	2.68	0.41
11:J:111:MET:O	11:J:114:PRO:HD3	2.20	0.41
12:K:39:VAL:HG12	12:K:40:ASN:CG	2.45	0.41
15:N:93:ARG:H	15:N:93:ARG:HG2	1.54	0.41
15:N:155:HIS:ND1	15:N:158:ARG:NE	2.55	0.41
16:O:67:ALA:O	16:O:69:TYR:N	2.54	0.41
28:1:77:LYS:HA	28:1:80:MET:CE	2.43	0.41
1:A:590:A:C2'	1:A:591:A:H5'	2.51	0.41
1:A:596:C:H2'	1:A:597:A:C8	2.55	0.41
1:A:638:C:H2'	1:A:639:A:H8	1.85	0.41
1:A:710:G:OP1	17:P:24:ALA:HB3	2.20	0.41
1:A:1217:G:H2'	1:A:1218:U:C6	2.55	0.41
1:A:1506:U:H6	1:A:1506:U:H5'	1.86	0.41
1:A:1513:C:O2'	1:A:1514:C:H5'	2.19	0.41
38:A:3268:HOH:O	23:V:17:THR:CG2	2.69	0.41
4:C:36:ASP:CB	4:C:85:ASP:H	2.32	0.41
4:C:42:VAL:HG11	4:C:75:GLY:O	2.21	0.41
5:D:238:ASN:HD22	5:D:240:GLY:N	2.14	0.41
7:F:169:THR:C	7:F:170:TYR:CD1	2.98	0.41
11:J:62:GLU:CD	38:J:8385:HOH:O	2.64	0.41
13:L:78:LYS:HA	13:L:79:PRO:HD3	1.88	0.41
13:L:118:ALA:O	13:L:120:ARG:N	2.54	0.41
14:M:93:VAL:HG12	14:M:97:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:37:ARG:HD3	16:O:37:ARG:HA	1.84	0.41
17:P:80:ASP:OD1	17:P:81:PHE:N	2.53	0.41
26:Y:12:ILE:HG23	26:Y:36:HIS:CG	2.55	0.41
1:A:292:G:N2	38:A:5231:HOH:O	2.30	0.41
1:A:736:A:H2'	1:A:737:A:O4'	2.20	0.41
1:A:920:C:H5'	1:A:921:G:C4	2.55	0.41
1:A:1524:U:O2'	1:A:1525:G:P	2.78	0.41
1:A:1600:G:H8	1:A:1600:G:OP2	2.03	0.41
1:A:2346:C:O3'	7:F:52:THR:HG23	2.20	0.41
1:A:2547:C:H2'	1:A:2548:C:C6	2.56	0.41
5:D:280:VAL:HG13	5:D:333:GLU:O	2.20	0.41
5:D:280:VAL:HG11	5:D:335:ASN:H	1.86	0.41
7:F:101:THR:HG22	7:F:101:THR:O	2.20	0.41
12:K:6:PHE:O	12:K:8:ALA:N	2.53	0.41
12:K:107:ASN:ND2	12:K:107:ASN:C	2.78	0.41
15:N:74:ARG:HD3	15:N:88:VAL:HA	2.03	0.41
22:U:71:VAL:CG1	22:U:72:ILE:N	2.83	0.41
25:X:29:VAL:O	25:X:30:ASN:HB2	2.21	0.41
27:Z:107:PRO:HB3	27:Z:182:PHE:CD2	2.56	0.41
1:A:64:G:H2'	1:A:65:C:O4'	2.21	0.41
1:A:840:U:C2	1:A:2648:U:O4	2.73	0.41
1:A:1023:C:O2'	1:A:1024:G:H5'	2.21	0.41
1:A:1059:G:C8	1:A:2491:G:H4'	2.55	0.41
1:A:1161:A:O5'	1:A:1161:A:C8	2.73	0.41
1:A:1749:U:O2	1:A:1751:G:C8	2.74	0.41
1:A:1795:G:H2'	1:A:1796:A:O4'	2.21	0.41
1:A:2460:A:OP1	31:4:60:LYS:HB2	2.21	0.41
1:A:2837:U:H1'	5:D:307:ARG:HH12	1.85	0.41
1:A:2880:A:H2'	1:A:2881:C:O4'	2.20	0.41
6:E:40:ALA:CB	6:E:100:LEU:HD12	2.51	0.41
7:F:55:LYS:C	38:F:4069:HOH:O	2.62	0.41
7:F:60:GLU:O	7:F:62:ASP:N	2.53	0.41
7:F:163:VAL:HA	38:F:6326:HOH:O	2.20	0.41
8:G:158:ASP:OD1	8:G:160:ARG:HB2	2.20	0.41
9:H:4:VAL:HG13	9:H:76:PHE:CD1	2.55	0.41
10:I:65:THR:O	10:I:69:ARG:HB2	2.20	0.41
11:J:26:LYS:CD	11:J:28:ILE:HB	2.51	0.41
24:W:27:LEU:HA	24:W:49:LEU:HD13	2.02	0.41
1:A:328:U:O4'	6:E:202:THR:HG22	2.20	0.41
1:A:333:G:O2'	1:A:334:G:H5'	2.21	0.41
1:A:470:U:O2'	29:2:16:HIS:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:G:H4'	1:A:730:G:O3'	2.21	0.41
1:A:731:U:OP2	38:A:3515:HOH:O	2.22	0.41
1:A:1352:A:N1	6:E:48:SER:HB3	2.35	0.41
1:A:1383:U:H2'	1:A:1384:C:C6	2.56	0.41
1:A:1616:A:H5''	1:A:1617:C:OP1	2.20	0.41
1:A:1767:A:O2'	1:A:1768:C:H5'	2.21	0.41
1:A:1916:C:C2	1:A:1924:A:C2	3.08	0.41
1:A:2134:G:C6	1:A:2258:A:C8	3.09	0.41
1:A:2445:U:H2'	1:A:2446:G:H8	1.84	0.41
1:A:2651:C:H2'	1:A:2652:U:O4'	2.20	0.41
1:A:2825:C:H4'	1:A:2826:G:O5'	2.20	0.41
5:D:144:THR:CG2	5:D:145:HIS:N	2.83	0.41
5:D:168:GLY:H	5:D:174:ARG:HD3	1.83	0.41
6:E:114:ALA:HB1	6:E:223:LEU:HB3	2.02	0.41
7:F:94:ALA:O	7:F:95:THR:O	2.38	0.41
8:G:149:GLU:OE1	8:G:168:ILE:HG12	2.21	0.41
11:J:31:PHE:CD2	11:J:85:ILE:HG23	2.56	0.41
14:M:72:ASN:OD1	14:M:75:LEU:HD12	2.21	0.41
16:O:14:ARG:C	16:O:16:ALA:H	2.28	0.41
25:X:130:HIS:O	25:X:136:GLY:HA3	2.20	0.41
27:Z:109:LEU:HA	38:Z:8576:HOH:O	2.21	0.41
29:2:5:THR:N	29:2:6:PRO:HD2	2.35	0.41
30:3:36:ASN:HB3	30:3:39:ARG:NE	2.36	0.41
1:A:316:A:N3	1:A:336:G:O2'	2.49	0.41
1:A:397:A:P	38:A:3833:HOH:O	2.78	0.41
1:A:688:A:H62	14:M:111:ALA:HB2	1.85	0.41
1:A:920:C:H4'	1:A:921:G:N2	2.35	0.41
1:A:1477:C:H5'	1:A:1868:G:C5'	2.50	0.41
1:A:1603:A:H5'	1:A:1605:G:C4'	2.49	0.41
1:A:1855:G:O6	4:C:141:PRO:HG2	2.21	0.41
1:A:1880:C:C2	1:A:1881:A:C8	3.09	0.41
5:D:138:GLY:O	5:D:139:ASP:C	2.62	0.41
6:E:43:LYS:NZ	38:E:8392:HOH:O	2.41	0.41
7:F:146:LYS:HE2	16:O:107:ASN:ND2	2.36	0.41
11:J:1:LYS:HA	11:J:2:PRO:HD3	1.81	0.41
11:J:132:PHE:O	11:J:133:ILE:HD13	2.20	0.41
15:N:43:PRO:HG3	15:N:62:VAL:HG21	2.03	0.41
16:O:110:THR:HB	16:O:113:SER:OG	2.20	0.41
18:Q:115:SER:HG	18:Q:118:GLN:HG3	1.83	0.41
20:S:32:ALA:O	20:S:33:ARG:C	2.61	0.41
22:U:40:VAL:HA	22:U:119:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:12:THR:HG23	24:W:14:ALA:H	1.85	0.41
25:X:154:ARG:HE	25:X:154:ARG:HB3	1.64	0.41
26:Y:78:GLU:CG	26:Y:79:GLU:N	2.72	0.41
27:Z:116:LEU:HA	27:Z:116:LEU:HD23	1.82	0.41
28:1:39:CYS:SG	28:1:47:LEU:CD2	2.85	0.41
29:2:29:THR:O	29:2:32:LYS:NZ	2.53	0.41
29:2:31:LYS:O	29:2:32:LYS:HB2	2.21	0.41
1:A:10:U:O4	1:A:532:A:OP2	2.38	0.41
1:A:79:G:H22	1:A:97:G:H1'	1.86	0.41
1:A:123:U:O2'	1:A:124:C:H5'	2.21	0.41
1:A:151:A:C2	1:A:442:A:C8	3.09	0.41
1:A:154:C:O2'	1:A:155:C:H5'	2.20	0.41
1:A:861:A:H2'	1:A:862:U:C6	2.55	0.41
1:A:951:A:O2'	1:A:952:G:H5'	2.21	0.41
1:A:1003:U:O2	11:J:90:PHE:CZ	2.73	0.41
1:A:1162:G:H2'	1:A:1162:G:N3	2.36	0.41
1:A:1166:A:N3	1:A:1166:A:H2'	2.35	0.41
1:A:1218:U:H2'	1:A:1219:U:H6	1.85	0.41
1:A:1463:A:H2'	1:A:1464:U:C6	2.56	0.41
1:A:1566:C:O2'	1:A:1567:A:H5'	2.21	0.41
1:A:1609:C:H2'	1:A:1610:G:C8	2.56	0.41
1:A:1706:G:C6	1:A:1707:G:C6	3.08	0.41
1:A:1969:A:N7	1:A:1970:G:C6	2.88	0.41
1:A:2257:G:H4'	1:A:2259:C:C2	2.56	0.41
1:A:2398:A:H2'	1:A:2399:G:O4'	2.21	0.41
1:A:2473:U:O3'	1:A:2474:A:H3'	2.20	0.41
1:A:2501:G:H1'	38:A:4029:HOH:O	2.20	0.41
1:A:2506:A:H1'	38:A:5515:HOH:O	2.21	0.41
1:A:2834:G:C4	1:A:2847:G:N2	2.89	0.41
1:A:2839:C:H6	1:A:2839:C:O5'	2.04	0.41
2:B:3050:G:OP1	16:O:159:TYR:OH	2.37	0.41
4:C:93:THR:C	4:C:94:LEU:CD2	2.89	0.41
4:C:165:THR:O	4:C:165:THR:CG2	2.69	0.41
4:C:217:ARG:CG	4:C:217:ARG:NH1	2.84	0.41
4:C:231:LYS:O	4:C:232:ARG:HB3	2.21	0.41
5:D:14:GLY:HA3	38:D:8609:HOH:O	2.20	0.41
6:E:142:ASP:OD1	6:E:237:GLU:HB3	2.21	0.41
7:F:57:THR:HA	7:F:63:ILE:HA	2.01	0.41
7:F:87:ALA:O	7:F:88:LEU:C	2.64	0.41
7:F:99:ASP:HB2	7:F:103:ASN:H	1.86	0.41
8:G:154:ILE:HG13	8:G:156:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:115:VAL:O	9:H:118:LEU:N	2.54	0.41
11:J:26:LYS:HD2	11:J:28:ILE:CG1	2.50	0.41
11:J:129:ASN:N	11:J:129:ASN:HD22	2.18	0.41
13:L:37:TYR:CE2	13:L:45:PRO:HA	2.55	0.41
19:R:15:LYS:NZ	38:R:5620:HOH:O	2.50	0.41
25:X:122:ARG:HG2	25:X:122:ARG:NH1	2.27	0.41
25:X:122:ARG:CG	25:X:122:ARG:NH1	2.83	0.41
28:1:46:LYS:O	28:1:57:CYS:HA	2.20	0.41
31:4:42:ARG:HH11	31:4:42:ARG:CG	2.33	0.41
1:A:21:G:H5''	20:S:1:GLY:O	2.21	0.41
1:A:453:A:H4'	1:A:455:A:N7	2.36	0.41
1:A:658:C:O2'	1:A:662:U:OP1	2.34	0.41
1:A:1121:G:H21	1:A:1248:A:C4'	2.34	0.41
1:A:1151:G:OP1	10:I:63:ARG:NH1	2.54	0.41
1:A:1345:A:H2'	1:A:1346:U:C6	2.56	0.41
1:A:1656:A:H2'	1:A:1657:A:O4'	2.21	0.41
1:A:2462:G:O6	31:4:61:PRO:HG3	2.20	0.41
1:A:2786:G:O2'	1:A:2787:C:H5'	2.21	0.41
38:A:9692:HOH:O	14:M:4:LYS:HG3	2.21	0.41
38:B:8386:HOH:O	19:R:25:PRO:HB3	2.20	0.41
38:B:8525:HOH:O	16:O:107:ASN:HB3	2.21	0.41
4:C:179:MET:HG2	4:C:186:TRP:CG	2.56	0.41
6:E:118:THR:HG22	6:E:137:PRO:HB3	2.03	0.41
7:F:67:ASP:OD1	7:F:67:ASP:N	2.54	0.41
11:J:29:ALA:C	11:J:30:GLN:HG3	2.46	0.41
14:M:125:PHE:CE1	14:M:140:VAL:HG13	2.56	0.41
15:N:169:ARG:NH1	38:N:8576:HOH:O	2.54	0.41
