



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:36 PM UTC

PDB ID : 1K9M / pdb_00001k9m
Title : Co-crystal structure of tylosin bound to the 50S ribosomal subunit of *Haloarcula marismortui*
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-10-29
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

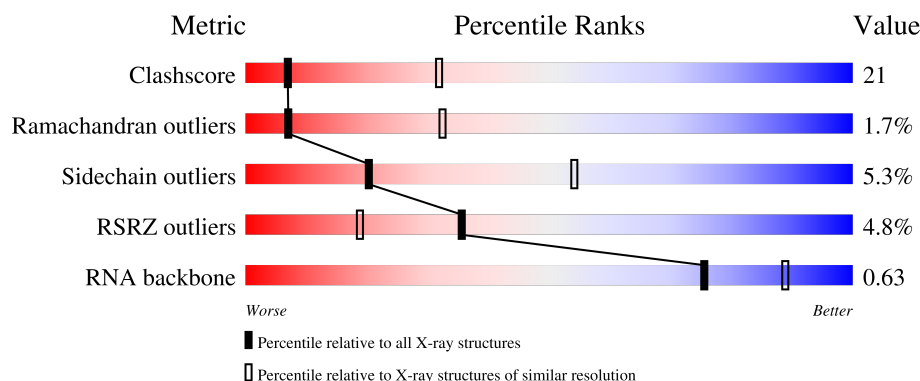
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	2922	4% 50% 36% 7% 6%
2	B	122	5% 44% 40% 11% 5%
3	C	239	2% 50% 41% 8% .
4	D	337	46% 46% 7%
5	E	246	57% 37% 6%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	NA	A	8377	-	-	-	X
34	CL	O	8507	-	-	X	-

2 Entry composition

There are 37 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 RRNA.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

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

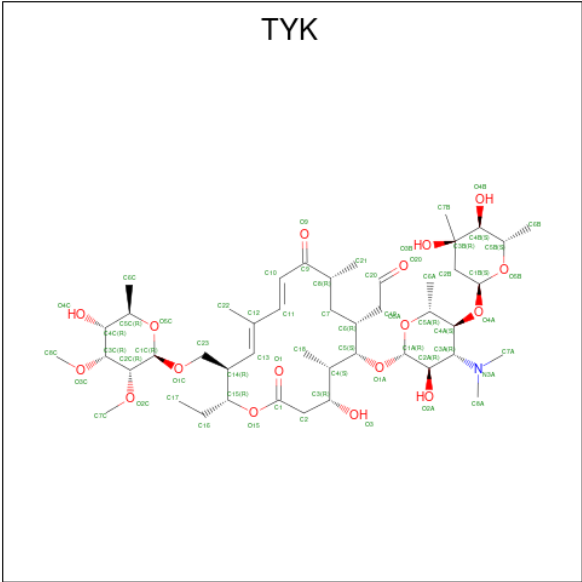
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

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

- Molecule 31 is TYLOSIN (CCD ID: TYK) (formula: C₄₆H₇₇NO₁₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			64	46	1	17		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	111	Total	Mg	0	0
			111	111		
32	B	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	D	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	1	1	Total	Mg	0	0
			1	1		
32	4	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	72	Total Na 72 72	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0
33	N	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	2	Total Na 2 2	0	0
33	T	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	8	Total Cl 8 8	0	0
34	C	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	4	Total Cl 4 4	0	0
34	M	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0
34	P	1	Total Cl 1 1	0	0
34	R	1	Total Cl 1 1	0	0

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

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

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

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

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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5921	Total 5921	O 5921	0	0
37	B	142	Total 142	O 142	0	0
37	C	126	Total 126	O 126	0	0
37	D	146	Total 146	O 146	0	0
37	E	174	Total 174	O 174	0	0
37	F	51	Total 51	O 51	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	26	Total 26	O 26	0	0
37	I	22	Total 22	O 22	0	0
37	J	79	Total 79	O 79	0	0
37	K	54	Total 54	O 54	0	0
37	L	60	Total 60	O 60	0	0
37	M	84	Total 84	O 84	0	0
37	N	127	Total 127	O 127	0	0
37	O	64	Total 64	O 64	0	0
37	P	42	Total 42	O 42	0	0
37	Q	66	Total 66	O 66	0	0
37	R	53	Total 53	O 53	0	0
37	S	84	Total 84	O 84	0	0
37	T	34	Total 34	O 34	0	0
37	U	39	Total 39	O 39	0	0
37	V	26	Total 26	O 26	0	0
37	W	12	Total 12	O 12	0	0
37	X	70	Total 70	O 70	0	0
37	Y	29	Total 29	O 29	0	0
37	Z	96	Total 96	O 96	0	0
37	1	37	Total 37	O 37	0	0

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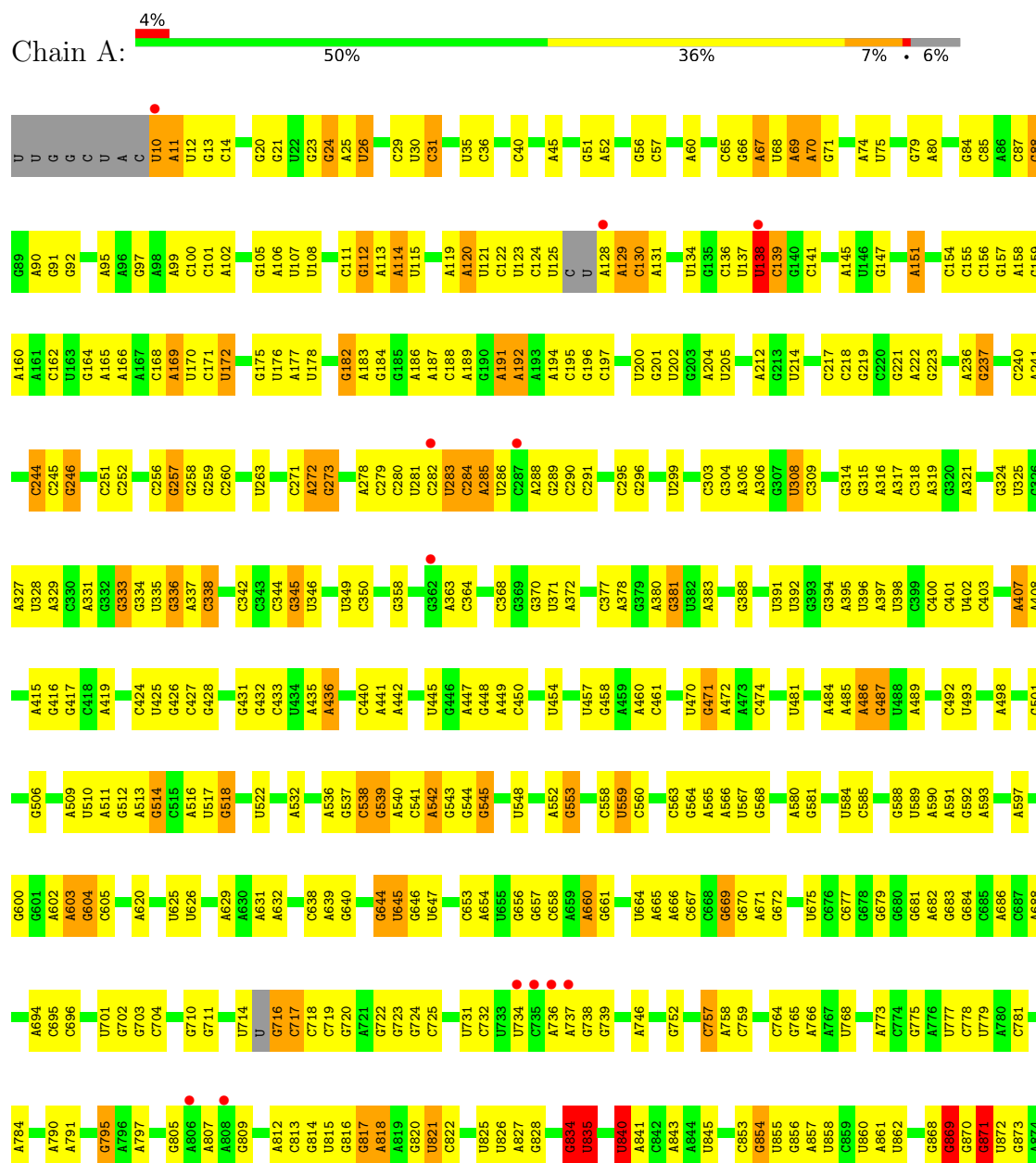
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	56	Total 56	O 56	0	0
37	3	43	Total 43	O 43	0	0
37	4	72	Total 72	O 72	0	0

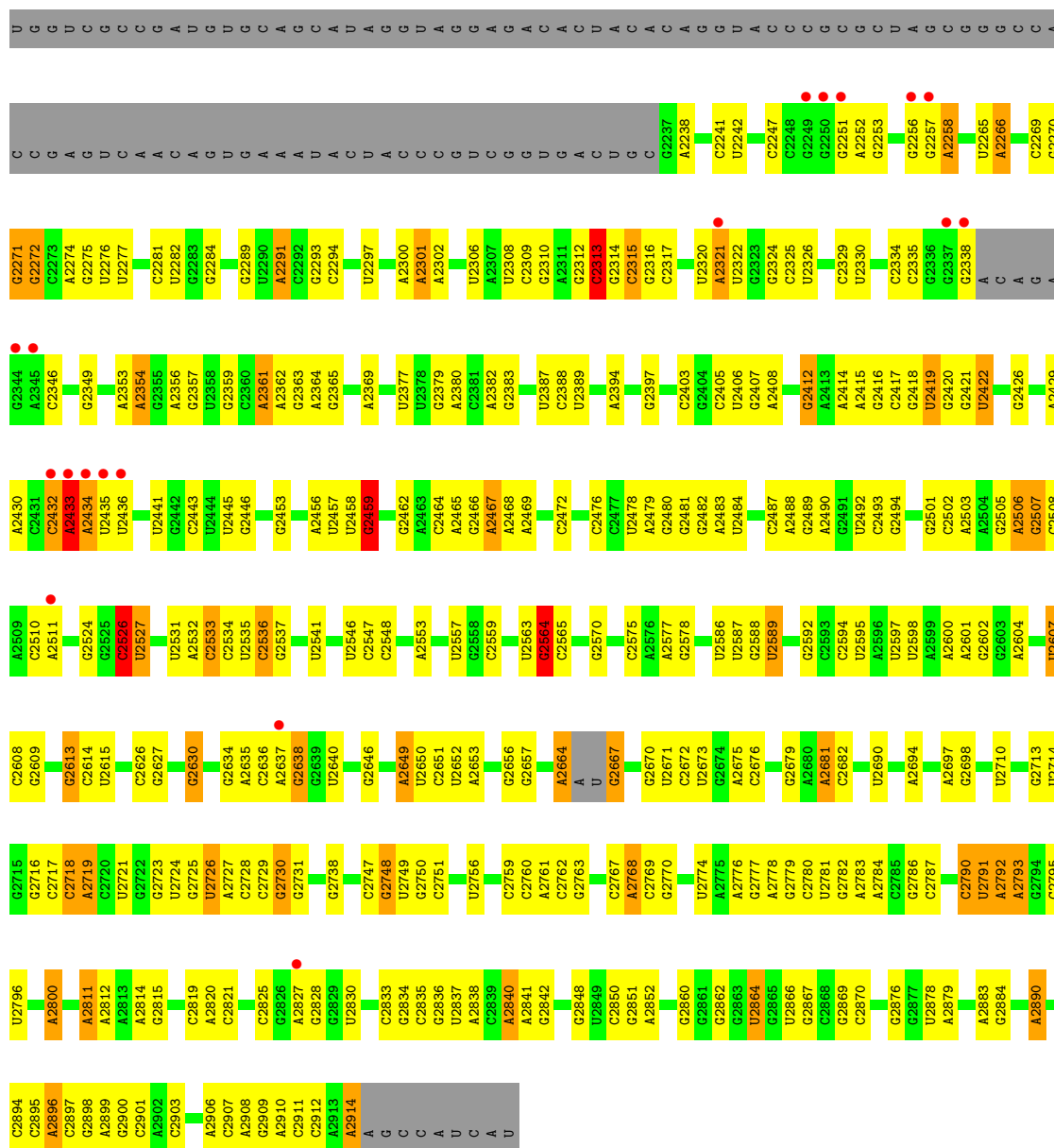
3 Residue-property plots

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

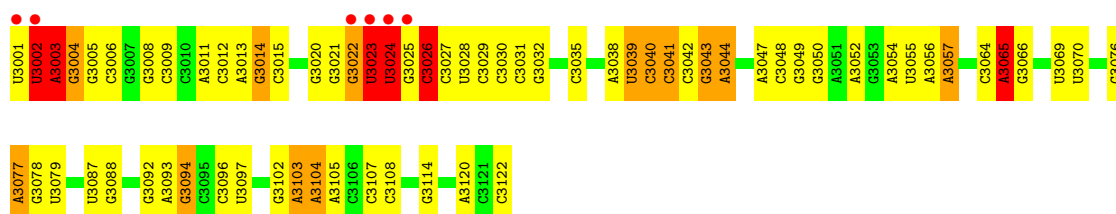
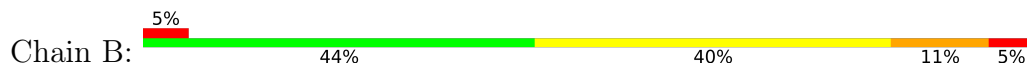
• Molecule 1: 23S rRNA



G2068	C1976	U1890	C1798	A1710	C1609	C1514	C1421	U1310	U1219	G1159	G1059	A875
G2071	U1977	C1894	A1711	A1712	C1610	A1515	U1422	G1311	C1229	G1160	C1060	A876
G2072	U1978	A1804	A1713	A1714	C1613	C1516	C1423	G1312	C1230	A1161	C	G877
A2074	U1979	G1805	A1715	A1716	A1614	G1523	A1424	G1325	U1234	G1162	U1066	G878
G2079	A1981	C1810	A1717	A1718	A1615	U1524	G1430	U1326	A1067	G1163	C	A882
G2080	C1982	A1815	C1721	C1722	U1625	G1525	G1433	A1328	G1072	A1164	C	U883
A2081	G1989	C1816	U1722	U1723	A1626	G1526	A1434	A1329	A1073	A1165	C	U884
G2082	C1990	G1817	G1724	G1725	A1630	A1527	U1435	A1330	U1079	G1166	C	G885
A2083	A1991	G1819	C1726	C1727	A1633	G1529	C1436	A1331	A1081	U1167	C	A886
G2087	U1992	G1820	A1730	A1731	G1634	U1530	G1441	U1332	A1082	U1170	A	G887
C2088	C1993	U1825	G1732	G1733	U1635	A1533	A1442	A1333	A1083	G1171	C	U888
A2089	A1994	C1826	A1734	A1735	G1636	G1534	G1443	U1334	A1084	G1172	A	C890
G2090	U1995	G1827	C1736	C1737	A1637	U1535	A1444	A1335	A1085	A1173	G	G891
G2091	U1996	G1828	A1738	A1739	A1638	G1536	G1445	A1337	A1086	G1174	G	G892
G2092	A1997	G1829	C1740	C1741	A1641	U1537	U1446	C1342	A1088	G1175	A	G898
G2093	G1998	A1830	A1742	A1743	A1642	G1543	U1447	A1349	U1096	A1177	C	G902
G2094	C2000	C1833	A1746	A1747	A1647	U1544	C1450	U1349	A1097	C1178	G	U903
A2095	G2001	U1834	A1748	A1749	G1647	G1545	A1451	U1350	A1098	U1180	C	U904
G2096	C2002	G1835	U1750	U1751	A1654	G1546	G1452	G1351	A1099	A1181	C	C905
G2097	U2003	U1836	A1752	A1753	G1655	U1549	C1456	A1352	C1103	C1182	C	G911
G2098	U2004	A1839	G1754	G1755	A1656	G1552	U1457	G1353	U1109	C1184	A	A912
G2099	G2005	C1841	A1756	A1757	A1657	U1553	A1458	A1354	G1110	U1185	C	G918
A2100	U2006	A1840	A1758	A1759	A1658	G1554	A1459	C1360	A1114	U1187	C	U919
G2101	G2007	U1845	U1760	U1761	A1659	U1555	C1462	C1366	C920	A1188	C	G921
A2102	A2010	U1846	A1762	A1763	G1660	U1559	A1463	A1372	U1115	A1189	A	A922
C2103	U2011	A1847	G1764	G1765	A1661	U1561	C1469	A1376	U1116	A1190	A	A923
G2104	U2012	U1850	A1766	A1767	A1662	U1562	A1470	A1377	A1117	A1191	C	A926
C2105	G2013	C1851	C1768	C1769	U1667	G1563	A1471	C1377	A1118	A1192	C	A929
C2106	U2107	G1855	U1770	U1771	U1668	U1564	A1472	U1378	U1120	A1193	C	C930
A2107	A2015	U1856	C1772	C1773	A1669	C1564	A1473	A1379	A1123	U1194	C	G931
U2109	U2016	C1857	G1774	G1775	G1670	U1573	C1474	U1380	C1127	U1195	C	U932
G2110	A2030	A1857	A1776	A1777	A1676	C1574	C1477	G1391	U1128	U1197	C	G941
A2111	U2031	U1860	C1768	C1769	A1677	A1580	U1478	A1392	U1129	A1200	C	U942
G2112	G2032	C1861	U1770	U1771	A1678	G1589	C1483	A1393	U1130	C1201	C	U949
C2113	U2033	G1862	U1772	U1773	A1681	G1592	G1484	C1394	A1131	A1202	C	A951
U2114	C2034	A1863	C1774	C1775	A1682	C1593	A1487	U1398	A1132	G1203	C	G950
U2115	C2035	G1868	A1774	A1775	G1683	C1594	U1488	A1399	A1133	C1204	C	G952
C2119	C2037	U1874	A1776	A1777	A1685	G1595	A1494	C1401	U1135	U1205	C	U954
U2120	A2038	G1877	A1778	A1779	C1686	U1596	C1495	G1407	G1136	A1207	C	G959
G2121	G2044	U1878	A1780	A1781	A1687	A1597	U1500	A1408	U1137	C1208	C	G960
C2122	C2045	G1879	U1782	U1783	A1688	A1598	A1501	G1409	U1138	G1209	C	A961
A2123	G2046	U1882	C1784	C1785	C1690	G1601	A1502	U1412	C1140	G1210	C	G962
U2127	G2050	C1883	U1786	U1787	A1691	G1602	A1503	U1417	G1151	C1211	C	C963
G2128	A2054	G1884	A1788	A1789	C1692	G1604	A1504	U1418	A1152	C1212	C	U970
U2133	U2055	A1885	G1789	G1790	C1699	G1605	U1505	G1417	C1156	U1214	C	G
G2134	A2056	U1886	C1790	C1791	A1700	A1606	U1506	U1419	C1157	U1215	C	U1056
A2135	U2059	U1887	A1791	A1792	A1702	G1608	C1513	C1420	G1216	A1057	C	A1058
G2136	A								G1158	U1218	C	U

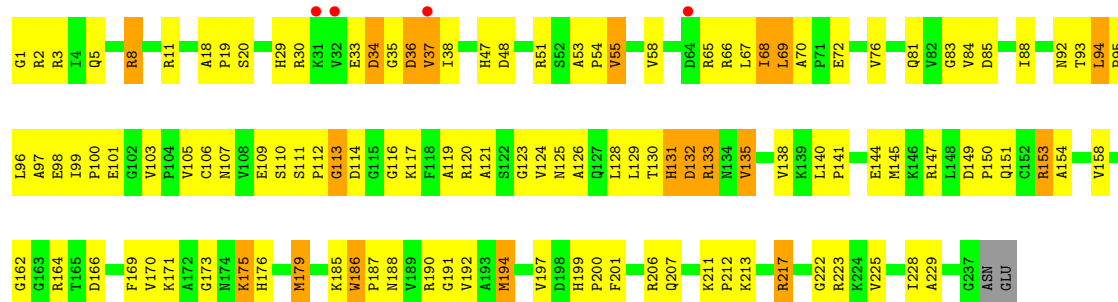


• Molecule 2: 5S RRNA



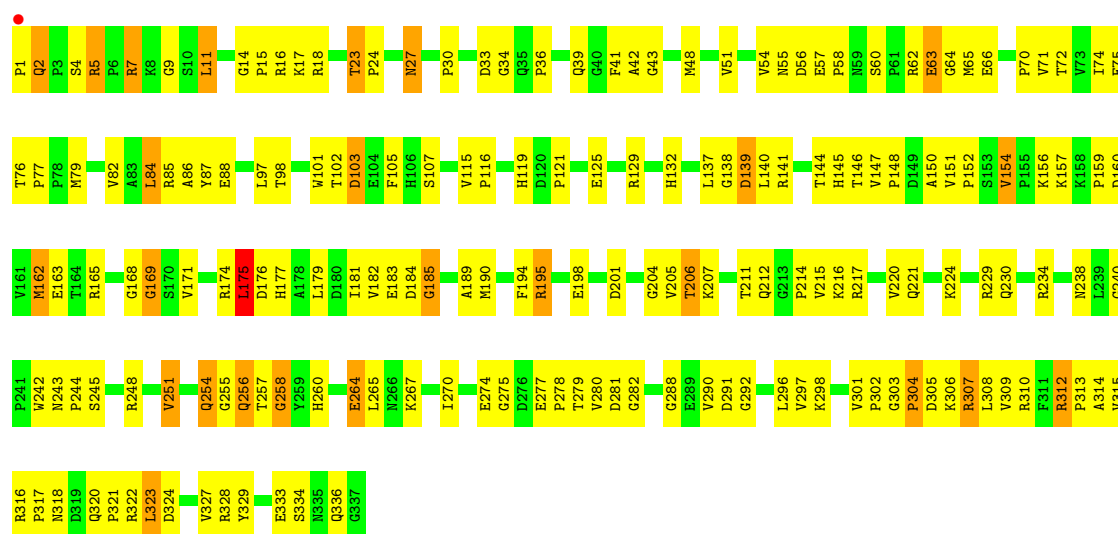
• Molecule 3: RIBOSOMAL PROTEIN L2





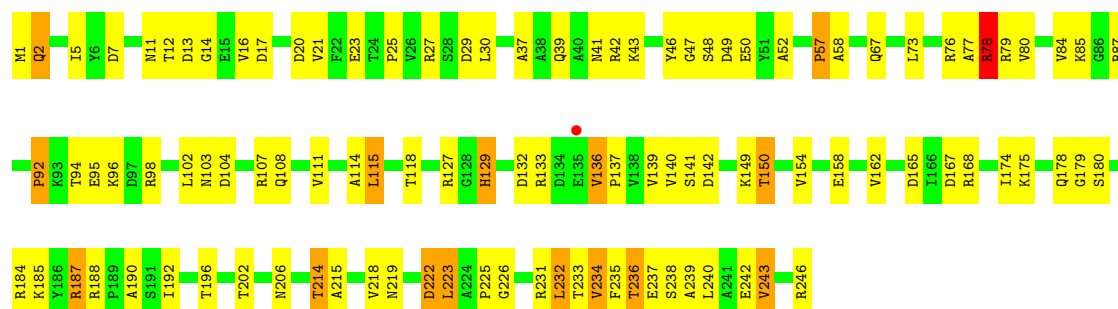
• Molecule 4: RIBOSOMAL PROBLEM L3

Chain D: 46% 46% 7%



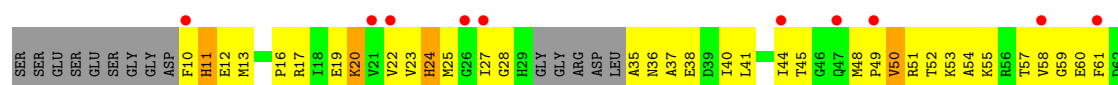
• Molecule 5: RIBOSOMAL PROBLEM L4

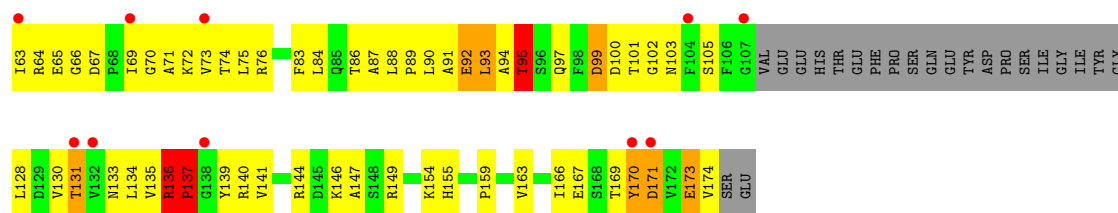
Chain E: 57% 37% 6%



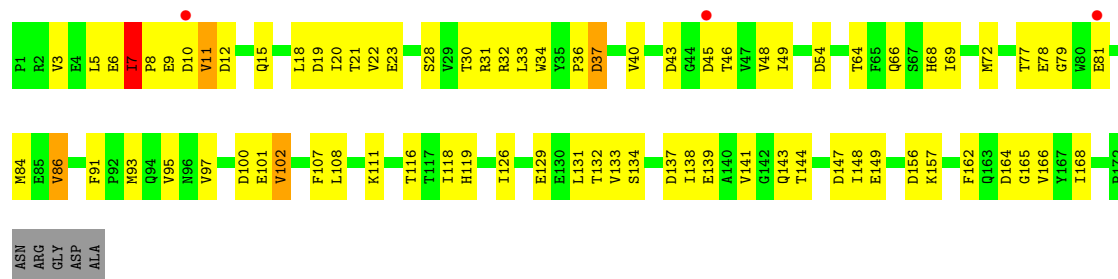
• Molecule 6: RIBOSOMAL PROBLEM L5

Chain F: 11% 27% 45% 6% 20%

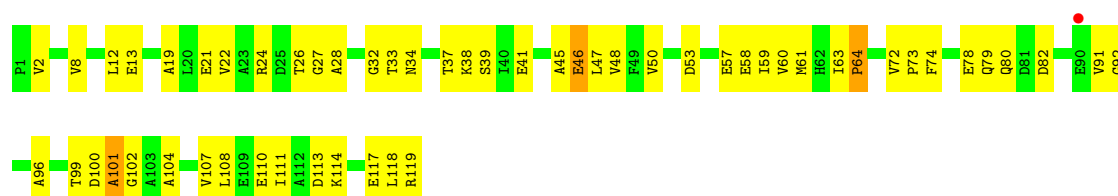




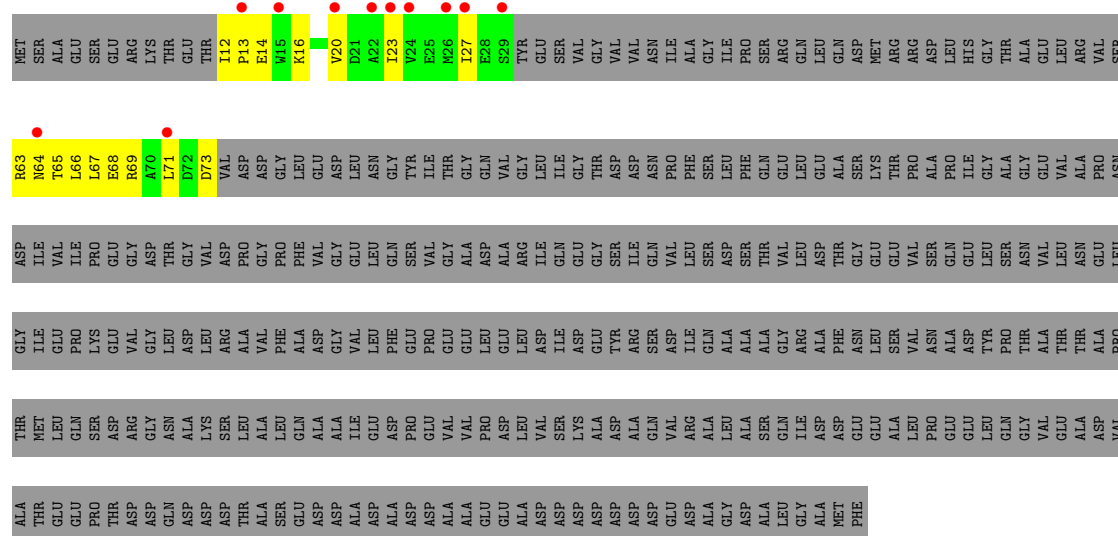
● Molecule 7: RIBOSOMAL PROTEIN L6



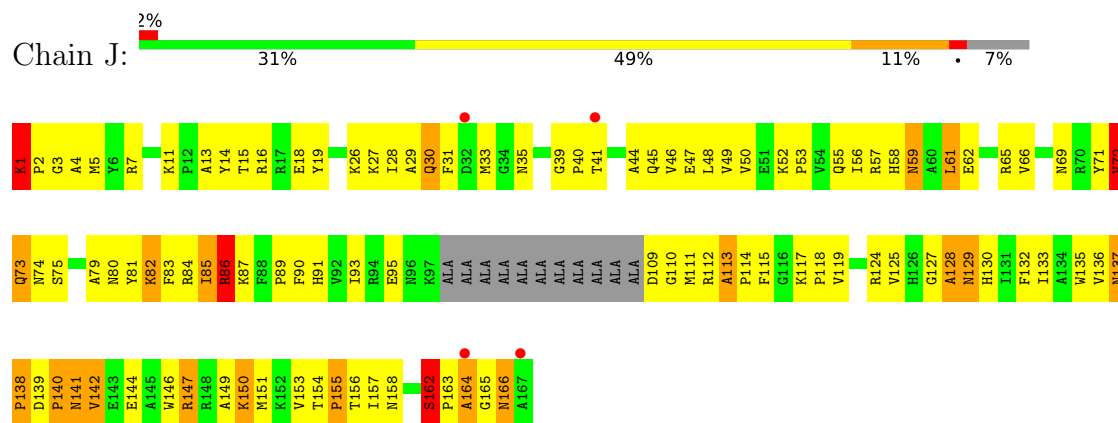
● Molecule 8: RIBOSOMAL PROTEIN L7AE



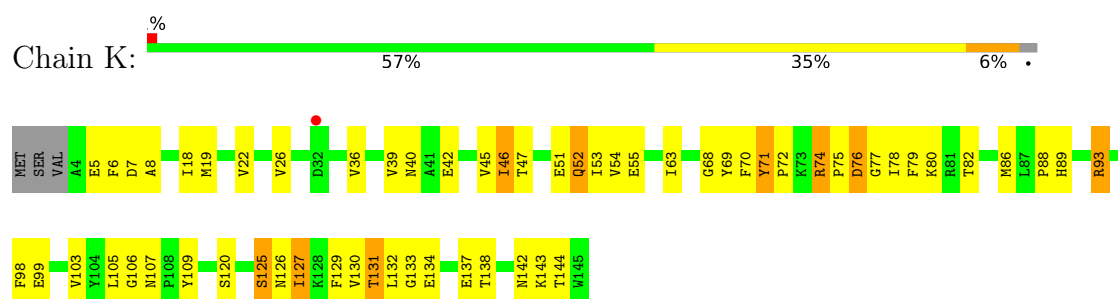
● Molecule 9: RIBOSOMAL PROTEIN L10



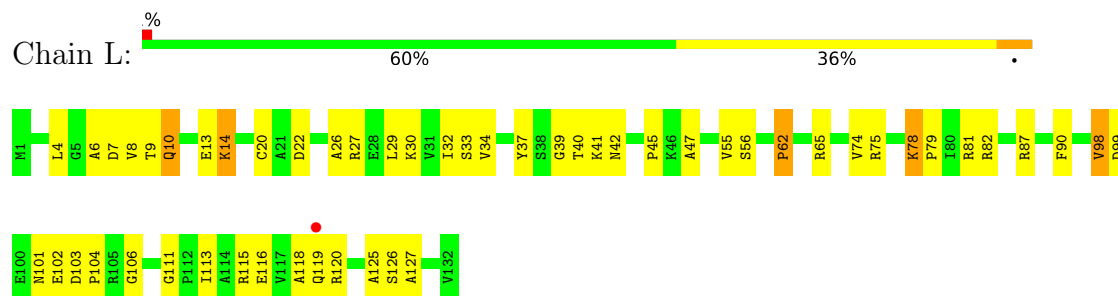
- Molecule 10: RIBOSOMAL PROTEIN L10E



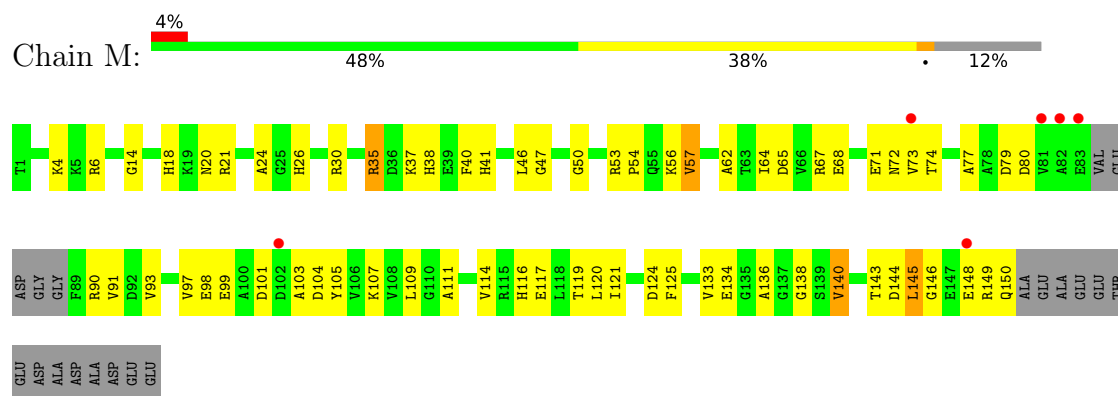
- Molecule 11: RIBOSOMAL PROTEIN L13



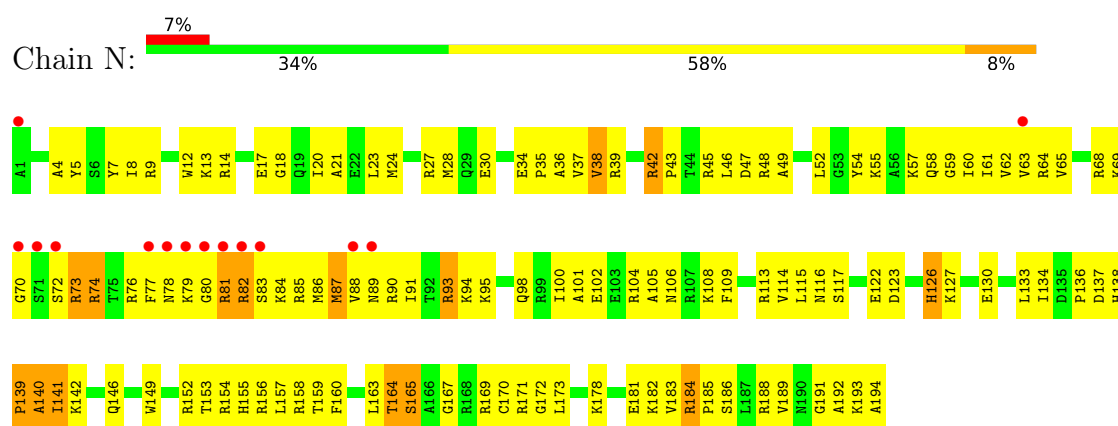
- Molecule 12: RIBOSOMAL PROTEIN L14



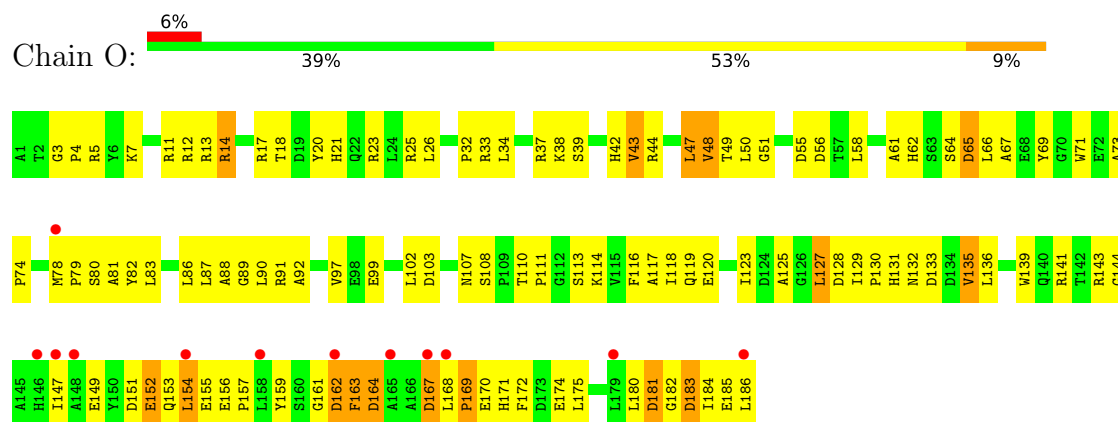
- Molecule 13: RIBOSOMAL PROTEIN L15



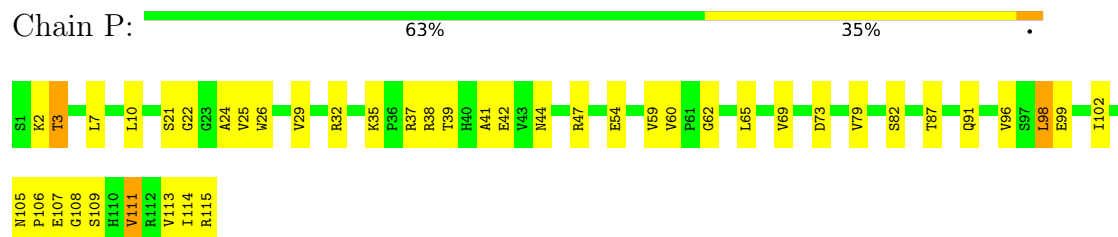
- Molecule 14: RIBOSOMAL PROTEIN L15E



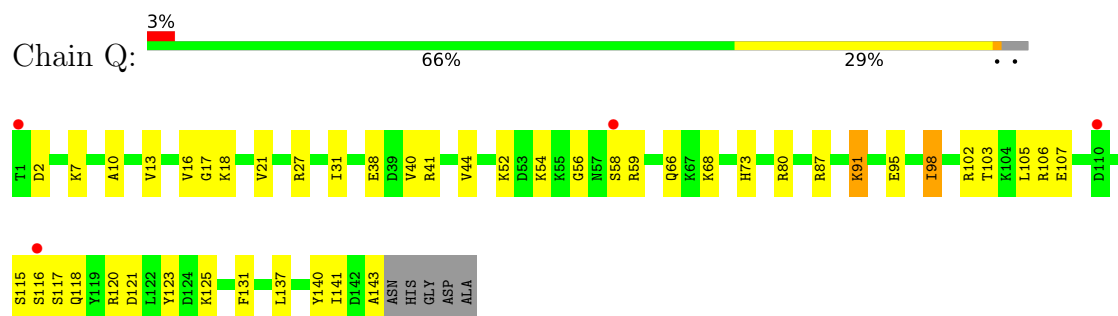
● Molecule 15: RIBOSOMAL PROTEIN L18



● Molecule 16: RIBOSOMAL PROTEIN L18E



● Molecule 17: RIBOSOMAL PROTEIN L19E



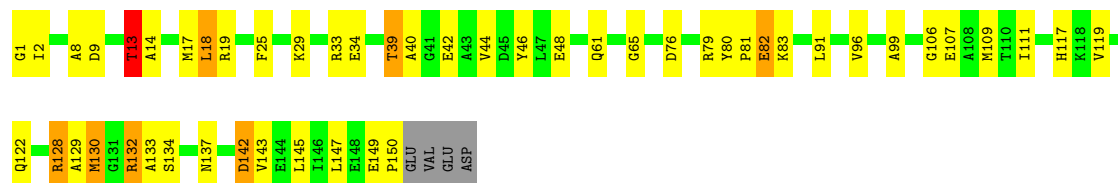
● Molecule 18: RIBOSOMAL PROTEIN L21E





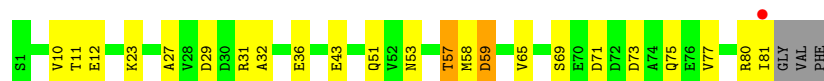
• Molecule 19: RIBOSOMAL PROTEIN L22

Chain S: 65% 27% 5% . .