17:P:35:LYS:HD3	38:P:3360:HOH:O	2.20	0.41
19:R:25:PRO:HA	19:R:26:PRO:HD3	1.86	0.41
19:R:40:HIS:CE1	19:R:94:GLN:HA	2.56	0.41
21:T:10:VAL:HG11	24:W:36:ALA:HA	2.02	0.41
22:U:14:ALA:HA	22:U:15:PRO:HD3	1.93	0.41
25:X:132:VAL:C	25:X:134:GLU:N	2.78	0.41
1:A:78:G:C6	1:A:79:G:C6	3.09	0.40
1:A:164:G:C6	1:A:165:A:C5	3.08	0.40
1:A:243:A:H61	1:A:269:G:H1'	1.86	0.40
1:A:506:G:N2	1:A:509:A:C5'	2.71	0.40
1:A:593:A:N7	38:A:3887:HOH:O	2.53	0.40
1:A:724:G:O2'	1:A:725:C:H5'	2.21	0.40
1:A:1191:A:N1	1:A:1206:U:O4	2.54	0.40
1:A:1611:G:O2'	1:A:1612:A:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1861:C:H4'	4:C:6:GLY:O	2.21	0.40
1:A:2047:C:H5'	38:A:9316:HOH:O	2.21	0.40
1:A:2090:G:H2'	1:A:2091:G:C8	2.56	0.40
1:A:2588:G:H2'	1:A:2589:U:H4'	2.03	0.40
1:A:2846:C:OP1	5:D:158:LYS:HD3	2.21	0.40
5:D:222:LYS:HE2	38:D:8547:HOH:O	2.21	0.40
5:D:265:LEU:CD2	5:D:316:ARG:HD3	2.51	0.40
6:E:127:ARG:NH2	6:E:225:PRO:O	2.53	0.40
7:F:168:SER:O	7:F:168:SER:OG	2.35	0.40
8:G:132:THR:HB	38:G:2227:HOH:O	2.21	0.40
11:J:26:LYS:HD2	11:J:28:ILE:HB	2.03	0.40
11:J:62:GLU:OE2	11:J:66:VAL:CG2	2.69	0.40
11:J:113:ALA:N	11:J:114:PRO:CD	2.84	0.40
15:N:97:ILE:CD1	15:N:127:LYS:HD2	2.51	0.40
17:P:49:GLU:HB2	17:P:70:LEU:HD12	2.03	0.40
25:X:58:SER:OG	25:X:147:ASP:OD2	2.34	0.40
31:4:54:LYS:NZ	38:4:8526:HOH:O	2.52	0.40
1:A:88:G:H2'	1:A:89:G:C8	2.55	0.40
1:A:329:A:C5	1:A:347:A:C2	3.10	0.40
1:A:585:C:H6	38:A:5555:HOH:O	2.04	0.40
1:A:587:A:H5''	38:A:6745:HOH:O	2.19	0.40
1:A:958:G:O2'	1:A:959:C:H5'	2.21	0.40
1:A:1498:G:O2'	1:A:1499:U:H5'	2.21	0.40
1:A:1594:C:C2	1:A:1601:G:C2	3.09	0.40
1:A:1850:U:H2'	1:A:1851:G:C8	2.56	0.40
1:A:1886:A:C5'	38:1:8405:HOH:O	2.69	0.40
1:A:2004:U:H2'	1:A:2005:G:OP1	2.21	0.40
1:A:2364:A:H5''	19:R:15:LYS:HD3	2.03	0.40
1:A:2590:U:H2'	1:A:2591:C:H5'	2.03	0.40
1:A:2620:U:O4	36:5:76:PPU:CA	2.69	0.40
1:A:2649:A:H5'	1:A:2649:A:H8	1.86	0.40
1:A:2868:C:H2'	1:A:2869:G:O4'	2.21	0.40
38:A:8866:HOH:O	29:2:1:THR:HA	2.20	0.40
2:B:3050:G:OP1	16:O:147:ILE:CD1	2.68	0.40
2:B:3078:G:O2'	2:B:3079:U:OP2	2.39	0.40
4:C:105:VAL:HG11	4:C:154:ALA:CB	2.51	0.40
5:D:223:ARG:HG3	5:D:232:TRP:C	2.46	0.40
5:D:265:LEU:HD21	5:D:316:ARG:HD3	2.02	0.40
6:E:85:LYS:CE	38:E:8328:HOH:O	2.67	0.40
7:F:96:SER:C	7:F:98:PHE:H	2.27	0.40
9:H:58:GLU:HA	9:H:61:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:66:LEU:HA	9:H:66:LEU:HD12	1.85	0.40
10:I:71:LEU:C	10:I:73:ASP:N	2.79	0.40
11:J:14:TYR:HB2	38:J:8353:HOH:O	2.21	0.40
11:J:35:ASN:HD21	11:J:80:ASN:HA	1.83	0.40
15:N:137:ASP:HA	15:N:142:LYS:HE3	2.03	0.40
24:W:57:LYS:HA	24:W:60:GLN:HE21	1.85	0.40
25:X:151:GLU:O	25:X:154:ARG:HB3	2.20	0.40
26:Y:14:LEU:HD12	26:Y:67:PRO:O	2.21	0.40
1:A:39:G:C2	1:A:444:C:C2	3.10	0.40
1:A:138:U:OP2	1:A:139:C:H5	2.04	0.40
1:A:590:A:H2'	1:A:591:A:O4'	2.21	0.40
1:A:860:U:C2'	38:A:5151:HOH:O	2.69	0.40
1:A:1309:U:OP2	6:E:189:PRO:HA	2.21	0.40
1:A:1517:U:C2	1:A:1670:G:N2	2.89	0.40
1:A:1815:A:H4'	1:A:2751:C:O4'	2.22	0.40
1:A:2355:G:H5''	1:A:2356:A:OP2	2.22	0.40
1:A:2541:U:O2'	1:A:2542:C:H5'	2.21	0.40
38:A:3897:HOH:O	4:C:11:ARG:CZ	2.70	0.40
2:B:3034:A:H2'	2:B:3035:C:O4'	2.21	0.40
5:D:54:VAL:O	5:D:55:ASN:C	2.63	0.40
7:F:48:MET:HA	7:F:49:PRO:HD3	1.81	0.40
7:F:128:LEU:N	38:F:5495:HOH:O	2.54	0.40
11:J:31:PHE:HE2	11:J:87:LYS:O	2.04	0.40
11:J:35:ASN:ND2	11:J:79:ALA:O	2.54	0.40
14:M:107:LYS:HD2	14:M:124:ASP:OD2	2.21	0.40
15:N:69:LYS:HD3	15:N:124:GLY:O	2.21	0.40
18:Q:143:ALA:CA	38:Q:197:HOH:O	2.70	0.40
22:U:101:LEU:HD13	22:U:112:LEU:HD11	2.03	0.40
27:Z:144:ARG:NH1	38:Z:8581:HOH:O	2.51	0.40
1:A:220:C:C4'	38:A:5208:HOH:O	2.69	0.40
1:A:269:G:C2	1:A:270:U:O4	2.73	0.40
1:A:682:A:H2'	1:A:683:G:O4'	2.21	0.40
1:A:690:G:H4'	1:A:741:C:O2	2.22	0.40
1:A:1235:G:C1'	12:K:63:ILE:HG23	2.51	0.40
1:A:1816:C:H2'	1:A:1817:U:O4'	2.21	0.40
1:A:1972:U:H2'	1:A:1973:A:C5'	2.49	0.40
1:A:2011:A:H4'	1:A:2012:U:O5'	2.22	0.40
1:A:2255:A:H2'	1:A:2256:G:O4'	2.21	0.40
1:A:2481:G:C3'	1:A:2482:G:H5''	2.51	0.40
1:A:2533:C:O2'	1:A:2534:C:H5'	2.21	0.40
1:A:2821:C:H4'	5:D:116:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:16:ARG:NH1	38:D:8617:HOH:O	2.53	0.40
5:D:224:LYS:O	5:D:227:HIS:HB2	2.22	0.40
5:D:279:THR:OG1	5:D:290:VAL:HB	2.22	0.40
6:E:80:VAL:HA	6:E:81:PRO:HD3	1.94	0.40
6:E:123:LEU:HD23	6:E:123:LEU:HA	1.92	0.40
13:L:66:ARG:HG2	13:L:66:ARG:HH11	1.86	0.40
16:O:5:ARG:HG3	19:R:18:PRO:HB3	2.02	0.40
16:O:37:ARG:CZ	38:O:8534:HOH:O	2.69	0.40
17:P:59:VAL:CG2	17:P:111:VAL:HG23	2.52	0.40
17:P:63:LYS:HG3	17:P:80:ASP:O	2.22	0.40
18:Q:131:PHE:CD1	18:Q:137:LEU:HD13	2.56	0.40
29:2:25:LYS:CD	30:3:49:GLU:H	2.33	0.40
1:A:101:C:O2'	1:A:102:A:H5'	2.21	0.40
1:A:299:U:C5'	38:A:6794:HOH:O	2.60	0.40
1:A:382:U:C5	1:A:406:G:C2	3.09	0.40
1:A:545:G:H2'	1:A:546:C:O4'	2.21	0.40
1:A:853:C:H2'	1:A:854:G:O4'	2.21	0.40
1:A:953:G:H2'	38:A:7145:HOH:O	2.22	0.40
1:A:1215:A:O3'	1:A:1216:G:C4'	2.69	0.40
1:A:1252:A:H2'	1:A:1253:C:O4'	2.21	0.40
1:A:1266:U:H4'	27:Z:115:ARG:HH21	1.85	0.40
1:A:1316:G:H1'	1:A:1340:G:N2	2.37	0.40
1:A:2123:A:P	15:N:89:ASN:ND2	2.95	0.40
1:A:2269:C:C2'	1:A:2270:G:H5'	2.51	0.40
1:A:2348:C:C5'	7:F:22:VAL:HG21	2.51	0.40
1:A:2554:U:C6	1:A:2577:A:N6	2.90	0.40
2:B:3058:G:H3'	2:B:3059:C:C6	2.56	0.40
5:D:215:VAL:HA	5:D:220:VAL:HG22	2.02	0.40
6:E:3:ALA:N	6:E:16:VAL:O	2.53	0.40
6:E:7:ASP:O	6:E:9:ASP:N	2.55	0.40
7:F:51:ARG:HA	38:F:7636:HOH:O	2.22	0.40
8:G:108:LEU:HD11	8:G:164:ASP:HB2	2.04	0.40
10:I:23:ILE:CD1	10:I:67:LEU:HD23	2.41	0.40
11:J:73:GLN:OE1	11:J:73:GLN:CA	2.69	0.40
14:M:72:ASN:HB2	38:M:8585:HOH:O	2.21	0.40
15:N:77:PHE:O	15:N:77:PHE:CD1	2.75	0.40
16:O:114:LYS:O	16:O:117:ALA:HB3	2.21	0.40
16:O:167:ASP:O	16:O:168:LEU:HD23	2.22	0.40
18:Q:10:ALA:C	18:Q:13:VAL:HG12	2.46	0.40
18:Q:16:VAL:CG1	18:Q:17:GLY:N	2.85	0.40
31:4:70:ARG:HD3	38:4:8537:HOH:O	2.21	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	
4	C	235/239 (98%)	202 (86%)	29 (12%)	4 (2%)	7	30
5	D	335/337 (99%)	299 (89%)	28 (8%)	8 (2%)	4	22
6	E	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	30	62
7	F	134/176 (76%)	93 (69%)	29 (22%)	12 (9%)	0	2
8	G	170/177 (96%)	158 (93%)	11 (6%)	1 (1%)	21	53
9	H	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	4	20
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	2	12
11	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	3	15
12	K	140/145 (97%)	129 (92%)	6 (4%)	5 (4%)	2	14
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	8	33
14	M	141/164 (86%)	122 (86%)	18 (13%)	1 (1%)	18	50
15	N	192/194 (99%)	173 (90%)	18 (9%)	1 (0%)	24	58
16	O	184/186 (99%)	163 (89%)	13 (7%)	8 (4%)	2	11
17	P	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
18	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	18	50
19	R	93/95 (98%)	85 (91%)	5 (5%)	3 (3%)	3	16
20	S	148/154 (96%)	135 (91%)	12 (8%)	1 (1%)	18	50
21	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
22	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	16
25	X	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Y	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	2	13
27	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
28	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	4	19
29	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	5	24
All	All	3633/4235 (86%)	3276 (90%)	289 (8%)	68 (2%)	6	27