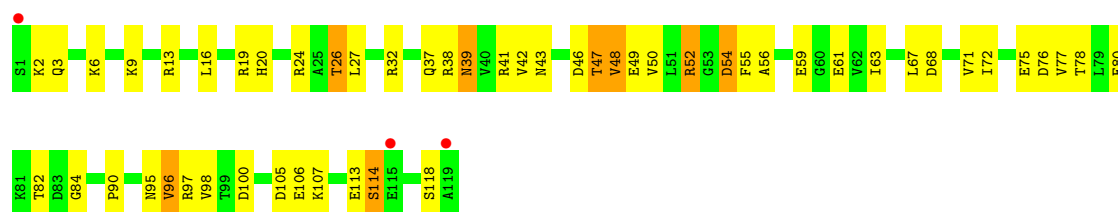
• Molecule 20: RIBOSOMAL PROTEIN L23

Chain T: 69% 25% . .



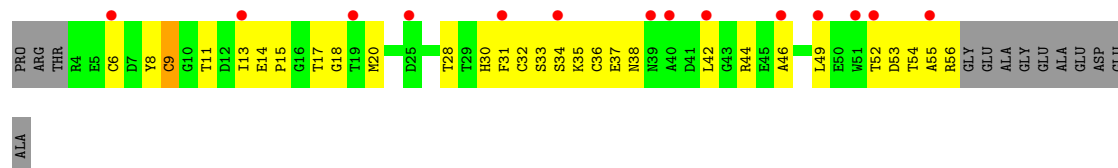
• Molecule 21: RIBOSOMAL PROTEIN L24

Chain U: 55% 38% 7%



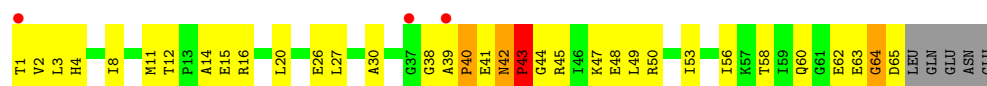
• Molecule 22: RIBOSOMAL PROTEIN L24E

Chain V: 21% 36% 42% 20%

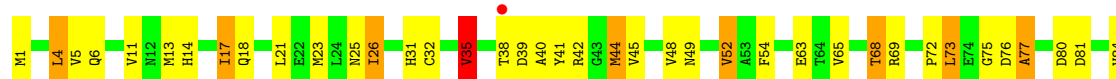


• Molecule 23: RIBOSOMAL PROTEIN L29

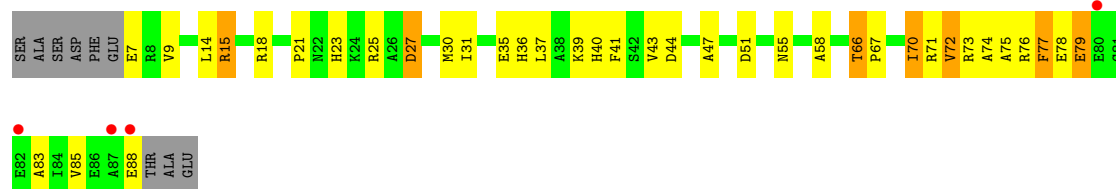
Chain W: 4% 44% 43% 7%



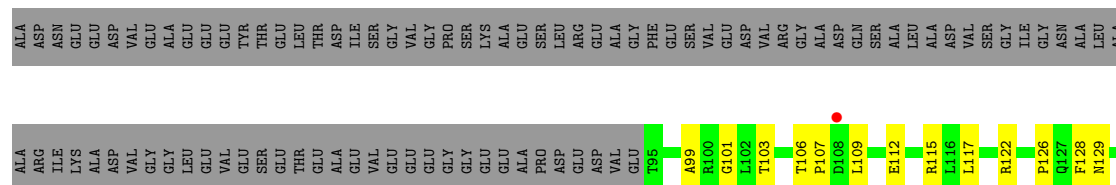
• Molecule 24: RIBOSOMAL PROTEIN L30



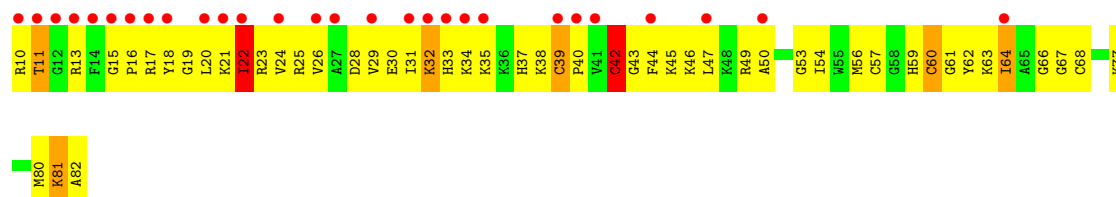
• Molecule 25: RIBOSOMAL PROTEIN L31E



• Molecule 26: RIBOSOMAL PROTEIN L32E

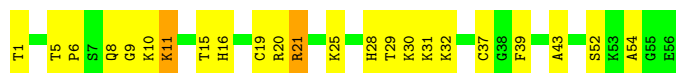


• Molecule 27: RIBOSOMAL PROTEIN L37Ae



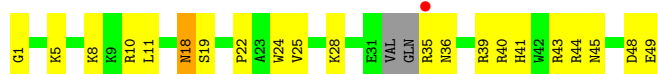
• Molecule 28: RIBOSOMAL PROTEIN L37E

Chain 2:  59% 38% .



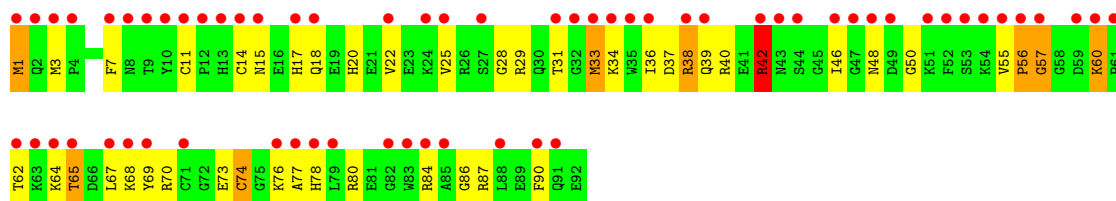
• Molecule 29: RIBOSOMAL PROTEIN L39E

Chain 3:  2% 52% 42% . .



• Molecule 30: RIBOSOMAL PROTEIN L44E

Chain 4:  68% 50% 40% 9% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-3.00) 92.5 (19.99-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.262 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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, K, CD, TYK, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	5/66076 (0.0%)	0.74	57/103052 (0.1%)
2	B	0.75	10/2905 (0.3%)	0.86	12/4528 (0.3%)
3	C	0.75	5/1787 (0.3%)	1.15	12/2409 (0.5%)
4	D	0.62	0/2689	1.12	20/3652 (0.5%)
5	E	0.64	0/1883	1.09	10/2551 (0.4%)
6	F	0.49	0/1111	0.98	4/1498 (0.3%)
7	G	0.57	0/1382	0.96	5/1880 (0.3%)
8	H	0.53	0/896	0.98	2/1219 (0.2%)
9	I	0.63	0/241	0.90	1/324 (0.3%)
10	J	0.65	0/1246	1.31	17/1686 (1.0%)
11	K	0.62	0/1135	1.01	4/1530 (0.3%)
12	L	0.62	0/1003	1.12	6/1351 (0.4%)
13	M	0.54	0/1126	1.12	5/1504 (0.3%)
14	N	0.75	0/1633	1.23	13/2180 (0.6%)
15	O	0.55	0/1473	1.20	17/1999 (0.9%)
16	P	0.62	0/873	1.07	4/1181 (0.3%)
17	Q	0.58	0/1143	0.99	1/1521 (0.1%)
18	R	0.64	0/748	1.18	8/1005 (0.8%)
19	S	0.86	5/1172 (0.4%)	1.14	7/1578 (0.4%)
20	T	0.55	0/648	1.01	3/875 (0.3%)
21	U	0.55	0/957	1.04	6/1289 (0.5%)
22	V	0.91	0/417	1.17	2/562 (0.4%)
23	W	0.53	0/502	1.06	4/675 (0.6%)
24	X	0.73	1/1218 (0.1%)	1.10	9/1655 (0.5%)
25	Y	0.64	0/664	1.06	3/895 (0.3%)
26	Z	0.61	0/1146	1.05	2/1536 (0.1%)
27	1	1.00	2/575 (0.3%)	1.21	3/763 (0.4%)
28	2	0.59	0/437	1.08	3/578 (0.5%)
29	3	0.54	0/398	0.86	0/527
30	4	1.22	2/771 (0.3%)	1.14	4/1024 (0.4%)
All	All	0.56	30/98255 (0.0%)	0.86	244/147027 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	150
2	B	0	4
All	All	1	154

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2104	C	O5'-C5'	-13.18	1.22	1.42
2	B	3023	U	C2'-O2'	10.11	1.57	1.42
3	C	186	TRP	C-O	-9.89	1.12	1.24
2	B	3023	U	O5'-C5'	8.70	1.55	1.42
3	C	186	TRP	CA-CB	-8.61	1.39	1.53
19	S	132	ARG	N-CA	8.20	1.55	1.45
19	S	132	ARG	CA-CB	-7.68	1.40	1.53
2	B	3025	G	O3'-P	7.37	1.72	1.61
2	B	3025	G	C4'-O4'	7.33	1.56	1.45
2	B	3026	C	P-OP2	-7.11	1.34	1.49
30	4	1	MET	SD-CE	6.89	1.96	1.79
2	B	3024	U	P-OP2	-6.63	1.35	1.49
1	A	2106	C	O3'-P	-6.54	1.51	1.61
2	B	3025	G	P-OP2	-6.51	1.35	1.49
2	B	3025	G	C3'-O3'	-6.49	1.32	1.42
30	4	33	MET	SD-CE	6.45	1.95	1.79
24	X	44	MET	SD-CE	-6.44	1.63	1.79
3	C	194	MET	SD-CE	-6.33	1.63	1.79
19	S	129	ALA	C-O	-6.32	1.15	1.23
3	C	186	TRP	CA-C	6.22	1.59	1.52
1	A	2100	A	O5'-C5'	6.08	1.51	1.42
2	B	3026	C	P-O5'	-5.64	1.51	1.59
27	1	22	ILE	CA-CB	5.56	1.60	1.54
2	B	3004	G	O5'-C5'	5.48	1.50	1.42
3	C	186	TRP	N-CA	5.43	1.57	1.45
1	A	1206	U	P-OP2	5.39	1.59	1.49
19	S	130	MET	CB-CG	-5.25	1.36	1.52
19	S	128	ARG	CA-C	-5.16	1.46	1.52
1	A	2099	G	C3'-O3'	5.11	1.49	1.42
27	1	24	VAL	CA-CB	5.07	1.60	1.54

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-14.92	63.25	108.00
1	A	1563	G	C2'-C3'-O3'	14.11	130.66	109.50
10	J	74	ASN	N-CA-C	-14.03	94.62	114.12
1	A	1164	U	OP2-P-O3'	-13.98	66.05	108.00
10	J	141	ASN	N-CA-C	-12.24	98.05	113.23
14	N	141	ILE	N-CA-C	-11.78	102.36	111.90
15	O	135	VAL	N-CA-C	-11.53	101.83	113.47
1	A	1979	G	C2'-C3'-O3'	10.02	124.53	109.50
14	N	139	PRO	N-CA-C	-9.52	97.72	111.33
4	D	23	THR	CA-C-N	9.26	129.32	119.78
4	D	23	THR	C-N-CA	9.26	129.32	119.78
1	A	1563	G	C4'-C3'-O3'	9.05	122.97	109.40
1	A	1942	A	C5'-C4'-C3'	8.96	129.45	116.00
2	B	3025	G	C1'-C2'-O2'	-8.93	95.01	108.40
6	F	136	ARG	CA-C-N	8.78	130.81	119.84
6	F	136	ARG	C-N-CA	8.78	130.81	119.84
1	A	2103	A	C5'-C4'-O4'	8.77	122.25	109.10
18	R	17	LYS	N-CA-C	-8.59	98.23	110.08
24	X	35	VAL	N-CA-C	8.35	117.55	107.61
2	B	3025	G	O3'-P-O5'	8.26	116.38	104.00
2	B	3026	C	C3'-C2'-O2'	8.15	122.93	110.70
10	J	1	LYS	CA-C-N	7.99	127.92	119.85
10	J	1	LYS	C-N-CA	7.99	127.92	119.85
7	G	11	VAL	N-CA-C	7.92	121.48	109.20
4	D	323	LEU	N-CA-C	7.82	120.40	110.24
10	J	156	THR	N-CA-C	-7.80	98.94	110.48
20	T	27	ALA	N-CA-C	-7.74	96.63	109.24
2	B	3024	U	C4'-C3'-O3'	7.70	124.55	113.00
13	M	57	VAL	N-CA-C	-7.65	105.39	112.43
1	A	2104	C	C3'-C2'-O2'	-7.63	99.25	110.70
15	O	51	GLY	CA-C-N	7.62	127.66	119.28
15	O	51	GLY	C-N-CA	7.62	127.66	119.28
18	R	47	VAL	CA-C-N	7.53	127.07	119.24
18	R	47	VAL	C-N-CA	7.53	127.07	119.24
15	O	133	ASP	N-CA-C	7.52	120.43	111.33
15	O	169	PRO	N-CA-C	-7.51	104.13	114.27
5	E	175	LYS	N-CA-C	7.50	120.55	110.35
30	4	55	VAL	CA-C-N	7.49	129.20	119.84
30	4	55	VAL	C-N-CA	7.49	129.20	119.84
10	J	147	ARG	N-CA-C	-7.49	103.10	111.71
18	R	86	VAL	N-CA-C	7.41	118.13	108.35
4	D	157	LYS	N-CA-C	-7.29	105.00	114.04
15	O	153	GLN	N-CA-C	-7.22	103.38	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	113	ALA	CA-C-N	7.14	127.76	120.04
10	J	113	ALA	C-N-CA	7.14	127.76	120.04
23	W	42	ASN	CA-C-N	6.96	128.53	119.84
23	W	42	ASN	C-N-CA	6.96	128.53	119.84
3	C	70	ALA	N-CA-C	6.84	119.55	109.42
4	D	154	VAL	CA-C-N	6.82	127.10	119.32
4	D	154	VAL	C-N-CA	6.82	127.10	119.32
15	O	117	ALA	N-CA-C	-6.79	103.95	111.36
13	M	145	LEU	N-CA-C	-6.79	103.94	111.82
10	J	155	PRO	N-CA-C	6.79	121.59	111.41
14	N	42	ARG	CA-C-N	6.75	126.51	119.76
14	N	42	ARG	C-N-CA	6.75	126.51	119.76
2	B	3026	C	O3'-P-O5'	6.75	114.13	104.00
14	N	74	ARG	N-CA-C	6.71	119.84	108.90
4	D	147	VAL	CA-C-N	6.67	127.20	119.47
4	D	147	VAL	C-N-CA	6.67	127.20	119.47
24	X	143	THR	N-CA-C	-6.66	104.10	111.36
10	J	137	ASN	N-CA-C	-6.63	101.47	110.36
15	O	13	ARG	N-CA-C	-6.63	105.32	113.41
2	B	3039	U	N1-C1'-C2'	6.59	121.89	112.00
19	S	18	LEU	N-CA-C	-6.59	99.18	109.72
6	F	100	ASP	N-CA-C	-6.57	105.27	113.28
15	O	3	GLY	CA-C-N	6.57	126.19	119.56
15	O	3	GLY	C-N-CA	6.57	126.19	119.56
7	G	48	VAL	N-CA-C	6.55	117.34	108.17
16	P	79	VAL	N-CA-C	-6.52	104.14	110.72
2	B	3025	G	C3'-C2'-O2'	6.50	120.45	110.70
24	X	115	THR	N-CA-C	6.50	119.49	108.90
4	D	265	LEU	N-CA-C	6.49	119.31	110.55
28	2	21	ARG	N-CA-C	6.48	119.31	111.40
3	C	8	ARG	N-CA-C	-6.46	104.24	111.28
3	C	48	ASP	CA-C-N	6.42	126.34	119.28
3	C	48	ASP	C-N-CA	6.42	126.34	119.28
1	A	2419	U	N1-C1'-C2'	6.40	121.61	112.00
5	E	78	ARG	N-CA-C	6.40	117.86	108.14
4	D	175	LEU	N-CA-C	-6.33	104.30	111.07
7	G	7	ILE	CA-C-N	6.32	126.27	119.76
7	G	7	ILE	C-N-CA	6.32	126.27	119.76
22	V	18	GLY	N-CA-C	6.32	119.98	112.33
28	2	43	ALA	N-CA-C	-6.32	104.47	111.36
20	T	57	THR	N-CA-C	6.30	119.06	110.55
12	L	8	VAL	N-CA-C	6.29	117.53	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	68	GLY	N-CA-C	6.25	120.04	112.48
19	S	142	ASP	N-CA-C	-6.25	99.98	109.85
24	X	126	ASP	N-CA-C	6.23	120.61	113.19
3	C	222	GLY	N-CA-C	-6.19	106.56	114.37
1	A	1721	C	N1-C1'-C2'	6.16	121.24	112.00
19	S	130	MET	CB-CG-SD	6.16	131.17	112.70
30	4	42	ARG	N-CA-C	6.15	117.65	111.07
16	P	82	SER	N-CA-C	-6.13	102.40	110.43
14	N	73	ARG	N-CA-C	-6.10	96.89	108.17
25	Y	79	GLU	N-CA-C	6.10	120.56	113.18
15	O	102	LEU	N-CA-C	6.06	118.06	108.67
2	B	3002	U	C4'-C3'-O3'	6.05	118.47	109.40
10	J	162	SER	CA-C-N	-6.05	112.28	119.84
10	J	162	SER	C-N-CA	-6.05	112.28	119.84
1	A	2432	C	N1-C1'-C2'	6.02	121.03	112.00
1	A	1592	G	N9-C1'-C2'	6.02	121.03	112.00
21	U	54	ASP	N-CA-C	-6.00	105.45	112.89
18	R	68	GLY	N-CA-C	-6.00	101.15	111.47
3	C	5	GLN	N-CA-C	5.98	117.80	111.28
3	C	166	ASP	N-CA-C	5.98	118.59	111.71
12	L	78	LYS	CA-C-N	5.98	126.32	119.92
12	L	78	LYS	C-N-CA	5.98	126.32	119.92
10	J	86	ARG	N-CA-C	5.97	120.40	113.18
10	J	129	ASN	CA-C-N	-5.96	114.50	122.72
10	J	129	ASN	C-N-CA	-5.96	114.50	122.72
14	N	90	ARG	N-CA-C	5.96	120.55	113.28
1	A	2096	A	C4'-C3'-O3'	-5.96	104.07	113.00
13	M	20	ASN	N-CA-C	5.92	120.61	111.56
1	A	2103	A	O3'-P-O5'	5.90	112.86	104.00
11	K	89	HIS	N-CA-C	5.90	119.95	112.87
1	A	2726	U	N1-C1'-C2'	5.89	120.83	112.00
27	1	39	CYS	N-CA-C	5.87	117.10	109.64
1	A	1819	G	C5'-C4'-C3'	5.87	124.81	116.00
1	A	388	G	C3'-C2'-O2'	5.87	119.50	110.70
1	A	129	A	C2'-C3'-O3'	5.87	122.50	113.70
2	B	3039	U	C4'-C3'-O3'	-5.87	104.20	113.00
1	A	2459	G	C3'-C2'-O2'	5.86	119.48	110.70
11	K	71	TYR	CA-C-N	5.83	125.59	119.76
11	K	71	TYR	C-N-CA	5.83	125.59	119.76
28	2	11	LYS	N-CA-C	5.77	118.56	108.52
4	D	151	VAL	CA-C-N	5.77	124.97	118.97
4	D	151	VAL	C-N-CA	5.77	124.97	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	75	GLY	N-CA-C	5.77	117.92	112.04
2	B	3003	A	C4'-C3'-C2'	-5.76	96.84	102.60
19	S	137	ASN	N-CA-C	5.76	119.34	110.42
5	E	179	GLY	N-CA-C	-5.75	105.62	113.27
24	X	68	THR	N-CA-C	5.72	117.59	111.36
14	N	8	ILE	N-CA-C	-5.69	104.96	110.42
1	A	1942	A	C5'-C4'-O4'	5.69	118.33	109.80
13	M	37	LYS	N-CA-C	5.68	117.16	108.12
1	A	1723	G	C4'-C3'-O3'	-5.67	104.49	113.00
21	U	52	ARG	N-CA-C	5.66	122.86	110.80
1	A	840	U	N1-C1'-C2'	5.66	120.48	112.00
2	B	3023	U	P-O5'-C5'	5.65	129.38	120.90
5	E	80	VAL	CA-C-N	5.65	125.76	119.32
5	E	80	VAL	C-N-CA	5.65	125.76	119.32
22	V	36	CYS	CA-CB-SG	-5.63	101.44	114.40
1	A	2291	A	C4'-C3'-O3'	-5.63	104.56	113.00
17	Q	56	GLY	N-CA-C	-5.63	102.29	110.90
1	A	2293	G	C3'-C2'-O2'	5.60	119.10	110.70
15	O	14	ARG	N-CA-C	-5.60	105.08	111.07
5	E	92	PRO	N-CA-C	-5.59	102.32	111.21
23	W	64	GLY	N-CA-C	-5.59	107.28	115.72
19	S	122	GLN	N-CA-C	-5.56	100.05	108.67
9	I	14	GLU	N-CA-C	5.56	117.42	111.36
19	S	76	ASP	N-CA-C	5.55	119.83	112.72
1	A	2102	G	C3'-C2'-O2'	-5.54	106.29	114.60
18	R	13	LYS	N-CA-C	5.54	119.54	112.34
7	G	37	ASP	N-CA-C	5.53	119.31	112.24
1	A	2526	C	N1-C1'-C2'	5.52	120.28	112.00
1	A	843	A	C4'-C3'-O3'	-5.51	104.73	113.00
18	R	49	ASN	N-CA-C	5.51	117.96	110.35
26	Z	143	TRP	N-CA-C	5.51	118.22	109.96
1	A	2835	C	C4'-C3'-O3'	-5.50	104.75	113.00
3	C	186	TRP	O-C-N	5.49	127.66	122.06
24	X	25	ASN	CA-C-N	-5.47	115.82	123.10
24	X	25	ASN	C-N-CA	-5.47	115.82	123.10
15	O	48	VAL	N-CA-C	5.47	116.85	108.71
21	U	3	GLN	CA-C-N	5.46	126.66	119.84
21	U	3	GLN	C-N-CA	5.46	126.66	119.84
1	A	854	G	C4'-C3'-O3'	-5.45	104.83	113.00
12	L	14	LYS	N-CA-C	-5.45	102.23	110.24
16	P	69	VAL	N-CA-C	5.44	116.31	108.48
4	D	230	GLN	N-CA-C	5.44	119.63	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	32	LYS	N-CA-C	-5.44	105.44	111.36
10	J	7	ARG	N-CA-C	5.43	119.52	113.01
1	A	2315	C	C5'-C4'-C3'	-5.40	107.90	116.00
30	4	60	LYS	N-CA-C	-5.40	103.24	109.93
24	X	17	ILE	N-CA-C	-5.39	105.87	111.58
18	R	51	ARG	N-CA-C	5.38	117.47	110.53
1	A	1450	C	C2'-C3'-O3'	-5.36	105.66	113.70
1	A	1504	A	N9-C1'-C2'	5.36	120.04	112.00
25	Y	51	ASP	CA-C-N	5.35	126.53	119.84
25	Y	51	ASP	C-N-CA	5.35	126.53	119.84
1	A	959	C	C4'-C3'-O3'	-5.35	104.98	113.00
13	M	47	GLY	N-CA-C	5.33	117.50	111.85
1	A	1738	C	O4'-C4'-C3'	-5.33	98.67	104.00
1	A	834	G	C2'-C3'-O3'	-5.32	105.72	113.70
1	A	2103	A	N9-C1'-C2'	-5.32	106.02	114.00
16	P	2	LYS	N-CA-C	-5.32	102.61	110.48
10	J	110	GLY	N-CA-C	-5.32	100.58	113.18
3	C	135	VAL	N-CA-C	5.30	115.75	108.12
2	B	3026	C	C5'-C4'-O4'	5.29	117.74	109.80
1	A	2103	A	C4'-C3'-O3'	-5.29	101.47	109.40
6	F	137	PRO	N-CA-C	5.28	123.34	112.47
14	N	70	GLY	N-CA-C	5.28	121.82	112.53
20	T	59	ASP	N-CA-C	-5.26	106.88	113.72
4	D	48	MET	N-CA-C	5.25	117.80	109.50
1	A	1120	U	C5'-C4'-C3'	-5.25	108.13	116.00
1	A	244	C	C3'-C2'-O2'	5.24	118.56	110.70
3	C	110	SER	N-CA-C	-5.24	105.24	111.69
5	E	150	THR	N-CA-C	-5.24	105.46	111.07
1	A	138	U	C2'-C3'-O3'	-5.22	105.88	113.70
1	A	1917	G	C3'-C2'-O2'	5.22	118.53	110.70
1	A	2275	G	C3'-C2'-O2'	5.21	118.52	110.70
21	U	46	ASP	N-CA-C	5.21	117.25	110.43
4	D	242	TRP	N-CA-C	-5.20	105.52	111.14
26	Z	202	ALA	N-CA-C	-5.20	101.63	109.85
1	A	903	U	C3'-C2'-O2'	5.20	118.50	110.70
19	S	13	THR	N-CA-C	5.20	117.90	109.06
15	O	108	SER	CA-C-N	5.20	126.34	119.84
15	O	108	SER	C-N-CA	5.20	126.34	119.84
5	E	129	HIS	N-CA-C	5.20	117.56	110.24
12	L	111	GLY	CA-C-N	5.20	125.20	120.21
12	L	111	GLY	C-N-CA	5.20	125.20	120.21
1	A	2103	A	C3'-C2'-O2'	5.18	122.38	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	82	ARG	N-CA-C	-5.17	102.82	110.48
14	N	100	ILE	N-CA-C	-5.17	105.45	110.42
1	A	2301	A	N9-C1'-C2'	5.17	119.76	112.00
1	A	2667	G	O5'-C5'-C4'	5.17	119.26	111.50
5	E	215	ALA	N-CA-C	5.17	118.37	111.75
1	A	2433	A	N9-C1'-C2'	5.16	119.75	112.00
4	D	303	GLY	CA-C-N	5.16	126.28	119.84
4	D	303	GLY	C-N-CA	5.16	126.28	119.84
15	O	168	LEU	N-CA-C	5.15	119.87	108.64
5	E	167	ASP	N-CA-C	-5.13	105.69	111.28
4	D	258	GLY	N-CA-C	-5.12	106.13	112.33
3	C	113	GLY	N-CA-C	5.12	121.86	115.21
21	U	78	THR	N-CA-C	5.10	116.43	109.18
1	A	2291	A	N9-C1'-C2'	5.09	119.64	112.00
23	W	26	GLU	N-CA-C	-5.09	105.73	111.28
1	A	2864	U	C4'-C3'-O3'	-5.09	105.37	113.00
8	H	8	VAL	N-CA-C	5.09	112.19	107.56
3	C	133	ARG	N-CA-C	-5.08	106.93	113.23
14	N	126	HIS	CB-CA-C	-5.08	101.32	110.36
27	1	42	CYS	N-CA-C	-5.07	102.12	109.31
1	A	1730	G	C5'-C4'-C3'	5.06	122.80	115.20
1	A	1738	C	C5'-C4'-C3'	5.06	123.60	116.00
1	A	2664	A	N9-C1'-C2'	5.06	119.58	112.00
1	A	335	U	C4'-C3'-O3'	-5.05	105.42	113.00
4	D	282	GLY	N-CA-C	-5.05	109.07	115.08
14	N	184	ARG	N-CA-C	-5.05	103.32	110.29
15	O	131	HIS	N-CA-C	5.04	114.80	108.45
4	D	270	ILE	N-CA-C	5.04	115.76	110.62
1	A	1165	G	N9-C1'-C2'	5.03	119.55	112.00
1	A	2313	C	C5'-C4'-C3'	5.02	123.53	116.00
1	A	1474	C	N1-C1'-C2'	5.02	119.53	112.00
1	A	1189	A	N9-C1'-C2'	5.01	119.51	112.00
8	H	118	LEU	N-CA-C	-5.00	107.24	113.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (154) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	G	Sidechain
1	A	1039	G	Sidechain
1	A	1053	G	Sidechain
1	A	1072	G	Sidechain
1	A	1119	G	Sidechain
1	A	112	G	Sidechain
1	A	1134	G	Sidechain
1	A	1140	C	Sidechain
1	A	1206	U	Sidechain
1	A	1229	C	Sidechain
1	A	1264	U	Sidechain
1	A	1309	U	Sidechain
1	A	1336	U	Sidechain
1	A	1348	A	Sidechain
1	A	1350	U	Sidechain
1	A	1376	G	Sidechain
1	A	138	U	Sidechain
1	A	1400	C	Sidechain
1	A	1408	U	Sidechain
1	A	1417	G	Sidechain
1	A	1423	C	Sidechain
1	A	1430	G	Sidechain
1	A	1433	G	Sidechain
1	A	1447	U	Sidechain
1	A	1452	G	Sidechain
1	A	1458	A	Sidechain
1	A	1470	A	Sidechain
1	A	1487	A	Sidechain
1	A	1501	A	Sidechain
1	A	1503	U	Sidechain
1	A	1535	G	Sidechain
1	A	1595	G	Sidechain
1	A	1614	G	Sidechain
1	A	162	C	Sidechain
1	A	1647	G	Sidechain
1	A	1677	U	Sidechain
1	A	1681	G	Sidechain
1	A	1685	A	Sidechain
1	A	1688	G	Sidechain
1	A	170	U	Sidechain
1	A	171	C	Sidechain
1	A	172	U	Sidechain
1	A	1736	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1747	A	Sidechain
1	A	1748	U	Sidechain
1	A	1758	U	Sidechain
1	A	176	U	Sidechain
1	A	1819	G	Sidechain
1	A	182	G	Sidechain
1	A	1833	U	Sidechain
1	A	1835	U	Sidechain
1	A	1839	A	Sidechain
1	A	1846	U	Sidechain
1	A	1860	U	Sidechain
1	A	1861	C	Sidechain
1	A	1878	G	Sidechain
1	A	1879	U	Sidechain
1	A	1908	G	Sidechain
1	A	191	A	Sidechain
1	A	197	C	Sidechain
1	A	1972	U	Sidechain
1	A	1993	C	Sidechain
1	A	2001	G	Sidechain
1	A	2035	C	Sidechain
1	A	2059	U	Sidechain
1	A	2073	G	Sidechain
1	A	2103	A	Sidechain
1	A	2106	C	Sidechain
1	A	2110	G	Sidechain
1	A	2127	U	Sidechain
1	A	2128	G	Sidechain
1	A	2133	U	Sidechain
1	A	2266	A	Sidechain
1	A	2294	C	Sidechain
1	A	2297	U	Sidechain
1	A	2308	U	Sidechain
1	A	2312	G	Sidechain
1	A	2313	C	Sidechain
1	A	2364	A	Sidechain
1	A	24	G	Sidechain
1	A	2412	G	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	2436	U	Sidechain
1	A	2441	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2458	U	Sidechain
1	A	2459	G	Sidechain
1	A	246	G	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain
1	A	2506	A	Sidechain
1	A	2557	U	Sidechain
1	A	2564	G	Sidechain
1	A	257	G	Sidechain
1	A	2575	C	Sidechain
1	A	2597	U	Sidechain
1	A	26	U	Sidechain
1	A	2607	U	Sidechain
1	A	2615	U	Sidechain
1	A	2630	G	Sidechain
1	A	2640	U	Sidechain
1	A	2673	U	Sidechain
1	A	2675	A	Sidechain
1	A	2730	G	Sidechain
1	A	2774	U	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	2800	A	Sidechain
1	A	2811	A	Sidechain
1	A	2840	A	Sidechain
1	A	2842	G	Sidechain
1	A	2864	U	Sidechain
1	A	333	G	Sidechain
1	A	398	U	Sidechain
1	A	407	A	Sidechain
1	A	436	A	Sidechain
1	A	458	G	Sidechain
1	A	471	G	Sidechain
1	A	481	U	Sidechain
1	A	486	A	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	552	A	Sidechain
1	A	589	U	Sidechain
1	A	626	U	Sidechain
1	A	669	G	Sidechain
1	A	720	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	722	G	Sidechain
1	A	723	G	Sidechain
1	A	757	C	Sidechain
1	A	768	U	Sidechain
1	A	773	A	Sidechain
1	A	781	C	Sidechain
1	A	784	A	Sidechain
1	A	791	A	Sidechain
1	A	795	G	Sidechain
1	A	815	U	Sidechain
1	A	817	G	Sidechain
1	A	818	A	Sidechain
1	A	835	U	Sidechain
1	A	840	U	Sidechain
1	A	855	U	Sidechain
1	A	869	G	Sidechain
1	A	871	G	Sidechain
1	A	877	G	Sidechain
1	A	882	A	Sidechain
1	A	887	G	Sidechain
1	A	898	G	Sidechain
1	A	919	U	Sidechain
1	A	954	U	Sidechain
2	B	3005	G	Sidechain
2	B	3065	A	Sidechain
2	B	3094	G	Sidechain
2	B	3120	A	Sidechain

5.2 Too-close contacts [i](#)

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	1181	0
2	B	2600	0	1326	80	0
3	C	1754	0	1763	143	0
4	D	2624	0	2533	202	0
5	E	1858	0	1816	125	0
6	F	1094	0	1085	141	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1357	0	1266	83	0
8	H	885	0	854	65	0
9	I	240	0	231	23	0
10	J	1215	0	1215	167	0
11	K	1119	0	1098	69	0
12	L	993	0	1027	59	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	181	0
15	O	1444	0	1401	135	0
16	P	864	0	873	42	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	26	0
19	S	1149	0	1122	59	0
20	T	641	0	605	25	0
21	U	949	0	923	57	0
22	V	410	0	368	38	0
23	W	499	0	511	33	0
24	X	1195	0	1137	103	0
25	Y	654	0	653	51	0
26	Z	1130	0	1133	64	0
27	1	563	0	601	80	0
28	2	430	0	426	28	0
29	3	393	0	406	27	0
30	4	755	0	732	58	0
31	A	64	0	76	2	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	111	0	0	0	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	72	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
34	4	1	0	0	0	0
34	A	8	0	0	1	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	4	0	0	2	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	2	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	37	0	0	10	0
37	2	56	0	0	4	0
37	3	43	0	0	5	0
37	4	72	0	0	4	0
37	A	5921	0	0	269	0
37	B	142	0	0	14	0
37	C	126	0	0	22	0
37	D	146	0	0	28	0
37	E	174	0	0	34	0
37	F	51	0	0	20	0
37	G	42	0	0	9	0
37	H	26	0	0	11	0
37	I	22	0	0	6	0
37	J	79	0	0	18	0
37	K	54	0	0	5	0
37	L	60	0	0	10	0
37	M	84	0	0	18	0
37	N	127	0	0	30	0
37	O	64	0	0	18	0
37	P	42	0	0	12	0
37	Q	66	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	R	53	0	0	3	0
37	S	84	0	0	9	0
37	T	34	0	0	4	0
37	U	39	0	0	5	0
37	V	26	0	0	5	0
37	W	12	0	0	1	0
37	X	70	0	0	10	0
37	Y	29	0	0	12	0
37	Z	96	0	0	17	0
All	All	98593	0	59582	3164	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 21.

All (3164) 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)
6:F:25:MET:HE2	6:F:41:LEU:HG	1.26	1.16
1:A:1160:G:H5'	1:A:1161:A:H5'	1.25	1.15
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.30	1.13
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.64	1.13
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.20	1.12
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.14	1.10
1:A:1134:G:H4'	10:J:151:MET:HE1	1.34	1.09
14:N:87:MET:CG	30:4:46:ILE:HG21	1.84	1.08
5:E:236:THR:HG22	5:E:239:ALA:H	1.11	1.07
1:A:871:G:H5'	1:A:871:G:H8	1.17	1.07
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.33	1.06
14:N:164:THR:HG22	14:N:167:GLY:H	1.23	1.04
14:N:87:MET:HG2	30:4:46:ILE:CG2	1.88	1.03
4:D:140:LEU:HA	37:D:8577:HOH:O	1.59	1.02
1:A:871:G:H5'	1:A:871:G:C8	1.94	1.02
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.38	1.01
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.40	1.01
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.43	1.01
1:A:962:C:H1'	15:O:5:ARG:NH1	1.75	1.01
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.41	1.01
2:B:3056:A:H2'	2:B:3057:A:H5''	1.43	1.00
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.83	1.00
14:N:64:ARG:HD2	37:N:8584:HOH:O	1.59	1.00
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.27	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:162:MET:HE1	4:D:308:LEU:HD21	1.40	0.99
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.44	0.99
11:K:76:ASP:HA	37:K:8563:HOH:O	1.62	0.99
1:A:2122:C:OP2	37:A:6559:HOH:O	1.80	0.99
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.43	0.99
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.45	0.98
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.45	0.98
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.44	0.98
1:A:856:G:H2'	37:A:5402:HOH:O	1.65	0.97
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.47	0.97
37:A:6752:HOH:O	15:O:4:PRO:HD2	1.65	0.97
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.47	0.97
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.47	0.97
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.63	0.97
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.78	0.96
14:N:24:MET:HE3	14:N:28:MET:HE3	1.47	0.96
1:A:542:A:H5'	1:A:542:A:H8	1.28	0.96
10:J:165:GLY:HA3	37:J:8399:HOH:O	1.64	0.96
1:A:541:C:H2'	1:A:542:A:H5''	1.44	0.96
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.79	0.96
1:A:2717:C:H2'	1:A:2718:C:H5''	1.47	0.96
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.45	0.96
17:Q:115:SER:H	17:Q:118:GLN:HE21	0.97	0.95
2:B:3076:G:H3'	2:B:3077:A:H5''	1.49	0.94
12:L:10:GLN:HE21	12:L:10:GLN:H	1.15	0.94
3:C:223:ARG:HG3	37:C:8605:HOH:O	1.68	0.94
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.49	0.94
4:D:86:ALA:HA	37:D:8577:HOH:O	1.67	0.94
5:E:140:VAL:HB	37:E:8456:HOH:O	1.65	0.94
6:F:105:SER:HB2	6:F:131:THR:HG23	1.50	0.93
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.50	0.93
1:A:1835:U:H5	1:A:1840:A:N7	1.65	0.93
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.48	0.93
1:A:1751:G:H2'	1:A:1752:G:H5''	1.51	0.93
24:X:149:LEU:HG	24:X:153:MET:HE2	1.51	0.92
14:N:52:LEU:HD11	37:N:8615:HOH:O	1.68	0.92
16:P:7:LEU:HD22	37:P:5650:HOH:O	1.70	0.92
37:A:6854:HOH:O	14:N:178:LYS:HB2	1.70	0.92
5:E:2:GLN:HB3	37:E:8335:HOH:O	1.70	0.91
12:L:10:GLN:H	12:L:10:GLN:NE2	1.68	0.91
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2121:G:OP2	37:A:3491:HOH:O	1.89	0.91
1:A:871:G:H8	1:A:871:G:C5'	1.84	0.91
13:M:68:GLU:HA	37:M:8549:HOH:O	1.70	0.90
1:A:156:C:H5''	14:N:171:ARG:HD3	1.52	0.90
24:X:88:THR:HB	37:X:6679:HOH:O	1.70	0.90
1:A:962:C:H1'	15:O:5:ARG:HH12	1.32	0.90
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.50	0.90
2:B:3023:U:H5''	2:B:3024:U:OP2	1.69	0.90
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.34	0.90
1:A:1474:C:H6	1:A:1474:C:H5'	1.35	0.89
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.53	0.89
20:T:57:THR:HG22	20:T:59:ASP:H	1.37	0.89
10:J:27:LYS:H	10:J:58:HIS:HD2	1.15	0.89
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.53	0.89
13:M:133:VAL:HA	37:M:8577:HOH:O	1.72	0.89
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.53	0.88
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.08	0.88
4:D:62:ARG:HA	4:D:65:MET:HE3	1.52	0.88
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.07	0.88
10:J:150:LYS:HE2	37:J:8385:HOH:O	1.73	0.88
5:E:236:THR:HG21	37:E:8375:HOH:O	1.72	0.88
1:A:870:G:H2'	1:A:871:G:H5''	1.54	0.88
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.38	0.88
1:A:1116:U:HO2'	1:A:1118:A:H2	0.91	0.87
15:O:144:GLY:O	15:O:147:ILE:HG22	1.74	0.87
37:A:3656:HOH:O	14:N:79:LYS:HD3	1.73	0.87
10:J:59:ASN:H	10:J:59:ASN:HD22	1.20	0.87
1:A:2432:C:O4'	37:A:9716:HOH:O	1.93	0.87
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.38	0.87
1:A:1242:A:H5'	11:K:82:THR:HG23	1.53	0.87
4:D:321:PRO:HA	37:D:8656:HOH:O	1.72	0.86
1:A:1634:G:H3'	37:A:3866:HOH:O	1.75	0.86
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.56	0.86
1:A:1166:A:H1'	1:A:1192:A:C2	2.10	0.86
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.75	0.86
1:A:1116:U:H3	1:A:1246:A:H62	1.23	0.86
1:A:1667:A:H5'	1:A:1667:A:H8	1.38	0.86
10:J:2:PRO:HB2	37:J:8367:HOH:O	1.74	0.85
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.58	0.85
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.76	0.85
10:J:162:SER:HB2	10:J:163:PRO:CD	2.04	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:47:ARG:HH11	16:P:47:ARG:HG3	1.41	0.85
1:A:541:C:C2'	1:A:542:A:H5''	2.06	0.85
1:A:2812:A:H2	1:A:2814:A:H62	1.25	0.85
1:A:2004:U:H4'	37:A:5282:HOH:O	1.76	0.85
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.75	0.85
14:N:87:MET:CB	30:4:46:ILE:HD13	2.07	0.85
1:A:645:U:OP2	13:M:4:LYS:HE2	1.77	0.85
22:V:20:MET:HE2	22:V:30:HIS:NE2	1.91	0.85
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.76	0.85
13:M:79:ASP:HB3	37:M:8564:HOH:O	1.77	0.85
1:A:1118:A:H8	1:A:1118:A:H3'	1.42	0.84
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.75	0.84
1:A:2506:A:HO2'	1:A:2507:G:H8	0.85	0.84
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.41	0.84
29:3:41:HIS:H	29:3:45:ASN:HD22	1.24	0.84
24:X:88:THR:HG22	24:X:89:ASP:H	1.42	0.84
1:A:1886:A:N3	37:A:4792:HOH:O	2.10	0.84
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.60	0.84
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.59	0.84
13:M:67:ARG:O	13:M:71:GLU:HG3	1.78	0.84
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.59	0.84
1:A:1209:C:H4'	37:A:5255:HOH:O	1.78	0.83
37:A:4493:HOH:O	14:N:94:LYS:HE3	1.77	0.83
19:S:99:ALA:CB	19:S:109:MET:HE1	2.07	0.83
1:A:2123:A:OP2	37:A:5264:HOH:O	1.96	0.83
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.59	0.83
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.24	0.83
5:E:246:ARG:HB3	5:E:246:ARG:NH1	1.93	0.83
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.77	0.83
14:N:172:GLY:O	14:N:183:VAL:HG11	1.79	0.83
26:Z:141:THR:HG23	37:Z:8589:HOH:O	1.78	0.83
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.61	0.83
1:A:172:U:OP2	37:A:6192:HOH:O	1.97	0.82
5:E:236:THR:HG22	5:E:239:ALA:N	1.94	0.82
1:A:346:U:H4'	37:A:6824:HOH:O	1.79	0.82
1:A:2274:A:N3	14:N:86:MET:HE1	1.94	0.82
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.94	0.82
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.44	0.82
30:4:73:GLU:HB3	37:4:8563:HOH:O	1.77	0.82
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.61	0.82
15:O:7:LYS:HE3	18:R:21:ARG:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:30:MET:HE1	25:Y:58:ALA:HB3	1.61	0.82
1:A:31:C:H2'	37:A:7684:HOH:O	1.78	0.82
1:A:2466:G:OP1	37:A:3621:HOH:O	1.96	0.82
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.60	0.82
4:D:162:MET:HE2	4:D:310:ARG:HD3	1.59	0.82
1:A:2533:C:H6	1:A:2533:C:H5'	1.43	0.81
1:A:2717:C:C2'	1:A:2718:C:H5''	2.10	0.81
6:F:154:LYS:H	6:F:154:LYS:HD2	1.45	0.81
10:J:59:ASN:HD22	10:J:59:ASN:N	1.77	0.81
1:A:544:G:H2'	1:A:545:G:H5''	1.61	0.81
37:A:3760:HOH:O	14:N:189:VAL:HG21	1.81	0.81
5:E:76:ARG:HD2	37:E:8436:HOH:O	1.80	0.81
8:H:96:ALA:HA	37:H:3111:HOH:O	1.80	0.81
21:U:55:PHE:HB2	37:U:6384:HOH:O	1.78	0.81
22:V:9:CYS:HA	22:V:52:THR:HG23	1.60	0.81
23:W:1:THR:HG23	23:W:2:VAL:H	1.45	0.81
1:A:1184:C:H1'	37:A:7456:HOH:O	1.81	0.81
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.10	0.81
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.61	0.81
2:B:3056:A:C2'	2:B:3057:A:H5''	2.11	0.81
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.14	0.81
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.62	0.81
1:A:545:G:H5'	1:A:545:G:H8	1.46	0.80
1:A:1118:A:H3'	1:A:1118:A:C8	2.15	0.80
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.64	0.80
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.47	0.80
1:A:797:A:H4'	27:1:10:ARG:N	1.97	0.80
37:A:7549:HOH:O	30:4:60:LYS:HG3	1.81	0.80
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.28	0.80
14:N:87:MET:CB	30:4:46:ILE:HG21	2.11	0.80
24:X:122:ARG:NH2	24:X:154:ARG:HD2	1.97	0.80
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.64	0.80
14:N:61:ILE:HG13	37:N:8621:HOH:O	1.80	0.80
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.64	0.80
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.21	0.79
1:A:797:A:C4'	27:1:10:ARG:N	2.45	0.79
27:1:54:ILE:HD12	37:1:8416:HOH:O	1.82	0.79
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.62	0.79
1:A:1120:U:H6	1:A:1120:U:H5''	1.47	0.79
25:Y:31:ILE:O	25:Y:35:GLU:HG3	1.83	0.79
1:A:21:G:H5'	19:S:2:ILE:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:C:H4'	1:A:1451:C:OP2	1.82	0.79
10:J:139:ASP:N	10:J:140:PRO:HD3	1.98	0.79
1:A:559:U:H6	1:A:559:U:H5'	1.47	0.79
26:Z:133:HIS:HD2	37:Z:8582:HOH:O	1.65	0.79
1:A:1160:G:H5'	1:A:1161:A:C5'	2.11	0.79
1:A:1679:C:H5'	37:A:9314:HOH:O	1.83	0.79
2:B:3014:G:H5'	2:B:3014:G:H8	1.48	0.79
10:J:26:LYS:HG2	10:J:28:ILE:H	1.47	0.79
1:A:1160:G:C5'	1:A:1161:A:H5'	2.10	0.78
10:J:142:VAL:HG13	37:J:8383:HOH:O	1.83	0.78
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.18	0.78
37:A:5770:HOH:O	14:N:170:CYS:SG	2.41	0.78
1:A:2506:A:O2'	1:A:2507:G:H8	1.64	0.78
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.13	0.78
11:K:74:ARG:HB3	11:K:74:ARG:HH11	1.48	0.78
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.83	0.78
1:A:289:G:H22	1:A:363:A:H2	1.32	0.78
13:M:136:ALA:HB3	37:M:8577:HOH:O	1.83	0.78
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.13	0.78
5:E:246:ARG:HB3	5:E:246:ARG:HH11	1.47	0.78
16:P:32:ARG:O	16:P:32:ARG:HD3	1.83	0.78
1:A:381:G:H5''	37:A:4290:HOH:O	1.82	0.78
1:A:1134:G:C4'	10:J:151:MET:HE1	2.14	0.78
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.65	0.78
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.64	0.78
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.66	0.77
6:F:20:LYS:HA	6:F:75:LEU:O	1.85	0.77
1:A:1116:U:O2'	1:A:1118:A:H2	1.68	0.77
1:A:2586:U:H3	1:A:2592:G:H22	1.30	0.77
37:A:9547:HOH:O	4:D:267:LYS:HD3	1.84	0.77
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.65	0.77
2:B:3069:U:OP1	15:O:4:PRO:HG3	1.85	0.77
6:F:27:ILE:HG22	6:F:28:GLY:H	1.49	0.77
1:A:560:C:H42	1:A:597:A:H61	1.33	0.77
4:D:162:MET:HE2	4:D:310:ARG:CD	2.13	0.77
1:A:506:G:H22	1:A:509:A:C5'	1.97	0.77
3:C:191:GLY:HA2	3:C:194:MET:HE2	1.66	0.77
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.65	0.77
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.65	0.77
1:A:1205:U:H2'	1:A:1206:U:H5'	1.66	0.77
1:A:2426:G:H1'	37:A:6072:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.80	0.77
3:C:192:VAL:HB	37:C:8597:HOH:O	1.85	0.77
12:L:81:ARG:HB2	12:L:87:ARG:NH1	1.99	0.77
14:N:164:THR:HG23	14:N:165:SER:N	1.99	0.77
37:A:4924:HOH:O	2:B:3103:A:H4'	1.84	0.76
1:A:288:A:H61	1:A:364:C:H42	1.33	0.76
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.85	0.76
1:A:1164:U:H3	1:A:1192:A:H2	1.31	0.76
15:O:164:ASP:CG	15:O:167:ASP:HA	2.10	0.76
4:D:62:ARG:HA	4:D:65:MET:CE	2.14	0.76
20:T:57:THR:HG22	20:T:59:ASP:N	2.00	0.76
24:X:154:ARG:C	37:X:4276:HOH:O	2.28	0.76
1:A:1603:A:H5'	1:A:1605:G:O4'	1.85	0.76
37:A:6278:HOH:O	6:F:99:ASP:HA	1.84	0.76
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.66	0.76
8:H:91:VAL:HG12	8:H:92:GLY:N	2.00	0.76
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.68	0.76
22:V:9:CYS:SG	22:V:11:THR:HG23	2.26	0.76
24:X:88:THR:HG23	24:X:110:GLN:NE2	2.01	0.76
14:N:60:ILE:C	14:N:61:ILE:HD12	2.11	0.75
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.68	0.75
1:A:282:C:H1'	1:A:368:C:N4	2.00	0.75
1:A:542:A:H5'	1:A:542:A:C8	2.18	0.75
1:A:877:G:H5'	1:A:878:G:OP1	1.86	0.75
1:A:1474:C:H5'	1:A:1474:C:C6	2.19	0.75
10:J:137:ASN:O	10:J:139:ASP:N	2.19	0.75
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.17	0.75
26:Z:185:VAL:HA	37:Z:8564:HOH:O	1.85	0.75
1:A:1120:U:H5''	1:A:1120:U:C6	2.22	0.75
1:A:1625:U:H4'	37:A:4639:HOH:O	1.84	0.75
4:D:238:ASN:HD22	4:D:240:GLY:H	1.35	0.75
7:G:84:MET:HE2	7:G:133:VAL:CG2	2.16	0.75
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.68	0.75
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.86	0.75
1:A:1329:A:N1	34:A:8513:CL:CL	2.56	0.75
1:A:2054:A:N3	19:S:128:ARG:NH2	2.34	0.75
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.49	0.75
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.67	0.75
1:A:1165:G:H4'	1:A:1174:A:O2'	1.86	0.75
37:A:7413:HOH:O	21:U:9:LYS:HB2	1.86	0.75
1:A:1118:A:H62	1:A:1244:U:H3	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1666:C:O2'	1:A:1667:A:H5''	1.87	0.75
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.68	0.75
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.51	0.74
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.52	0.74
1:A:1187:U:H2'	37:A:6877:HOH:O	1.87	0.74
37:A:9075:HOH:O	4:D:214:PRO:HD2	1.87	0.74
8:H:58:GLU:HG3	8:H:61:MET:HE2	1.68	0.74
15:O:80:SER:HB2	37:O:8535:HOH:O	1.85	0.74
5:E:178:GLN:OE1	37:E:8470:HOH:O	2.05	0.74
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.84	0.74
1:A:1119:G:H22	1:A:1246:A:H2	1.31	0.74
1:A:1835:U:C5	1:A:1840:A:N7	2.53	0.74
1:A:960:G:H4'	37:A:7419:HOH:O	1.87	0.74
27:1:49:ARG:HD2	37:1:8427:HOH:O	1.88	0.74
1:A:1701:A:H5'	37:A:6266:HOH:O	1.87	0.74
4:D:62:ARG:CA	4:D:65:MET:HE3	2.18	0.74
10:J:140:PRO:HB3	37:J:8383:HOH:O	1.87	0.74
14:N:164:THR:HG22	14:N:167:GLY:N	2.00	0.74
27:1:39:CYS:SG	27:1:47:LEU:HD21	2.28	0.74
37:A:4833:HOH:O	14:N:14:ARG:HG2	1.87	0.74
24:X:129:LYS:HG2	37:X:1990:HOH:O	1.88	0.74
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.20	0.74
13:M:148:GLU:HA	37:M:8576:HOH:O	1.87	0.74
37:A:9383:HOH:O	14:N:94:LYS:HE2	1.88	0.73
5:E:107:ARG:NH1	5:E:107:ARG:HB3	2.03	0.73
8:H:91:VAL:HG12	8:H:92:GLY:H	1.51	0.73
26:Z:216:ARG:HD3	37:Z:8569:HOH:O	1.85	0.73
30:4:31:THR:HB	30:4:33:MET:HE3	1.69	0.73
9:I:12:ILE:HA	37:I:4499:HOH:O	1.88	0.73
1:A:111:C:O2'	28:2:20:ARG:HG2	1.89	0.73
1:A:1666:C:H2'	1:A:1667:A:H5'	1.69	0.73
19:S:39:THR:HB	19:S:42:GLU:HG3	1.70	0.73
24:X:110:GLN:NE2	24:X:110:GLN:HA	2.02	0.73
14:N:85:ARG:HA	14:N:87:MET:HE2	1.69	0.73
1:A:1151:G:OP1	9:I:16:LYS:NZ	2.20	0.73
37:A:7575:HOH:O	27:1:31:ILE:HG13	1.88	0.73
10:J:75:SER:O	10:J:79:ALA:HB2	1.88	0.73
1:A:1080:C:H4'	1:A:1081:A:OP1	1.88	0.73
37:B:5071:HOH:O	15:O:23:ARG:HD3	1.88	0.73
3:C:53:ALA:HB3	37:C:8609:HOH:O	1.89	0.73
30:4:65:THR:HG23	30:4:67:LEU:HG	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:C:H2'	1:A:542:A:C5'	2.16	0.73
1:A:1834:C:H2'	1:A:1840:A:N6	2.03	0.72
11:K:93:ARG:HB3	11:K:93:ARG:HH11	1.52	0.72
18:R:23:THR:HA	37:R:4792:HOH:O	1.89	0.72
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.22	0.72
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	1.88	0.72
37:A:4641:HOH:O	20:T:23:LYS:HE2	1.89	0.72
3:C:199:HIS:CD2	3:C:201:PHE:H	2.06	0.72
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.19	0.72
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.71	0.72
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.19	0.72
4:D:179:LEU:O	4:D:183:GLU:HG2	1.88	0.72
8:H:46:GLU:O	8:H:73:PRO:HD2	1.89	0.72
1:A:1372:A:H3'	37:A:7173:HOH:O	1.88	0.72
1:A:2421:G:H3'	1:A:2422:U:H5''	1.70	0.72
1:A:2638:G:H1'	37:A:7756:HOH:O	1.89	0.72
37:A:7444:HOH:O	4:D:211:THR:HG21	1.89	0.72
11:K:19:MET:HE2	11:K:79:PHE:HA	1.70	0.72
19:S:17:MET:HE1	19:S:19:ARG:NH2	2.04	0.72
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.71	0.72
1:A:1191:A:H3'	1:A:1192:A:H5''	1.70	0.72
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.54	0.72
1:A:284:C:H4'	1:A:285:A:O5'	1.89	0.72
1:A:1213:C:O2'	1:A:1214:G:H5'	1.89	0.72
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.71	0.72
5:E:27:ARG:HG3	5:E:29:ASP:OD1	1.88	0.72
9:I:12:ILE:N	9:I:13:PRO:HD3	2.04	0.72
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.89	0.72
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.20	0.72
1:A:1119:G:H8	11:K:52:GLN:HE22	1.36	0.72
1:A:2382:A:H5'	37:A:4714:HOH:O	1.89	0.72
10:J:162:SER:CB	10:J:163:PRO:HD3	2.17	0.72
1:A:236:A:H4'	1:A:237:G:H5'	1.73	0.71
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.20	0.71
10:J:141:ASN:HA	37:J:8369:HOH:O	1.90	0.71
15:O:12:ARG:HD3	15:O:18:THR:OG1	1.90	0.71
15:O:113:SER:HB2	37:O:8556:HOH:O	1.89	0.71
1:A:338:C:H4'	5:E:174:ILE:CD1	2.20	0.71
1:A:1701:A:H4'	1:A:1702:U:H5''	1.71	0.71
1:A:2346:C:O2'	6:F:52:THR:HG21	1.91	0.71
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:143:THR:HG22	13:M:144:ASP:N	2.05	0.71
26:Z:220:GLU:HG2	37:Z:8551:HOH:O	1.89	0.71
1:A:870:G:C2'	1:A:871:G:H5''	2.20	0.71
1:A:1329:A:H2	37:A:4657:HOH:O	1.72	0.71
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.59	0.71
6:F:97:GLN:HG2	6:F:97:GLN:O	1.89	0.71
10:J:71:TYR:C	10:J:73:GLN:H	1.98	0.71
14:N:85:ARG:NE	37:N:8519:HOH:O	2.19	0.71
29:3:41:HIS:N	29:3:45:ASN:HD22	1.88	0.71
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.72	0.71
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.73	0.71
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.71	0.71
1:A:2420:G:O2'	1:A:2421:G:H5'	1.91	0.71
2:B:3013:A:O2'	2:B:3014:G:H5''	1.91	0.71
11:K:19:MET:HE3	11:K:132:LEU:CD1	2.18	0.71
14:N:138:HIS:ND1	14:N:139:PRO:O	2.19	0.71
19:S:39:THR:HG23	19:S:107:GLU:O	1.90	0.71
1:A:2434:A:O3'	30:4:28:GLY:HA3	1.90	0.71
23:W:39:ALA:N	23:W:40:PRO:HD2	2.06	0.71
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.53	0.71
3:C:194:MET:HE3	3:C:199:HIS:HB2	1.73	0.71
14:N:186:SER:O	14:N:189:VAL:HG12	1.90	0.71
2:B:3029:C:H2'	2:B:3030:C:H5'	1.73	0.70
4:D:175:LEU:HD23	4:D:175:LEU:C	2.15	0.70
12:L:10:GLN:HE21	12:L:10:GLN:N	1.89	0.70
1:A:553:G:P	26:Z:204:ARG:HH22	2.14	0.70
21:U:47:THR:HB	21:U:100:ASP:HB3	1.72	0.70
19:S:106:GLY:HA2	19:S:109:MET:CE	2.20	0.70
26:Z:235:GLU:H	26:Z:235:GLU:CD	1.99	0.70
27:1:30:GLU:HA	27:1:33:HIS:CB	2.21	0.70
1:A:2419:U:H5''	1:A:2420:G:H5'	1.73	0.70
8:H:99:THR:HA	37:H:3461:HOH:O	1.91	0.70
10:J:139:ASP:HA	37:J:8373:HOH:O	1.91	0.70
24:X:80:ASP:O	24:X:84:VAL:HG23	1.90	0.70
1:A:1353:C:P	37:A:4652:HOH:O	2.50	0.70
14:N:139:PRO:O	14:N:140:ALA:HB3	1.92	0.70
1:A:338:C:H4'	5:E:174:ILE:HD11	1.73	0.70
5:E:1:MET:HG2	5:E:2:GLN:H	1.55	0.70
10:J:14:TYR:H	10:J:91:HIS:CE1	2.09	0.70
3:C:121:ALA:O	3:C:124:VAL:HG22	1.92	0.70
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:G:C2'	1:A:545:G:H5''	2.21	0.70
1:A:1160:G:N3	37:A:5610:HOH:O	2.24	0.70
1:A:2768:A:H2'	1:A:2769:C:O4'	1.91	0.70
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.73	0.70
8:H:53:ASP:OD1	8:H:80:GLN:HB2	1.92	0.70
10:J:41:THR:HA	37:J:8397:HOH:O	1.91	0.70
1:A:1753:C:O2	4:D:229:ARG:NH2	2.25	0.69
1:A:2748:G:H2'	37:A:7534:HOH:O	1.92	0.69
1:A:871:G:C8	1:A:871:G:C5'	2.65	0.69
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.74	0.69
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.22	0.69
1:A:214:U:H5'	37:A:6120:HOH:O	1.91	0.69
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.26	0.69
1:A:2467:A:H2'	37:A:5431:HOH:O	1.92	0.69
14:N:172:GLY:C	14:N:183:VAL:HG11	2.18	0.69
19:S:9:ASP:O	19:S:13:THR:HB	1.92	0.69
1:A:1209:C:H2'	1:A:1210:G:H8	1.58	0.69
1:A:1810:C:OP1	22:V:44:ARG:NE	2.18	0.69
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.22	0.69
25:Y:25:ARG:NH1	37:Y:3861:HOH:O	2.25	0.69
1:A:516:A:OP2	37:A:5623:HOH:O	2.10	0.69
37:A:3698:HOH:O	14:N:157:LEU:HD11	1.93	0.69
6:F:55:LYS:HA	37:F:6752:HOH:O	1.93	0.69
1:A:131:A:OP2	37:A:3135:HOH:O	2.10	0.69
1:A:281:U:H2'	1:A:282:C:O4'	1.92	0.69
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.57	0.69
5:E:214:THR:HG21	37:E:8403:HOH:O	1.91	0.69
14:N:104:ARG:O	14:N:108:LYS:HG2	1.92	0.69
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.75	0.69
30:4:48:ASN:ND2	30:4:50:GLY:H	1.91	0.69
37:A:5197:HOH:O	12:L:39:GLY:HA2	1.93	0.69
3:C:200:PRO:O	37:C:8590:HOH:O	2.10	0.69
5:E:139:VAL:HG13	37:E:8453:HOH:O	1.92	0.69
6:F:23:VAL:HG23	6:F:23:VAL:O	1.92	0.69
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.90	0.69
19:S:44:VAL:O	19:S:48:GLU:HG3	1.92	0.69
1:A:1073:A:OP2	37:A:4235:HOH:O	2.11	0.69
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.58	0.69
3:C:35:GLY:O	3:C:36:ASP:HB3	1.92	0.69
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.75	0.69
11:K:131:THR:HG22	11:K:134:GLU:H	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.26	0.69
1:A:1741:U:H5'	1:A:1742:A:OP1	1.92	0.69
7:G:101:GLU:HB2	7:G:116:THR:O	1.92	0.69
14:N:152:ARG:HG3	37:N:8554:HOH:O	1.93	0.69
1:A:204:A:H2'	1:A:205:U:H5'	1.74	0.69
1:A:820:G:O2'	1:A:856:G:H4'	1.92	0.69
1:A:2468:A:H61	30:4:48:ASN:HD21	1.40	0.69
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.09	0.69
26:Z:155:ARG:NH1	37:Z:8559:HOH:O	2.24	0.69
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.58	0.68
1:A:2526:C:O2'	1:A:2527:U:H5'	1.93	0.68
3:C:101:GLU:OE2	3:C:131:HIS:HB2	1.93	0.68
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.75	0.68
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.75	0.68
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.06	0.68
1:A:20:G:H21	19:S:117:HIS:HD2	1.40	0.68
37:A:9116:HOH:O	14:N:82:ARG:HD2	1.93	0.68
1:A:1919:A:H4'	37:A:4819:HOH:O	1.92	0.68
1:A:2467:A:OP1	37:A:9040:HOH:O	2.12	0.68
7:G:11:VAL:HG12	7:G:12:ASP:N	2.07	0.68
10:J:27:LYS:H	10:J:58:HIS:CD2	2.06	0.68
24:X:65:VAL:HA	24:X:68:THR:HG22	1.76	0.68
22:V:14:GLU:O	22:V:17:THR:HB	1.93	0.68
1:A:2578:G:H5'	1:A:2578:G:H8	1.58	0.68
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.09	0.68
25:Y:15:ARG:HB3	25:Y:15:ARG:HH11	1.59	0.68
1:A:1667:A:H5'	1:A:1667:A:C8	2.27	0.68
16:P:87:THR:O	16:P:91:GLN:HG3	1.94	0.68
23:W:39:ALA:C	23:W:41:GLU:H	2.02	0.68
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.59	0.68
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.11	0.68
1:A:1751:G:C2'	1:A:1752:G:H5''	2.24	0.68
2:B:3023:U:C5'	2:B:3024:U:OP2	2.42	0.68
1:A:2508:C:H2'	37:A:6734:HOH:O	1.94	0.67
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.94	0.67
3:C:105:VAL:HG12	3:C:106:CYS:N	2.10	0.67
6:F:95:THR:C	6:F:97:GLN:H	2.02	0.67
7:G:93:MET:HE1	7:G:165:GLY:N	2.09	0.67
10:J:49:VAL:O	10:J:157:ILE:HG23	1.94	0.67
24:X:5:VAL:HG11	24:X:153:MET:HE1	1.77	0.67
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:THR:O	6:F:97:GLN:N	2.24	0.67
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.76	0.67
27:1:29:VAL:O	27:1:33:HIS:HB2	1.95	0.67
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.77	0.67
23:W:56:ILE:O	23:W:60:GLN:HG3	1.95	0.67