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	93	LEU
7	F	95	THR
7	F	137	PRO
7	F	173	GLU
9	H	101	ALA
11	J	162	SER
14	M	80	ASP
16	O	154	LEU
16	O	162	ASP
16	O	164	ASP
16	O	183	ASP
26	Y	87	ALA
4	C	34	ASP
5	D	34	GLY
5	D	169	GLY
6	E	8	LEU
7	F	36	ASN
11	J	138	PRO
11	J	164	ALA
12	K	5	GLU
12	K	143	LYS
13	L	119	GLN
16	O	167	ASP
18	Q	116	SER
19	R	89	ALA
24	W	43	PRO
25	X	77	ALA
28	1	81	LYS

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Mol	Chain	Res	Type
31	4	57	GLY
4	C	132	ASP
5	D	184	ASP
7	F	16	PRO
7	F	20	LYS
7	F	61	PHE
7	F	171	ASP
8	G	44	GLY
11	J	40	PRO
12	K	76	ASP
15	N	140	ALA
16	O	181	ASP
25	X	49	ASN
26	Y	77	PHE
31	4	56	PRO
4	C	62	ASP
5	D	107	SER
7	F	11	HIS
7	F	96	SER
7	F	170	TYR
10	I	72	ASP
13	L	126	SER
26	Y	78	GLU
5	D	2	GLN
5	D	185	GLY
9	H	64	PRO
12	K	7	ASP
12	K	50	GLU
16	O	68	GLU
16	O	155	GLU
4	C	37	VAL
9	H	61	MET
19	R	18	PRO
19	R	54	PRO
24	W	40	PRO
11	J	72	VAL
20	S	106	GLY
28	1	41	VAL
5	D	5	ARG

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	
4	C	179/181 (99%)	167 (93%)	12 (7%)	15	44
5	D	282/282 (100%)	264 (94%)	18 (6%)	16	45
6	E	193/193 (100%)	176 (91%)	17 (9%)	9	33
7	F	117/147 (80%)	110 (94%)	7 (6%)	17	48
8	G	152/155 (98%)	148 (97%)	4 (3%)	40	70
9	H	92/92 (100%)	91 (99%)	1 (1%)	65	82
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	108 (88%)	14 (12%)	5	22
12	K	118/121 (98%)	112 (95%)	6 (5%)	21	53
13	L	106/106 (100%)	103 (97%)	3 (3%)	38	69
14	M	112/126 (89%)	108 (96%)	4 (4%)	31	63
15	N	166/166 (100%)	157 (95%)	9 (5%)	20	51
16	O	149/149 (100%)	140 (94%)	9 (6%)	17	48
17	P	93/93 (100%)	89 (96%)	4 (4%)	26	58
18	Q	113/116 (97%)	110 (97%)	3 (3%)	39	70
19	R	79/79 (100%)	75 (95%)	4 (5%)	21	53
20	S	117/121 (97%)	113 (97%)	4 (3%)	32	64
21	T	71/73 (97%)	70 (99%)	1 (1%)	59	80
22	U	105/105 (100%)	100 (95%)	5 (5%)	23	55
23	V	44/52 (85%)	43 (98%)	1 (2%)	44	72
24	W	51/56 (91%)	50 (98%)	1 (2%)	48	75
25	X	130/130 (100%)	120 (92%)	10 (8%)	12	38
26	Y	66/73 (90%)	62 (94%)	4 (6%)	17	47
27	Z	120/195 (62%)	112 (93%)	8 (7%)	15	44
28	1	56/56 (100%)	49 (88%)	7 (12%)	4	19
29	2	46/46 (100%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	3	42/44 (96%)	41 (98%)	1 (2%)	43 72
31	4	79/79 (100%)	71 (90%)	8 (10%)	7 27
All	All	3027/3441 (88%)	2862 (94%)	165 (6%)	19 51