1:A:1119:G:N2	1:A:1246:A:C2	2.58	0.67
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.09	0.67
21:U:32:ARG:NH1	21:U:38:ARG:HH12	1.92	0.67
24:X:88:THR:HG22	24:X:89:ASP:N	2.10	0.67
1:A:88:G:N7	29:3:28:LYS:HD2	2.09	0.67
1:A:447:A:OP1	21:U:2:LYS:HG2	1.95	0.67
1:A:506:G:H22	1:A:509:A:H5'	1.59	0.67
1:A:869:G:OP1	14:N:79:LYS:HE2	1.94	0.67
4:D:248:ARG:HG2	37:K:8541:HOH:O	1.94	0.67
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.76	0.67
14:N:69:LYS:O	14:N:73:ARG:NH2	2.25	0.67
5:E:237:GLU:HB2	37:E:8433:HOH:O	1.94	0.67
1:A:711:G:H1'	37:A:7079:HOH:O	1.93	0.67
1:A:2420:G:H4'	37:A:4067:HOH:O	1.95	0.67
1:A:2646:G:H1'	31:A:9000:TYK:H221	1.76	0.67
6:F:69:ILE:HG22	6:F:69:ILE:O	1.95	0.67
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.77	0.67
22:V:6:CYS:SG	22:V:31:PHE:HA	2.35	0.67
1:A:2830:U:H3'	37:A:5204:HOH:O	1.94	0.67
1:A:450:C:OP1	5:E:184:ARG:NH2	2.22	0.67
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.75	0.67
20:T:43:GLU:HB3	37:T:8343:HOH:O	1.95	0.67
22:V:14:GLU:OE1	22:V:15:PRO:HD2	1.94	0.67
1:A:1909:A:N1	1:A:2128:G:H1'	2.10	0.66
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.77	0.66
5:E:233:THR:HG22	5:E:234:VAL:N	2.09	0.66
1:A:1170:U:O2'	1:A:1172:G:N7	2.24	0.66
30:4:7:PHE:HE2	30:4:22:VAL:HG21	1.60	0.66
1:A:1766:U:O2	1:A:1778:A:H5'	1.95	0.66
27:1:42:CYS:SG	27:1:44:PHE:N	2.60	0.66
1:A:21:G:C5'	19:S:2:ILE:HA	2.24	0.66
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.76	0.66
9:I:63:ARG:N	37:I:2569:HOH:O	2.28	0.66
11:K:133:GLY:O	11:K:137:GLU:HG3	1.96	0.66
1:A:282:C:H1'	1:A:368:C:H42	1.60	0.66
1:A:338:C:H5''	37:E:8423:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:U:H2'	1:A:1131:G:O4'	1.95	0.66
1:A:2716:G:H5''	4:D:206:THR:HG21	1.78	0.66
1:A:2862:G:H4'	4:D:336:GLN:O	1.95	0.66
37:A:9380:HOH:O	27:1:34:LYS:HD3	1.94	0.66
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.31	0.66
1:A:1878:G:H1'	37:A:6101:HOH:O	1.96	0.66
27:1:10:ARG:HA	37:1:8414:HOH:O	1.94	0.66
1:A:664:U:OP1	37:A:3755:HOH:O	2.13	0.66
5:E:214:THR:HG23	37:E:8441:HOH:O	1.94	0.66
13:M:145:LEU:O	13:M:148:GLU:HG3	1.96	0.66
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.94	0.66
7:G:84:MET:HE1	7:G:148:ILE:CD1	2.26	0.66
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.30	0.66
20:T:53:ASN:ND2	37:T:8322:HOH:O	2.28	0.66
1:A:2729:C:H2'	1:A:2730:G:H8	1.61	0.66
1:A:2827:A:H2'	1:A:2828:G:O4'	1.95	0.66
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.93	0.66
23:W:12:THR:HG22	23:W:15:GLU:CG	2.16	0.66
1:A:603:A:H5''	1:A:604:G:OP1	1.95	0.66
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.77	0.66
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.26	0.66
14:N:30:GLU:O	14:N:34:GLU:HG3	1.96	0.66
1:A:820:G:OP1	27:1:17:ARG:NH2	2.23	0.65
1:A:845:U:OP2	37:A:9197:HOH:O	2.14	0.65
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.31	0.65
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.77	0.65
5:E:236:THR:CG2	5:E:239:ALA:H	2.01	0.65
7:G:132:THR:HB	37:G:2227:HOH:O	1.96	0.65
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.96	0.65
1:A:1328:A:OP1	26:Z:169:ARG:HD2	1.96	0.65
1:A:2320:U:H4'	1:A:2321:A:O4'	1.96	0.65
37:A:4360:HOH:O	14:N:84:LYS:HE2	1.96	0.65
10:J:27:LYS:N	10:J:58:HIS:HD2	1.92	0.65
10:J:59:ASN:H	10:J:59:ASN:ND2	1.94	0.65
1:A:506:G:H22	1:A:509:A:H5''	1.61	0.65
5:E:236:THR:H	5:E:239:ALA:HB3	1.61	0.65
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.44	0.65
37:A:9495:HOH:O	4:D:18:ARG:HD3	1.97	0.65
5:E:234:VAL:HG22	5:E:234:VAL:O	1.97	0.65
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.32	0.65
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:GLU:O	3:C:34:ASP:HB2	1.95	0.65
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.59	0.65
1:A:2329:C:O2'	1:A:2330:U:H5'	1.96	0.65
4:D:145:HIS:HD2	4:D:146:THR:O	1.79	0.65
13:M:53:ARG:NH2	13:M:57:VAL:HG12	2.10	0.65
1:A:2310:G:OP2	10:J:114:PRO:HD2	1.96	0.65
6:F:166:ILE:HD12	37:F:6326:HOH:O	1.96	0.65
14:N:52:LEU:HD21	37:N:8615:HOH:O	1.97	0.65
24:X:149:LEU:CG	24:X:153:MET:HE2	2.27	0.65
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.25	0.65
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.62	0.65
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.31	0.65
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.79	0.65
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.27	0.65
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.79	0.65
1:A:2421:G:H3'	1:A:2422:U:C5'	2.27	0.65
22:V:9:CYS:CA	22:V:52:THR:HG23	2.26	0.65
1:A:2908:A:H2'	1:A:2909:G:O4'	1.97	0.65
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.43	0.65
14:N:139:PRO:O	14:N:140:ALA:CB	2.45	0.65
4:D:258:GLY:H	4:D:260:HIS:CE1	2.14	0.64
14:N:154:ARG:NE	37:N:8639:HOH:O	2.31	0.64
23:W:64:GLY:O	23:W:65:ASP:HB2	1.96	0.64
24:X:130:HIS:O	24:X:136:GLY:HA3	1.97	0.64
28:2:25:LYS:HE2	37:3:7213:HOH:O	1.95	0.64
1:A:2432:C:O2'	1:A:2433:A:H5'	1.98	0.64
1:A:2637:A:H5'	37:A:9265:HOH:O	1.97	0.64
5:E:236:THR:HA	37:E:8456:HOH:O	1.96	0.64
6:F:135:VAL:HG22	6:F:136:ARG:H	1.60	0.64
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.26	0.64
11:K:107:ASN:ND2	11:K:109:TYR:H	1.95	0.64
1:A:962:C:C1'	15:O:5:ARG:NH1	2.59	0.64
1:A:2281:C:H2'	1:A:2282:U:H5'	1.80	0.64
37:A:6951:HOH:O	23:W:4:HIS:HB3	1.97	0.64
14:N:104:ARG:O	14:N:108:LYS:HE2	1.97	0.64
29:3:41:HIS:H	29:3:45:ASN:ND2	1.95	0.64
1:A:31:C:H4'	37:A:7413:HOH:O	1.97	0.64
1:A:272:A:H3'	37:A:7522:HOH:O	1.97	0.64
1:A:1700:C:OP2	37:A:6013:HOH:O	2.14	0.64
1:A:1123:A:C6	1:A:1238:C:H5'	2.33	0.64
1:A:1185:U:H2'	1:A:1186:C:C6	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.12	0.64
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.31	0.64
11:K:99:GLU:HA	37:K:8573:HOH:O	1.97	0.64
1:A:2359:G:N7	37:A:3675:HOH:O	2.29	0.64
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.30	0.64
3:C:175:LYS:HE2	37:C:8578:HOH:O	1.98	0.64
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.63	0.64
14:N:154:ARG:CZ	37:N:8639:HOH:O	2.45	0.64
4:D:305:ASP:O	4:D:306:LYS:HB2	1.98	0.64
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.96	0.64
1:A:1329:A:C2	37:A:4657:HOH:O	2.49	0.64
3:C:94:LEU:N	3:C:94:LEU:HD23	2.12	0.64
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.80	0.64
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.33	0.64
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.96	0.64
6:F:174:VAL:HG13	37:F:6555:HOH:O	1.98	0.64
1:A:2912:C:OP2	37:A:5528:HOH:O	2.15	0.63
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.78	0.63
1:A:188:C:H5''	14:N:163:LEU:HD21	1.80	0.63
2:B:3020:G:O2'	2:B:3021:G:H5'	1.98	0.63
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.81	0.63
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.63	0.63
27:1:46:LYS:O	27:1:57:CYS:HA	1.98	0.63
27:1:47:LEU:HD23	27:1:57:CYS:HB2	1.80	0.63
28:2:10:LYS:HG3	37:2:2979:HOH:O	1.98	0.63
1:A:157:G:OP2	37:A:9466:HOH:O	2.15	0.63
1:A:263:U:O4'	8:H:59:ILE:HD13	1.98	0.63
1:A:282:C:O2'	1:A:283:U:H5'	1.99	0.63
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.62	0.63
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.80	0.63
10:J:139:ASP:H	10:J:140:PRO:HD3	1.64	0.63
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.80	0.63
27:1:18:TYR:HB3	27:1:22:ILE:HG21	1.79	0.63
1:A:272:A:H5'	1:A:273:G:OP2	1.99	0.63
1:A:1159:G:P	37:A:4264:HOH:O	2.56	0.63
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.13	0.63
6:F:25:MET:CE	6:F:37:ALA:HB1	2.28	0.63
15:O:58:LEU:HD12	15:O:58:LEU:N	2.14	0.63
24:X:4:LEU:O	24:X:32:CYS:HA	1.99	0.63
26:Z:186:ARG:HG2	26:Z:186:ARG:HH11	1.64	0.63
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2281:C:C2'	1:A:2282:U:H5'	2.29	0.63
2:B:3039:U:H1'	2:B:3044:A:H61	1.62	0.63
1:A:251:C:O2'	1:A:252:C:H5'	1.99	0.63
1:A:1187:U:O2'	1:A:1189:A:H2	1.82	0.63
16:P:47:ARG:HG3	16:P:47:ARG:NH1	2.12	0.63
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.80	0.63
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.79	0.63
1:A:941:G:O2'	1:A:942:U:H5'	1.98	0.63
14:N:39:ARG:NH2	37:N:8621:HOH:O	2.31	0.63
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.80	0.63
1:A:656:G:OP2	16:P:37:ARG:HD2	1.98	0.62
12:L:115:ARG:HG3	12:L:116:GLU:N	2.14	0.62
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.81	0.62
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.29	0.62
1:A:2094:G:H4'	4:D:245:SER:HB3	1.81	0.62
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.28	0.62
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.80	0.62
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.81	0.62
24:X:38:THR:HG22	37:X:3580:HOH:O	1.99	0.62
6:F:19:GLU:O	6:F:20:LYS:HG2	1.99	0.62
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.80	0.62
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.15	0.62
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.81	0.62
1:A:2005:G:O2'	1:A:2008:U:OP2	2.16	0.62
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.40	0.62
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.62	0.62
5:E:12:THR:HB	37:E:8446:HOH:O	1.98	0.62
10:J:75:SER:C	10:J:79:ALA:HB2	2.24	0.62
10:J:166:ASN:N	10:J:166:ASN:HD22	1.97	0.62
14:N:154:ARG:HG3	37:N:8612:HOH:O	1.99	0.62
24:X:13:MET:CE	24:X:17:ILE:HG22	2.29	0.62
28:2:28:HIS:CD2	28:2:31:LYS:HG3	2.34	0.62
6:F:99:ASP:CB	6:F:103:ASN:H	2.13	0.62
7:G:23:GLU:HG2	7:G:28:SER:CB	2.30	0.62
1:A:1119:G:H2'	11:K:52:GLN:NE2	2.15	0.62
1:A:2064:U:H5'	1:A:2652:U:H4'	1.82	0.62
4:D:14:GLY:HA2	4:D:15:PRO:C	2.25	0.62
6:F:101:THR:HG22	37:F:7400:HOH:O	1.99	0.62
7:G:93:MET:HE1	7:G:165:GLY:H	1.62	0.62
18:R:25:PRO:HB2	37:R:4350:HOH:O	2.00	0.62
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.29	0.62
1:A:299:U:H5'	37:A:7324:HOH:O	1.99	0.62
1:A:885:G:OP2	37:A:9389:HOH:O	2.16	0.62
1:A:902:G:N7	13:M:18:HIS:HD2	1.97	0.62
1:A:1119:G:H8	11:K:52:GLN:NE2	1.97	0.62
1:A:1241:G:N2	11:K:86:MET:HE2	2.15	0.62
7:G:7:ILE:HD11	7:G:11:VAL:C	2.25	0.62
21:U:19:ARG:HD3	21:U:67:LEU:O	2.00	0.62
1:A:2291:A:C8	1:A:2309:C:H5'	2.34	0.62
1:A:2878:U:H2'	1:A:2879:A:O4'	2.00	0.62
3:C:199:HIS:HD2	3:C:201:PHE:H	1.46	0.62
27:1:31:ILE:O	27:1:35:LYS:HG3	1.98	0.62
27:1:46:LYS:HB2	27:1:57:CYS:SG	2.38	0.62
27:1:77:LYS:HA	27:1:80:MET:HE2	1.82	0.62
1:A:1735:C:O2'	1:A:1736:A:H5'	1.99	0.62
1:A:2346:C:O5'	1:A:2346:C:H6	1.83	0.62
4:D:2:GLN:CD	37:D:8618:HOH:O	2.42	0.62
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.82	0.62
23:W:58:THR:O	23:W:62:GLU:HG3	2.00	0.62
1:A:960:G:H2'	1:A:960:G:N3	2.15	0.62
3:C:11:ARG:HD3	37:C:8517:HOH:O	1.99	0.62
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.81	0.62
1:A:1377:C:H6	1:A:1377:C:H5'	1.65	0.61
37:A:4806:HOH:O	11:K:47:THR:HB	1.99	0.61
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.65	0.61
15:O:64:SER:C	15:O:66:LEU:H	2.08	0.61
16:P:42:GLU:HB2	37:P:2176:HOH:O	1.97	0.61
1:A:2408:A:H2	37:A:3073:HOH:O	1.83	0.61
8:H:110:GLU:HG2	37:H:6926:HOH:O	2.00	0.61
27:1:61:GLY:HA3	37:1:8425:HOH:O	1.99	0.61
1:A:2044:G:OP1	25:Y:23:HIS:HE1	1.83	0.61
1:A:2769:C:H2'	1:A:2770:G:O4'	2.00	0.61
3:C:131:HIS:O	3:C:132:ASP:HB2	1.98	0.61
3:C:179:MET:HA	3:C:179:MET:HE3	1.83	0.61
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.14	0.61
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.35	0.61
1:A:821:U:H2'	1:A:822:C:H6	1.64	0.61
1:A:155:C:OP2	14:N:188:ARG:NH1	2.28	0.61
37:A:4162:HOH:O	26:Z:186:ARG:HD2	2.00	0.61
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.83	0.61
5:E:133:ARG:HD2	37:E:8411:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.81	0.61
14:N:164:THR:CG2	14:N:165:SER:N	2.62	0.61
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.81	0.61
1:A:119:A:H2'	1:A:120:A:H5''	1.83	0.61
1:A:558:C:C2'	1:A:559:U:H5''	2.31	0.61
37:A:6229:HOH:O	22:V:56:ARG:HB3	2.00	0.61
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.31	0.61
5:E:132:ASP:HB3	37:E:8365:HOH:O	2.01	0.61
24:X:110:GLN:HA	24:X:110:GLN:HE21	1.62	0.61
26:Z:189:ASN:ND2	26:Z:192:ASP:H	1.97	0.61
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.99	0.61
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.82	0.61
25:Y:41:PHE:O	25:Y:43:VAL:HG23	2.01	0.61
1:A:396:U:OP2	30:4:38:ARG:NH1	2.34	0.61
37:A:6017:HOH:O	30:4:62:THR:HB	2.00	0.61
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.81	0.61
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.00	0.61
27:1:53:GLY:HA2	27:1:67:GLY:O	2.00	0.61
1:A:625:U:H5''	1:A:1044:C:N4	2.15	0.61
2:B:3107:C:H5	37:B:3167:HOH:O	1.84	0.61
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.83	0.61
10:J:46:VAL:O	10:J:146:TRP:HH2	1.84	0.61
1:A:2324:G:H4'	1:A:2418:G:O2'	2.01	0.60
1:A:2649:A:H5'	1:A:2649:A:H8	1.66	0.60
2:B:3049:G:H5''	37:B:4707:HOH:O	2.00	0.60
12:L:29:LEU:HB3	12:L:55:VAL:CG1	2.27	0.60
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.31	0.60
30:4:57:GLY:HA2	37:4:8529:HOH:O	2.00	0.60
1:A:121:U:OP2	29:3:10:ARG:NH2	2.34	0.60
12:L:55:VAL:HG12	12:L:56:SER:N	2.16	0.60
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.66	0.60
24:X:122:ARG:HH11	24:X:122:ARG:CG	2.13	0.60
27:1:42:CYS:SG	27:1:43:GLY:N	2.74	0.60
1:A:661:G:C5	1:A:686:A:C2	2.89	0.60
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.81	0.60
5:E:78:ARG:HG3	5:E:78:ARG:NH1	2.12	0.60
13:M:26:HIS:HB2	37:M:8512:HOH:O	2.00	0.60
14:N:48:ARG:NH2	37:N:8561:HOH:O	2.32	0.60
15:O:169:PRO:O	15:O:172:PHE:HB3	2.01	0.60
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.82	0.60
29:3:18:ASN:HD21	29:3:40:ARG:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:G:OP1	28:2:16:HIS:HE1	1.85	0.60
1:A:2780:C:H2'	1:A:2781:U:C6	2.37	0.60
7:G:69:ILE:HA	7:G:72:MET:CE	2.32	0.60
8:H:58:GLU:HA	8:H:61:MET:HE2	1.82	0.60
14:N:133:LEU:O	14:N:134:ILE:HD13	2.01	0.60
15:O:141:ARG:HB3	37:O:8566:HOH:O	2.02	0.60
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.82	0.60
1:A:204:A:C2'	1:A:205:U:H5'	2.30	0.60
1:A:2533:C:H5'	1:A:2533:C:C6	2.32	0.60
37:A:4540:HOH:O	5:E:50:GLU:HG2	2.00	0.60
5:E:16:VAL:HG12	5:E:17:ASP:N	2.16	0.60
5:E:115:LEU:O	5:E:118:THR:HB	2.01	0.60
9:I:12:ILE:N	9:I:13:PRO:CD	2.65	0.60
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.83	0.60
7:G:81:GLU:HG2	7:G:134:SER:CB	2.32	0.60
7:G:84:MET:HE1	7:G:148:ILE:HD12	1.82	0.60
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.82	0.60
1:A:283:U:H5''	1:A:284:C:P	2.42	0.60
1:A:474:C:O3'	5:E:73:LEU:HD21	2.01	0.60
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.83	0.60
6:F:37:ALA:O	6:F:40:ILE:HG12	2.02	0.60
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.82	0.60
1:A:212:A:O4'	1:A:214:U:C6	2.55	0.60
1:A:558:C:H5'	37:A:5233:HOH:O	2.02	0.60
1:A:2361:A:H2'	1:A:2362:A:C8	2.35	0.60
1:A:2768:A:O2'	1:A:2769:C:H5'	2.02	0.60
4:D:36:PRO:HA	4:D:168:GLY:CA	2.31	0.60
6:F:136:ARG:HD2	6:F:155:HIS:O	2.01	0.60
21:U:6:LYS:NZ	37:U:644:HOH:O	2.35	0.60
30:4:74:CYS:SG	30:4:76:LYS:HB2	2.42	0.60
1:A:280:C:H2'	1:A:281:U:O4'	2.02	0.60
10:J:127:GLY:O	10:J:128:ALA:HB3	1.99	0.60
1:A:2429:A:H2'	1:A:2430:A:C8	2.37	0.60
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.31	0.60
1:A:1422:U:H2'	1:A:1423:C:C6	2.36	0.59
1:A:2088:C:H1'	1:A:2841:A:N1	2.17	0.59
1:A:2748:G:H5'	37:A:7534:HOH:O	2.02	0.59
1:A:2851:G:O2'	1:A:2852:A:H5'	2.01	0.59
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.02	0.59
34:K:8501:CL:CL	37:K:8547:HOH:O	2.53	0.59
19:S:119:VAL:O	19:S:119:VAL:HG12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.27	0.59
1:A:151:A:C2	1:A:442:A:C8	2.90	0.59
15:O:163:PHE:HA	37:O:8520:HOH:O	2.02	0.59
19:S:39:THR:HB	19:S:42:GLU:CG	2.31	0.59
23:W:39:ALA:O	23:W:41:GLU:N	2.35	0.59
24:X:13:MET:HE2	24:X:18:GLN:HA	1.84	0.59
5:E:118:THR:O	5:E:136:VAL:HG13	2.02	0.59
6:F:25:MET:HE1	6:F:37:ALA:O	2.02	0.59
6:F:135:VAL:HG22	6:F:136:ARG:N	2.16	0.59
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.83	0.59
23:W:44:GLY:O	23:W:48:GLU:HG2	2.01	0.59
1:A:739:G:C5	37:A:7536:HOH:O	2.51	0.59
37:A:9111:HOH:O	5:E:103:ASN:HB3	2.01	0.59
4:D:75:GLU:C	4:D:77:PRO:HD3	2.28	0.59
14:N:38:VAL:C	14:N:63:VAL:HG13	2.28	0.59
15:O:154:LEU:O	15:O:155:GLU:HB3	2.00	0.59
1:A:951:A:C2'	1:A:952:G:H5'	2.33	0.59
1:A:2505:G:O2'	1:A:2506:A:H5'	2.02	0.59
37:A:3960:HOH:O	21:U:82:THR:HA	2.02	0.59
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.84	0.59
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.32	0.59
1:A:514:G:OP1	1:A:514:G:H2'	2.03	0.59
1:A:2284:G:H1'	37:A:9555:HOH:O	2.00	0.59
3:C:129:LEU:CD1	3:C:145:MET:HE1	2.33	0.59
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.32	0.59
10:J:136:VAL:HG22	10:J:137:ASN:O	2.02	0.59
14:N:74:ARG:NH2	37:N:8629:HOH:O	2.32	0.59
15:O:151:ASP:O	15:O:154:LEU:HB2	2.03	0.59
1:A:1819:G:H2'	1:A:1820:G:H4'	1.84	0.59
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.84	0.59
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.84	0.59
1:A:820:G:H5'	1:A:821:U:H5'	1.84	0.59
2:B:3003:A:N6	2:B:3022:G:H1'	2.18	0.59
10:J:136:VAL:HG23	37:J:8345:HOH:O	2.03	0.59
15:O:152:GLU:C	15:O:154:LEU:H	2.09	0.59
1:A:182:G:H4'	14:N:157:LEU:HD13	1.83	0.59
1:A:485:A:N3	1:A:487:G:H5''	2.17	0.59
1:A:2635:A:O2'	1:A:2636:C:H5'	2.03	0.59
1:A:2690:U:O2'	7:G:111:LYS:HE3	2.03	0.59
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.32	0.59
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:C:H5''	37:A:6739:HOH:O	2.02	0.59
3:C:188:ASN:OD1	37:C:8559:HOH:O	2.16	0.59
6:F:59:GLY:C	6:F:61:PHE:H	2.11	0.59
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.02	0.59
10:J:144:GLU:OE1	10:J:144:GLU:HA	2.03	0.59
30:4:40:ARG:HD2	37:4:8553:HOH:O	2.02	0.59
2:B:3042:C:H2'	37:B:6700:HOH:O	2.02	0.58
4:D:7:ARG:HD3	4:D:9:GLY:O	2.02	0.58
4:D:254:GLN:HG2	4:D:255:GLY:N	2.18	0.58
6:F:105:SER:CB	6:F:131:THR:HG23	2.30	0.58
7:G:32:ARG:O	7:G:33:LEU:HD23	2.03	0.58
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.84	0.58
20:T:51:GLN:NE2	20:T:53:ASN:HD21	2.01	0.58
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.33	0.58
1:A:485:A:O2'	1:A:487:G:H5'	2.03	0.58
1:A:559:U:H5'	1:A:559:U:C6	2.36	0.58
9:I:64:ASN:HD22	9:I:64:ASN:N	2.01	0.58
10:J:44:ALA:HA	10:J:163:PRO:O	2.04	0.58
37:L:7438:HOH:O	22:V:20:MET:HE1	2.03	0.58
19:S:33:ARG:NH1	37:S:8544:HOH:O	2.36	0.58
2:B:3055:U:H4'	2:B:3056:A:C8	2.38	0.58
3:C:37:VAL:HG22	37:C:8601:HOH:O	2.03	0.58
4:D:168:GLY:N	4:D:174:ARG:HD3	2.18	0.58
6:F:50:VAL:O	6:F:71:ALA:HA	2.03	0.58
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.33	0.58
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.15	0.58
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.04	0.58
1:A:391:U:OP2	14:N:84:LYS:NZ	2.36	0.58
1:A:542:A:H2'	1:A:543:G:O4'	2.03	0.58
1:A:1615:A:H4'	37:A:5863:HOH:O	2.02	0.58
37:A:3731:HOH:O	21:U:9:LYS:CD	2.51	0.58
2:B:3001:U:O3'	2:B:3003:A:H5''	2.03	0.58
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.18	0.58
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.43	0.58
1:A:2064:U:OP1	37:A:3324:HOH:O	2.17	0.58
1:A:2241:C:O2'	1:A:2242:U:H5'	2.02	0.58
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.84	0.58
5:E:219:ASN:O	5:E:222:ASP:OD1	2.20	0.58
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.86	0.58
7:G:84:MET:HE2	7:G:133:VAL:HG21	1.85	0.58
8:H:58:GLU:HA	8:H:61:MET:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:149:ALA:C	10:J:151:MET:H	2.10	0.58
14:N:68:ARG:O	14:N:68:ARG:HD3	2.04	0.58
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.66	0.58
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.86	0.58
24:X:41:TYR:O	24:X:45:VAL:HG13	2.04	0.58
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.33	0.58
1:A:157:G:H4'	14:N:95:LYS:HE3	1.85	0.58
1:A:2394:A:OP1	37:A:7078:HOH:O	2.17	0.58
1:A:2502:C:C2'	1:A:2503:A:H5'	2.33	0.58
2:B:3044:A:O4'	6:F:76:ARG:NE	2.37	0.58
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.84	0.58
1:A:797:A:O4'	27:1:10:ARG:N	2.36	0.58
1:A:1127:C:H2'	1:A:1128:U:H5'	1.85	0.58
1:A:1200:A:H4'	37:A:7328:HOH:O	2.02	0.58
1:A:1333:U:H2'	1:A:1334:C:C6	2.39	0.58
1:A:2415:A:C2	15:O:25:ARG:HB3	2.39	0.58
1:A:2443:C:H3'	37:A:3453:HOH:O	2.03	0.58
1:A:2456:A:H5'	37:A:5671:HOH:O	2.02	0.58
1:A:2897:C:H2'	1:A:2898:G:H8	1.68	0.58
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.03	0.58
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.34	0.58
13:M:73:VAL:HG23	13:M:74:THR:H	1.67	0.58
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.85	0.58
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.38	0.58
1:A:281:U:O2'	1:A:282:C:H5'	2.04	0.58
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.36	0.58
3:C:211:LYS:NZ	37:C:8575:HOH:O	2.37	0.58
25:Y:30:MET:HE3	25:Y:55:ASN:OD1	2.03	0.58
1:A:1118:A:C8	1:A:1118:A:C3'	2.81	0.58
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.85	0.58
10:J:71:TYR:C	10:J:73:GLN:N	2.59	0.58
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.84	0.58
25:Y:25:ARG:CZ	37:Y:3861:HOH:O	2.50	0.58
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.04	0.58
26:Z:212:ARG:HD2	37:Z:8601:HOH:O	2.03	0.58
1:A:240:C:H4'	14:N:146:GLN:NE2	2.19	0.58
1:A:2587:U:H2'	1:A:2589:U:H5''	1.85	0.58
1:A:2783:A:H3'	37:A:5208:HOH:O	2.03	0.58
4:D:141:ARG:HD2	4:D:163:GLU:OE2	2.03	0.58
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.86	0.58
11:K:74:ARG:O	11:K:78:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:39:ALA:N	23:W:40:PRO:CD	2.66	0.58
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.17	0.58
1:A:1825:U:O4'	1:A:1999:C:H5''	2.04	0.57
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.52	0.57
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.36	0.57
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.39	0.57
1:A:289:G:N2	1:A:363:A:H2	1.99	0.57
1:A:1241:G:H21	11:K:86:MET:HE2	1.68	0.57
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.04	0.57
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.87	0.57
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.04	0.57
22:V:52:THR:CG2	22:V:54:THR:HB	2.34	0.57
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.67	0.57
1:A:1641:A:H2'	1:A:1642:A:H5'	1.85	0.57
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.66	0.57
19:S:132:ARG:CZ	37:S:8583:HOH:O	2.52	0.57
1:A:182:G:H5'	37:A:5132:HOH:O	2.04	0.57
1:A:1923:G:H4'	30:4:31:THR:O	2.05	0.57
3:C:97:ALA:HB2	3:C:150:PRO:HB2	1.86	0.57
19:S:39:THR:HG22	19:S:42:GLU:H	1.69	0.57
23:W:64:GLY:O	23:W:65:ASP:CB	2.52	0.57
24:X:26:ILE:O	24:X:26:ILE:CG1	2.52	0.57
1:A:513:A:N3	37:A:3635:HOH:O	2.33	0.57
1:A:1200:A:C4'	37:A:7328:HOH:O	2.52	0.57
1:A:1972:U:H2'	1:A:1973:A:H5'	1.87	0.57
6:F:27:ILE:HG22	6:F:28:GLY:N	2.20	0.57
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.20	0.57
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.86	0.57
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.05	0.57
1:A:184:G:H5''	14:N:153:THR:HG22	1.87	0.57
1:A:1773:G:C8	27:1:16:PRO:HA	2.40	0.57
2:B:3039:U:H1'	2:B:3044:A:N6	2.19	0.57
8:H:107:VAL:O	8:H:111:ILE:HG13	2.04	0.57
11:K:19:MET:HE1	11:K:78:ILE:HG22	1.86	0.57
14:N:72:SER:OG	14:N:74:ARG:HB2	2.04	0.57
27:1:25:ARG:O	27:1:29:VAL:HG23	2.05	0.57
3:C:171:LYS:NZ	37:C:8526:HOH:O	2.34	0.57
6:F:86:THR:O	6:F:90:LEU:HG	2.05	0.57
7:G:6:GLU:HA	7:G:46:THR:HG22	1.87	0.57
7:G:15:GLN:HG2	7:G:19:ASP:O	2.05	0.57
14:N:87:MET:HE1	37:N:8530:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:39:THR:O	16:P:115:ARG:NH2	2.38	0.57
1:A:136:C:H2'	1:A:137:U:O4'	2.04	0.57
1:A:1505:U:H6	1:A:1505:U:H5'	1.68	0.57
1:A:1827:G:H2'	1:A:1828:G:C8	2.40	0.57
1:A:2729:C:O2'	1:A:2730:G:H5'	2.05	0.57
4:D:275:GLY:O	4:D:291:ASP:HA	2.05	0.57
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.70	0.57
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.40	0.57
1:A:1192:A:O2'	1:A:1193:A:OP1	2.20	0.57
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.39	0.57
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.86	0.57
1:A:681:G:H5'	1:A:681:G:N3	2.20	0.57
1:A:2484:U:C2	37:A:9601:HOH:O	2.52	0.57
3:C:36:ASP:OD2	3:C:85:ASP:HB2	2.04	0.57
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.68	0.57
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.05	0.57
8:H:99:THR:O	8:H:99:THR:HG23	2.04	0.57
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.35	0.57
18:R:40:HIS:HD2	18:R:60:THR:OG1	1.88	0.57
19:S:39:THR:HB	19:S:42:GLU:CD	2.29	0.57
1:A:183:A:H5'	14:N:157:LEU:HD12	1.87	0.56
1:A:545:G:H5'	1:A:545:G:C8	2.35	0.56
1:A:1855:G:H8	3:C:144:GLU:OE2	1.88	0.56
1:A:2466:G:H5''	37:A:3621:HOH:O	2.05	0.56
2:B:3014:G:H5'	2:B:3014:G:C8	2.34	0.56
4:D:280:VAL:CG1	4:D:334:SER:HA	2.35	0.56
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.18	0.56
13:M:143:THR:HG22	13:M:144:ASP:H	1.70	0.56
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.34	0.56
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.86	0.56
28:2:25:LYS:HG2	28:2:25:LYS:O	2.04	0.56
1:A:2414:A:H2'	1:A:2415:A:C8	2.40	0.56
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.40	0.56
37:A:3731:HOH:O	21:U:9:LYS:HD2	2.04	0.56
4:D:125:GLU:O	4:D:129:ARG:HG3	2.05	0.56
7:G:137:ASP:O	7:G:141:VAL:HG23	2.05	0.56
14:N:24:MET:O	14:N:28:MET:HG3	2.05	0.56
15:O:110:THR:HB	15:O:113:SER:OG	2.04	0.56
30:4:3:MET:O	30:4:90:PHE:HA	2.04	0.56
1:A:394:G:H1	14:N:181:GLU:CD	2.14	0.56
1:A:470:U:O2'	28:2:16:HIS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:G:H5'	1:A:1598:A:H4'	1.86	0.56
1:A:1523:G:H2'	1:A:1524:U:C6	2.40	0.56
1:A:1947:G:N2	1:A:1966:U:C2	2.73	0.56
1:A:2010:A:H2'	37:A:5935:HOH:O	2.05	0.56
1:A:2657:G:OP1	4:D:17:LYS:HB2	2.06	0.56
37:A:5504:HOH:O	14:N:58:GLN:HG3	2.03	0.56
5:E:84:VAL:O	5:E:85:LYS:HB2	2.04	0.56
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.87	0.56
8:H:2:VAL:HG22	8:H:57:GLU:OE1	2.04	0.56
15:O:37:ARG:NE	37:O:8533:HOH:O	2.38	0.56
16:P:25:VAL:HG23	16:P:26:TRP:N	2.21	0.56
19:S:132:ARG:HG2	19:S:133:ALA:N	2.20	0.56
22:V:52:THR:HG22	22:V:54:THR:HB	1.88	0.56
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.87	0.56
26:Z:185:VAL:HG12	37:Z:8570:HOH:O	2.04	0.56
28:2:28:HIS:HD2	28:2:31:LYS:H	1.52	0.56
1:A:1189:A:H1'	1:A:1209:C:C1'	2.36	0.56
2:B:3002:U:OP2	2:B:3002:U:H4'	2.05	0.56
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.69	0.56
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.20	0.56
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.86	0.56
28:2:8:GLN:HE22	28:2:11:LYS:NZ	2.03	0.56
1:A:88:G:H5'	1:A:88:G:H8	1.70	0.56
1:A:558:C:O2'	1:A:559:U:H5''	2.06	0.56
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.39	0.56
1:A:2710:U:H1'	37:A:7618:HOH:O	2.06	0.56
10:J:28:ILE:HA	10:J:62:GLU:OE1	2.06	0.56
14:N:38:VAL:O	14:N:63:VAL:HG13	2.06	0.56
1:A:1234:U:N3	4:D:244:PRO:HB3	2.20	0.56
4:D:156:LYS:HZ1	4:D:160:ASP:CG	2.14	0.56
1:A:1162:G:H2'	37:A:6565:HOH:O	2.05	0.56
1:A:1205:U:H2'	1:A:1206:U:C5'	2.34	0.56
1:A:1308:A:H5'	37:A:6916:HOH:O	2.06	0.56
1:A:1636:G:O2'	1:A:1637:A:H5'	2.05	0.56
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.06	0.56
37:A:4515:HOH:O	10:J:151:MET:HE2	2.04	0.56
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.88	0.56
8:H:19:ALA:O	8:H:22:VAL:HG22	2.06	0.56
8:H:110:GLU:O	8:H:114:LYS:HG3	2.06	0.56
21:U:37:GLN:OE1	21:U:118:SER:HA	2.05	0.56
1:A:283:U:H5''	1:A:284:C:OP2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:A:H3'	37:A:5022:HOH:O	2.05	0.56
1:A:1025:C:H5'	24:X:23:MET:O	2.06	0.56
1:A:1423:C:O2'	1:A:1424:A:H5'	2.06	0.56
1:A:2472:C:O2'	1:A:2634:G:H4'	2.05	0.56
37:A:5494:HOH:O	4:D:298:LYS:HD3	2.04	0.56
4:D:190:MET:HE2	4:D:194:PHE:HD1	1.63	0.56
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.88	0.56
14:N:149:TRP:O	14:N:152:ARG:HG2	2.06	0.56
14:N:154:ARG:HD3	37:N:8639:HOH:O	2.03	0.56
17:Q:143:ALA:HA	37:Q:2178:HOH:O	2.06	0.56
1:A:1086:A:C6	24:X:11:VAL:HG11	2.40	0.56
1:A:1528:A:H2'	1:A:1529:G:O4'	2.06	0.56
1:A:1918:U:OP2	37:A:3996:HOH:O	2.18	0.56
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.87	0.56
6:F:11:HIS:C	6:F:13:MET:H	2.13	0.56
1:A:168:C:O2'	1:A:169:A:H5'	2.06	0.56
1:A:2362:A:H2'	1:A:2363:G:C8	2.40	0.56
37:A:6687:HOH:O	26:Z:165:GLU:HB3	2.05	0.56
2:B:3028:U:H2'	2:B:3029:C:C6	2.41	0.56
8:H:28:ALA:HB3	8:H:99:THR:O	2.05	0.56
11:K:74:ARG:HH11	11:K:74:ARG:CB	2.17	0.56
28:2:1:THR:HB	37:2:6858:HOH:O	2.06	0.56
1:A:660:A:H4'	1:A:661:G:O5'	2.06	0.55
1:A:926:A:O2'	13:M:41:HIS:HD2	1.88	0.55
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.55
3:C:194:MET:HE3	3:C:199:HIS:CB	2.35	0.55
15:O:155:GLU:O	15:O:156:GLU:HG3	2.06	0.55
26:Z:144:ARG:CZ	37:Z:8612:HOH:O	2.53	0.55
1:A:1134:G:C5'	10:J:151:MET:HE1	2.36	0.55
1:A:2038:A:OP2	4:D:224:LYS:NZ	2.32	0.55
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.22	0.55
11:K:52:GLN:HG3	11:K:53:ILE:N	2.21	0.55
14:N:35:PRO:O	37:N:8537:HOH:O	2.18	0.55
2:B:3055:U:H4'	2:B:3056:A:H8	1.70	0.55
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.88	0.55
14:N:154:ARG:CD	37:N:8639:HOH:O	2.55	0.55
20:T:51:GLN:HE21	20:T:53:ASN:ND2	2.03	0.55
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.41	0.55
1:A:1044:C:H5''	37:A:9022:HOH:O	2.07	0.55
1:A:1166:A:H1'	1:A:1192:A:N1	2.20	0.55
1:A:1249:U:H2'	1:A:1250:C:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ARG:O	10:J:61:LEU:HD22	2.06	0.55
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.36	0.55
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.87	0.55
1:A:1659:A:H2'	1:A:1660:G:O4'	2.07	0.55
1:A:2301:A:H5''	1:A:2302:A:H5'	1.88	0.55
5:E:37:ALA:O	5:E:41:ASN:ND2	2.39	0.55
7:G:79:GLY:HA3	37:G:7046:HOH:O	2.06	0.55
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.51	0.55
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.42	0.55
24:X:21:LEU:HD13	24:X:26:ILE:HD11	1.87	0.55
1:A:447:A:O2'	1:A:448:G:H5'	2.07	0.55
24:X:119:HIS:HD2	24:X:120:PRO:O	1.89	0.55
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.42	0.55
4:D:7:ARG:NH1	4:D:11:LEU:HD21	2.22	0.55
5:E:107:ARG:CB	5:E:107:ARG:HH11	2.19	0.55
8:H:91:VAL:CG1	8:H:92:GLY:N	2.70	0.55
13:M:104:ASP:O	13:M:105:TYR:HB3	2.05	0.55
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.89	0.55
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.06	0.55
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.07	0.55
1:A:564:G:H1'	37:A:6293:HOH:O	2.07	0.55
1:A:1116:U:O2'	1:A:1118:A:C2	2.51	0.55
1:A:2649:A:H5'	1:A:2649:A:C8	2.42	0.55
37:A:4432:HOH:O	14:N:146:GLN:HG2	2.06	0.55
6:F:99:ASP:HB3	6:F:103:ASN:H	1.71	0.55
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.22	0.55
21:U:19:ARG:NH1	21:U:68:ASP:O	2.40	0.55
24:X:88:THR:O	37:X:2374:HOH:O	2.18	0.55
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.07	0.55
1:A:158:A:O2'	1:A:159:G:H5'	2.07	0.55
1:A:327:A:OP1	5:E:149:LYS:NZ	2.25	0.55
1:A:1456:C:H2'	1:A:1457:U:C6	2.42	0.55
1:A:2115:U:H2'	1:A:2116:U:C6	2.42	0.55
5:E:168:ARG:NH2	5:E:190:ALA:O	2.40	0.55
24:X:76:ASP:O	24:X:77:ALA:C	2.50	0.55
1:A:625:U:H5'	37:A:3162:HOH:O	2.05	0.55
1:A:1311:G:C2	1:A:1312:G:C8	2.95	0.55
1:A:2082:G:O2'	1:A:2083:A:H5'	2.06	0.55
4:D:248:ARG:O	4:D:251:VAL:CG1	2.55	0.55
4:D:305:ASP:O	4:D:306:LYS:CB	2.55	0.55
37:L:408:HOH:O	22:V:37:GLU:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:73:ALA:N	37:O:8563:HOH:O	2.40	0.55
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.42	0.55
24:X:13:MET:HE3	24:X:17:ILE:CG2	2.37	0.55
1:A:371:U:H2'	1:A:372:A:H8	1.72	0.54
1:A:669:G:O2'	1:A:670:G:H5'	2.07	0.54
1:A:671:A:O2'	1:A:672:G:H2'	2.08	0.54
1:A:2316:G:H8	37:A:5631:HOH:O	1.90	0.54
1:A:2787:C:H5	37:A:4605:HOH:O	1.88	0.54
4:D:7:ARG:CD	4:D:9:GLY:O	2.54	0.54
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.20	0.54
13:M:104:ASP:HB3	37:M:8569:HOH:O	2.07	0.54
13:M:114:VAL:HG11	37:M:8577:HOH:O	2.08	0.54
27:1:39:CYS:CB	27:1:47:LEU:HD21	2.36	0.54
1:A:484:A:N1	1:A:506:G:H4'	2.21	0.54
1:A:567:U:H5''	37:X:5817:HOH:O	2.07	0.54
1:A:710:G:OP1	16:P:24:ALA:HB3	2.07	0.54
1:A:1393:A:H2'	1:A:1394:C:C6	2.43	0.54
1:A:1477:C:O2'	1:A:1478:U:H5'	2.06	0.54
1:A:1741:U:O2'	1:A:2723:G:H4'	2.07	0.54
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.89	0.54
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.72	0.54
16:P:26:TRP:N	37:P:3062:HOH:O	2.39	0.54
18:R:32:GLU:HA	18:R:71:TYR:OH	2.07	0.54
21:U:106:GLU:HG3	37:U:4913:HOH:O	2.07	0.54
22:V:9:CYS:HA	22:V:52:THR:CG2	2.35	0.54
27:1:22:ILE:O	27:1:26:VAL:HG23	2.08	0.54
1:A:134:U:C2	1:A:145:A:C2	2.95	0.54
1:A:2779:G:H21	7:G:143:GLN:NE2	2.05	0.54
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.90	0.54
5:E:236:THR:O	5:E:237:GLU:C	2.49	0.54
6:F:10:PHE:CG	6:F:11:HIS:N	2.75	0.54
8:H:104:ALA:HA	37:H:6617:HOH:O	2.08	0.54
10:J:31:PHE:HE2	10:J:87:LYS:O	1.89	0.54
10:J:154:THR:HB	10:J:155:PRO:HD3	1.89	0.54
19:S:29:LYS:HB3	37:S:8533:HOH:O	2.07	0.54
25:Y:37:LEU:CD1	25:Y:85:VAL:HG21	2.28	0.54
1:A:558:C:H2'	1:A:559:U:C5'	2.36	0.54
1:A:590:A:H2'	1:A:591:A:H5'	1.90	0.54
1:A:1527:A:H1'	1:A:1528:A:C8	2.42	0.54
1:A:2383:G:N3	37:A:6686:HOH:O	2.33	0.54
4:D:24:PRO:HG3	4:D:204:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:14:TYR:N	10:J:91:HIS:CE1	2.76	0.54
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.42	0.54
13:M:143:THR:HG22	13:M:145:LEU:H	1.71	0.54
1:A:1165:G:OP1	1:A:1165:G:H3'	2.08	0.54
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.39	0.54
1:A:2325:C:H1'	37:A:4122:HOH:O	2.08	0.54
1:A:2494:G:H4'	10:J:5:MET:SD	2.47	0.54
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.08	0.54
37:A:4330:HOH:O	16:P:37:ARG:HG3	2.07	0.54
6:F:140:ARG:O	6:F:144:ARG:HG2	2.08	0.54
12:L:30:LYS:O	12:L:55:VAL:HG13	2.07	0.54
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.35	0.54
24:X:90:TYR:N	24:X:90:TYR:CD1	2.75	0.54
26:Z:133:HIS:CD2	37:Z:8582:HOH:O	2.50	0.54
1:A:305:A:C5	1:A:329:A:C2	2.96	0.54
1:A:1118:A:H8	1:A:1119:G:H5''	1.72	0.54
1:A:2672:C:H1'	37:D:8634:HOH:O	2.08	0.54
4:D:43:GLY:O	4:D:308:LEU:HD12	2.07	0.54
5:E:76:ARG:HD3	37:E:8368:HOH:O	2.07	0.54
6:F:86:THR:C	6:F:89:PRO:HD2	2.32	0.54
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.22	0.54
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.23	0.54
1:A:221:G:H2'	1:A:222:A:C8	2.42	0.54
1:A:349:U:O2'	1:A:350:C:H5'	2.08	0.54
1:A:431:G:P	14:N:48:ARG:HH12	2.31	0.54
1:A:2502:C:H2'	1:A:2503:A:H5'	1.89	0.54
2:B:3054:A:O2'	2:B:3055:U:H5'	2.08	0.54
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.08	0.54
4:D:146:THR:O	4:D:159:PRO:HB3	2.07	0.54
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.32	0.54
5:E:104:ASP:O	5:E:108:GLN:HG3	2.08	0.54
6:F:170:TYR:O	6:F:171:ASP:HB3	2.07	0.54
7:G:37:ASP:OD1	11:K:125:SER:HB3	2.08	0.54
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.72	0.54
24:X:139:GLY:O	24:X:141:HIS:HD2	1.90	0.54
1:A:138:U:H5''	1:A:139:C:OP2	2.08	0.54
14:N:79:LYS:HD2	37:N:8555:HOH:O	2.08	0.54
26:Z:186:ARG:HG2	26:Z:186:ARG:NH1	2.22	0.54
1:A:2906:A:H5'	1:A:2907:C:O4'	2.07	0.54
4:D:72:THR:HB	37:D:8603:HOH:O	2.07	0.54
4:D:82:VAL:O	4:D:82:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.06	0.54
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.23	0.54
25:Y:71:ARG:CD	37:Y:2171:HOH:O	2.55	0.54
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.43	0.54
27:1:34:LYS:HE2	37:1:8424:HOH:O	2.07	0.54
30:4:34:LYS:HB2	30:4:37:ASP:OD2	2.07	0.54
1:A:316:A:H5'	21:U:54:ASP:OD2	2.07	0.54
1:A:1293:U:O2'	26:Z:149:GLN:NE2	2.28	0.54
1:A:2507:G:H2'	1:A:2510:C:H42	1.73	0.54
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.38	0.54
9:I:12:ILE:HG22	9:I:12:ILE:O	2.06	0.54
9:I:16:LYS:O	9:I:20:VAL:HG23	2.08	0.54
14:N:79:LYS:NZ	37:N:8565:HOH:O	2.41	0.54
23:W:8:ILE:HA	23:W:11:MET:HE3	1.90	0.54
27:1:19:GLY:O	27:1:23:ARG:HG2	2.07	0.54
1:A:926:A:O2'	13:M:41:HIS:CD2	2.61	0.53
1:A:1168:C:H2'	1:A:1169:U:O4'	2.07	0.53
1:A:1559:A:H1'	37:A:5842:HOH:O	2.07	0.53
1:A:1711:A:O2'	1:A:1712:A:H5'	2.08	0.53
1:A:2123:A:H5'	14:N:89:ASN:HD21	1.73	0.53
1:A:2256:G:H2'	1:A:2257:G:H5'	1.90	0.53
1:A:2769:C:C2'	1:A:2770:G:H5'	2.38	0.53
4:D:119:HIS:O	4:D:121:PRO:HD3	2.07	0.53
4:D:204:GLY:HA3	37:D:8652:HOH:O	2.07	0.53
5:E:107:ARG:NH1	5:E:107:ARG:CB	2.70	0.53
7:G:15:GLN:NE2	7:G:40:VAL:O	2.41	0.53
10:J:69:ASN:O	10:J:72:VAL:HG12	2.08	0.53
13:M:73:VAL:HG23	13:M:74:THR:N	2.23	0.53
1:A:1182:C:H1'	1:A:1192:A:H8	1.73	0.53
1:A:1422:U:H2'	1:A:1423:C:H6	1.72	0.53
1:A:2011:A:H4'	1:A:2012:U:O5'	2.09	0.53
3:C:211:LYS:NZ	37:C:8622:HOH:O	2.39	0.53
6:F:57:THR:HG23	6:F:63:ILE:CB	2.38	0.53
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.90	0.53
10:J:139:ASP:N	10:J:140:PRO:CD	2.70	0.53
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.43	0.53
29:3:35:ARG:HB2	37:3:2691:HOH:O	2.08	0.53
1:A:821:U:O2'	1:A:822:C:H5'	2.09	0.53
1:A:1733:A:H4'	4:D:212:GLN:HA	1.88	0.53
1:A:1887:U:OP1	27:1:21:LYS:HE3	2.09	0.53
1:A:2276:U:H2'	1:A:2277:U:C6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.90	0.53
3:C:179:MET:HG2	3:C:186:TRP:CB	2.39	0.53
10:J:109:ASP:HB2	37:J:8348:HOH:O	2.08	0.53
1:A:56:G:H5''	23:W:50:ARG:NH1	2.23	0.53
1:A:631:A:N3	1:A:2073:G:O2'	2.38	0.53
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.34	0.53
6:F:35:ALA:N	37:F:5576:HOH:O	2.41	0.53
7:G:22:VAL:O	7:G:28:SER:HA	2.08	0.53
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.90	0.53
10:J:118:PRO:HD2	37:J:8341:HOH:O	2.09	0.53
13:M:143:THR:CG2	13:M:144:ASP:N	2.70	0.53
14:N:186:SER:OG	14:N:189:VAL:HG12	2.09	0.53
1:A:1060:C:H6	1:A:1060:C:H5'	1.73	0.53
1:A:1299:G:O6	13:M:6:ARG:HD3	2.08	0.53
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.09	0.53
1:A:2433:A:H2'	1:A:2434:A:C8	2.43	0.53
1:A:2860:G:H1'	37:A:6782:HOH:O	2.09	0.53
4:D:51:VAL:HG21	4:D:327:VAL:HG13	1.90	0.53
6:F:146:LYS:NZ	15:O:107:ASN:ND2	2.54	0.53
8:H:46:GLU:N	37:H:3461:HOH:O	2.41	0.53
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.24	0.53
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.72	0.53
21:U:9:LYS:HE3	21:U:13:ARG:NH1	2.24	0.53
22:V:52:THR:HG22	22:V:54:THR:H	1.74	0.53
1:A:489:A:C8	21:U:82:THR:HG22	2.44	0.53
1:A:1172:G:H1'	37:A:4947:HOH:O	2.08	0.53
1:A:1741:U:HO2'	1:A:2723:G:H4'	1.74	0.53
1:A:2256:G:H2'	1:A:2257:G:C5'	2.38	0.53
1:A:2349:G:OP1	6:F:20:LYS:NZ	2.34	0.53
4:D:88:GLU:O	4:D:88:GLU:HG3	2.08	0.53
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.24	0.53
13:M:57:VAL:HG12	13:M:57:VAL:O	2.09	0.53
19:S:82:GLU:HG3	19:S:83:LYS:N	2.23	0.53
26:Z:112:GLU:OE1	26:Z:112:GLU:HA	2.09	0.53
1:A:45:A:N6	1:A:147:G:C4	2.77	0.53
1:A:51:G:O2'	1:A:52:A:H5'	2.08	0.53
1:A:1189:A:H1'	1:A:1209:C:H1'	1.91	0.53
1:A:1441:G:O2'	1:A:1442:A:H5'	2.09	0.53
1:A:1525:G:H5'	1:A:1526:A:OP2	2.09	0.53
1:A:1778:A:H2'	1:A:1779:A:H5'	1.90	0.53
1:A:1787:C:H4'	1:A:2883:A:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1857:A:N6	1:A:2247:C:H1'	2.24	0.53
1:A:2001:G:O2'	1:A:2002:C:H5'	2.09	0.53
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.09	0.53
37:A:7662:HOH:O	26:Z:172:THR:HB	2.08	0.53
2:B:3096:C:H2'	2:B:3097:U:C6	2.44	0.53
5:E:142:ASP:OD1	5:E:236:THR:HG23	2.08	0.53
14:N:87:MET:SD	37:N:8530:HOH:O	2.59	0.53
15:O:37:ARG:HD3	34:O:8507:CL:CL	2.46	0.53
22:V:33:SER:O	22:V:37:GLU:HG3	2.08	0.53
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.90	0.53
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.08	0.53
30:4:7:PHE:HE2	30:4:22:VAL:CG2	2.21	0.53
1:A:2321:A:O2'	1:A:2322:U:H3'	2.09	0.53
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.07	0.53
26:Z:144:ARG:NE	37:Z:8612:HOH:O	2.41	0.53
1:A:113:A:OP2	1:A:114:A:H5''	2.09	0.53
1:A:1209:C:C2	1:A:1210:G:C8	2.97	0.53
2:B:3041:C:C6	6:F:50:VAL:HG21	2.44	0.53
4:D:162:MET:CE	4:D:308:LEU:HD21	2.27	0.53
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.91	0.53
6:F:86:THR:HG23	37:F:7477:HOH:O	2.09	0.53
10:J:163:PRO:O	10:J:164:ALA:HB2	2.09	0.53
14:N:123:ASP:C	14:N:123:ASP:OD1	2.52	0.53
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.39	0.53
23:W:11:MET:HB3	23:W:15:GLU:HB2	1.90	0.53
27:1:28:ASP:O	27:1:31:ILE:HG22	2.09	0.53
1:A:21:G:H4'	19:S:2:ILE:HG22	1.90	0.53
1:A:256:C:H2'	1:A:257:G:O4'	2.08	0.53
1:A:516:A:P	37:A:5623:HOH:O	2.67	0.53
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.41	0.53
1:A:2089:A:O2'	1:A:2090:G:H5'	2.09	0.53
3:C:18:ALA:O	3:C:20:SER:N	2.38	0.53
4:D:54:VAL:O	4:D:55:ASN:C	2.51	0.53
14:N:76:ARG:HG2	14:N:76:ARG:HH11	1.73	0.53
1:A:512:G:O3'	1:A:513:A:H8	1.92	0.52
1:A:1159:G:H21	1:A:1189:A:H8	1.55	0.52
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.73	0.52
1:A:2478:U:O2'	1:A:2479:A:H5'	2.09	0.52
2:B:3006:C:P	15:O:37:ARG:NH1	2.82	0.52
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.90	0.52
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:149:ARG:O	13:M:150:GLN:HB2	2.09	0.52
15:O:89:GLY:O	15:O:92:ALA:HB3	2.09	0.52
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.73	0.52
29:3:48:ASP:O	29:3:49:GLU:HB2	2.10	0.52
1:A:415:A:O2'	1:A:416:G:H5'	2.09	0.52
1:A:1166:A:H61	1:A:1180:U:H3	1.56	0.52
1:A:1268:C:O2'	26:Z:169:ARG:HB2	2.08	0.52
1:A:1353:C:O5'	37:A:4652:HOH:O	2.19	0.52
1:A:1675:C:H5''	29:3:5:LYS:HD2	1.91	0.52
1:A:2015:A:H2'	1:A:2016:U:O4'	2.09	0.52
1:A:2911:C:H3'	37:A:5528:HOH:O	2.09	0.52
37:A:3818:HOH:O	10:J:11:LYS:HE2	2.08	0.52
4:D:74:ILE:HG13	37:D:8603:HOH:O	2.08	0.52
4:D:215:VAL:HB	4:D:234:ARG:HH12	1.75	0.52
6:F:64:ARG:O	6:F:67:ASP:OD2	2.26	0.52
8:H:117:GLU:C	8:H:119:ARG:H	2.17	0.52
16:P:10:LEU:HD13	16:P:99:GLU:HG3	1.91	0.52
16:P:21:SER:OG	16:P:106:PRO:HB2	2.09	0.52
26:Z:144:ARG:NH2	37:Z:8612:HOH:O	2.42	0.52
1:A:1180:U:H2'	1:A:1181:A:O4'	2.09	0.52
1:A:1192:A:H3'	1:A:1193:A:H5'	1.90	0.52
6:F:84:LEU:C	6:F:86:THR:H	2.17	0.52
9:I:63:ARG:O	9:I:67:LEU:HG	2.09	0.52
1:A:1535:G:H2'	1:A:1536:C:C6	2.44	0.52
1:A:2004:U:H5''	1:A:2005:G:C8	2.45	0.52
1:A:2604:A:H5'	37:A:5768:HOH:O	2.10	0.52
1:A:2780:C:H2'	1:A:2781:U:H6	1.73	0.52
37:A:6303:HOH:O	6:F:55:LYS:HB2	2.10	0.52
37:A:9312:HOH:O	27:1:16:PRO:HG3	2.10	0.52
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.91	0.52
5:E:242:GLU:HG3	37:E:8383:HOH:O	2.09	0.52
7:G:11:VAL:CG1	7:G:12:ASP:N	2.72	0.52
7:G:69:ILE:HA	7:G:72:MET:HE3	1.91	0.52
12:L:40:THR:O	12:L:41:LYS:C	2.52	0.52
15:O:119:GLN:O	15:O:123:ILE:HG13	2.09	0.52
20:T:81:ILE:HG23	37:T:8335:HOH:O	2.09	0.52
1:A:834:G:H5''	1:A:835:U:O5'	2.10	0.52
1:A:1058:A:H2'	1:A:1060:C:H5''	1.90	0.52
1:A:1450:C:C4'	1:A:1451:C:OP2	2.57	0.52
1:A:1666:C:C2'	1:A:1667:A:C5'	2.88	0.52
1:A:1829:A:H2'	1:A:1830:C:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2833:C:C2	1:A:2848:G:N2	2.78	0.52
3:C:93:THR:C	3:C:94:LEU:HD23	2.34	0.52
4:D:27:ASN:HD22	4:D:27:ASN:H	1.57	0.52
4:D:76:THR:N	4:D:77:PRO:HD3	2.25	0.52
4:D:297:VAL:HB	37:D:8603:HOH:O	2.10	0.52
6:F:11:HIS:O	6:F:12:GLU:HB3	2.09	0.52
6:F:163:VAL:HA	37:F:6326:HOH:O	2.09	0.52
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.39	0.52
11:K:45:VAL:HG23	11:K:130:VAL:O	2.08	0.52
17:Q:115:SER:O	17:Q:117:SER:N	2.43	0.52
21:U:32:ARG:NH1	21:U:38:ARG:NH1	2.57	0.52
24:X:13:MET:HE2	24:X:18:GLN:CA	2.40	0.52
1:A:92:G:H4'	23:W:44:GLY:HA3	1.91	0.52
1:A:160:A:C4	1:A:177:A:C2	2.98	0.52
1:A:285:A:H2'	1:A:286:U:O4'	2.09	0.52
1:A:1003:U:O2	10:J:90:PHE:CZ	2.62	0.52
1:A:1119:G:C8	11:K:52:GLN:NE2	2.78	0.52
1:A:2382:A:OP1	30:4:80:ARG:HG2	2.10	0.52
1:A:2638:G:H5'	37:A:4902:HOH:O	2.09	0.52
7:G:157:LYS:NZ	37:G:2401:HOH:O	2.43	0.52
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.45	0.52
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.10	0.52
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.40	0.52
1:A:344:C:H2'	1:A:345:G:O4'	2.09	0.52
1:A:1269:G:H2'	1:A:1270:U:C6	2.45	0.52
1:A:1847:A:OP1	3:C:175:LYS:HG3	2.10	0.52
1:A:2795:C:O2'	1:A:2796:U:H5'	2.09	0.52
4:D:41:PHE:CE1	4:D:79:MET:HG3	2.43	0.52
4:D:62:ARG:CB	4:D:65:MET:HE3	2.39	0.52
4:D:87:TYR:O	4:D:138:GLY:N	2.36	0.52
6:F:94:ALA:O	6:F:95:THR:O	2.28	0.52
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.27	0.52
16:P:25:VAL:HG23	16:P:26:TRP:H	1.74	0.52
20:T:57:THR:C	20:T:59:ASP:H	2.17	0.52
1:A:920:C:H5'	1:A:921:G:C4	2.45	0.52
1:A:1015:C:H2'	1:A:1016:U:H6	1.74	0.52
1:A:2819:C:H2'	1:A:2820:A:C8	2.44	0.52
1:A:2866:U:H4'	1:A:2867:G:H5'	1.92	0.52
37:A:5053:HOH:O	4:D:216:LYS:HA	2.09	0.52
8:H:2:VAL:HG11	14:N:23:LEU:HD23	1.91	0.52
10:J:5:MET:HG3	37:J:8367:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:77:GLY:O	11:K:78:ILE:C	2.53	0.52
13:M:146:GLY:C	13:M:148:GLU:H	2.18	0.52
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.74	0.52
27:1:11:THR:HG21	27:1:23:ARG:HB2	1.91	0.52
1:A:283:U:H5	1:A:284:C:N4	2.07	0.52
1:A:454:U:O4	37:A:9155:HOH:O	2.19	0.52
1:A:1752:G:H2'	37:A:7541:HOH:O	2.10	0.52
2:B:3107:C:C5	37:B:3167:HOH:O	2.54	0.52
37:B:5071:HOH:O	15:O:20:TYR:CE2	2.54	0.52
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.91	0.52
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.91	0.52
7:G:21:THR:HG23	7:G:30:THR:OG1	2.10	0.52
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.90	0.52
1:A:1119:G:N2	1:A:1246:A:H2	2.04	0.52
1:A:1139:U:H2'	1:A:1140:C:C6	2.45	0.52
1:A:1666:C:C2'	1:A:1667:A:H5'	2.38	0.52
1:A:2256:G:C2'	1:A:2257:G:H5'	2.40	0.52
3:C:105:VAL:CG1	3:C:106:CYS:N	2.72	0.52
4:D:41:PHE:HB3	4:D:190:MET:HE1	1.91	0.52
6:F:25:MET:HE2	6:F:41:LEU:CG	2.18	0.52
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.09	0.52
12:L:37:TYR:CD2	37:L:7169:HOH:O	2.55	0.52
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.45	0.52
14:N:164:THR:HB	37:N:8520:HOH:O	2.10	0.52
1:A:1056:U:H2'	1:A:1057:A:O4'	2.10	0.51
1:A:1555:G:H4'	1:A:1630:A:H2	1.75	0.51
1:A:2453:G:H4'	13:M:50:GLY:C	2.35	0.51
1:A:2536:C:OP1	37:A:3089:HOH:O	2.19	0.51
1:A:2760:C:H5''	37:A:5303:HOH:O	2.10	0.51
37:A:7212:HOH:O	14:N:13:LYS:HE2	2.10	0.51
2:B:3029:C:C2'	2:B:3030:C:H5'	2.40	0.51
7:G:68:HIS:O	7:G:72:MET:HG3	2.10	0.51
13:M:21:ARG:N	37:M:8536:HOH:O	2.43	0.51
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.40	0.51
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.39	0.51
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.45	0.51
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.92	0.51
27:1:13:ARG:NH1	37:1:8420:HOH:O	2.37	0.51
27:1:47:LEU:CD2	27:1:57:CYS:HB2	2.40	0.51
1:A:952:G:H4'	37:A:4002:HOH:O	2.11	0.51
1:A:1209:C:O2	1:A:1210:G:C8	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1701:A:H4'	1:A:1702:U:C5'	2.40	0.51
37:A:7009:HOH:O	3:C:211:LYS:HG2	2.09	0.51
5:E:85:LYS:NZ	37:E:8325:HOH:O	2.42	0.51
7:G:77:THR:OG1	7:G:78:GLU:N	2.41	0.51
16:P:35:LYS:HD3	37:P:3360:HOH:O	2.09	0.51
19:S:132:ARG:NH2	37:S:8583:HOH:O	2.41	0.51
20:T:23:LYS:HD3	20:T:65:VAL:HG12	1.91	0.51
24:X:122:ARG:HH22	24:X:154:ARG:C	2.19	0.51
1:A:189:A:OP1	14:N:171:ARG:NH2	2.44	0.51
1:A:1164:U:C4'	1:A:1165:G:OP1	2.54	0.51
1:A:1189:A:H1'	1:A:1209:C:O4'	2.11	0.51
1:A:2010:A:C2'	37:A:5935:HOH:O	2.58	0.51
2:B:3092:G:H2'	2:B:3093:A:C8	2.45	0.51
3:C:192:VAL:O	3:C:192:VAL:CG1	2.58	0.51
4:D:79:MET:HE3	4:D:144:THR:HG21	1.92	0.51
10:J:4:ALA:HB3	37:J:8367:HOH:O	2.11	0.51
10:J:71:TYR:O	10:J:73:GLN:N	2.43	0.51
10:J:150:LYS:HE2	37:J:8381:HOH:O	2.10	0.51
10:J:151:MET:HA	10:J:151:MET:HE3	1.92	0.51