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	ARG
4	C	33	GLU
4	C	36	ASP
4	C	55	VAL
4	C	68	ILE
4	C	69	LEU
4	C	94	LEU
4	C	131	HIS
4	C	153	ARG
4	C	175	LYS
4	C	179	MET
4	C	217	ARG
5	D	7	ARG
5	D	11	LEU
5	D	27	ASN
5	D	33	ASP
5	D	63	GLU
5	D	84	LEU
5	D	97	LEU
5	D	98	THR
5	D	103	ASP
5	D	195	ARG
5	D	245	SER
5	D	251	VAL
5	D	254	GLN
5	D	256	GLN
5	D	264	GLU
5	D	304	PRO
5	D	307	ARG
5	D	312	ARG
6	E	2	GLN
6	E	67	GLN
6	E	76	ARG
6	E	81	PRO

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Mol	Chain	Res	Type
6	E	91	PRO
6	E	94	THR
6	E	101	ASP
6	E	115	LEU
6	E	136	VAL
6	E	187	ARG
6	E	214	THR
6	E	222	ASP
6	E	223	LEU
6	E	234	VAL
6	E	236	THR
6	E	240	LEU
6	E	243	VAL
7	F	24	HIS
7	F	50	VAL
7	F	99	ASP
7	F	131	THR
7	F	136	ARG
7	F	137	PRO
7	F	149	ARG
8	G	7	ILE
8	G	54	ASP
8	G	86	VAL
8	G	102	VAL
9	H	12	LEU
11	J	1	LYS
11	J	18	GLU
11	J	30	GLN
11	J	59	ASN
11	J	61	LEU
11	J	72	VAL
11	J	73	GLN
11	J	82	LYS
11	J	85	ILE
11	J	86	ARG
11	J	94	ARG
11	J	142	VAL
11	J	150	LYS
11	J	166	ASN
12	K	46	ILE
12	K	74	ARG
12	K	93	ARG

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Mol	Chain	Res	Type
12	K	125	SER
12	K	127	ILE
12	K	131	THR
13	L	7	ASP
13	L	10	GLN
13	L	98	VAL
14	M	35	ARG
14	M	75	LEU
14	M	117	GLU
14	M	140	VAL
15	N	38	VAL
15	N	46	LEU
15	N	81	ARG
15	N	87	MET
15	N	93	ARG
15	N	99	ARG
15	N	130	GLU
15	N	136	PRO
15	N	164	THR
16	O	12	ARG
16	O	17	ARG
16	O	26	LEU
16	O	43	VAL
16	O	47	LEU
16	O	127	LEU
16	O	128	ASP
16	O	152	GLU
16	O	163	PHE
17	P	3	THR
17	P	28	ASP
17	P	98	LEU
17	P	111	VAL
18	Q	52	LYS
18	Q	91	LYS
18	Q	98	ILE
19	R	11	ARG
19	R	16	ASN
19	R	57	ASP
19	R	95	GLU
20	S	13	THR
20	S	39	THR
20	S	82	GLU

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Mol	Chain	Res	Type
20	S	132	ARG
21	T	10	VAL
22	U	26	THR
22	U	39	ASN
22	U	47	THR
22	U	48	VAL
22	U	96	VAL
23	V	9	CYS
24	W	43	PRO
25	X	4	LEU
25	X	26	ILE
25	X	35	VAL
25	X	52	VAL
25	X	73	LEU
25	X	120	PRO
25	X	122	ARG
25	X	142	ASP
25	X	146	ILE
25	X	154	ARG
26	Y	15	ARG
26	Y	52	PRO
26	Y	66	THR
26	Y	72	VAL
27	Z	103	THR
27	Z	154	ARG
27	Z	163	THR
27	Z	172	THR
27	Z	189	ASN
27	Z	200	THR
27	Z	203	VAL
27	Z	235	GLU
28	1	11	THR
28	1	22	ILE
28	1	32	LYS
28	1	42	CYS
28	1	60	CYS
28	1	64	ILE
28	1	68	CYS
30	3	18	ASN
31	4	3	MET
31	4	14	CYS
31	4	34	LYS

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Mol	Chain	Res	Type
31	4	38	ARG
31	4	42	ARG
31	4	56	PRO
31	4	65	THR
31	4	74	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	29	HIS
4	C	47	HIS
4	C	92	ASN
4	C	127	GLN
4	C	151	GLN
4	C	177	HIS
4	C	199	HIS
4	C	218	ASN
5	D	27	ASN
5	D	55	ASN
5	D	145	HIS
5	D	221	GLN
5	D	238	ASN
5	D	256	GLN
5	D	260	HIS
5	D	332	ASN
6	E	2	GLN
6	E	39	GLN
6	E	67	GLN
6	E	108	GLN
6	E	129	HIS
6	E	163	HIS
7	F	103	ASN
7	F	133	ASN
8	G	96	ASN
8	G	106	ASN
8	G	143	GLN
10	I	17	GLN
10	I	64	ASN
11	J	35	ASN
11	J	45	GLN
11	J	55	GLN
11	J	58	HIS

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Mol	Chain	Res	Type
11	J	59	ASN
11	J	74	ASN
11	J	80	ASN
11	J	91	HIS
11	J	129	ASN
11	J	130	HIS
11	J	137	ASN
11	J	166	ASN
12	K	52	GLN
12	K	89	HIS
12	K	107	ASN
13	L	10	GLN
14	M	18	HIS
14	M	41	HIS
14	M	58	GLN
14	M	116	HIS
15	N	26	HIS
15	N	58	GLN
15	N	89	ASN
15	N	176	GLN
16	O	107	ASN
16	O	119	GLN
16	O	140	GLN
16	O	153	GLN
18	Q	50	GLN
18	Q	66	GLN
18	Q	73	HIS
18	Q	118	GLN
19	R	16	ASN
19	R	40	HIS
19	R	67	GLN
20	S	61	GLN
20	S	94	ASN
20	S	98	ASN
20	S	117	HIS
20	S	122	GLN
20	S	140	GLN
21	T	51	GLN
21	T	53	ASN
21	T	55	GLN
21	T	56	ASN
22	U	39	ASN

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Mol	Chain	Res	Type
22	U	73	HIS
23	V	39	ASN
23	V	48	ASN
24	W	4	HIS
24	W	60	GLN
25	X	6	GLN
25	X	28	HIS
25	X	31	HIS
25	X	87	HIS
25	X	110	GLN
25	X	119	HIS
25	X	125	HIS
25	X	141	HIS
26	Y	23	HIS
27	Z	133	HIS
27	Z	134	HIS
27	Z	149	GLN
27	Z	189	ASN
28	1	33	HIS
28	1	70	GLN
29	2	8	GLN
29	2	16	HIS
29	2	28	HIS
30	3	16	ASN
30	3	17	GLN
30	3	18	ASN
30	3	37	HIS
30	3	41	HIS
30	3	45	ASN
31	4	30	GLN
31	4	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	255 (9%)	36 (1%)
2	B	121/122 (99%)	20 (16%)	5 (4%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	275 (9%)	41 (1%)

All (275) 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
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	318	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	461	C
1	A	487	G
1	A	498	A

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Mol	Chain	Res	Type
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
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	882	A
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	920	C
1	A	921	G

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Mol	Chain	Res	Type
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	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	G
1	A	1161	A
1	A	1162	G
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	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C

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Mol	Chain	Res	Type
1	A	1380	U
1	A	1407	A
1	A	1409	G
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	1524	U
1	A	1525	G
1	A	1526	A
1	A	1528	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
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	1737	A
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

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Mol	Chain	Res	Type
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	1982	C
1	A	1996	U
1	A	2004	U
1	A	2006	C
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
1	A	2074	A
1	A	2096	A
1	A	2101	A
1	A	2102	G
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	2346	C
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2466	G
1	A	2467	A
1	A	2469	A

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Mol	Chain	Res	Type
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
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	2590	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G
1	A	2649	A
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

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Mol	Chain	Res	Type
1	A	2896	A
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	3023	U
2	B	3024	U
2	B	3025	G
2	B	3026	C
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	3103	A
2	B	3104	A
2	B	3114	G
2	B	3122	C

All (41) 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	603	A
1	A	644	G
1	A	699	C
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

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Mol	Chain	Res	Type
1	A	1237	U
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1563	G
1	A	1685	A
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2466	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	3023	U
2	B	3024	U
2	B	3043	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 233 ligands modelled in this entry, 232 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
36	PPU	5	76	3	37,40,41	2.23	13 (35%)	47,57,60	1.52	7 (14%)

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
36	PPU	5	76	3	-	2/25/43/44	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	CB-CG	4.86	1.62	1.51
36	5	76	PPU	C-N3'	4.51	1.43	1.34
36	5	76	PPU	CE2-CD2	-4.26	1.31	1.38
36	5	76	PPU	C10-N6	-4.23	1.36	1.45
36	5	76	PPU	CD1-CG	-3.88	1.31	1.38
36	5	76	PPU	C9-N6	-3.73	1.37	1.45
36	5	76	PPU	O-C	3.70	1.30	1.23
36	5	76	PPU	CE1-CD1	-3.42	1.33	1.38
36	5	76	PPU	CE1-CZ	2.53	1.43	1.38
36	5	76	PPU	CA-N	2.40	1.61	1.48
36	5	76	PPU	C2-N1	2.40	1.38	1.33
36	5	76	PPU	O2'-C2'	-2.28	1.37	1.43
36	5	76	PPU	C2-N3	-2.24	1.30	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	76	PPU	CA-C-N3'	-4.38	110.28	116.21
36	5	76	PPU	C3'-N3'-C	-4.02	117.09	123.20
36	5	76	PPU	CG-CB-CA	-3.98	105.98	114.13
36	5	76	PPU	CM-OC-CZ	3.24	124.45	117.50
36	5	76	PPU	C2-N1-C6	2.71	118.45	111.83
36	5	76	PPU	CE2-CZ-CE1	-2.26	116.86	120.16
36	5	76	PPU	O4'-C1'-C2'	2.18	111.29	106.62

There are no chirality outliers.