15:O:82:TYR:C	15:O:82:TYR:CD2	2.88	0.51
15:O:157:PRO:HA	37:O:8527:HOH:O	2.09	0.51
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.75	0.51
21:U:20:HIS:ND1	21:U:41:ARG:NE	2.55	0.51
23:W:16:ARG:NH2	23:W:63:GLU:HG3	2.25	0.51
1:A:113:A:OP2	1:A:114:A:H2'	2.10	0.51
1:A:440:C:H2'	1:A:441:A:C8	2.45	0.51
1:A:558:C:H2'	1:A:559:U:H5''	1.92	0.51
1:A:629:A:C2	1:A:2074:A:C2	2.99	0.51
1:A:1494:A:O2'	1:A:1505:U:O2	2.24	0.51
1:A:2768:A:H3'	37:A:4392:HOH:O	2.11	0.51
4:D:175:LEU:C	4:D:175:LEU:CD2	2.82	0.51
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.10	0.51
13:M:77:ALA:HB3	37:M:8535:HOH:O	2.09	0.51
13:M:148:GLU:HB2	37:M:8592:HOH:O	2.09	0.51
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.40	0.51
14:N:137:ASP:HA	14:N:142:LYS:HE3	1.92	0.51
23:W:4:HIS:O	23:W:8:ILE:HG13	2.11	0.51
26:Z:115:ARG:NE	37:Z:8557:HOH:O	2.43	0.51
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.44	0.51
1:A:661:G:C4	1:A:686:A:C2	2.99	0.51
1:A:1667:A:H2'	1:A:1668:U:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1768:C:H2'	1:A:1769:C:O4'	2.10	0.51
1:A:2812:A:H1'	37:A:5767:HOH:O	2.09	0.51
5:E:16:VAL:HG12	5:E:17:ASP:H	1.74	0.51
5:E:233:THR:CG2	5:E:234:VAL:N	2.74	0.51
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.39	0.51
10:J:157:ILE:CG2	10:J:158:ASN:N	2.73	0.51
10:J:166:ASN:N	10:J:166:ASN:ND2	2.58	0.51
17:Q:131:PHE:CD1	17:Q:137:LEU:HD13	2.44	0.51
18:R:93:ARG:HH11	18:R:93:ARG:HG3	1.75	0.51
27:1:39:CYS:HA	27:1:47:LEU:CD1	2.38	0.51
1:A:51:G:N2	1:A:111:C:C2	2.78	0.51
1:A:657:G:OP1	5:E:27:ARG:NH2	2.40	0.51
1:A:920:C:H5''	1:A:921:G:O5'	2.10	0.51
1:A:963:C:O5'	1:A:963:C:H6	1.93	0.51
4:D:333:GLU:HB2	22:V:14:GLU:OE2	2.11	0.51
8:H:57:GLU:O	8:H:61:MET:HG3	2.09	0.51
10:J:127:GLY:O	10:J:128:ALA:CB	2.58	0.51
10:J:162:SER:CB	10:J:163:PRO:CD	2.79	0.51
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.09	0.51
12:L:34:VAL:HB	37:L:7169:HOH:O	2.11	0.51
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.92	0.51
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.75	0.51
1:A:1097:A:H5''	24:X:125:HIS:NE2	2.26	0.51
1:A:1827:G:C6	1:A:1828:G:C6	2.99	0.51
4:D:146:THR:C	4:D:148:PRO:HD3	2.35	0.51
4:D:175:LEU:HD23	4:D:175:LEU:O	2.10	0.51
5:E:1:MET:HG2	5:E:2:GLN:N	2.24	0.51
11:K:131:THR:HG22	11:K:133:GLY:N	2.26	0.51
11:K:142:ASN:O	11:K:144:THR:N	2.44	0.51
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.93	0.51
22:V:35:LYS:NZ	37:V:6621:HOH:O	2.27	0.51
24:X:38:THR:HG22	24:X:39:ASP:H	1.76	0.51
1:A:1625:U:H5''	37:A:5999:HOH:O	2.11	0.51
1:A:2314:G:C2'	1:A:2315:C:H5'	2.40	0.51
1:A:2487:C:H5	37:A:4859:HOH:O	1.94	0.51
1:A:2506:A:O2'	1:A:2507:G:O5'	2.29	0.51
1:A:2613:G:O2'	1:A:2614:C:H5'	2.11	0.51
10:J:65:ARG:HB3	37:J:8387:HOH:O	2.10	0.51
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.92	0.51
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.40	0.51
1:A:21:G:H5''	19:S:1:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:A:H5''	21:U:52:ARG:HD2	1.93	0.51
1:A:694:A:H2'	1:A:695:C:H5'	1.92	0.51
1:A:795:G:N3	1:A:817:G:C2	2.79	0.51
1:A:1862:C:C2'	1:A:1863:G:H5'	2.41	0.51
1:A:1942:A:H3'	37:A:7334:HOH:O	2.10	0.51
1:A:2459:G:OP2	30:4:64:LYS:HD2	2.11	0.51
4:D:162:MET:HG3	4:D:310:ARG:CZ	2.41	0.51
8:H:59:ILE:O	8:H:59:ILE:HG22	2.10	0.51
10:J:81:TYR:CD1	10:J:81:TYR:C	2.88	0.51
27:1:30:GLU:CA	27:1:33:HIS:HB3	2.37	0.51
29:3:18:ASN:ND2	29:3:40:ARG:H	2.09	0.51
1:A:1118:A:C8	1:A:1119:G:H5''	2.45	0.51
1:A:2326:U:H4'	1:A:2412:G:C4'	2.41	0.51
3:C:173:GLY:O	3:C:176:HIS:HB3	2.10	0.51
4:D:205:VAL:O	4:D:307:ARG:NE	2.44	0.51
6:F:23:VAL:O	6:F:23:VAL:CG2	2.59	0.51
7:G:7:ILE:HD11	7:G:11:VAL:O	2.11	0.51
8:H:100:ASP:O	8:H:101:ALA:O	2.29	0.51
16:P:26:TRP:HB2	37:P:3062:HOH:O	2.11	0.51
27:1:10:ARG:HG3	27:1:11:THR:N	2.26	0.51
28:2:15:THR:O	28:2:29:THR:HG22	2.11	0.51
1:A:1595:G:O2'	1:A:1596:U:H5'	2.11	0.50
1:A:2730:G:O2'	1:A:2731:G:H5'	2.12	0.50
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.58	0.50
10:J:35:ASN:ND2	10:J:79:ALA:O	2.44	0.50
10:J:147:ARG:HA	10:J:150:LYS:HZ2	1.76	0.50
15:O:182:GLY:O	15:O:183:ASP:O	2.29	0.50
22:V:20:MET:CG	22:V:28:THR:HG23	2.41	0.50
1:A:1819:G:H5'	37:A:4684:HOH:O	2.12	0.50
1:A:2679:G:H2'	1:A:2681:A:OP2	2.11	0.50
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.76	0.50
10:J:129:ASN:HD22	10:J:129:ASN:N	2.09	0.50
11:K:45:VAL:HG22	11:K:46:ILE:N	2.25	0.50
16:P:25:VAL:O	16:P:29:VAL:HG23	2.10	0.50
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.41	0.50
1:A:306:A:P	21:U:38:ARG:HH21	2.34	0.50
1:A:922:A:N7	1:A:2281:C:H5'	2.25	0.50
1:A:952:G:OP1	18:R:42:LYS:HE2	2.11	0.50
1:A:1015:C:H2'	1:A:1016:U:C6	2.46	0.50
5:E:133:ARG:NH2	37:E:8428:HOH:O	2.43	0.50
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:30:ARG:NH2	37:M:8525:HOH:O	2.33	0.50
14:N:78:ASN:ND2	37:N:8642:HOH:O	2.37	0.50
14:N:113:ARG:HH21	14:N:156:ARG:HG2	1.73	0.50
19:S:34:GLU:HG2	19:S:46:TYR:OH	2.11	0.50
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.46	0.50
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.92	0.50
1:A:257:G:O2'	1:A:258:G:H5'	2.10	0.50
1:A:539:G:H2'	1:A:540:A:C8	2.46	0.50
1:A:2121:G:O2'	1:A:2122:C:H5'	2.12	0.50
2:B:3008:G:O6	15:O:11:ARG:NH1	2.45	0.50
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.75	0.50
4:D:138:GLY:O	4:D:139:ASP:O	2.29	0.50
8:H:28:ALA:CB	8:H:99:THR:HG23	2.41	0.50
15:O:32:PRO:HD2	15:O:99:GLU:O	2.12	0.50
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.59	0.50
23:W:49:LEU:O	23:W:53:ILE:HG13	2.11	0.50
25:Y:25:ARG:CG	37:Y:5356:HOH:O	2.54	0.50
27:1:59:HIS:HA	37:1:8440:HOH:O	2.11	0.50
28:2:8:GLN:HE22	28:2:11:LYS:HZ1	1.59	0.50
1:A:522:U:O2'	1:A:1366:C:H5'	2.12	0.50
1:A:816:G:C6	1:A:817:G:N1	2.79	0.50
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.47	0.50
37:A:4036:HOH:O	4:D:27:ASN:HB2	2.12	0.50
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.17	0.50
11:K:22:VAL:O	11:K:26:VAL:HG23	2.12	0.50
14:N:61:ILE:HD12	14:N:61:ILE:N	2.26	0.50
15:O:163:PHE:HA	37:O:8564:HOH:O	2.09	0.50
16:P:44:ASN:HA	16:P:65:LEU:O	2.11	0.50
17:Q:41:ARG:O	17:Q:44:VAL:HB	2.12	0.50
26:Z:122:ARG:NH2	37:Z:8536:HOH:O	2.45	0.50
1:A:653:C:H2'	1:A:654:A:C8	2.45	0.50
1:A:1681:G:H5''	1:A:1682:A:H5'	1.93	0.50
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.76	0.50
1:A:2433:A:H2'	1:A:2434:A:H8	1.76	0.50
1:A:2713:G:O2'	1:A:2714:U:H5'	2.12	0.50
3:C:132:ASP:OD1	3:C:133:ARG:N	2.42	0.50
6:F:36:ASN:HA	37:F:7500:HOH:O	2.12	0.50
10:J:53:PRO:HG3	10:J:127:GLY:H	1.77	0.50
12:L:125:ALA:C	12:L:127:ALA:H	2.19	0.50
15:O:149:GLU:O	15:O:152:GLU:HB2	2.12	0.50
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:34:SER:O	22:V:38:ASN:ND2	2.45	0.50
25:Y:7:GLU:HA	25:Y:74:ALA:O	2.11	0.50
1:A:316:A:N3	1:A:336:G:O2'	2.43	0.50
1:A:514:G:H8	1:A:514:G:O5'	1.95	0.50
1:A:820:G:C5	3:C:171:LYS:HB2	2.47	0.50
1:A:1503:U:H2'	1:A:1504:A:O4'	2.12	0.50
3:C:8:ARG:NH1	37:C:8553:HOH:O	2.32	0.50
3:C:192:VAL:O	3:C:207:GLN:HG2	2.11	0.50
4:D:221:GLN:HE22	12:L:42:ASN:ND2	2.09	0.50
6:F:95:THR:C	6:F:97:GLN:N	2.67	0.50
10:J:26:LYS:HD2	10:J:28:ILE:HB	1.93	0.50
10:J:26:LYS:CD	10:J:28:ILE:HB	2.42	0.50
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.59	0.50
19:S:40:ALA:O	19:S:44:VAL:HG23	2.11	0.50
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.26	0.50
26:Z:184:GLU:OE1	26:Z:204:ARG:NH1	2.44	0.50
28:2:28:HIS:CD2	28:2:31:LYS:H	2.30	0.50
1:A:40:C:H6	1:A:40:C:O5'	1.95	0.50
1:A:703:G:O2'	1:A:704:C:H5'	2.11	0.50
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.94	0.50
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.94	0.50
6:F:10:PHE:CD1	6:F:11:HIS:N	2.80	0.50
9:I:23:ILE:O	9:I:27:ILE:HG13	2.11	0.50
1:A:590:A:C2'	1:A:591:A:H5'	2.42	0.50
1:A:1669:A:H2'	1:A:1670:G:C8	2.47	0.50
1:A:1783:A:O2'	1:A:1784:U:H5'	2.11	0.50
1:A:2073:G:OP2	1:A:2490:A:H5'	2.12	0.50
37:A:9870:HOH:O	11:K:46:ILE:HA	2.12	0.50
3:C:192:VAL:O	3:C:192:VAL:HG12	2.11	0.50
4:D:280:VAL:HG13	4:D:334:SER:HA	1.94	0.50
15:O:170:GLU:O	15:O:174:GLU:HG3	2.12	0.50
18:R:41:LEU:HB3	18:R:52:PHE:CZ	2.46	0.50
19:S:79:ARG:C	19:S:81:PRO:HD3	2.37	0.50
24:X:5:VAL:O	24:X:52:VAL:HG22	2.11	0.50
24:X:38:THR:HG22	24:X:39:ASP:N	2.27	0.50
24:X:88:THR:CG2	24:X:89:ASP:H	2.20	0.50
24:X:149:LEU:HG	24:X:153:MET:CE	2.35	0.50
29:3:39:ARG:NH1	37:3:6391:HOH:O	2.45	0.50
1:A:920:C:H4'	1:A:921:G:C2	2.47	0.49
1:A:949:U:O2'	18:R:40:HIS:HE1	1.95	0.49
1:A:1434:A:H2'	1:A:1436:C:C5	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3009:C:OP2	37:B:466:HOH:O	2.19	0.49
4:D:2:GLN:HA	37:D:8618:HOH:O	2.12	0.49
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.25	0.49
5:E:27:ARG:HG2	5:E:30:LEU:HG	1.92	0.49
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.46	0.49
14:N:14:ARG:HB3	14:N:17:GLU:HG3	1.94	0.49
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.39	0.49
1:A:603:A:H4'	1:A:604:G:O5'	2.12	0.49
1:A:1250:C:O2'	1:A:1251:C:H5'	2.11	0.49
1:A:2769:C:O2'	1:A:2770:G:H5'	2.12	0.49
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.26	0.49
3:C:191:GLY:HA2	3:C:194:MET:CE	2.40	0.49
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.47	0.49
5:E:236:THR:C	37:E:8453:HOH:O	2.55	0.49
16:P:59:VAL:HG23	16:P:111:VAL:HG23	1.94	0.49
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.12	0.49
1:A:639:A:H2'	1:A:640:G:C8	2.46	0.49
1:A:714:U:H3'	37:A:6924:HOH:O	2.12	0.49
1:A:1850:U:H2'	1:A:1851:G:H8	1.76	0.49
1:A:2256:G:O2'	1:A:2257:G:H5'	2.12	0.49
2:B:3064:C:H2'	2:B:3065:A:H5'	1.95	0.49
6:F:99:ASP:HB2	6:F:103:ASN:H	1.77	0.49
6:F:99:ASP:O	6:F:159:PRO:HG3	2.12	0.49
1:A:664:U:O4	1:A:681:G:H5''	2.12	0.49
1:A:1450:C:O2'	1:A:1494:A:H5'	2.13	0.49
1:A:1500:U:P	17:Q:41:ARG:HH22	2.35	0.49
37:B:7568:HOH:O	15:O:107:ASN:HB3	2.10	0.49
4:D:243:ASN:HA	4:D:244:PRO:C	2.36	0.49
6:F:58:VAL:HG12	6:F:59:GLY:N	2.27	0.49
15:O:58:LEU:N	15:O:58:LEU:CD1	2.75	0.49
15:O:71:TRP:N	37:O:8538:HOH:O	2.44	0.49
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.94	0.49
30:4:1:MET:N	30:4:87:ARG:O	2.41	0.49
1:A:400:C:O3'	37:A:5770:HOH:O	2.20	0.49
1:A:1209:C:H2'	1:A:1210:G:C8	2.44	0.49
1:A:2251:G:H2'	1:A:2252:A:C8	2.48	0.49
1:A:2359:G:H3'	37:A:5667:HOH:O	2.12	0.49
1:A:2756:U:H3	1:A:2896:A:H2	1.58	0.49
2:B:3023:U:C4'	2:B:3024:U:OP2	2.56	0.49
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.42	0.49
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.94	0.49
30:4:69:TYR:CB	30:4:78:HIS:CE1	2.95	0.49
1:A:449:A:N7	5:E:43:LYS:HG2	2.27	0.49
1:A:2064:U:H5'	1:A:2652:U:O3'	2.13	0.49
1:A:2265:U:H2'	1:A:2266:A:C8	2.48	0.49
1:A:2502:C:C4'	10:J:151:MET:HG2	2.43	0.49
3:C:55:VAL:HG22	3:C:68:ILE:O	2.12	0.49
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.47	0.49
8:H:37:THR:O	8:H:41:GLU:HG3	2.12	0.49
13:M:134:GLU:HA	13:M:138:GLY:O	2.13	0.49
1:A:154:C:H2'	1:A:155:C:H6	1.77	0.49
1:A:195:C:H2'	1:A:196:G:H5'	1.94	0.49
1:A:820:G:C6	3:C:171:LYS:HB2	2.48	0.49
1:A:960:G:N3	1:A:960:G:C2'	2.75	0.49
1:A:1174:A:C5	1:A:1201:C:H4'	2.47	0.49
1:A:1268:C:O2'	1:A:1269:G:H5'	2.12	0.49
1:A:2271:G:P	37:A:9418:HOH:O	2.70	0.49
1:A:2346:C:O3'	6:F:52:THR:HG23	2.11	0.49
1:A:2459:G:P	30:4:64:LYS:HB2	2.52	0.49
5:E:77:ALA:O	5:E:78:ARG:HG3	2.12	0.49
6:F:59:GLY:C	6:F:61:PHE:N	2.71	0.49
8:H:91:VAL:CG1	8:H:92:GLY:H	2.20	0.49
10:J:53:PRO:HA	10:J:125:VAL:O	2.13	0.49
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.12	0.49
20:T:80:ARG:NH1	37:T:8344:HOH:O	2.45	0.49
1:A:1657:A:H2'	1:A:1658:A:C8	2.47	0.49
1:A:1804:A:H2'	1:A:1805:G:C8	2.46	0.49
1:A:2488:A:H61	1:A:2534:C:H42	1.61	0.49
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.78	0.49
2:B:3031:C:H2'	2:B:3032:G:O4'	2.11	0.49
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.43	0.49
4:D:177:HIS:O	4:D:181:ILE:HG13	2.13	0.49
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.43	0.49
10:J:33:MET:SD	10:J:65:ARG:HD2	2.53	0.49
10:J:114:PRO:O	10:J:115:PHE:C	2.55	0.49
11:K:19:MET:CE	11:K:132:LEU:HD11	2.22	0.49
12:L:118:ALA:C	12:L:120:ARG:H	2.21	0.49
14:N:77:PHE:HD2	37:N:8527:HOH:O	1.94	0.49
23:W:12:THR:HG23	23:W:14:ALA:H	1.76	0.49
1:A:95:A:H5''	1:A:97:G:O4'	2.13	0.49
1:A:470:U:O2'	28:2:16:HIS:CD2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:U:H2'	1:A:1219:U:C6	2.47	0.49
1:A:1656:A:H2'	1:A:1657:A:O4'	2.13	0.49
1:A:1723:G:H2'	37:A:9608:HOH:O	2.13	0.49
1:A:1890:U:H4'	1:A:2010:A:C6	2.48	0.49
1:A:2011:A:P	37:A:5935:HOH:O	2.71	0.49
1:A:2083:A:C8	37:A:7572:HOH:O	2.54	0.49
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.93	0.49
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.12	0.49
6:F:102:GLY:O	6:F:134:LEU:HD12	2.13	0.49
7:G:7:ILE:HG22	7:G:45:ASP:O	2.13	0.49
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.95	0.49
18:R:28:ARG:HG2	37:R:4350:HOH:O	2.13	0.49
1:A:1213:C:C2'	1:A:1214:G:H5'	2.43	0.49
3:C:72:GLU:HG3	27:1:66:GLY:HA2	1.95	0.49
5:E:7:ASP:OD1	5:E:11:ASN:O	2.31	0.49
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.42	0.49
7:G:118:ILE:HG23	7:G:144:THR:HG21	1.95	0.49
14:N:77:PHE:CD1	14:N:77:PHE:O	2.65	0.49
15:O:43:VAL:HG11	15:O:81:ALA:HA	1.95	0.49
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.48	0.49
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.12	0.49
22:V:52:THR:HG22	22:V:54:THR:N	2.28	0.49
1:A:97:G:C2	21:U:107:LYS:HD2	2.47	0.48
1:A:432:G:O2'	1:A:433:C:H5'	2.13	0.48
1:A:739:G:N7	37:A:7536:HOH:O	2.44	0.48
1:A:812:A:H2'	1:A:813:C:C6	2.48	0.48
1:A:1594:C:O2'	1:A:1607:A:H4'	2.13	0.48
1:A:1829:A:N6	27:1:18:TYR:HA	2.28	0.48
1:A:2894:C:O2'	1:A:2895:C:H5'	2.13	0.48
4:D:140:LEU:HD23	37:D:8577:HOH:O	2.13	0.48
7:G:108:LEU:HD11	7:G:164:ASP:HB2	1.94	0.48
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.95	0.48
25:Y:36:HIS:CE1	25:Y:40:HIS:CD2	3.01	0.48
1:A:187:A:H3'	1:A:188:C:H6	1.77	0.48
1:A:201:G:N2	1:A:202:U:C2	2.81	0.48
1:A:428:G:OP1	37:A:6202:HOH:O	2.19	0.48
1:A:542:A:H1'	37:A:4650:HOH:O	2.13	0.48
1:A:1189:A:O2'	1:A:1208:C:H2'	2.13	0.48
1:A:1197:G:N2	37:A:6214:HOH:O	2.46	0.48
1:A:2269:C:C2'	1:A:2270:G:H5'	2.43	0.48
1:A:2459:G:OP1	30:4:64:LYS:N	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3049:G:H2'	2:B:3050:G:O4'	2.13	0.48
3:C:76:VAL:CG2	27:1:63:LYS:HB3	2.42	0.48
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.42	0.48
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.60	0.48
15:O:47:LEU:HD12	15:O:92:ALA:HB1	1.94	0.48
17:Q:115:SER:C	17:Q:117:SER:H	2.21	0.48
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.26	0.48
1:A:790:A:H1'	1:A:1710:A:H2'	1.95	0.48
1:A:1119:G:H2'	11:K:52:GLN:HE22	1.76	0.48
1:A:1205:U:C2'	1:A:1206:U:C5'	2.90	0.48
1:A:2365:G:H4'	18:R:45:PRO:O	2.13	0.48
1:A:2464:C:H5''	1:A:2465:A:OP1	2.13	0.48
1:A:2630:G:O6	3:C:206:ARG:NH2	2.46	0.48
37:A:6017:HOH:O	30:4:84:ARG:HB3	2.13	0.48
4:D:85:ARG:NH1	37:D:8634:HOH:O	2.46	0.48
4:D:301:VAL:HG13	4:D:302:PRO:HD2	1.95	0.48
6:F:59:GLY:O	6:F:61:PHE:N	2.36	0.48
10:J:57:ARG:C	10:J:59:ASN:N	2.70	0.48
14:N:36:ALA:HB1	37:N:8549:HOH:O	2.13	0.48
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.96	0.48
20:T:73:ASP:OD1	20:T:75:GLN:HB2	2.13	0.48
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.21	0.48
1:A:120:A:H2'	1:A:120:A:N3	2.27	0.48
1:A:1135:G:H5'	37:A:5905:HOH:O	2.12	0.48
1:A:1593:C:OP1	17:Q:117:SER:CB	2.62	0.48
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.94	0.48
1:A:2432:C:H4'	30:4:36:ILE:HG12	1.95	0.48
1:A:2524:G:H21	1:A:2526:C:N4	2.11	0.48
1:A:2598:U:O2	1:A:2600:A:H8	1.96	0.48
31:A:9000:TYK:H7A2	31:A:9000:TYK:O2A	2.13	0.48
4:D:4:SER:O	4:D:5:ARG:HB2	2.14	0.48
19:S:33:ARG:NH2	37:S:8533:HOH:O	2.37	0.48
24:X:48:VAL:CG1	24:X:48:VAL:O	2.59	0.48
25:Y:71:ARG:HD3	37:Y:2171:HOH:O	2.13	0.48
1:A:553:G:P	26:Z:204:ARG:NH2	2.86	0.48
1:A:1444:G:O2'	1:A:1445:G:H5'	2.13	0.48
1:A:1589:G:N2	1:A:1605:G:H1'	2.28	0.48
1:A:1862:C:H1'	37:A:7204:HOH:O	2.14	0.48
1:A:1909:A:H2'	1:A:1910:A:C8	2.48	0.48
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.43	0.48
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:274:GLU:HA	4:D:292:GLY:O	2.13	0.48
14:N:49:ALA:HB1	14:N:54:TYR:CB	2.43	0.48
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.13	0.48
24:X:26:ILE:O	24:X:26:ILE:HG13	2.11	0.48
1:A:182:G:O2'	1:A:183:A:H5'	2.14	0.48
1:A:281:U:H3'	37:A:7191:HOH:O	2.14	0.48
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.49	0.48
1:A:1699:C:H4'	37:A:6425:HOH:O	2.13	0.48
1:A:1840:A:OP1	37:A:9595:HOH:O	2.20	0.48
2:B:3042:C:O2	6:F:76:ARG:NH1	2.47	0.48
3:C:51:ARG:NH2	37:C:8609:HOH:O	2.47	0.48
5:E:95:GLU:H	5:E:95:GLU:CD	2.21	0.48
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.95	0.48
12:L:101:ASN:O	12:L:102:GLU:HB2	2.13	0.48
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.44	0.48
14:N:169:ARG:HD2	37:N:8590:HOH:O	2.14	0.48
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.42	0.48
1:A:1883:U:OP1	37:A:7834:HOH:O	2.20	0.48
1:A:1995:G:O2'	1:A:1997:A:N7	2.46	0.48
1:A:2501:G:H1'	37:A:4515:HOH:O	2.13	0.48
1:A:2815:G:OP2	11:K:99:GLU:HG2	2.14	0.48
3:C:149:ASP:OD1	3:C:151:GLN:HB2	2.14	0.48
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.95	0.48
14:N:12:TRP:CZ2	14:N:20:ILE:HD11	2.48	0.48
16:P:54:GLU:HG2	16:P:73:ASP:O	2.14	0.48
30:4:31:THR:HB	30:4:33:MET:CE	2.42	0.48
1:A:241:A:C2	1:A:378:A:H4'	2.49	0.48
1:A:716:G:H2'	1:A:717:C:O5'	2.14	0.48
1:A:2133:U:H4'	1:A:2134:G:H5'	1.96	0.48
37:B:4707:HOH:O	15:O:147:ILE:HB	2.14	0.48
3:C:105:VAL:HG12	3:C:106:CYS:H	1.79	0.48
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.43	0.48
11:K:93:ARG:HH11	11:K:93:ARG:CB	2.22	0.48
13:M:133:VAL:HB	37:M:8563:HOH:O	2.13	0.48
13:M:143:THR:CG2	13:M:144:ASP:H	2.26	0.48
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.74	0.48
1:A:1183:C:N4	37:A:4370:HOH:O	2.42	0.48
1:A:1328:A:N7	1:A:1329:A:C5	2.82	0.48
1:A:1976:G:O2'	1:A:1977:U:H5'	2.13	0.48
1:A:2089:A:C2'	1:A:2090:G:H5'	2.43	0.48
1:A:2361:A:H5''	37:A:9001:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:34:ASN:O	8:H:38:LYS:HG3	2.14	0.48
10:J:39:GLY:O	10:J:41:THR:N	2.47	0.48
13:M:101:ASP:C	13:M:103:ALA:H	2.21	0.48
14:N:115:LEU:HD13	14:N:116:ASN:HB2	1.95	0.48
15:O:67:ALA:C	15:O:69:TYR:H	2.22	0.48
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.79	0.48
1:A:559:U:H2'	1:A:560:C:O4'	2.14	0.48
1:A:602:A:O2'	1:A:605:C:H4'	2.14	0.48
1:A:1132:A:N6	1:A:1229:C:H2'	2.29	0.48
1:A:1191:A:C3'	1:A:1192:A:H5''	2.39	0.48
1:A:1925:G:OP1	30:4:29:ARG:NH2	2.47	0.48
1:A:2326:U:H4'	1:A:2412:G:H4'	1.96	0.48
1:A:2502:C:H4'	10:J:151:MET:HG2	1.96	0.48
7:G:36:PRO:HD3	11:K:127:ILE:HD12	1.96	0.48
14:N:49:ALA:C	14:N:54:TYR:HB3	2.38	0.48
15:O:171:HIS:CE1	37:O:8563:HOH:O	2.67	0.48
17:Q:2:ASP:C	17:Q:2:ASP:OD1	2.56	0.48
1:A:371:U:H2'	1:A:372:A:C8	2.47	0.47
1:A:450:C:H4'	5:E:46:TYR:CE1	2.49	0.47
1:A:731:U:O2'	1:A:732:C:H5'	2.14	0.47
1:A:737:A:H2'	1:A:738:G:O4'	2.14	0.47
1:A:918:G:C2	1:A:926:A:C2	3.02	0.47
1:A:1562:C:H42	1:A:2738:G:H1	1.62	0.47
1:A:2050:G:H5''	19:S:80:TYR:O	2.14	0.47
6:F:174:VAL:CG1	37:F:6555:HOH:O	2.61	0.47
15:O:113:SER:C	37:O:8556:HOH:O	2.58	0.47
15:O:161:GLY:O	15:O:162:ASP:C	2.56	0.47
23:W:27:LEU:O	23:W:30:ALA:N	2.47	0.47
24:X:76:ASP:O	24:X:77:ALA:O	2.32	0.47
24:X:142:ASP:HB3	24:X:145:GLY:H	1.78	0.47
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.49	0.47
27:1:37:HIS:O	27:1:45:LYS:HA	2.13	0.47
1:A:407:A:H5'	37:A:6003:HOH:O	2.13	0.47
1:A:1079:A:N1	1:A:2068:G:O2'	2.43	0.47
37:A:7447:HOH:O	5:E:188:ARG:HD3	2.14	0.47
5:E:180:SER:HB2	37:E:8450:HOH:O	2.14	0.47
10:J:65:ARG:CZ	37:J:8387:HOH:O	2.62	0.47
11:K:130:VAL:HG12	11:K:131:THR:N	2.29	0.47
1:A:457:U:H5	1:A:460:A:OP2	1.97	0.47
1:A:951:A:H2'	1:A:952:G:H5'	1.95	0.47
1:A:1462:C:H2'	1:A:1463:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1477:C:H5'	1:A:1868:G:C5'	2.45	0.47
1:A:2284:G:H5'	37:A:9440:HOH:O	2.13	0.47
37:A:9583:HOH:O	14:N:165:SER:HB3	2.14	0.47
4:D:248:ARG:O	4:D:251:VAL:HG12	2.14	0.47
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.90	0.47
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.96	0.47
14:N:47:ASP:CG	14:N:48:ARG:N	2.73	0.47
14:N:80:GLY:O	14:N:81:ARG:HD3	2.14	0.47
19:S:25:PHE:CE2	19:S:29:LYS:HE2	2.49	0.47
24:X:40:ALA:O	24:X:44:MET:HG3	2.14	0.47
27:1:47:LEU:HD23	27:1:57:CYS:CB	2.44	0.47
1:A:710:G:P	16:P:24:ALA:HB3	2.55	0.47
1:A:716:G:C2'	1:A:717:C:O5'	2.63	0.47
1:A:1773:G:H2'	1:A:1774:G:H5'	1.96	0.47
1:A:2724:U:H2'	1:A:2725:G:O4'	2.14	0.47
37:A:7447:HOH:O	5:E:188:ARG:CD	2.62	0.47
3:C:36:ASP:O	3:C:38:ILE:N	2.48	0.47
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.96	0.47
7:G:69:ILE:HA	7:G:72:MET:HE2	1.95	0.47
10:J:132:PHE:O	10:J:133:ILE:HD13	2.15	0.47
11:K:103:VAL:HG12	37:K:8563:HOH:O	2.15	0.47
15:O:141:ARG:N	37:O:8566:HOH:O	2.47	0.47
17:Q:58:SER:HB3	37:Q:4744:HOH:O	2.12	0.47
18:R:75:ILE:HD11	18:R:84:ILE:HD11	1.96	0.47
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.14	0.47
1:A:130:C:H5'	37:A:5189:HOH:O	2.13	0.47
1:A:445:U:H1'	37:A:7324:HOH:O	2.14	0.47
1:A:2000:G:O2'	1:A:2001:G:H5'	2.15	0.47
1:A:2353:A:H4'	1:A:2354:A:O5'	2.14	0.47
4:D:279:THR:CG2	4:D:280:VAL:N	2.77	0.47
11:K:107:ASN:C	11:K:107:ASN:HD22	2.22	0.47
24:X:137:GLN:HG3	24:X:137:GLN:O	2.15	0.47
1:A:764:C:H2'	1:A:765:G:O4'	2.15	0.47
1:A:1820:G:C6	1:A:2030:A:C2	3.03	0.47
1:A:1850:U:H2'	1:A:1851:G:C8	2.48	0.47
1:A:2896:A:H2'	1:A:2896:A:N3	2.30	0.47
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.49	0.47
4:D:55:ASN:HB3	4:D:64:GLY:H	1.79	0.47
4:D:162:MET:HE2	4:D:310:ARG:CG	2.44	0.47
5:E:20:ASP:O	5:E:23:GLU:HB2	2.15	0.47
5:E:165:ASP:O	5:E:168:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:113:ALA:N	10:J:114:PRO:CD	2.78	0.47
10:J:163:PRO:HG2	37:J:8340:HOH:O	2.14	0.47
14:N:61:ILE:HA	37:N:8621:HOH:O	2.15	0.47
14:N:138:HIS:C	14:N:139:PRO:O	2.50	0.47
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.44	0.47
18:R:75:ILE:HD13	18:R:84:ILE:HD11	1.97	0.47
22:V:44:ARG:CB	37:V:3805:HOH:O	2.61	0.47
1:A:101:C:H2'	1:A:102:A:H8	1.80	0.47
1:A:125:U:H2'	37:A:3740:HOH:O	2.15	0.47
1:A:1116:U:H3	1:A:1246:A:N6	2.03	0.47
1:A:1380:U:H5'	37:A:9211:HOH:O	2.14	0.47
1:A:2466:G:H8	37:A:9516:HOH:O	1.98	0.47
1:A:2718:C:H6	1:A:2718:C:H5'	1.79	0.47
37:A:7413:HOH:O	21:U:9:LYS:HD2	2.14	0.47
5:E:49:ASP:HB3	5:E:52:ALA:HB2	1.96	0.47
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.44	0.47
5:E:238:SER:HB3	37:E:8383:HOH:O	2.13	0.47
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.83	0.47
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.44	0.47
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.50	0.47
12:L:101:ASN:O	12:L:102:GLU:CB	2.63	0.47
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.30	0.47
14:N:137:ASP:C	14:N:142:LYS:HE3	2.40	0.47
15:O:67:ALA:C	15:O:69:TYR:N	2.73	0.47
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.50	0.47
17:Q:115:SER:C	17:Q:117:SER:N	2.73	0.47
21:U:55:PHE:CD2	21:U:77:VAL:HG13	2.49	0.47
21:U:80:GLU:OE2	21:U:84:GLY:HA2	2.15	0.47
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.14	0.47
30:4:74:CYS:SG	30:4:76:LYS:CB	3.03	0.47
1:A:222:A:H2'	1:A:223:G:O4'	2.14	0.47
1:A:1029:U:O2'	1:A:1273:C:OP1	2.30	0.47
1:A:1167:G:O2'	1:A:1168:C:H5'	2.15	0.47
1:A:2791:U:H1'	1:A:2792:A:H5''	1.96	0.47
3:C:88:ILE:HG22	3:C:88:ILE:O	2.14	0.47
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.14	0.47
10:J:59:ASN:N	10:J:59:ASN:ND2	2.50	0.47
29:3:24:TRP:CD1	37:3:6863:HOH:O	2.68	0.47
30:4:17:HIS:O	30:4:18:GLN:HG3	2.15	0.47
1:A:1333:U:H2'	1:A:1334:C:H6	1.78	0.47
1:A:1942:A:O2'	1:A:1943:C:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2269:C:H2'	1:A:2270:G:H5'	1.96	0.47
1:A:2667:G:H1'	1:A:2914:A:N3	2.29	0.47
37:A:5383:HOH:O	3:C:164:ARG:NE	2.47	0.47
2:B:3064:C:C2'	2:B:3065:A:H5'	2.45	0.47
3:C:2:ARG:NH1	37:C:8513:HOH:O	2.29	0.47
3:C:55:VAL:HG13	3:C:67:LEU:HD22	1.97	0.47
9:I:12:ILE:HG13	37:I:6833:HOH:O	2.15	0.47
15:O:154:LEU:HG	15:O:155:GLU:H	1.80	0.47
21:U:41:ARG:NH1	21:U:42:VAL:O	2.48	0.47
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.13	0.47
26:Z:129:ASN:OD1	26:Z:141:THR:OG1	2.29	0.47
27:1:30:GLU:HB3	27:1:34:LYS:HE3	1.97	0.47
28:2:5:THR:HB	28:2:6:PRO:CD	2.45	0.47
1:A:778:C:C4	1:A:779:U:C4	3.03	0.47
1:A:1003:U:O2	10:J:90:PHE:HZ	1.98	0.47
1:A:1887:U:OP1	27:1:21:LYS:HG3	2.14	0.47
1:A:2106:C:H2'	1:A:2107:U:C6	2.50	0.47
6:F:92:GLU:O	6:F:93:LEU:O	2.33	0.47
7:G:84:MET:HB2	7:G:131:LEU:HB2	1.96	0.47
12:L:20:CYS:HB3	12:L:26:ALA:O	2.15	0.47
25:Y:73:ARG:O	25:Y:85:VAL:HG13	2.14	0.47
26:Z:106:THR:CG2	26:Z:107:PRO:HD2	2.45	0.47
1:A:675:U:O2'	5:E:42:ARG:NH1	2.48	0.46
1:A:1114:A:H2'	1:A:1115:U:H6	1.79	0.46
1:A:1592:G:O2'	1:A:1593:C:O5'	2.33	0.46
1:A:1743:G:H1'	37:A:4863:HOH:O	2.15	0.46
1:A:1829:A:H61	27:1:18:TYR:HA	1.80	0.46
1:A:2064:U:H4'	1:A:2653:A:OP1	2.15	0.46
1:A:2533:C:H5'	37:A:6882:HOH:O	2.15	0.46
2:B:3008:G:C6	2:B:3009:C:C4	3.03	0.46
2:B:3057:A:C8	6:F:141:VAL:HG21	2.50	0.46
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.97	0.46
5:E:246:ARG:NE	37:E:8426:HOH:O	2.48	0.46
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.97	0.46
18:R:93:ARG:HG3	18:R:93:ARG:NH1	2.31	0.46
19:S:39:THR:O	19:S:40:ALA:C	2.58	0.46
21:U:27:LEU:HD23	21:U:98:VAL:HB	1.97	0.46
26:Z:134:HIS:CD2	26:Z:134:HIS:H	2.33	0.46
1:A:128:A:H3'	1:A:128:A:C8	2.50	0.46
1:A:818:A:O2'	27:1:13:ARG:HD3	2.15	0.46
1:A:1269:G:H2'	1:A:1270:U:H6	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:A:N1	5:E:48:SER:HB3	2.31	0.46
1:A:1594:C:C2	1:A:1601:G:C2	3.03	0.46
1:A:1996:U:O2'	1:A:1997:A:H5'	2.15	0.46
12:L:9:THR:O	12:L:10:GLN:C	2.56	0.46
13:M:148:GLU:HG2	37:M:8558:HOH:O	2.14	0.46
14:N:87:MET:HB3	30:4:46:ILE:CD1	2.32	0.46
14:N:89:ASN:HA	37:N:8551:HOH:O	2.14	0.46
16:P:105:ASN:HD21	16:P:109:SER:H	1.64	0.46
18:R:8:GLU:CD	18:R:8:GLU:C	2.83	0.46
21:U:38:ARG:NH1	37:U:6217:HOH:O	2.47	0.46
25:Y:79:GLU:OE2	37:Y:5564:HOH:O	2.21	0.46
30:4:69:TYR:O	30:4:77:ALA:HA	2.15	0.46
1:A:111:C:H2'	1:A:112:G:O4'	2.15	0.46
1:A:1191:A:N1	1:A:1206:U:O4	2.48	0.46
1:A:1562:C:O2	1:A:1562:C:H2'	2.15	0.46
3:C:58:VAL:O	3:C:65:ARG:HD2	2.16	0.46
5:E:84:VAL:O	5:E:85:LYS:CB	2.63	0.46
7:G:84:MET:HE1	7:G:148:ILE:HD13	1.95	0.46
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.45	0.46
13:M:14:GLY:N	37:M:8519:HOH:O	2.15	0.46
13:M:107:LYS:HE3	13:M:124:ASP:OD2	2.15	0.46
15:O:34:LEU:HA	15:O:47:LEU:CD2	2.45	0.46
28:2:29:THR:O	28:2:32:LYS:HE2	2.16	0.46
1:A:159:G:H2'	1:A:175:G:N2	2.31	0.46
1:A:567:U:O2'	1:A:568:G:H5'	2.14	0.46
3:C:111:SER:O	3:C:112:PRO:C	2.58	0.46
6:F:154:LYS:H	6:F:154:LYS:CD	2.22	0.46
7:G:34:TRP:O	11:K:127:ILE:HD11	2.14	0.46
15:O:37:ARG:HD3	15:O:37:ARG:HA	1.78	0.46
15:O:120:GLU:HG3	15:O:136:LEU:HD13	1.97	0.46
26:Z:109:LEU:HA	37:Z:8571:HOH:O	2.14	0.46
28:2:28:HIS:O	28:2:32:LYS:N	2.43	0.46
30:4:38:ARG:O	30:4:42:ARG:HB2	2.16	0.46
30:4:74:CYS:SG	30:4:76:LYS:CG	3.03	0.46
1:A:401:C:P	37:A:5770:HOH:O	2.74	0.46
1:A:1044:C:C5'	37:A:9022:HOH:O	2.61	0.46
1:A:2594:C:O2'	1:A:2595:U:H5'	2.16	0.46
2:B:3014:G:H2'	2:B:3015:C:H5'	1.98	0.46
2:B:3088:G:OP1	24:X:130:HIS:NE2	2.46	0.46
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.79	0.46
3:C:109:GLU:HG2	3:C:116:GLY:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:VAL:CG1	4:D:156:LYS:HG2	2.45	0.46
8:H:72:VAL:HA	8:H:73:PRO:HD3	1.84	0.46
8:H:79:GLN:HB2	8:H:82:ASP:OD2	2.16	0.46
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.16	0.46
15:O:154:LEU:HG	15:O:155:GLU:N	2.29	0.46
15:O:180:LEU:O	15:O:181:ASP:HB3	2.14	0.46
23:W:38:GLY:C	23:W:40:PRO:HD2	2.41	0.46
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.96	0.46
24:X:13:MET:O	24:X:14:HIS:C	2.58	0.46
1:A:383:A:H4'	37:A:5304:HOH:O	2.16	0.46
1:A:665:A:H2'	1:A:666:A:C8	2.50	0.46
1:A:1086:A:N6	24:X:11:VAL:HG11	2.31	0.46
1:A:1375:A:O2'	1:A:1376:G:H5'	2.16	0.46
5:E:111:VAL:HB	37:E:8321:HOH:O	2.15	0.46
7:G:18:LEU:HD13	7:G:34:TRP:CG	2.51	0.46
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.44	0.46
10:J:112:ARG:O	10:J:113:ALA:C	2.58	0.46
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.97	0.46
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.45	0.46
1:A:278:A:H2'	1:A:279:C:O4'	2.16	0.46
1:A:288:A:H2'	1:A:289:G:C8	2.51	0.46
1:A:1391:G:H2'	1:A:1392:A:H5'	1.98	0.46
1:A:1398:G:H2'	1:A:1399:A:C8	2.51	0.46
1:A:1615:A:H5'	37:A:4155:HOH:O	2.14	0.46
1:A:1815:A:H4'	1:A:2751:C:O4'	2.16	0.46
1:A:1989:G:O2'	1:A:1990:C:H5'	2.15	0.46
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.34	0.46
7:G:64:THR:HG22	7:G:68:HIS:CD2	2.51	0.46
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.98	0.46
11:K:131:THR:HB	11:K:134:GLU:HG3	1.97	0.46
15:O:154:LEU:O	15:O:155:GLU:CB	2.64	0.46
15:O:182:GLY:N	37:O:8567:HOH:O	2.49	0.46
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.74	0.46
21:U:113:GLU:O	21:U:114:SER:C	2.58	0.46
28:2:37:CYS:SG	28:2:39:PHE:HB2	2.55	0.46
1:A:175:G:H2'	14:N:192:ALA:HB3	1.96	0.46
1:A:2506:A:H1'	37:A:6034:HOH:O	2.16	0.46
2:B:3044:A:H1'	6:F:76:ARG:NH2	2.30	0.46
4:D:238:ASN:HD22	4:D:240:GLY:N	2.08	0.46
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.98	0.46
5:E:13:ASP:N	37:E:8446:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:THR:HG22	6:F:101:THR:O	2.16	0.46
6:F:169:THR:O	6:F:170:TYR:HB2	2.16	0.46
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.45	0.46
11:K:126:ASN:O	11:K:129:PHE:HE2	1.99	0.46
13:M:72:ASN:HB2	37:M:8585:HOH:O	2.15	0.46
14:N:63:VAL:O	14:N:130:GLU:HA	2.16	0.46
14:N:87:MET:SD	37:N:8532:HOH:O	2.61	0.46
15:O:64:SER:C	15:O:66:LEU:N	2.74	0.46
21:U:48:VAL:HG22	21:U:97:ARG:C	2.40	0.46
21:U:48:VAL:HG13	21:U:49:GLU:N	2.30	0.46
24:X:35:VAL:HG23	24:X:41:TYR:CD2	2.51	0.46
27:1:21:LYS:O	27:1:25:ARG:HG3	2.15	0.46
1:A:13:G:H2'	1:A:14:C:H6	1.80	0.46
1:A:259:G:H21	14:N:58:GLN:NE2	2.14	0.46
1:A:402:U:H2'	1:A:403:C:C6	2.50	0.46
1:A:544:G:H2'	1:A:545:G:C5'	2.41	0.46
1:A:677:C:H4'	5:E:246:ARG:NH2	2.31	0.46
1:A:1185:U:H5'	37:A:7456:HOH:O	2.16	0.46
1:A:1474:C:H6	1:A:1474:C:C5'	2.18	0.46
1:A:1730:G:H5'	1:A:1731:C:C5	2.51	0.46
1:A:1754:A:N7	37:A:7857:HOH:O	2.36	0.46
1:A:1894:C:C2	1:A:1939:U:C4	3.03	0.46
1:A:2087:C:O2'	1:A:2088:C:H5'	2.15	0.46
1:A:2488:A:H2	37:A:7264:HOH:O	1.98	0.46
1:A:2564:G:OP2	1:A:2565:C:H5''	2.16	0.46
2:B:3031:C:O2'	2:B:3032:G:H5'	2.15	0.46
3:C:125:ASN:CB	3:C:158:VAL:HG12	2.46	0.46
3:C:192:VAL:HG12	3:C:207:GLN:HB3	1.98	0.46
4:D:51:VAL:HG23	4:D:329:TYR:O	2.16	0.46
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.98	0.46
11:K:54:VAL:HG11	11:K:138:THR:HG21	1.97	0.46
12:L:87:ARG:NH1	37:L:4066:HOH:O	2.48	0.46
15:O:37:ARG:NH2	37:O:8533:HOH:O	2.49	0.46
15:O:50:LEU:HB2	37:O:8524:HOH:O	2.16	0.46
25:Y:14:LEU:HD12	25:Y:67:PRO:O	2.16	0.46
1:A:2121:G:H5''	37:A:3491:HOH:O	2.16	0.46
3:C:213:LYS:NZ	37:C:8528:HOH:O	2.41	0.46
4:D:168:GLY:O	4:D:169:GLY:O	2.34	0.46
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.77	0.46
6:F:84:LEU:HA	6:F:87:ALA:HB3	1.98	0.46
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:74:ARG:HD3	14:N:91:ILE:HD12	1.97	0.46
14:N:155:HIS:O	14:N:158:ARG:HG2	2.15	0.46
25:Y:21:PRO:HD3	37:Y:6179:HOH:O	2.15	0.46
1:A:303:C:H2'	1:A:304:G:O4'	2.16	0.45
1:A:308:U:C4	1:A:342:C:H1'	2.50	0.45
1:A:553:G:H5'	37:A:3479:HOH:O	2.15	0.45
1:A:646:G:H2'	1:A:647:U:C6	2.51	0.45
1:A:1398:G:O2'	1:A:1399:A:H5'	2.16	0.45
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.84	0.45
3:C:109:GLU:HG2	3:C:116:GLY:N	2.31	0.45
6:F:86:THR:CG2	37:F:7477:HOH:O	2.64	0.45
7:G:11:VAL:HG11	7:G:22:VAL:HG13	1.97	0.45
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.98	0.45
9:I:64:ASN:O	9:I:68:GLU:HG3	2.15	0.45
20:T:57:THR:HG22	20:T:59:ASP:HB2	1.97	0.45
1:A:1114:A:H2'	1:A:1115:U:C6	2.52	0.45
1:A:1407:A:O2'	1:A:1408:U:H3'	2.17	0.45
1:A:1441:G:H1'	37:A:7762:HOH:O	2.16	0.45
1:A:2435:U:P	30:4:28:GLY:HA3	2.56	0.45
1:A:2670:G:O2'	1:A:2671:U:H5'	2.17	0.45
6:F:128:LEU:HD23	6:F:128:LEU:C	2.42	0.45
14:N:98:GLN:NE2	14:N:117:SER:O	2.49	0.45
16:P:96:VAL:HA	37:P:4258:HOH:O	2.16	0.45
24:X:139:GLY:O	24:X:141:HIS:CD2	2.68	0.45
26:Z:115:ARG:CZ	37:Z:8557:HOH:O	2.64	0.45
1:A:517:U:H2'	1:A:518:G:H5'	1.97	0.45
1:A:657:G:H2'	1:A:658:C:C6	2.52	0.45
1:A:2719:A:C2	4:D:70:PRO:HG3	2.51	0.45
4:D:79:MET:HE1	37:D:8623:HOH:O	2.17	0.45
4:D:215:VAL:HA	4:D:220:VAL:HG22	1.97	0.45
4:D:304:PRO:HD2	4:D:307:ARG:HD2	1.98	0.45
4:D:316:ARG:N	4:D:317:PRO:HD3	2.32	0.45
6:F:53:LYS:HA	6:F:67:ASP:O	2.17	0.45
6:F:93:LEU:HG	37:F:3862:HOH:O	2.16	0.45
7:G:93:MET:HE2	7:G:107:PHE:CD1	2.51	0.45
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.52	0.45
10:J:157:ILE:HG22	10:J:158:ASN:N	2.31	0.45
11:K:42:GLU:O	11:K:131:THR:HG23	2.16	0.45
13:M:65:ASP:CG	13:M:111:ALA:HB3	2.41	0.45
14:N:57:LYS:HE2	14:N:140:ALA:O	2.16	0.45
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:A:H4'	1:A:338:C:C5	2.51	0.45
1:A:683:G:O2'	1:A:684:G:H5'	2.16	0.45
1:A:818:A:H2	27:1:13:ARG:HA	1.81	0.45
1:A:926:A:H1'	13:M:38:HIS:O	2.16	0.45
1:A:2112:A:H2'	1:A:2113:G:C8	2.52	0.45
1:A:2314:G:H2'	1:A:2315:C:H5'	1.98	0.45
1:A:2421:G:H4'	37:A:4751:HOH:O	2.17	0.45
1:A:2445:U:H2'	1:A:2446:G:C8	2.51	0.45
37:A:9401:HOH:O	14:N:52:LEU:HD23	2.17	0.45
3:C:29:HIS:HB2	3:C:153:ARG:HH12	1.82	0.45
4:D:198:GLU:HB3	37:D:8593:HOH:O	2.16	0.45
6:F:173:GLU:O	6:F:174:VAL:C	2.59	0.45
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.31	0.45
14:N:59:GLY:C	14:N:141:ILE:HD11	2.41	0.45
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.97	0.45
24:X:88:THR:CG2	24:X:89:ASP:N	2.79	0.45
25:Y:71:ARG:HD2	37:Y:7542:HOH:O	2.16	0.45
28:2:52:SER:HA	37:2:4248:HOH:O	2.15	0.45
1:A:1375:A:C2'	1:A:1376:G:H5'	2.46	0.45
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.16	0.45
1:A:2271:G:H2'	1:A:2271:G:N3	2.32	0.45
1:A:2403:C:H3'	37:A:5187:HOH:O	2.16	0.45
1:A:2406:U:C4	1:A:2407:G:N7	2.84	0.45
1:A:2577:A:H5'	37:A:7748:HOH:O	2.15	0.45
1:A:2776:A:H2'	1:A:2777:G:O4'	2.16	0.45
37:A:4700:HOH:O	15:O:21:HIS:HD2	2.00	0.45
19:S:82:GLU:HG3	19:S:83:LYS:H	1.82	0.45
21:U:71:VAL:HG11	21:U:90:PRO:CB	2.30	0.45
1:A:35:U:O2'	1:A:36:C:H5'	2.17	0.45
1:A:558:C:C2	1:A:600:G:N2	2.84	0.45
1:A:746:A:C6	16:P:65:LEU:HD13	2.52	0.45
1:A:1391:G:C5	1:A:1435:U:C4	3.04	0.45
1:A:1420:C:C2	1:A:1445:G:N2	2.84	0.45
1:A:1883:U:O2'	1:A:1884:G:H5'	2.17	0.45
1:A:2272:G:H5'	3:C:223:ARG:HB2	1.99	0.45
1:A:2505:G:H8	37:A:5616:HOH:O	2.00	0.45
1:A:2777:G:O2'	1:A:2778:A:H5'	2.16	0.45
37:A:6492:HOH:O	29:3:1:GLY:HA3	2.15	0.45
4:D:1:PRO:O	4:D:2:GLN:HB2	2.17	0.45
4:D:23:THR:HG23	4:D:162:MET:HE3	1.99	0.45
4:D:280:VAL:CG1	4:D:281:ASP:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:ILE:HG23	37:F:5583:HOH:O	2.15	0.45
14:N:134:ILE:O	14:N:136:PRO:HD3	2.17	0.45
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.31	0.45
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.49	0.45
24:X:63:GLU:HG2	24:X:93:ILE:HG22	1.98	0.45
1:A:164:G:H3'	37:A:3620:HOH:O	2.17	0.45
1:A:327:A:H2'	5:E:150:THR:OG1	2.16	0.45
1:A:424:C:H2'	1:A:425:U:C6	2.51	0.45
1:A:797:A:H5'	27:1:10:ARG:HG2	1.99	0.45
1:A:1161:A:H8	1:A:1161:A:O5'	2.00	0.45
1:A:1299:G:N2	37:A:4657:HOH:O	2.49	0.45
1:A:2456:A:H2'	1:A:2457:U:C6	2.52	0.45
37:A:9538:HOH:O	24:X:119:HIS:HE1	2.00	0.45
2:B:3093:A:C5	2:B:3094:G:H1'	2.52	0.45
3:C:228:ILE:O	3:C:229:ALA:C	2.60	0.45
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.15	0.45
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.45	0.45
9:I:12:ILE:HB	37:I:4714:HOH:O	2.16	0.45
17:Q:98:ILE:O	17:Q:98:ILE:HD13	2.16	0.45
1:A:12:U:H2'	1:A:13:G:H5'	1.98	0.45
1:A:69:A:H5'	1:A:69:A:C8	2.51	0.45
1:A:105:G:O2'	1:A:106:A:H5'	2.17	0.45
1:A:324:G:O2'	1:A:325:U:H5'	2.16	0.45
1:A:426:G:H2'	1:A:427:C:O4'	2.15	0.45
1:A:738:G:H3'	37:A:7031:HOH:O	2.16	0.45
1:A:766:A:H5'	37:A:4624:HOH:O	2.17	0.45
1:A:1592:G:C5	1:A:1593:C:C4	3.04	0.45
1:A:1878:G:O2'	1:A:1879:U:C6	2.68	0.45
1:A:2001:G:C2'	1:A:2002:C:H5'	2.47	0.45
1:A:2073:G:C6	1:A:2489:G:H4'	2.52	0.45
1:A:2356:A:H2'	1:A:2357:G:O4'	2.17	0.45
1:A:2456:A:H2'	1:A:2457:U:H6	1.82	0.45
1:A:2761:A:C4	1:A:2763:G:C8	3.04	0.45
2:B:3035:C:H5''	37:B:4078:HOH:O	2.16	0.45
3:C:105:VAL:CG1	3:C:106:CYS:H	2.30	0.45
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.46	0.45
17:Q:141:ILE:C	17:Q:143:ALA:H	2.25	0.45
1:A:565:A:OP2	1:A:592:G:N1	2.43	0.45
1:A:929:A:H8	1:A:929:A:O5'	2.00	0.45
1:A:1010:C:H4'	15:O:4:PRO:HB2	1.99	0.45
1:A:1687:C:O2	28:2:9:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1834:C:H2'	1:A:1840:A:H62	1.78	0.45
1:A:2032:U:O2'	1:A:2033:G:H5''	2.17	0.45
1:A:2896:A:H5''	37:A:6079:HOH:O	2.16	0.45
37:A:3749:HOH:O	22:V:17:THR:CG2	2.64	0.45
2:B:3056:A:C3'	2:B:3057:A:H5''	2.47	0.45
4:D:132:HIS:CE1	4:D:171:VAL:CG2	3.00	0.45
4:D:132:HIS:HB2	4:D:137:LEU:HD22	1.99	0.45
5:E:246:ARG:HH11	5:E:246:ARG:CB	2.24	0.45
7:G:11:VAL:HG12	7:G:12:ASP:H	1.82	0.45
7:G:43:ASP:HA	37:G:5864:HOH:O	2.16	0.45
10:J:84:ARG:CZ	10:J:135:TRP:CH2	3.00	0.45
14:N:84:LYS:O	14:N:87:MET:CG	2.65	0.45
24:X:41:TYR:HA	24:X:44:MET:HE3	1.99	0.45
24:X:48:VAL:O	24:X:48:VAL:HG12	2.15	0.45
1:A:251:C:H1'	14:N:58:GLN:HE22	1.81	0.45
1:A:333:G:O2'	1:A:334:G:H5'	2.17	0.45
1:A:558:C:H2'	1:A:559:U:H5'	1.99	0.45
1:A:584:U:H3'	37:A:6075:HOH:O	2.15	0.45
1:A:679:G:OP2	37:A:4408:HOH:O	2.20	0.45
1:A:1057:A:C6	1:A:1058:A:C6	3.05	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.17	0.45
4:D:2:GLN:NE2	37:D:8618:HOH:O	2.50	0.45
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.85	0.45
6:F:25:MET:HE3	6:F:37:ALA:HB1	1.97	0.45
9:I:12:ILE:HD12	37:I:692:HOH:O	2.16	0.45
10:J:26:LYS:HG2	10:J:28:ILE:N	2.24	0.45
10:J:117:LYS:O	10:J:119:VAL:HG13	2.17	0.45
19:S:106:GLY:CA	19:S:109:MET:HE3	2.34	0.45
24:X:14:HIS:HB2	24:X:17:ILE:HG13	1.99	0.45
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.51	0.45
24:X:122:ARG:CG	24:X:152:ALA:O	2.65	0.45
27:I:46:LYS:NZ	37:I:8440:HOH:O	2.49	0.45
1:A:328:U:O4'	5:E:202:THR:HG22	2.17	0.44
1:A:883:U:O2	1:A:883:U:H2'	2.17	0.44
1:A:1669:A:H2	37:A:3678:HOH:O	2.00	0.44
1:A:1829:A:C2'	1:A:1830:C:H5'	2.46	0.44
1:A:2559:C:H4'	37:A:7243:HOH:O	2.17	0.44
2:B:3020:G:H3'	37:B:2984:HOH:O	2.17	0.44
2:B:3092:G:C6	2:B:3093:A:C6	3.06	0.44
7:G:95:VAL:O	7:G:126:ILE:HD13	2.17	0.44
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:150:LYS:NZ	37:J:8381:HOH:O	2.49	0.44
23:W:42:ASN:O	23:W:44:GLY:N	2.50	0.44
1:A:84:G:O2'	1:A:85:C:H5'	2.17	0.44
1:A:558:C:C2'	1:A:559:U:C5'	2.95	0.44
1:A:1004:C:O2'	1:A:1005:A:H5'	2.17	0.44
1:A:1139:U:H2'	1:A:1140:C:H6	1.82	0.44
1:A:1242:A:H5'	11:K:82:THR:CG2	2.38	0.44
1:A:2546:U:OP1	37:A:3821:HOH:O	2.21	0.44
1:A:2607:U:O5'	1:A:2609:G:H4'	2.16	0.44
1:A:2697:A:H2'	1:A:2698:G:O4'	2.16	0.44
2:B:3038:A:H2	2:B:3043:G:H5''	1.83	0.44
3:C:95:PRO:HA	3:C:153:ARG:HA	2.00	0.44
4:D:212:GLN:HB2	4:D:257:THR:CG2	2.41	0.44
5:E:218:VAL:HG12	37:E:8426:HOH:O	2.17	0.44
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.32	0.44
24:X:26:ILE:HB	37:X:5420:HOH:O	2.16	0.44
1:A:88:G:C8	29:3:28:LYS:HB2	2.52	0.44
1:A:282:C:H2'	1:A:283:U:O4'	2.16	0.44
1:A:883:U:O2	1:A:883:U:C2'	2.65	0.44
1:A:1066:U:H2'	1:A:1067:A:C8	2.52	0.44
1:A:1412:U:O4	1:A:1681:G:H2'	2.18	0.44
1:A:2563:U:H2'	1:A:2565:C:O5'	2.17	0.44
2:B:3014:G:C2'	2:B:3015:C:H5'	2.47	0.44
3:C:33:GLU:H	3:C:33:GLU:CD	2.25	0.44
3:C:36:ASP:HB2	3:C:83:GLY:HA3	2.00	0.44
4:D:14:GLY:CA	4:D:15:PRO:C	2.90	0.44
5:E:79:ARG:O	5:E:87:ARG:HG2	2.18	0.44
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.46	0.44
10:J:62:GLU:OE2	10:J:66:VAL:CG2	2.66	0.44
14:N:108:LYS:N	14:N:108:LYS:HD3	2.32	0.44
37:N:8532:HOH:O	30:4:46:ILE:HB	2.17	0.44
16:P:44:ASN:OD1	16:P:65:LEU:HB2	2.17	0.44
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	1.99	0.44
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.80	0.44
1:A:10:U:O4	1:A:532:A:OP2	2.35	0.44
1:A:68:U:O2'	1:A:69:A:H5''	2.17	0.44
1:A:492:C:O2'	1:A:493:U:H5'	2.17	0.44
1:A:873:G:H2'	1:A:875:A:N7	2.32	0.44
1:A:1236:A:H2'	1:A:1237:U:O4'	2.16	0.44
1:A:2045:G:H2'	1:A:2046:G:O4'	2.17	0.44
1:A:2135:A:O2'	1:A:2136:G:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2346:C:H4'	6:F:52:THR:CG2	2.46	0.44
3:C:126:ALA:HB1	3:C:138:VAL:CG1	2.47	0.44
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.47	0.44
7:G:162:PHE:CD1	7:G:162:PHE:N	2.85	0.44
14:N:182:LYS:HB2	14:N:194:ALA:HB2	1.99	0.44
20:T:11:THR:O	20:T:12:GLU:C	2.60	0.44
24:X:42:ARG:O	24:X:45:VAL:HG22	2.18	0.44
27:1:57:CYS:O	27:1:61:GLY:N	2.47	0.44
29:3:40:ARG:HG2	29:3:40:ARG:HH11	1.82	0.44
1:A:67:A:H5'	1:A:69:A:C8	2.53	0.44
1:A:245:C:C2'	1:A:246:G:H5'	2.48	0.44
1:A:694:A:C2'	1:A:695:C:H5'	2.47	0.44
1:A:902:G:N7	13:M:18:HIS:CD2	2.84	0.44
1:A:2334:C:O2'	1:A:2335:C:H5'	2.18	0.44
1:A:2338:G:H1'	6:F:105:SER:OG	2.17	0.44
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.48	0.44
8:H:22:VAL:HG21	8:H:104:ALA:HB2	2.00	0.44
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.18	0.44
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.29	0.44
26:Z:106:THR:HG22	26:Z:107:PRO:O	2.17	0.44
26:Z:107:PRO:HD3	26:Z:182:PHE:CE1	2.53	0.44
1:A:245:C:H2'	1:A:246:G:H5'	1.98	0.44
1:A:1081:A:C6	1:A:1082:A:N1	2.85	0.44
1:A:1099:G:OP1	2:B:3087:U:O2'	2.33	0.44
2:B:3107:C:H2'	2:B:3108:C:C6	2.52	0.44
4:D:240:GLY:HA3	37:D:8654:HOH:O	2.17	0.44
5:E:21:VAL:C	5:E:23:GLU:H	2.25	0.44
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.77	0.44
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.30	0.44
14:N:115:LEU:HD13	14:N:115:LEU:C	2.43	0.44
17:Q:27:ARG:O	17:Q:31:ILE:HG13	2.18	0.44
23:W:1:THR:HG23	23:W:2:VAL:N	2.23	0.44
24:X:126:ASP:HB3	24:X:135:GLY:O	2.18	0.44
25:Y:27:ASP:OD2	25:Y:27:ASP:N	2.51	0.44
1:A:204:A:H2'	1:A:205:U:C5'	2.45	0.44
1:A:449:A:C8	5:E:43:LYS:HG2	2.52	0.44
1:A:1127:C:C2'	1:A:1128:U:H5'	2.48	0.44
1:A:1409:G:H5'	37:A:3700:HOH:O	2.17	0.44
1:A:1515:A:H2'	1:A:1516:C:C6	2.53	0.44
1:A:1969:A:N7	1:A:1970:G:C6	2.85	0.44
1:A:2289:G:H21	1:A:2291:A:H2	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2727:A:H2'	1:A:2728:C:H5'	1.99	0.44
5:E:25:PRO:HD2	37:E:8431:HOH:O	2.15	0.44
5:E:235:PHE:CE2	5:E:243:VAL:HG21	2.48	0.44
10:J:72:VAL:CG1	10:J:81:TYR:CZ	3.01	0.44
12:L:55:VAL:CG1	12:L:56:SER:N	2.80	0.44
15:O:152:GLU:C	15:O:154:LEU:N	2.75	0.44
16:P:99:GLU:CG	37:P:6044:HOH:O	2.66	0.44
24:X:65:VAL:HA	24:X:68:THR:CG2	2.47	0.44
1:A:259:G:O2'	1:A:260:C:H5'	2.18	0.44
1:A:538:C:H5''	1:A:539:G:C8	2.53	0.44
1:A:853:C:H2'	1:A:854:G:O4'	2.17	0.44
1:A:1690:C:C5	1:A:1692:C:C4	3.06	0.44
1:A:1902:G:H2'	1:A:1903:U:O4'	2.18	0.44
1:A:1925:G:O2'	1:A:1926:G:H5'	2.18	0.44
1:A:2050:G:OP1	19:S:79:ARG:HB3	2.18	0.44
1:A:2055:A:H5'	19:S:134:SER:HB2	2.00	0.44
1:A:2506:A:C1'	37:A:6034:HOH:O	2.65	0.44
6:F:103:ASN:ND2	6:F:134:LEU:H	2.16	0.44
10:J:31:PHE:CD2	10:J:85:ILE:HG23	2.53	0.44
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.53	0.44
11:K:107:ASN:HD22	11:K:109:TYR:H	1.62	0.44
19:S:132:ARG:NH1	37:S:8559:HOH:O	2.51	0.44
21:U:26:THR:HA	21:U:39:ASN:HB3	1.99	0.44
1:A:435:A:O2'	1:A:436:A:H5'	2.18	0.44
1:A:861:A:H2'	1:A:862:U:C6	2.52	0.44
1:A:875:A:C2	3:C:194:MET:SD	3.11	0.44
1:A:2090:G:H2'	1:A:2091:G:C8	2.52	0.44
1:A:2134:G:C6	1:A:2258:A:C8	3.06	0.44
1:A:2482:G:O2'	1:A:2535:U:OP2	2.29	0.44
10:J:31:PHE:HD2	10:J:85:ILE:O	2.01	0.44
10:J:149:ALA:C	10:J:151:MET:N	2.76	0.44
14:N:84:LYS:O	14:N:87:MET:HG2	2.18	0.44
15:O:154:LEU:HD12	15:O:156:GLU:O	2.18	0.44
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.18	0.44
18:R:31:GLU:CD	18:R:93:ARG:HH12	2.26	0.44
19:S:65:GLY:C	37:S:8517:HOH:O	2.61	0.44
26:Z:112:GLU:CD	26:Z:115:ARG:NH1	2.75	0.44
1:A:51:G:C2	1:A:111:C:C2	3.06	0.43
1:A:244:C:O5'	1:A:244:C:H6	2.00	0.43
1:A:445:U:C1'	37:A:7324:HOH:O	2.66	0.43
1:A:870:G:C3'	1:A:871:G:H5''	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:U:C5	1:A:1170:U:C4	3.06	0.43
1:A:1666:C:H2'	1:A:1667:A:H8	1.83	0.43
1:A:2408:A:H4'	30:4:15:ASN:O	2.17	0.43
1:A:2724:U:O4	1:A:2725:G:N1	2.51	0.43
6:F:58:VAL:CG1	6:F:59:GLY:N	2.80	0.43
10:J:46:VAL:O	10:J:146:TRP:CH2	2.68	0.43
12:L:34:VAL:CG2	12:L:47:ALA:HB2	2.47	0.43
13:M:65:ASP:HA	13:M:109:LEU:O	2.17	0.43
14:N:57:LYS:HB3	14:N:60:ILE:HD12	2.00	0.43
14:N:106:ASN:ND2	34:N:8518:CL:CL	2.88	0.43
14:N:184:ARG:HB2	14:N:184:ARG:NH1	2.33	0.43
16:P:41:ALA:HA	37:P:5104:HOH:O	2.18	0.43
17:Q:27:ARG:HA	37:Q:3969:HOH:O	2.18	0.43
1:A:13:G:H2'	1:A:14:C:C6	2.53	0.43
1:A:69:A:H5'	1:A:69:A:H8	1.83	0.43
1:A:244:C:OP2	8:H:38:LYS:HE3	2.18	0.43
1:A:892:G:H5''	28:2:54:ALA:HB2	2.00	0.43
1:A:912:A:C4	1:A:1294:A:C2	3.06	0.43
1:A:1096:U:H5''	1:A:1258:G:O6	2.18	0.43
1:A:1173:A:H4'	1:A:1174:A:C8	2.53	0.43
1:A:1419:U:O2	1:A:1419:U:H3'	2.18	0.43
1:A:2265:U:H2'	1:A:2266:A:H8	1.84	0.43
5:E:162:VAL:HG12	5:E:162:VAL:O	2.18	0.43
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.46	0.43
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.49	0.43
8:H:99:THR:O	8:H:100:ASP:HB2	2.17	0.43
13:M:98:GLU:O	13:M:99:GLU:CB	2.66	0.43
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.47	0.43
20:T:57:THR:CG2	20:T:58:MET:N	2.81	0.43
1:A:1097:A:H5''	24:X:125:HIS:CE1	2.53	0.43
1:A:1215:A:O3'	1:A:1216:G:C4'	2.66	0.43
1:A:2119:C:O2'	1:A:2120:U:H5'	2.18	0.43
37:A:6175:HOH:O	29:3:44:ARG:HG2	2.18	0.43
3:C:69:LEU:C	3:C:69:LEU:HD12	2.42	0.43
4:D:11:LEU:C	37:D:8614:HOH:O	2.62	0.43
4:D:103:ASP:HB2	37:D:8590:HOH:O	2.17	0.43
4:D:144:THR:HG22	4:D:145:HIS:N	2.33	0.43
14:N:62:VAL:C	14:N:63:VAL:HG23	2.43	0.43
14:N:76:ARG:HG2	14:N:76:ARG:NH1	2.34	0.43
15:O:37:ARG:CD	34:O:8507:CL:CL	3.03	0.43
17:Q:143:ALA:HA	37:Q:5521:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:43:VAL:HG12	25:Y:47:ALA:HB3	2.00	0.43
1:A:329:A:OP2	5:E:206:ASN:HB2	2.18	0.43
1:A:538:C:OP2	26:Z:134:HIS:HE1	2.01	0.43
1:A:580:A:N1	1:A:1253:C:O2'	2.47	0.43
1:A:1205:U:C2'	1:A:1206:U:H5'	2.42	0.43
1:A:2004:U:O2	1:A:2004:U:H2'	2.17	0.43
1:A:2092:G:H2'	1:A:2613:G:OP1	2.18	0.43
1:A:2759:C:OP1	4:D:207:LYS:NZ	2.43	0.43
37:A:7395:HOH:O	21:U:2:LYS:HE2	2.17	0.43
2:B:3047:A:C2	2:B:3048:C:C2	3.06	0.43
37:B:4707:HOH:O	15:O:147:ILE:HD12	2.18	0.43
5:E:185:LYS:NZ	37:E:8423:HOH:O	2.49	0.43
11:K:6:PHE:O	11:K:8:ALA:N	2.51	0.43
14:N:169:ARG:NH1	37:N:8572:HOH:O	2.52	0.43
16:P:107:GLU:O	16:P:108:GLY:C	2.61	0.43
19:S:39:THR:CB	19:S:42:GLU:HG3	2.42	0.43
19:S:96:VAL:HG13	19:S:106:GLY:HA3	2.00	0.43
21:U:48:VAL:HG22	21:U:97:ARG:O	2.19	0.43
1:A:65:C:O2'	1:A:66:G:H5'	2.18	0.43
1:A:101:C:H2'	1:A:102:A:C8	2.53	0.43
1:A:566:A:H2'	1:A:567:U:O4'	2.18	0.43
1:A:1257:C:H2'	1:A:1258:G:O4'	2.18	0.43
1:A:1609:C:H2'	1:A:1610:G:H8	1.82	0.43
1:A:1666:C:O2'	1:A:1667:A:C5'	2.62	0.43
1:A:1783:A:C2'	1:A:1784:U:H5'	2.48	0.43
1:A:2095:A:C2	1:A:2651:C:C2	3.06	0.43
1:A:2468:A:N6	30:4:50:GLY:O	2.52	0.43
2:B:3104:A:O2'	2:B:3105:A:H5'	2.19	0.43
3:C:211:LYS:CB	3:C:212:PRO:HD2	2.36	0.43
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.18	0.43
8:H:27:GLY:HA3	37:H:5413:HOH:O	2.19	0.43
9:I:71:LEU:C	9:I:73:ASP:H	2.26	0.43
10:J:45:GLN:HE21	10:J:135:TRP:NE1	2.17	0.43
13:M:93:VAL:HG12	13:M:97:VAL:HG23	2.01	0.43
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.36	0.43
15:O:37:ARG:CZ	37:O:8533:HOH:O	2.67	0.43
15:O:67:ALA:HA	15:O:71:TRP:H	1.83	0.43