All (2) torsion outliers are listed below:

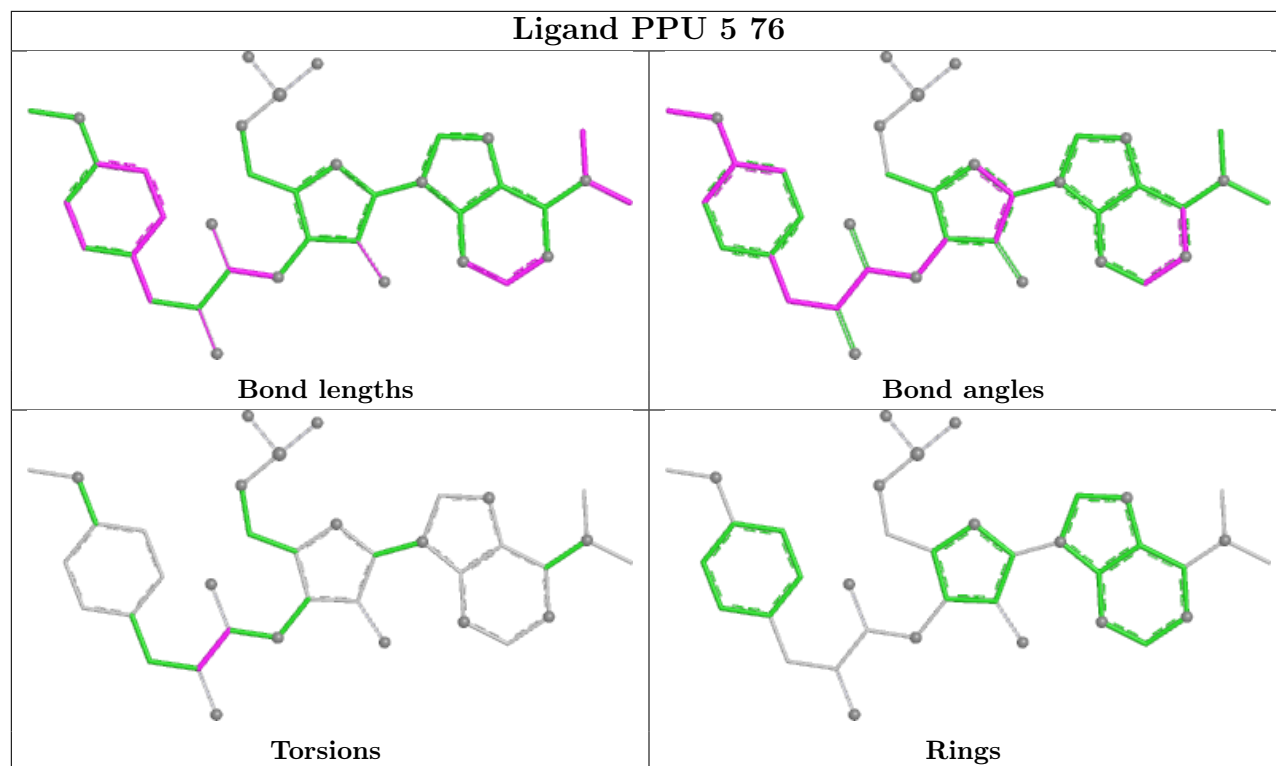
Mol	Chain	Res	Type	Atoms
36	5	76	PPU	O-C-CA-CB
36	5	76	PPU	N3'-C-CA-CB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	76	PPU	4	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(Å²)	Q<0.9
1	A	2754/2922 (94%)	-0.12	87 (3%)	50	33	19, 45, 94, 144	0
2	B	122/122 (100%)	0.49	7 (5%)	29	17	33, 67, 97, 147	0
3	5	2/2 (100%)	2.25	1 (50%)	0	0	65, 65, 65, 87	0
4	C	237/239 (99%)	0.41	14 (5%)	28	17	30, 62, 97, 109	0
5	D	337/337 (100%)	0.10	3 (0%)	81	65	22, 50, 77, 89	0
6	E	246/246 (100%)	0.03	1 (0%)	88	79	20, 44, 69, 78	0
7	F	140/176 (79%)	1.52	34 (24%)	2	1	65, 101, 122, 128	0
8	G	172/177 (97%)	0.42	4 (2%)	61	42	38, 62, 84, 89	0
9	H	119/119 (100%)	0.65	5 (4%)	40	25	51, 76, 99, 107	0
10	I	29/348 (8%)	1.52	7 (24%)	2	1	66, 87, 95, 99	0
11	J	156/167 (93%)	0.62	15 (9%)	13	9	35, 59, 82, 89	0
12	K	142/145 (97%)	-0.02	1 (0%)	84	70	32, 44, 67, 78	0
13	L	132/132 (100%)	0.17	1 (0%)	82	67	33, 49, 75, 82	0
14	M	145/164 (88%)	0.89	20 (13%)	6	4	26, 79, 106, 111	0
15	N	194/194 (100%)	0.55	25 (12%)	7	5	28, 47, 106, 118	0
16	O	186/186 (100%)	0.92	23 (12%)	8	6	46, 73, 112, 125	0
17	P	115/115 (100%)	0.27	1 (0%)	81	65	36, 53, 68, 72	0
18	Q	143/148 (96%)	0.26	2 (1%)	73	55	34, 53, 76, 85	0
19	R	95/95 (100%)	0.13	1 (1%)	78	61	36, 47, 63, 82	0
20	S	150/154 (97%)	-0.23	0	100	100	26, 40, 61, 72	0
21	T	81/84 (96%)	0.34	1 (1%)	76	59	44, 62, 82, 88	0
22	U	119/119 (100%)	0.37	3 (2%)	58	39	40, 55, 84, 104	0
23	V	53/66 (80%)	1.27	6 (11%)	10	7	77, 92, 100, 108	0
24	W	65/70 (92%)	0.86	8 (12%)	8	6	46, 76, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	154/154 (100%)	-0.12	0 100 100	28, 42, 59, 70	0
26	Y	82/91 (90%)	0.40	5 (6%) 27 16	37, 53, 77, 91	0
27	Z	142/240 (59%)	-0.15	1 (0%) 84 70	25, 40, 64, 82	0
28	1	73/73 (100%)	2.82	46 (63%) 0 0	93, 115, 125, 127	0
29	2	56/56 (100%)	-0.45	0 100 100	22, 32, 40, 45	0
30	3	46/48 (95%)	0.55	4 (8%) 16 10	34, 63, 96, 105	0
31	4	92/92 (100%)	3.04	63 (68%) 0 0	110, 125, 133, 136	0
All	All	6579/7281 (90%)	0.23	389 (5%) 28 17	19, 52, 105, 147	0

All (389) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	10.2
15	N	80	GLY	8.8
15	N	89	ASN	8.2
31	4	60	LYS	7.2
1	A	1173	A	7.2
28	1	16	PRO	7.1
15	N	81	ARG	7.0
15	N	70	GLY	6.5
31	4	79	LEU	6.1
31	4	33	MET	6.0
28	1	26	VAL	6.0
28	1	22	ILE	6.0
28	1	20	LEU	5.8
31	4	83	TRP	5.7
28	1	40	PRO	5.7
1	A	1176	C	5.5
31	4	12	PRO	5.5
15	N	82	ARG	5.4
31	4	62	THR	5.3
31	4	76	LYS	5.2
28	1	41	VAL	5.2
19	R	95	GLU	5.2
31	4	84	ARG	5.2
28	1	18	TYR	5.2
2	B	3025	G	5.1
28	1	12	GLY	5.1
15	N	71	SER	5.0
1	A	1175	G	5.0

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Mol	Chain	Res	Type	RSRZ
7	F	63	ILE	4.9
14	M	37	LYS	4.9
15	N	83	SER	4.8
31	4	61	PRO	4.8
14	M	36	ASP	4.8
28	1	44	PHE	4.8
2	B	3001	U	4.7
31	4	48	ASN	4.7
31	4	88	LEU	4.6
7	F	10	PHE	4.5
31	4	46	ILE	4.5
28	1	35	LYS	4.5
28	1	32	LYS	4.5
31	4	43	ASN	4.5
28	1	29	VAL	4.4
1	A	1925	G	4.4
28	1	34	LYS	4.4
15	N	73	ARG	4.4
31	4	67	LEU	4.3
16	O	167	ASP	4.3
15	N	90	ARG	4.3
31	4	11	CYS	4.3
15	N	88	VAL	4.3
31	4	51	LYS	4.3
31	4	85	ALA	4.3
31	4	2	GLN	4.2
31	4	3	MET	4.2
28	1	31	ILE	4.2
28	1	13	ARG	4.2
28	1	15	GLY	4.2
16	O	168	LEU	4.1
15	N	79	LYS	4.1
31	4	34	LYS	4.1
1	A	1162	G	4.1
31	4	7	PHE	4.1
31	4	9	THR	4.0
15	N	68	ARG	4.0
31	4	17	HIS	4.0
1	A	1168	C	4.0
28	1	17	ARG	4.0
16	O	179	LEU	4.0
31	4	1	MET	4.0

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Mol	Chain	Res	Type	RSRZ
28	1	64	ILE	4.0
1	A	2433	A	4.0
8	G	45	ASP	3.9
31	4	36	ILE	3.9
15	N	77	PHE	3.9
31	4	10	TYR	3.9
1	A	2432	C	3.9
15	N	75	THR	3.9
31	4	63	LYS	3.9
15	N	72	SER	3.9
31	4	35	TRP	3.8
15	N	78	ASN	3.8
31	4	42	ARG	3.8
14	M	46	LEU	3.8
10	I	26	MET	3.8
26	Y	88	GLU	3.8
18	Q	110	ASP	3.8
7	F	69	ILE	3.8
31	4	54	LYS	3.8
31	4	82	GLY	3.8
7	F	21	VAL	3.7
1	A	1198	U	3.7
31	4	52	PHE	3.7
24	W	39	ALA	3.7
28	1	19	GLY	3.7
1	A	735	C	3.7
1	A	1177	A	3.6
28	1	39	CYS	3.6
28	1	54	ILE	3.6
1	A	10	U	3.6
2	B	3024	U	3.6
31	4	38	ARG	3.6
1	A	1171	A	3.6
3	5	74	C	3.6
14	M	83	GLU	3.5
16	O	148	ALA	3.5
4	C	36	ASP	3.5
28	1	42	CYS	3.5
2	B	3023	U	3.5
4	C	52	SER	3.5
31	4	77	ALA	3.5
31	4	64	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
31	4	39	GLN	3.4
1	A	1160	G	3.4
31	4	69	TYR	3.4
16	O	163	PHE	3.4
1	A	1193	A	3.4
1	A	2748	G	3.3
31	4	22	VAL	3.3
31	4	31	THR	3.3
1	A	1170	U	3.3
8	G	10	ASP	3.3
31	4	59	ASP	3.3
4	C	37	VAL	3.3
11	J	40	PRO	3.3
28	1	24	VAL	3.3
1	A	1172	G	3.3
5	D	1	PRO	3.2
10	I	27	ILE	3.2
28	1	23	ARG	3.2
28	1	52	THR	3.2
31	4	75	GLY	3.2
31	4	56	PRO	3.2
11	J	135	TRP	3.2
15	N	86	MET	3.2
31	4	68	LYS	3.2
9	H	106	THR	3.2
1	A	2345	A	3.1
31	4	65	THR	3.1
14	M	82	ALA	3.1
1	A	806	A	3.1
28	1	48	LYS	3.1
1	A	2466	G	3.1
10	I	20	VAL	3.1
30	3	49	GLU	3.1
10	I	71	LEU	3.1
23	V	55	ALA	3.1
1	A	1192	A	3.1
7	F	96	SER	3.0
14	M	146	GLY	3.0
1	A	1169	U	3.0
11	J	114	PRO	3.0
1	A	1924	A	3.0
11	J	110	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
30	3	39	ARG	3.0
1	A	1190	G	3.0
28	1	21	LYS	3.0
26	Y	82	GLU	3.0
28	1	14	PHE	3.0
1	A	1181	A	3.0
1	A	2249	G	3.0
11	J	38	ALA	3.0
31	4	13	HIS	3.0
1	A	1166	A	2.9
16	O	147	ILE	2.9
7	F	47	GLN	2.9
14	M	34	GLY	2.9
11	J	36	ASN	2.9
24	W	40	PRO	2.9
31	4	15	ASN	2.9
31	4	74	CYS	2.9
14	M	133	VAL	2.9
14	M	38	HIS	2.9
2	B	3002	U	2.9
31	4	81	GLU	2.9
14	M	77	ALA	2.9
7	F	95	THR	2.9
15	N	76	ARG	2.9
31	4	29	ARG	2.9
7	F	131	THR	2.9
16	O	154	LEU	2.9
1	A	1165	G	2.9
1	A	2250	G	2.9
18	Q	116	SER	2.9
31	4	53	SER	2.9
31	4	90	PHE	2.9
31	4	50	GLY	2.8
31	4	4	PRO	2.8
7	F	35	ALA	2.8
4	C	60	PHE	2.8
7	F	107	GLY	2.8
1	A	1184	C	2.8
4	C	51	ARG	2.8
15	N	74	ARG	2.8
7	F	171	ASP	2.8
28	1	33	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1167	G	2.8
1	A	2421	G	2.8
28	1	11	THR	2.8
1	A	1174	A	2.8
9	H	102	GLY	2.8
11	J	39	GLY	2.8
31	4	14	CYS	2.8
6	E	135	GLU	2.8
1	A	138	U	2.8
1	A	1205	U	2.8
31	4	55	VAL	2.8
16	O	169	PRO	2.8
16	O	186	LEU	2.8
31	4	44	SER	2.8
7	F	49	PRO	2.8
7	F	159	PRO	2.8
28	1	27	ALA	2.7
1	A	2637	A	2.7
11	J	167	ALA	2.7
31	4	78	HIS	2.7
1	A	736	A	2.7
1	A	1185	U	2.7
28	1	30	GLU	2.7
7	F	57	THR	2.7
7	F	138	GLY	2.7
31	4	47	GLY	2.7
1	A	2254	G	2.6
16	O	56	ASP	2.6
9	H	101	ALA	2.6
1	A	2338	G	2.6
15	N	84	LYS	2.6
26	Y	65	ASN	2.6
14	M	148	GLU	2.6
7	F	59	GLY	2.6
24	W	43	PRO	2.6
31	4	45	GLY	2.6
1	A	1917	G	2.6
2	B	3022	G	2.6
14	M	99	GLU	2.6
22	U	119	ALA	2.6
1	A	1161	A	2.6
7	F	50	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
11	J	59	ASN	2.6
1	A	1206	U	2.5
16	O	136	LEU	2.5
28	1	53	GLY	2.5
23	V	40	ALA	2.5
11	J	140	PRO	2.5
4	C	63	GLY	2.5
31	4	25	VAL	2.5
16	O	138	ASP	2.5
28	1	28	ASP	2.5
28	1	45	LYS	2.5
1	A	1964	U	2.5
15	N	165	SER	2.5
28	1	47	LEU	2.5
4	C	32	VAL	2.5
7	F	22	VAL	2.5
1	A	2379	G	2.5
7	F	97	GLN	2.5
16	O	1	ALA	2.5
30	3	37	HIS	2.5
7	F	13	MET	2.5
24	W	44	GLY	2.5
28	1	51	GLY	2.5
1	A	1163	G	2.5
1	A	2257	G	2.5
4	C	38	ILE	2.4
1	A	714	U	2.4
23	V	51	TRP	2.4
28	1	10	ARG	2.4
2	B	3021	G	2.4
16	O	184	ILE	2.4
7	F	93	LEU	2.4
7	F	100	ASP	2.4
22	U	116	ASP	2.4
14	M	40	PHE	2.4
4	C	31	LYS	2.4
7	F	105	SER	2.4
7	F	75	LEU	2.4
17	P	80	ASP	2.3
28	1	75	ALA	2.3
1	A	1182	C	2.3
31	4	91	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1202	A	2.3
1	A	1525	G	2.3
14	M	81	VAL	2.3
4	C	236	GLY	2.3
16	O	162	ASP	2.3
1	A	368	C	2.3
1	A	1204	C	2.3
23	V	13	ILE	2.3
11	J	37	GLY	2.3
14	M	47	GLY	2.3
12	K	70	PHE	2.3
1	A	960	G	2.3
1	A	1923	G	2.3
1	A	1926	G	2.3
7	F	12	GLU	2.3
9	H	105	ALA	2.3
23	V	49	LEU	2.3
1	A	737	A	2.3
24	W	37	GLY	2.3
7	F	61	PHE	2.3
28	1	65	ALA	2.3
8	G	100	ASP	2.3
11	J	32	ASP	2.3
1	A	1605	G	2.3
1	A	2459	G	2.3
31	4	58	GLY	2.3
1	A	2376	C	2.2
11	J	83	PHE	2.2
10	I	67	LEU	2.2
14	M	45	PRO	2.2
4	C	91	GLY	2.2
1	A	1180	U	2.2
1	A	2419	U	2.2
1	A	2436	U	2.2
16	O	185	GLU	2.2
26	Y	80	GLU	2.2
5	D	319	ASP	2.2
11	J	139	ASP	2.2
14	M	149	ARG	2.2
1	A	1951	G	2.2
1	A	1915	U	2.2
15	N	85	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
27	Z	108	ASP	2.2
4	C	27	LEU	2.2
1	A	970	U	2.2
7	F	76	ARG	2.2
31	4	8	ASN	2.2
1	A	2344	G	2.2
1	A	2507	G	2.2
1	A	1194	A	2.2
1	A	2321	A	2.2
1	A	2511	A	2.2
10	I	13	PRO	2.2
7	F	104	PHE	2.2
24	W	45	ARG	2.1
7	F	11	HIS	2.1
7	F	174	VAL	2.1
24	W	2	VAL	2.1
28	1	79	VAL	2.1
1	A	1195	G	2.1
28	1	46	LYS	2.1
14	M	111	ALA	2.1
5	D	57	GLU	2.1
7	F	130	VAL	2.1
16	O	78	MET	2.1
8	G	39	ASP	2.1
16	O	158	LEU	2.1
1	A	128	A	2.1
1	A	1191	A	2.1
28	1	25	ARG	2.1
28	1	62	TYR	2.1
1	A	1197	G	2.1
1	A	1916	C	2.1
9	H	107	VAL	2.1
28	1	74	VAL	2.1
1	A	1561	U	2.1
1	A	2322	U	2.1
16	O	180	LEU	2.1
4	C	41	THR	2.1
7	F	101	THR	2.1
16	O	172	PHE	2.1
15	N	156	ARG	2.1
15	N	91	ILE	2.1
1	A	1188	A	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2460	A	2.1
13	L	130	MET	2.1
26	Y	85	VAL	2.1
28	1	36	LYS	2.1
1	A	1279	U	2.1
1	A	2378	U	2.1
7	F	17	ARG	2.1
23	V	54	THR	2.1
14	M	91	VAL	2.0
1	A	1186	C	2.0
1	A	1929	G	2.0
10	I	73	ASP	2.0
14	M	102	ASP	2.0
16	O	165	ALA	2.0
16	O	166	ALA	2.0
22	U	5	ASP	2.0
11	J	84	ARG	2.0
30	3	36	ASN	2.0
1	A	999	C	2.0
7	F	87	ALA	2.0
15	N	192	ALA	2.0
21	T	19	ASP	2.0
1	A	1178	G	2.0
16	O	69	TYR	2.0
4	C	82	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	NA	B	8351	1/1	0.36	0.16	75,75,75,75	0
34	NA	A	8384	1/1	0.44	0.17	82,82,82,82	0
34	NA	A	8340	1/1	0.45	0.17	58,58,58,58	0
35	CL	4	8504	1/1	0.46	0.14	101,101,101,101	0
34	NA	T	8312	1/1	0.49	0.16	80,80,80,80	0
34	NA	A	8328	1/1	0.54	0.26	47,47,47,47	0
32	MG	A	8049	1/1	0.63	0.22	95,95,95,95	0
34	NA	A	8302	1/1	0.63	0.16	31,31,31,31	0
34	NA	B	8383	1/1	0.66	0.43	77,77,77,77	0
34	NA	A	8341	1/1	0.66	0.16	55,55,55,55	0
34	NA	A	8381	1/1	0.66	0.10	46,46,46,46	0
34	NA	A	8301	1/1	0.67	0.13	31,31,31,31	0
34	NA	A	8373	1/1	0.68	0.15	54,54,54,54	0
34	NA	A	8382	1/1	0.71	0.47	79,79,79,79	0
34	NA	A	8329	1/1	0.71	0.23	61,61,61,61	0
34	NA	A	8357	1/1	0.71	0.15	49,49,49,49	0
34	NA	A	8365	1/1	0.73	0.28	46,46,46,46	0
34	NA	S	8337	1/1	0.73	0.11	52,52,52,52	0
32	MG	B	8095	1/1	0.74	0.13	72,72,72,72	0
34	NA	A	8352	1/1	0.75	0.15	39,39,39,39	0
34	NA	A	8366	1/1	0.75	0.17	47,47,47,47	0
34	NA	A	8368	1/1	0.75	0.19	56,56,56,56	0
34	NA	A	8332	1/1	0.75	0.22	68,68,68,68	0
32	MG	A	8102	1/1	0.76	0.51	135,135,135,135	0
35	CL	C	8509	1/1	0.76	0.18	86,86,86,86	0
34	NA	A	8363	1/1	0.76	0.22	48,48,48,48	0
34	NA	A	8327	1/1	0.77	0.16	40,40,40,40	0
34	NA	A	8344	1/1	0.77	0.07	27,27,27,27	0
35	CL	M	8510	1/1	0.78	0.22	97,97,97,97	0
37	CD	4	8404	1/1	0.78	0.19	203,203,203,203	0
34	NA	A	8385	1/1	0.79	0.21	46,46,46,46	0
35	CL	A	8522	1/1	0.79	0.38	83,83,83,83	0
32	MG	A	8076	1/1	0.79	0.14	79,79,79,79	0
34	NA	A	8319	1/1	0.79	0.11	44,44,44,44	0
34	NA	A	8374	1/1	0.79	0.35	60,60,60,60	0
34	NA	S	8386	1/1	0.79	0.23	70,70,70,70	0
34	NA	A	8356	1/1	0.80	0.29	57,57,57,57	0
34	NA	A	8377	1/1	0.81	0.40	86,86,86,86	0
32	MG	A	8045	1/1	0.81	0.09	50,50,50,50	0
37	CD	1	8403	1/1	0.81	0.16	203,203,203,203	0
34	NA	A	8371	1/1	0.81	0.27	54,54,54,54	0
34	NA	A	8354	1/1	0.82	0.14	51,51,51,51	0
32	MG	1	8105	1/1	0.83	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8067	1/1	0.83	0.14	41,41,41,41	0
32	MG	A	8114	1/1	0.83	0.31	124,124,124,124	0
34	NA	A	8355	1/1	0.83	0.30	64,64,64,64	0
35	CL	D	8519	1/1	0.83	0.17	70,70,70,70	0
34	NA	A	8303	1/1	0.83	0.18	51,51,51,51	0
32	MG	A	8089	1/1	0.83	0.10	82,82,82,82	0
34	NA	R	8348	1/1	0.83	0.10	57,57,57,57	0
34	NA	A	8326	1/1	0.83	0.20	60,60,60,60	0
32	MG	A	8046	1/1	0.84	0.07	53,53,53,53	0
34	NA	A	8362	1/1	0.84	0.36	74,74,74,74	0
35	CL	N	8518	1/1	0.84	0.11	46,46,46,46	0
35	CL	K	8502	1/1	0.85	0.11	71,71,71,71	0
32	MG	A	8101	1/1	0.85	0.10	50,50,50,50	0
32	MG	A	8050	1/1	0.85	0.07	52,52,52,52	0
34	NA	A	8379	1/1	0.86	0.13	48,48,48,48	0
34	NA	A	8307	1/1	0.86	0.15	58,58,58,58	0
32	MG	A	8092	1/1	0.86	0.20	91,91,91,91	0
32	MG	A	8047	1/1	0.86	0.08	31,31,31,31	0
32	MG	A	8024	1/1	0.86	0.37	110,110,110,110	0
34	NA	A	8378	1/1	0.87	0.24	52,52,52,52	0
34	NA	A	8316	1/1	0.87	0.13	45,45,45,45	0
34	NA	J	8309	1/1	0.87	0.13	42,42,42,42	0
32	MG	A	8116	1/1	0.87	0.10	55,55,55,55	0
35	CL	A	8505	1/1	0.88	0.18	74,74,74,74	0
34	NA	A	8318	1/1	0.88	0.15	43,43,43,43	0
35	CL	R	8511	1/1	0.88	0.13	67,67,67,67	0
32	MG	A	8066	1/1	0.88	0.11	65,65,65,65	0
34	NA	A	8331	1/1	0.88	0.34	76,76,76,76	0
34	NA	A	8372	1/1	0.88	0.24	80,80,80,80	0
34	NA	A	8308	1/1	0.89	0.16	63,63,63,63	0
32	MG	A	8057	1/1	0.89	0.10	46,46,46,46	0
32	MG	U	8073	1/1	0.90	0.06	48,48,48,48	0
32	MG	A	8093	1/1	0.90	0.13	44,44,44,44	0
36	PPU	5	76	37/38	0.90	0.14	60,64,69,71	0
32	MG	A	8075	1/1	0.90	0.08	45,45,45,45	0
35	CL	O	8507	1/1	0.90	0.09	65,65,65,65	0
32	MG	4	8078	1/1	0.91	0.08	74,74,74,74	0
32	MG	A	8111	1/1	0.91	0.07	61,61,61,61	0
34	NA	A	8310	1/1	0.91	0.17	40,40,40,40	0
35	CL	K	8516	1/1	0.91	0.15	61,61,61,61	0
32	MG	A	8070	1/1	0.91	0.23	69,69,69,69	0
32	MG	A	8053	1/1	0.91	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8090	1/1	0.92	0.18	70,70,70,70	0
34	NA	A	8306	1/1	0.92	0.18	44,44,44,44	0
34	NA	A	8370	1/1	0.92	0.22	52,52,52,52	0
34	NA	A	8321	1/1	0.92	0.15	48,48,48,48	0
34	NA	A	8358	1/1	0.92	0.25	105,105,105,105	0
35	CL	A	8503	1/1	0.92	0.12	57,57,57,57	0
34	NA	A	8349	1/1	0.92	0.16	67,67,67,67	0
34	NA	A	8334	1/1	0.92	0.10	46,46,46,46	0
34	NA	A	8335	1/1	0.92	0.16	57,57,57,57	0
34	NA	C	8345	1/1	0.92	0.08	35,35,35,35	0
32	MG	A	8042	1/1	0.93	0.07	34,34,34,34	0
32	MG	A	8117	1/1	0.93	0.05	33,33,33,33	0
32	MG	A	8088	1/1	0.93	0.09	65,65,65,65	0
34	NA	A	8375	1/1	0.93	0.17	55,55,55,55	0
32	MG	D	8055	1/1	0.93	0.09	81,81,81,81	0
32	MG	A	8051	1/1	0.93	0.09	86,86,86,86	0
32	MG	A	8062	1/1	0.93	0.07	49,49,49,49	0
34	NA	A	8330	1/1	0.93	0.08	35,35,35,35	0
35	CL	S	8506	1/1	0.93	0.10	60,60,60,60	0
34	NA	4	8369	1/1	0.93	0.28	66,66,66,66	0
34	NA	A	8353	1/1	0.93	0.15	53,53,53,53	0
32	MG	A	8113	1/1	0.93	0.07	54,54,54,54	0
32	MG	A	8064	1/1	0.93	0.16	24,24,24,24	0
35	CL	K	8501	1/1	0.94	0.08	58,58,58,58	0
34	NA	A	8339	1/1	0.94	0.06	30,30,30,30	0
32	MG	A	8041	1/1	0.94	0.06	55,55,55,55	0
35	CL	K	8521	1/1	0.94	0.10	60,60,60,60	0
32	MG	A	8103	1/1	0.94	0.07	45,45,45,45	0
34	NA	A	8342	1/1	0.94	0.06	28,28,28,28	0
34	NA	A	8325	1/1	0.94	0.16	40,40,40,40	0
34	NA	A	8313	1/1	0.94	0.09	74,74,74,74	0
34	NA	A	8350	1/1	0.94	0.11	37,37,37,37	0
35	CL	Z	8517	1/1	0.94	0.07	61,61,61,61	0
35	CL	Z	8520	1/1	0.94	0.10	35,35,35,35	0
35	CL	A	8515	1/1	0.94	0.16	68,68,68,68	0
33	K	A	8202	1/1	0.94	0.12	89,89,89,89	0
37	CD	V	8401	1/1	0.94	0.12	129,129,129,129	0
32	MG	Z	8109	1/1	0.94	0.07	38,38,38,38	0
34	NA	J	8322	1/1	0.94	0.24	72,72,72,72	0
32	MG	A	8082	1/1	0.95	0.07	56,56,56,56	0
33	K	A	8201	1/1	0.95	0.22	71,71,71,71	0
32	MG	A	8096	1/1	0.95	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8333	1/1	0.95	0.13	33,33,33,33	0
32	MG	A	8100	1/1	0.95	0.13	79,79,79,79	0
34	NA	K	8346	1/1	0.95	0.08	37,37,37,37	0
34	NA	N	8347	1/1	0.95	0.05	24,24,24,24	0
32	MG	A	8023	1/1	0.95	0.07	45,45,45,45	0
34	NA	A	8323	1/1	0.95	0.13	45,45,45,45	0
32	MG	A	8071	1/1	0.95	0.04	93,93,93,93	0
34	NA	A	8360	1/1	0.95	0.16	61,61,61,61	0
34	NA	U	8343	1/1	0.95	0.04	27,27,27,27	0
34	NA	A	8361	1/1	0.95	0.13	62,62,62,62	0
32	MG	A	8043	1/1	0.95	0.06	32,32,32,32	0
32	MG	A	8104	1/1	0.95	0.06	52,52,52,52	0
35	CL	A	8513	1/1	0.95	0.09	56,56,56,56	0
32	MG	A	8052	1/1	0.95	0.06	51,51,51,51	0
32	MG	A	8112	1/1	0.95	0.12	57,57,57,57	0
32	MG	A	8040	1/1	0.96	0.17	100,100,100,100	0
34	NA	A	8338	1/1	0.96	0.05	44,44,44,44	0
32	MG	A	8094	1/1	0.96	0.11	65,65,65,65	0
34	NA	A	8314	1/1	0.96	0.08	43,43,43,43	0
32	MG	A	8008	1/1	0.96	0.09	42,42,42,42	0
35	CL	P	8508	1/1	0.96	0.07	82,82,82,82	0
35	CL	A	8512	1/1	0.96	0.07	31,31,31,31	0
34	NA	A	8305	1/1	0.96	0.06	27,27,27,27	0
35	CL	A	8514	1/1	0.96	0.08	50,50,50,50	0
32	MG	A	8106	1/1	0.96	0.07	76,76,76,76	0
34	NA	A	8320	1/1	0.96	0.08	42,42,42,42	0
32	MG	A	8044	1/1	0.96	0.09	54,54,54,54	0
32	MG	A	8087	1/1	0.96	0.05	49,49,49,49	0
34	NA	A	8324	1/1	0.96	0.17	51,51,51,51	0
34	NA	A	8367	1/1	0.96	0.08	43,43,43,43	0
32	MG	A	8039	1/1	0.97	0.06	51,51,51,51	0
32	MG	A	8014	1/1	0.97	0.06	20,20,20,20	0
32	MG	A	8115	1/1	0.97	0.07	59,59,59,59	0
32	MG	A	8108	1/1	0.97	0.06	53,53,53,53	0
32	MG	A	8056	1/1	0.97	0.04	56,56,56,56	0
34	NA	A	8336	1/1	0.97	0.03	49,49,49,49	0
37	CD	P	8405	1/1	0.97	0.04	89,89,89,89	0
32	MG	A	8099	1/1	0.97	0.09	68,68,68,68	0
34	NA	A	8359	1/1	0.97	0.15	60,60,60,60	0
34	NA	E	8304	1/1	0.97	0.05	25,25,25,25	0
32	MG	A	8059	1/1	0.98	0.04	47,47,47,47	0
34	NA	A	8315	1/1	0.98	0.08	43,43,43,43	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	0.09	44,44,44,44	0
34	NA	A	8317	1/1	0.98	0.03	32,32,32,32	0
34	NA	A	8376	1/1	0.98	0.09	79,79,79,79	0
32	MG	A	8034	1/1	0.98	0.04	36,36,36,36	0
32	MG	A	8063	1/1	0.98	0.05	85,85,85,85	0
32	MG	A	8035	1/1	0.98	0.04	48,48,48,48	0
32	MG	A	8005	1/1	0.98	0.04	38,38,38,38	0
32	MG	L	8069	1/1	0.98	0.03	81,81,81,81	0
32	MG	A	8019	1/1	0.98	0.07	30,30,30,30	0
32	MG	A	8097	1/1	0.98	0.09	32,32,32,32	0
32	MG	A	8098	1/1	0.98	0.12	33,33,33,33	0
32	MG	A	8068	1/1	0.98	0.04	46,46,46,46	0
32	MG	A	8022	1/1	0.98	0.05	32,32,32,32	0
32	MG	A	8002	1/1	0.98	0.05	36,36,36,36	0
32	MG	A	8072	1/1	0.98	0.04	53,53,53,53	0
32	MG	A	8012	1/1	0.98	0.05	44,44,44,44	0
32	MG	A	8054	1/1	0.98	0.05	33,33,33,33	0
34	NA	M	8380	1/1	0.98	0.06	65,65,65,65	0
34	NA	A	8364	1/1	0.98	0.12	54,54,54,54	0
32	MG	A	8079	1/1	0.98	0.05	48,48,48,48	0
32	MG	A	8027	1/1	0.98	0.04	54,54,54,54	0
32	MG	A	8110	1/1	0.98	0.09	30,30,30,30	0
32	MG	A	8083	1/1	0.98	0.07	37,37,37,37	0
32	MG	A	8085	1/1	0.98	0.06	95,95,95,95	0
32	MG	A	8029	1/1	0.98	0.03	38,38,38,38	0
32	MG	A	8017	1/1	0.99	0.08	35,35,35,35	0
32	MG	A	8018	1/1	0.99	0.03	42,42,42,42	0
32	MG	A	8091	1/1	0.99	0.06	67,67,67,67	0
32	MG	A	8061	1/1	0.99	0.04	45,45,45,45	0
32	MG	A	8006	1/1	0.99	0.04	57,57,57,57	0
32	MG	A	8021	1/1	0.99	0.03	32,32,32,32	0
32	MG	A	8003	1/1	0.99	0.03	23,23,23,23	0
32	MG	A	8010	1/1	0.99	0.03	30,30,30,30	0
32	MG	A	8004	1/1	0.99	0.05	53,53,53,53	0
32	MG	A	8026	1/1	0.99	0.02	33,33,33,33	0
32	MG	A	8013	1/1	0.99	0.04	42,42,42,42	0
32	MG	A	8048	1/1	0.99	0.03	33,33,33,33	0
32	MG	A	8028	1/1	0.99	0.04	37,37,37,37	0
32	MG	A	8074	1/1	0.99	0.05	42,42,42,42	0
32	MG	A	8001	1/1	0.99	0.03	33,33,33,33	0
34	NA	A	8311	1/1	0.99	0.04	31,31,31,31	0
32	MG	A	8030	1/1	0.99	0.04	34,34,34,34	0

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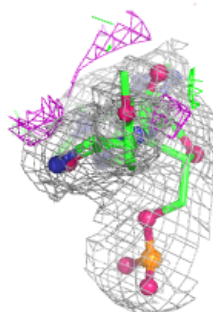
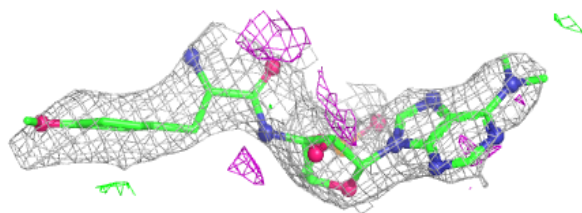
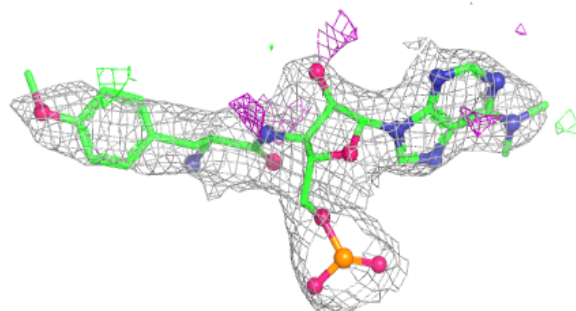
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8107	1/1	0.99	0.03	36,36,36,36	0
32	MG	A	8077	1/1	0.99	0.04	32,32,32,32	0
32	MG	A	8032	1/1	0.99	0.07	34,34,34,34	0
32	MG	A	8080	1/1	0.99	0.04	35,35,35,35	0
32	MG	A	8081	1/1	0.99	0.03	39,39,39,39	0
32	MG	A	8015	1/1	0.99	0.03	50,50,50,50	0
32	MG	A	8016	1/1	0.99	0.03	36,36,36,36	0
32	MG	A	8084	1/1	0.99	0.07	50,50,50,50	0
32	MG	A	8036	1/1	0.99	0.04	38,38,38,38	0
32	MG	A	8086	1/1	0.99	0.04	49,49,49,49	0
32	MG	A	8037	1/1	0.99	0.05	43,43,43,43	0
32	MG	C	8065	1/1	0.99	0.03	68,68,68,68	0
32	MG	A	8058	1/1	0.99	0.07	39,39,39,39	0
32	MG	A	8033	1/1	1.00	0.03	25,25,25,25	0
32	MG	A	8009	1/1	1.00	0.02	32,32,32,32	0
32	MG	A	8007	1/1	1.00	0.06	28,28,28,28	0
32	MG	A	8020	1/1	1.00	0.04	46,46,46,46	0
32	MG	A	8025	1/1	1.00	0.02	40,40,40,40	0
32	MG	A	8038	1/1	1.00	0.04	33,33,33,33	0
32	MG	A	8031	1/1	1.00	0.02	32,32,32,32	0
37	CD	2	8402	1/1	1.00	0.03	57,57,57,57	0
32	MG	A	8011	1/1	1.00	0.04	24,24,24,24	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.

Electron density around PPU 5 76:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.