15:O:91:ARG:HG3	15:O:186:LEU:HD23	2.01	0.43
15:O:116:PHE:HB2	37:O:8556:HOH:O	2.19	0.43
17:Q:13:VAL:CG2	17:Q:41:ARG:HG2	2.46	0.43
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:U:H1'	37:A:7626:HOH:O	2.17	0.43
1:A:563:C:H2'	1:A:564:G:O4'	2.19	0.43
1:A:734:U:O2'	1:A:737:A:N6	2.51	0.43
1:A:1164:U:O4'	1:A:1165:G:OP1	2.35	0.43
1:A:2036:C:OP1	37:A:6682:HOH:O	2.21	0.43
1:A:2054:A:H2	19:S:128:ARG:HH22	1.62	0.43
1:A:2346:C:H4'	6:F:52:THR:HG22	2.01	0.43
1:A:2598:U:O2	1:A:2600:A:C8	2.72	0.43
1:A:2900:G:H2'	1:A:2901:C:O4'	2.19	0.43
1:A:2911:C:H2'	1:A:2912:C:C6	2.54	0.43
2:B:3092:G:H22	10:J:52:LYS:NZ	2.16	0.43
3:C:109:GLU:CD	3:C:113:GLY:H	2.26	0.43
3:C:170:VAL:HG13	27:1:22:ILE:CG2	2.48	0.43
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.34	0.43
5:E:114:ALA:HB1	5:E:223:LEU:HB3	2.01	0.43
6:F:63:ILE:C	37:F:5728:HOH:O	2.62	0.43
11:K:39:VAL:CG1	11:K:107:ASN:HB2	2.49	0.43
14:N:35:PRO:HD2	14:N:38:VAL:HG21	2.01	0.43
14:N:87:MET:CE	37:N:8530:HOH:O	2.63	0.43
15:O:114:LYS:O	15:O:118:ILE:HG13	2.18	0.43
20:T:73:ASP:O	20:T:77:VAL:HG23	2.19	0.43
24:X:110:GLN:HE21	24:X:110:GLN:CA	2.27	0.43
1:A:820:G:H5'	1:A:821:U:C5'	2.49	0.43
1:A:929:A:C8	1:A:930:C:C5	3.07	0.43
1:A:1332:C:O2'	1:A:1333:U:H5'	2.19	0.43
1:A:2055:A:H4'	19:S:132:ARG:NH2	2.33	0.43
1:A:2300:A:H4'	1:A:2301:A:O5'	2.19	0.43
1:A:2898:G:O2'	1:A:2899:A:H5'	2.18	0.43
3:C:8:ARG:HG2	37:C:8553:HOH:O	2.17	0.43
4:D:162:MET:HG3	4:D:310:ARG:NH1	2.33	0.43
5:E:39:GLN:O	5:E:43:LYS:HD3	2.19	0.43
5:E:129:HIS:CE1	5:E:232:LEU:H	2.37	0.43
9:I:73:ASP:C	37:I:2994:HOH:O	2.62	0.43
13:M:35:ARG:O	13:M:40:PHE:HA	2.18	0.43
13:M:91:VAL:HG13	13:M:91:VAL:O	2.18	0.43
14:N:42:ARG:HA	14:N:43:PRO:HD3	1.79	0.43
18:R:53:HIS:O	18:R:55:ARG:N	2.52	0.43
21:U:75:GLU:O	21:U:76:ASP:HB2	2.18	0.43
26:Z:187:VAL:CG1	26:Z:205:ILE:HA	2.47	0.43
27:1:46:LYS:HB3	37:1:8438:HOH:O	2.17	0.43
27:1:50:ALA:HB3	27:1:54:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.53	0.43
1:A:392:U:H4'	14:N:193:LYS:HB3	2.01	0.43
1:A:489:A:C8	21:U:82:THR:CG2	3.02	0.43
1:A:757:C:H2'	1:A:758:A:C8	2.54	0.43
1:A:1308:A:O4'	5:E:226:GLY:HA3	2.19	0.43
1:A:1992:U:H2'	1:A:1994:A:OP2	2.19	0.43
1:A:2416:G:H2'	1:A:2417:C:C6	2.54	0.43
1:A:2837:U:H2'	37:A:6820:HOH:O	2.19	0.43
2:B:3078:G:N2	2:B:3103:A:OP2	2.48	0.43
3:C:94:LEU:N	3:C:94:LEU:CD2	2.82	0.43
3:C:169:PHE:O	3:C:170:VAL:HB	2.18	0.43
3:C:211:LYS:HD3	37:C:8613:HOH:O	2.18	0.43
5:E:187:ARG:O	5:E:187:ARG:HG3	2.16	0.43
7:G:7:ILE:HA	7:G:8:PRO:HD3	1.82	0.43
7:G:49:ILE:HD11	7:G:69:ILE:HD12	2.00	0.43
8:H:117:GLU:C	8:H:119:ARG:N	2.77	0.43
10:J:15:THR:HG22	10:J:91:HIS:HA	1.99	0.43
12:L:118:ALA:O	12:L:120:ARG:N	2.52	0.43
14:N:24:MET:HE3	14:N:28:MET:CE	2.33	0.43
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.81	0.43
20:T:58:MET:SD	29:3:8:LYS:HE3	2.59	0.43
25:Y:15:ARG:HB3	25:Y:15:ARG:NH1	2.29	0.43
1:A:69:A:H2'	1:A:70:A:OP2	2.18	0.43
1:A:221:G:OP2	13:M:46:LEU:HB3	2.19	0.43
1:A:321:A:H1'	37:A:7016:HOH:O	2.19	0.43
1:A:553:G:O2'	26:Z:179:PRO:HG3	2.19	0.43
1:A:1176:C:H1'	37:A:3901:HOH:O	2.18	0.43
1:A:1301:C:O2'	1:A:1331:A:H4'	2.19	0.43
1:A:1679:C:O2'	1:A:1685:A:N1	2.51	0.43
1:A:1921:A:C6	1:A:1922:A:C2	3.07	0.43
1:A:2626:C:H2'	1:A:2627:G:C8	2.54	0.43
1:A:2681:A:N6	1:A:2714:U:H4'	2.33	0.43
1:A:2781:U:C2'	1:A:2782:G:H5'	2.49	0.43
5:E:115:LEU:HD12	5:E:115:LEU:HA	1.83	0.43
37:E:8360:HOH:O	16:P:3:THR:HG21	2.19	0.43
6:F:35:ALA:C	6:F:37:ALA:N	2.76	0.43
8:H:80:GLN:HB3	37:H:2563:HOH:O	2.19	0.43
10:J:50:VAL:HA	10:J:157:ILE:HG12	2.00	0.43
14:N:37:VAL:HG21	14:N:108:LYS:HG3	2.01	0.43
15:O:66:LEU:HD12	15:O:66:LEU:HA	1.92	0.43
15:O:71:TRP:CE3	15:O:175:LEU:CD2	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:129:ILE:HA	15:O:130:PRO:HD3	1.93	0.43
1:A:192:A:N6	1:A:194:A:C2	2.87	0.43
1:A:542:A:C8	1:A:542:A:C5'	2.98	0.43
1:A:1021:G:O2'	1:A:1022:A:H5'	2.18	0.43
1:A:1023:C:H2'	1:A:1024:G:O4'	2.19	0.43
1:A:1235:G:C1'	11:K:63:ILE:HG23	2.49	0.43
1:A:1543:G:N1	1:A:1641:A:OP2	2.40	0.43
2:B:3039:U:H3'	2:B:3040:C:H5''	2.00	0.43
2:B:3057:A:N3	2:B:3057:A:H5'	2.33	0.43
3:C:101:GLU:HG2	3:C:131:HIS:ND1	2.34	0.43
3:C:217:ARG:HH11	3:C:217:ARG:CG	2.30	0.43
3:C:223:ARG:NH1	37:C:8518:HOH:O	2.50	0.43
4:D:11:LEU:HA	37:D:8614:HOH:O	2.18	0.43
4:D:41:PHE:N	37:D:8647:HOH:O	2.52	0.43
4:D:279:THR:HG22	4:D:280:VAL:N	2.33	0.43
6:F:48:MET:HE2	6:F:48:MET:HB3	1.96	0.43
8:H:113:ASP:O	8:H:117:GLU:HG3	2.19	0.43
10:J:95:GLU:HB3	10:J:119:VAL:HG11	2.01	0.43
13:M:30:ARG:NH1	37:M:8511:HOH:O	2.42	0.43
18:R:77:ASP:N	18:R:80:LYS:O	2.52	0.43
27:1:30:GLU:O	27:1:33:HIS:HB3	2.18	0.43
1:A:100:C:H4'	21:U:16:LEU:HB2	2.01	0.42
1:A:818:A:C2	27:1:13:ARG:HA	2.54	0.42
1:A:1137:G:H1'	37:A:3851:HOH:O	2.19	0.42
1:A:1513:C:O2'	1:A:1514:C:H5'	2.18	0.42
1:A:2656:G:C2'	1:A:2657:G:H5'	2.48	0.42
2:B:3078:G:O2'	2:B:3079:U:P	2.77	0.42
4:D:23:THR:CG2	4:D:162:MET:HE3	2.49	0.42
5:E:14:GLY:N	37:E:8446:HOH:O	2.52	0.42
6:F:17:ARG:NH2	37:F:3723:HOH:O	2.40	0.42
9:I:12:ILE:O	9:I:13:PRO:C	2.61	0.42
10:J:136:VAL:HG22	10:J:137:ASN:N	2.34	0.42
14:N:77:PHE:CE2	14:N:86:MET:HG2	2.53	0.42
20:T:57:THR:CG2	20:T:59:ASP:HB2	2.49	0.42
22:V:49:LEU:O	22:V:55:ALA:CB	2.67	0.42
24:X:6:GLN:HA	24:X:52:VAL:HG23	2.00	0.42
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.18	0.42
24:X:90:TYR:N	37:X:6679:HOH:O	2.52	0.42
1:A:164:G:C6	1:A:165:A:C5	3.06	0.42
1:A:1717:A:H5''	17:Q:54:LYS:HB2	2.01	0.42
1:A:1746:A:N3	1:A:1748:U:C4	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1947:G:N2	1:A:1966:U:O2	2.51	0.42
2:B:3006:C:P	15:O:37:ARG:HH11	2.42	0.42
3:C:55:VAL:CG1	3:C:67:LEU:HD22	2.49	0.42
4:D:129:ARG:NH2	4:D:176:ASP:OD1	2.51	0.42
4:D:254:GLN:HG2	4:D:255:GLY:H	1.83	0.42
5:E:98:ARG:NH1	37:E:8358:HOH:O	2.45	0.42
11:K:88:PRO:HA	34:K:8502:CL:CL	2.55	0.42
12:L:103:ASP:O	12:L:104:PRO:C	2.60	0.42
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.97	0.42
19:S:61:GLN:CD	37:S:8540:HOH:O	2.62	0.42
23:W:12:THR:O	23:W:15:GLU:N	2.51	0.42
1:A:29:C:O2'	1:A:30:U:H5'	2.19	0.42
1:A:120:A:OP1	28:2:32:LYS:NZ	2.47	0.42
1:A:407:A:C2	1:A:408:A:C4	3.07	0.42
1:A:1123:A:C2	1:A:1129:C:H4'	2.54	0.42
1:A:1532:G:C6	1:A:1533:A:C6	3.08	0.42
1:A:1701:A:H5''	1:A:1702:U:H3'	2.01	0.42
1:A:1733:A:C6	1:A:1734:C:C2	3.07	0.42
1:A:1773:G:C2'	1:A:1774:G:H5'	2.49	0.42
1:A:2113:G:C6	1:A:2114:C:C4	3.07	0.42
1:A:2481:G:C3'	1:A:2482:G:H5''	2.49	0.42
1:A:2833:C:O2	1:A:2848:G:C2	2.72	0.42
2:B:3003:A:H2'	37:B:2430:HOH:O	2.19	0.42
3:C:81:GLN:CB	3:C:92:ASN:ND2	2.81	0.42
4:D:84:LEU:O	4:D:84:LEU:HD13	2.19	0.42
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.81	0.42
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.49	0.42
7:G:20:ILE:O	7:G:30:THR:HA	2.19	0.42
12:L:22:ASP:C	12:L:22:ASP:OD1	2.62	0.42
14:N:18:GLY:O	14:N:21:ALA:HB3	2.20	0.42
14:N:191:GLY:O	14:N:192:ALA:HB3	2.17	0.42
16:P:60:VAL:C	16:P:62:GLY:H	2.28	0.42
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.48	0.42
24:X:122:ARG:HG3	24:X:152:ALA:O	2.20	0.42
1:A:23:G:C6	1:A:24:G:N1	2.88	0.42
1:A:585:C:H6	37:A:6075:HOH:O	2.01	0.42
1:A:1573:A:H2'	1:A:1574:C:O4'	2.19	0.42
1:A:1804:A:H2'	1:A:1805:G:H8	1.84	0.42
1:A:1862:C:O2'	1:A:1863:G:H5'	2.20	0.42
1:A:2405:C:H5'	37:A:6578:HOH:O	2.18	0.42
1:A:2432:C:C4'	37:A:9716:HOH:O	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2637:A:C4'	37:A:4335:HOH:O	2.67	0.42
1:A:2656:G:O2'	1:A:2657:G:H5'	2.18	0.42
3:C:170:VAL:HG13	27:1:22:ILE:HG21	2.01	0.42
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.55	0.42
7:G:137:ASP:OD1	7:G:139:GLU:HB2	2.19	0.42
10:J:150:LYS:HA	10:J:153:VAL:CG2	2.49	0.42
21:U:38:ARG:HH11	21:U:38:ARG:HG3	1.83	0.42
25:Y:25:ARG:CD	37:Y:3861:HOH:O	2.47	0.42
28:2:19:CYS:SG	28:2:21:ARG:N	2.93	0.42
1:A:80:A:H3'	21:U:43:ASN:OD1	2.18	0.42
1:A:380:A:OP2	14:N:9:ARG:HD2	2.20	0.42
1:A:661:G:C6	1:A:686:A:C2	3.08	0.42
1:A:911:G:H5'	1:A:932:U:OP1	2.19	0.42
1:A:1215:A:O3'	1:A:1216:G:H4'	2.19	0.42
1:A:1253:C:H5'	37:A:7728:HOH:O	2.19	0.42
1:A:1459:A:OP2	37:A:9229:HOH:O	2.22	0.42
1:A:1506:U:H6	1:A:1506:U:H5'	1.85	0.42
1:A:1751:G:C3'	1:A:1752:G:H5''	2.49	0.42
1:A:1863:G:OP2	37:A:3122:HOH:O	2.22	0.42
1:A:2121:G:C2'	1:A:2122:C:H5'	2.50	0.42
1:A:2769:C:H2'	1:A:2770:G:C5'	2.49	0.42
4:D:307:ARG:HH11	4:D:307:ARG:HG3	1.83	0.42
15:O:47:LEU:HD23	15:O:47:LEU:HA	1.79	0.42
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.82	0.42
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.49	0.42
23:W:45:ARG:C	23:W:47:LYS:N	2.76	0.42
1:A:69:A:C2'	1:A:70:A:OP2	2.68	0.42
1:A:168:C:C2'	1:A:169:A:H5'	2.49	0.42
1:A:370:G:O2'	1:A:371:U:H5'	2.20	0.42
1:A:492:C:C2'	1:A:493:U:H5'	2.49	0.42
1:A:666:A:H2'	1:A:667:C:O4'	2.20	0.42
1:A:736:A:H2'	1:A:737:A:O4'	2.19	0.42
1:A:1166:A:N3	1:A:1166:A:H2'	2.34	0.42
1:A:2079:G:C6	1:A:2080:G:C5	3.08	0.42
1:A:2387:U:H2'	1:A:2388:C:C6	2.54	0.42
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.53	0.42
1:A:2812:A:C2	1:A:2814:A:N6	2.75	0.42
2:B:3012:C:H5'	2:B:3070:U:O4'	2.20	0.42
4:D:16:ARG:NE	37:D:8553:HOH:O	2.19	0.42
4:D:162:MET:CE	4:D:310:ARG:HD3	2.41	0.42
4:D:168:GLY:H	4:D:174:ARG:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:24:HIS:HB2	6:F:72:LYS:CB	2.50	0.42
6:F:64:ARG:HD3	6:F:67:ASP:HB3	2.02	0.42
10:J:47:GLU:HG2	10:J:133:ILE:HD12	2.00	0.42
10:J:137:ASN:O	10:J:138:PRO:C	2.62	0.42
12:L:99:ASP:C	12:L:99:ASP:OD1	2.62	0.42
15:O:38:LYS:HE3	15:O:38:LYS:HB2	1.71	0.42
24:X:122:ARG:CZ	37:X:5817:HOH:O	2.67	0.42
26:Z:112:GLU:OE1	26:Z:115:ARG:NH1	2.52	0.42
1:A:581:G:H5'	37:A:7679:HOH:O	2.20	0.42
1:A:710:G:N2	1:A:719:C:C2	2.88	0.42
1:A:1123:A:N6	1:A:1238:C:H5'	2.33	0.42
1:A:1211:G:O2'	1:A:1212:C:H5'	2.19	0.42
1:A:2833:C:C2	1:A:2848:G:C2	3.08	0.42
1:A:2909:G:H2'	1:A:2910:A:H8	1.84	0.42
4:D:277:GLU:N	4:D:278:PRO:HD2	2.34	0.42
7:G:11:VAL:HG13	7:G:23:GLU:O	2.18	0.42
8:H:26:THR:HB	8:H:102:GLY:C	2.45	0.42
10:J:55:GLN:HE21	10:J:124:ARG:NE	2.08	0.42
12:L:37:TYR:CE2	12:L:45:PRO:HA	2.55	0.42
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.19	0.42
14:N:186:SER:OG	14:N:189:VAL:CG1	2.67	0.42
15:O:86:LEU:O	15:O:90:LEU:HG	2.18	0.42
26:Z:101:GLY:HA3	37:Z:8561:HOH:O	2.20	0.42
30:4:7:PHE:CE2	30:4:22:VAL:CG2	3.00	0.42
1:A:177:A:C8	1:A:178:U:C5	3.07	0.42
1:A:394:G:HO2'	1:A:395:A:H8	1.63	0.42
1:A:472:A:N1	1:A:888:U:O2'	2.49	0.42
1:A:752:G:O6	37:A:4299:HOH:O	2.22	0.42
1:A:1163:G:H3'	1:A:1164:U:H2'	2.02	0.42
1:A:1191:A:C2	1:A:1207:A:C2	3.08	0.42
1:A:1886:A:H4'	37:1:8405:HOH:O	2.19	0.42
1:A:1934:A:C8	1:A:1935:C:C5	3.07	0.42
1:A:2432:C:C2'	1:A:2433:A:H5'	2.50	0.42
1:A:2883:A:H2'	1:A:2884:G:O4'	2.20	0.42
37:A:4546:HOH:O	14:N:83:SER:HA	2.19	0.42
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.31	0.42
2:B:3078:G:N2	2:B:3102:G:H2'	2.34	0.42
3:C:123:GLY:HA3	3:C:162:GLY:HA2	2.01	0.42
4:D:60:SER:C	4:D:62:ARG:H	2.27	0.42
4:D:101:TRP:HB2	4:D:119:HIS:CD2	2.55	0.42
5:E:107:ARG:HB3	5:E:107:ARG:CZ	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:SER:HA	37:E:8381:HOH:O	2.19	0.42
6:F:10:PHE:CE1	6:F:11:HIS:HB3	2.54	0.42
6:F:173:GLU:HG3	6:F:174:VAL:N	2.35	0.42
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.55	0.42
17:Q:120:ARG:NH2	17:Q:123:TYR:HD2	2.12	0.42
24:X:88:THR:HG23	24:X:110:GLN:HB3	2.02	0.42
29:3:19:SER:O	29:3:36:ASN:ND2	2.53	0.42
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.34	0.42
1:A:25:A:C2'	1:A:26:U:H5'	2.50	0.42
1:A:218:C:P	30:4:39:GLN:HE21	2.42	0.42
1:A:724:G:O2'	1:A:725:C:H5'	2.20	0.42
1:A:1185:U:O4'	37:A:7456:HOH:O	2.21	0.42
1:A:1299:G:N7	13:M:6:ARG:NH1	2.67	0.42
1:A:1400:C:O2'	1:A:1401:G:H5'	2.20	0.42
1:A:1483:C:O2'	1:A:1484:G:H5'	2.20	0.42
1:A:1692:C:H1'	37:A:9450:HOH:O	2.19	0.42
1:A:2012:U:H2'	1:A:2013:G:OP1	2.19	0.42
1:A:2501:G:O2'	10:J:151:MET:HE2	2.20	0.42
1:A:2531:U:O2'	1:A:2532:A:H5'	2.19	0.42
1:A:2897:C:O2'	1:A:2898:G:H5'	2.20	0.42
37:A:3731:HOH:O	21:U:9:LYS:HD3	2.18	0.42
2:B:3030:C:OP1	6:F:137:PRO:O	2.37	0.42
2:B:3040:C:N4	6:F:51:ARG:HB2	2.34	0.42
3:C:69:LEU:CD2	3:C:120:ARG:HB3	2.44	0.42
4:D:16:ARG:NH1	37:D:8614:HOH:O	2.53	0.42
4:D:215:VAL:HB	4:D:234:ARG:NH1	2.34	0.42
4:D:248:ARG:NH2	37:D:8522:HOH:O	2.52	0.42
5:E:27:ARG:CG	5:E:29:ASP:OD1	2.63	0.42
12:L:14:LYS:CB	12:L:45:PRO:HG2	2.45	0.42
13:M:145:LEU:O	13:M:145:LEU:HD23	2.20	0.42
22:V:49:LEU:CD1	37:V:3805:HOH:O	2.68	0.42
1:A:818:A:H5''	37:A:6570:HOH:O	2.20	0.42
1:A:827:A:H2'	1:A:828:G:O4'	2.19	0.42
1:A:841:A:OP2	19:S:128:ARG:HD2	2.20	0.42
1:A:889:C:H2'	1:A:890:C:C6	2.55	0.42
1:A:1773:G:O2'	27:1:15:GLY:HA2	2.20	0.42
1:A:2415:A:C2	15:O:25:ARG:CB	3.03	0.42
37:A:7050:HOH:O	19:S:33:ARG:HD3	2.20	0.42
2:B:3026:C:O2'	2:B:3027:C:H5'	2.20	0.42
7:G:5:LEU:HD21	7:G:66:GLN:HG3	2.02	0.42
7:G:23:GLU:HG2	7:G:28:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:81:GLU:HA	7:G:133:VAL:O	2.19	0.42
8:H:33:THR:HG21	8:H:59:ILE:O	2.19	0.42
9:I:64:ASN:N	9:I:64:ASN:ND2	2.67	0.42
10:J:111:MET:O	10:J:114:PRO:HD3	2.20	0.42
12:L:6:ALA:HB3	12:L:116:GLU:HG2	2.01	0.42
12:L:118:ALA:HA	12:L:125:ALA:HB2	2.02	0.42
15:O:39:SER:HB3	15:O:42:HIS:H	1.85	0.42
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.48	0.42
27:1:47:LEU:HA	27:1:56:MET:O	2.20	0.42
30:4:62:THR:HG23	30:4:86:GLY:HA2	2.02	0.42
1:A:201:G:N1	1:A:202:U:C4	2.88	0.41
1:A:217:C:OP1	1:A:395:A:O2'	2.36	0.41
1:A:825:U:H5''	1:A:826:U:OP1	2.20	0.41
1:A:1098:A:H2'	1:A:1099:G:O4'	2.20	0.41
1:A:1469:C:N3	1:A:1472:C:OP2	2.53	0.41
1:A:2044:G:OP1	25:Y:23:HIS:CE1	2.69	0.41
1:A:2379:G:N7	1:A:2408:A:N1	2.67	0.41
1:A:2443:C:O3'	13:M:56:LYS:HE3	2.20	0.41
1:A:2869:G:H2'	1:A:2870:C:C6	2.55	0.41
2:B:3039:U:HO2'	2:B:3042:C:H5	1.58	0.41
3:C:51:ARG:HB2	37:C:8609:HOH:O	2.19	0.41
3:C:88:ILE:CD1	3:C:100:PRO:HD3	2.39	0.41
4:D:17:LYS:O	4:D:260:HIS:HD2	2.03	0.41
6:F:57:THR:HA	6:F:63:ILE:HA	2.01	0.41
8:H:60:VAL:O	8:H:61:MET:C	2.63	0.41
10:J:154:THR:HB	10:J:155:PRO:CD	2.50	0.41
12:L:78:LYS:HA	12:L:79:PRO:HD3	1.85	0.41
13:M:54:PRO:HG2	13:M:57:VAL:HG21	2.01	0.41
13:M:98:GLU:O	13:M:99:GLU:HB2	2.20	0.41
13:M:148:GLU:CG	37:M:8558:HOH:O	2.67	0.41
14:N:98:GLN:O	14:N:101:ALA:HB3	2.19	0.41
15:O:38:LYS:HE2	15:O:107:ASN:ND2	2.34	0.41
15:O:184:ILE:HG22	15:O:185:GLU:N	2.33	0.41
24:X:38:THR:O	24:X:42:ARG:HB2	2.20	0.41
30:4:87:ARG:HD2	37:4:8528:HOH:O	2.21	0.41
1:A:315:G:C6	1:A:316:A:C6	3.08	0.41
1:A:593:A:N7	37:A:4369:HOH:O	2.52	0.41
37:A:5662:HOH:O	15:O:21:HIS:HE1	2.04	0.41
3:C:186:TRP:CG	3:C:187:PRO:HA	2.55	0.41
4:D:307:ARG:NH1	4:D:307:ARG:HG3	2.35	0.41
5:E:102:LEU:HD12	37:E:8315:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:23:VAL:HG12	6:F:130:VAL:HG22	2.01	0.41
7:G:138:ILE:HG22	37:G:5404:HOH:O	2.19	0.41
23:W:1:THR:C	23:W:3:LEU:N	2.78	0.41
25:Y:74:ALA:HB2	25:Y:85:VAL:HG13	2.01	0.41
1:A:99:A:H3'	1:A:100:C:C6	2.56	0.41
1:A:517:U:C2'	1:A:518:G:H5'	2.50	0.41
1:A:1014:A:H2'	1:A:1015:C:H5'	2.02	0.41
4:D:150:ALA:O	4:D:152:PRO:HD3	2.20	0.41
6:F:167:GLU:C	6:F:169:THR:H	2.28	0.41
10:J:56:ILE:HG21	10:J:61:LEU:HD13	2.02	0.41
12:L:98:VAL:HG13	12:L:99:ASP:O	2.21	0.41
13:M:64:ILE:O	13:M:64:ILE:HG23	2.19	0.41
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.50	0.41
15:O:132:ASN:O	15:O:135:VAL:HG12	2.20	0.41
16:P:39:THR:HB	37:P:3360:HOH:O	2.19	0.41
16:P:113:VAL:O	16:P:114:ILE:HD13	2.20	0.41
19:S:149:GLU:HA	19:S:150:PRO:HD3	1.92	0.41
21:U:96:VAL:HG13	21:U:97:ARG:N	2.36	0.41
22:V:6:CYS:C	22:V:8:TYR:H	2.28	0.41
26:Z:189:ASN:C	26:Z:189:ASN:ND2	2.78	0.41
29:3:40:ARG:HG2	29:3:40:ARG:NH1	2.35	0.41
1:A:159:G:H2'	1:A:175:G:H22	1.85	0.41
1:A:377:C:H5	37:A:3286:HOH:O	2.03	0.41
1:A:380:A:H5''	14:N:48:ARG:NH2	2.35	0.41
1:A:454:U:C2	37:A:9027:HOH:O	2.57	0.41
1:A:492:C:C2	1:A:501:G:N2	2.88	0.41
1:A:711:G:C2	1:A:718:C:C2	3.08	0.41
1:A:1846:U:H2'	1:A:1847:A:C4	2.56	0.41
1:A:1943:C:O4'	3:C:212:PRO:HA	2.19	0.41
37:A:4806:HOH:O	11:K:47:THR:CB	2.64	0.41
3:C:135:VAL:N	37:C:8600:HOH:O	2.52	0.41
6:F:44:ILE:HG12	6:F:83:PHE:CE1	2.52	0.41
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.50	0.41
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.55	0.41
10:J:26:LYS:HE3	10:J:28:ILE:HB	2.02	0.41
12:L:4:LEU:HD22	12:L:116:GLU:HB3	2.02	0.41
14:N:173:LEU:HA	14:N:183:VAL:HG11	2.03	0.41
19:S:61:GLN:NE2	37:S:8540:HOH:O	2.54	0.41
22:V:38:ASN:O	22:V:42:LEU:HG	2.20	0.41
23:W:12:THR:HG23	23:W:14:ALA:N	2.36	0.41
1:A:79:G:H22	1:A:97:G:H1'	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:U:H2'	1:A:124:C:C6	2.56	0.41
1:A:654:A:OP2	16:P:38:ARG:HD3	2.20	0.41
1:A:695:C:H2'	1:A:696:C:C6	2.55	0.41
1:A:1132:A:H2'	1:A:1133:A:C8	2.55	0.41
1:A:1305:C:O2'	1:A:1306:U:H5'	2.19	0.41
1:A:1609:C:H2'	1:A:1610:G:C8	2.56	0.41
1:A:1969:A:O2'	1:A:1970:G:H5'	2.20	0.41
1:A:1992:U:C2	1:A:1994:A:OP2	2.74	0.41
1:A:2488:A:H1'	37:A:9092:HOH:O	2.20	0.41
1:A:2767:C:OP1	4:D:318:ASN:ND2	2.53	0.41
1:A:2836:G:C6	1:A:2838:A:C2	3.08	0.41
2:B:3057:A:H8	6:F:141:VAL:HG21	1.85	0.41
5:E:154:VAL:O	5:E:158:GLU:HG3	2.20	0.41
10:J:84:ARG:NH2	10:J:135:TRP:CH2	2.82	0.41
10:J:86:ARG:H	10:J:86:ARG:HG2	1.63	0.41
17:Q:13:VAL:HG11	17:Q:40:VAL:HG12	2.03	0.41
23:W:42:ASN:N	23:W:43:PRO:HD3	2.35	0.41
24:X:110:GLN:NE2	24:X:110:GLN:CA	2.69	0.41
25:Y:9:VAL:HG22	25:Y:88:GLU:OE2	2.20	0.41
26:Z:235:GLU:CD	26:Z:235:GLU:N	2.73	0.41
27:1:30:GLU:C	27:1:33:HIS:HB3	2.45	0.41
1:A:107:U:H2'	1:A:108:U:H5'	2.02	0.41
1:A:168:C:H6	1:A:168:C:O5'	2.03	0.41
1:A:644:G:N3	1:A:644:G:H5'	2.35	0.41
1:A:682:A:H2'	1:A:683:G:O4'	2.21	0.41
1:A:790:A:H1'	1:A:1710:A:O2'	2.21	0.41
1:A:2251:G:H4'	37:A:7398:HOH:O	2.21	0.41
1:A:2252:A:C5	1:A:2253:G:H1'	2.55	0.41
1:A:2435:U:H1'	37:A:5404:HOH:O	2.19	0.41
1:A:2505:G:C2'	1:A:2506:A:H5'	2.50	0.41
1:A:2570:G:H5''	37:A:4885:HOH:O	2.20	0.41
37:A:9678:HOH:O	4:D:254:GLN:HG3	2.19	0.41
3:C:51:ARG:CZ	37:C:8609:HOH:O	2.68	0.41
4:D:7:ARG:HH11	4:D:7:ARG:CG	2.25	0.41
4:D:7:ARG:NH1	4:D:7:ARG:CG	2.81	0.41
4:D:105:PHE:CD1	4:D:115:VAL:HG11	2.56	0.41
5:E:57:PRO:O	5:E:58:ALA:C	2.63	0.41
5:E:196:THR:HG23	37:E:8400:HOH:O	2.20	0.41
6:F:52:THR:N	6:F:70:GLY:O	2.53	0.41
10:J:82:LYS:NZ	10:J:82:LYS:CB	2.84	0.41
12:L:118:ALA:C	12:L:120:ARG:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:52:LEU:HD13	14:N:116:ASN:CG	2.45	0.41
15:O:154:LEU:C	15:O:156:GLU:H	2.26	0.41
16:P:98:LEU:O	16:P:102:ILE:HG13	2.20	0.41
19:S:119:VAL:O	19:S:119:VAL:CG1	2.68	0.41
21:U:16:LEU:HD23	21:U:16:LEU:HA	1.85	0.41
24:X:73:LEU:HD12	24:X:73:LEU:HA	1.90	0.41
24:X:122:ARG:NH1	24:X:152:ALA:O	2.54	0.41
27:1:42:CYS:HG	27:1:44:PHE:HB2	1.82	0.41
1:A:90:A:H2'	1:A:91:G:O4'	2.21	0.41
1:A:470:U:H2'	1:A:471:G:O4'	2.21	0.41
1:A:805:G:O2'	1:A:807:A:N7	2.51	0.41
1:A:1789:G:O6	17:Q:73:HIS:HE1	2.04	0.41
1:A:2434:A:O3'	30:4:28:GLY:CA	2.63	0.41
37:A:5876:HOH:O	3:C:185:LYS:HE2	2.20	0.41
37:A:9657:HOH:O	26:Z:163:THR:HG23	2.21	0.41
3:C:53:ALA:HB1	3:C:54:PRO:HD2	2.02	0.41
4:D:189:ALA:HB1	37:D:8564:HOH:O	2.20	0.41
4:D:312:ARG:HG2	4:D:313:PRO:N	2.33	0.41
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.50	0.41
7:G:9:GLU:HG3	7:G:10:ASP:N	2.36	0.41
8:H:34:ASN:HA	14:N:4:ALA:HB2	2.03	0.41
10:J:30:GLN:H	10:J:65:ARG:NH1	2.18	0.41
10:J:165:GLY:C	10:J:166:ASN:HD22	2.27	0.41
12:L:90:PHE:N	12:L:90:PHE:CD1	2.89	0.41
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.51	0.41
14:N:74:ARG:O	14:N:88:VAL:HG13	2.20	0.41
15:O:74:PRO:HG2	15:O:159:TYR:CZ	2.56	0.41
21:U:48:VAL:CG1	21:U:96:VAL:HG13	2.51	0.41
25:Y:9:VAL:HG13	25:Y:88:GLU:CD	2.45	0.41
25:Y:70:ILE:O	25:Y:70:ILE:HG23	2.20	0.41
28:2:10:LYS:CB	37:2:2979:HOH:O	2.68	0.41
1:A:177:A:H2'	1:A:178:U:O4'	2.21	0.41
1:A:331:A:H1'	37:A:4765:HOH:O	2.19	0.41
1:A:396:U:H5'	30:4:42:ARG:NH1	2.35	0.41
1:A:904:U:O2	1:A:1354:G:H3'	2.20	0.41
1:A:1188:A:C5	1:A:1189:A:C2	3.09	0.41
1:A:1951:G:N2	37:A:6241:HOH:O	2.52	0.41
1:A:1973:A:H5'	1:A:1973:A:H8	1.85	0.41
1:A:2011:A:O4'	1:A:2013:G:C8	2.74	0.41
1:A:2094:G:H4'	4:D:245:SER:CB	2.50	0.41
1:A:2363:G:O2'	18:R:11:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2397:G:C5	1:A:2465:A:C6	3.09	0.41
1:A:2896:A:OP1	25:Y:15:ARG:NH1	2.54	0.41
3:C:130:THR:HG22	3:C:131:HIS:O	2.20	0.41
4:D:84:LEU:HD13	4:D:84:LEU:C	2.46	0.41
4:D:313:PRO:O	4:D:314:ALA:C	2.64	0.41
7:G:11:VAL:HG11	7:G:22:VAL:CG1	2.51	0.41
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.53	0.41
17:Q:125:LYS:NZ	17:Q:140:TYR:OH	2.46	0.41
24:X:85:ALA:HB2	24:X:91:ASP:O	2.21	0.41
1:A:74:A:H2'	1:A:75:U:C6	2.56	0.41
1:A:314:G:N2	1:A:316:A:H3'	2.36	0.41
1:A:485:A:H4'	1:A:486:A:OP1	2.21	0.41
1:A:553:G:O4'	1:A:1325:G:H5'	2.20	0.41
1:A:814:G:H8	37:A:7194:HOH:O	2.02	0.41
1:A:860:U:H2'	1:A:861:A:C8	2.56	0.41
1:A:1103:C:O2'	11:K:86:MET:HB3	2.21	0.41
1:A:1352:A:P	5:E:92:PRO:HG3	2.61	0.41
1:A:1545:C:H2'	1:A:1546:G:O4'	2.21	0.41
1:A:1684:A:O2'	1:A:1685:A:H5''	2.21	0.41
1:A:1815:A:H2'	1:A:1816:C:O4'	2.21	0.41
1:A:1840:A:H4'	1:A:1841:C:O5'	2.21	0.41
1:A:1882:C:O2'	1:A:2012:U:OP2	2.31	0.41
1:A:2012:U:C2'	1:A:2013:G:OP1	2.69	0.41
1:A:2072:G:C6	1:A:2533:C:H1'	2.56	0.41
1:A:2453:G:H3'	37:A:5897:HOH:O	2.20	0.41
2:B:3004:G:O2'	15:O:44:ARG:NH2	2.54	0.41
2:B:3014:G:H2'	2:B:3015:C:C5'	2.51	0.41
3:C:19:PRO:HD3	37:C:8604:HOH:O	2.21	0.41
3:C:30:ARG:HE	3:C:30:ARG:HB3	1.68	0.41
3:C:55:VAL:HG11	3:C:67:LEU:HD13	2.02	0.41
3:C:114:ASP:HB2	3:C:117:LYS:HE2	2.02	0.41
4:D:55:ASN:HB3	4:D:64:GLY:N	2.35	0.41
4:D:60:SER:C	4:D:62:ARG:N	2.78	0.41
4:D:185:GLY:HA2	37:D:8633:HOH:O	2.21	0.41
4:D:279:THR:OG1	4:D:290:VAL:HB	2.21	0.41
4:D:321:PRO:HG3	37:D:8597:HOH:O	2.20	0.41
5:E:25:PRO:HG2	37:E:8322:HOH:O	2.20	0.41
6:F:64:ARG:HG2	6:F:66:GLY:O	2.21	0.41
7:G:156:ASP:OD2	7:G:157:LYS:NZ	2.42	0.41
8:H:32:GLY:N	37:H:3111:HOH:O	2.53	0.41
8:H:58:GLU:HG3	8:H:61:MET:CE	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:65:THR:O	9:I:69:ARG:HB2	2.20	0.41
9:I:66:LEU:O	9:I:69:ARG:HB3	2.21	0.41
11:K:74:ARG:NH1	11:K:76:ASP:HB2	2.35	0.41
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.03	0.41
15:O:73:ALA:HB1	15:O:74:PRO:HD2	2.02	0.41
15:O:86:LEU:HD12	15:O:125:ALA:CB	2.42	0.41
15:O:110:THR:HA	15:O:111:PRO:HD3	1.95	0.41
16:P:105:ASN:O	16:P:105:ASN:CG	2.64	0.41
20:T:69:SER:C	20:T:71:ASP:N	2.79	0.41
21:U:71:VAL:CG1	21:U:72:ILE:N	2.83	0.41
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.21	0.41
24:X:21:LEU:HB3	24:X:26:ILE:HG12	2.03	0.41
30:4:74:CYS:SG	30:4:76:LYS:HD2	2.61	0.41
1:A:746:A:N6	16:P:65:LEU:HD13	2.36	0.41
1:A:932:U:O2'	1:A:1296:A:H1'	2.21	0.41
1:A:1234:U:C4	4:D:244:PRO:HB3	2.56	0.41
1:A:1304:U:H2'	1:A:1305:C:C6	2.56	0.41
1:A:1444:G:O2'	1:A:1502:A:N1	2.46	0.41
1:A:1641:A:C2'	1:A:1642:A:H5'	2.50	0.41
1:A:1973:A:H2'	1:A:1974:G:O4'	2.21	0.41
1:A:2325:C:H2'	1:A:2326:U:C6	2.56	0.41
1:A:2781:U:H2'	1:A:2782:G:H5'	2.03	0.41
1:A:2793:A:H2'	37:A:4464:HOH:O	2.19	0.41
3:C:83:GLY:O	3:C:94:LEU:HB3	2.20	0.41
4:D:102:THR:HG23	4:D:182:VAL:CG1	2.51	0.41
4:D:275:GLY:C	4:D:291:ASP:HA	2.46	0.41
5:E:78:ARG:HH11	5:E:78:ARG:CG	2.27	0.41
6:F:25:MET:SD	6:F:40:ILE:HD11	2.61	0.41
7:G:102:VAL:HG11	7:G:148:ILE:HD11	2.02	0.41
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.51	0.41
7:G:149:GLU:OE1	7:G:168:ILE:HG12	2.21	0.41
8:H:59:ILE:O	8:H:59:ILE:CG2	2.69	0.41
10:J:139:ASP:O	10:J:139:ASP:CG	2.63	0.41
14:N:5:TYR:C	14:N:7:TYR:N	2.79	0.41
15:O:50:LEU:HD12	15:O:50:LEU:HA	1.80	0.41
16:P:32:ARG:HD3	16:P:32:ARG:C	2.45	0.41
20:T:69:SER:C	20:T:71:ASP:H	2.29	0.41
22:V:14:GLU:OE1	22:V:15:PRO:CD	2.65	0.41
24:X:5:VAL:O	24:X:52:VAL:CG2	2.69	0.41
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.36	0.41
1:A:119:A:C2	1:A:122:C:C4	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:A:C5'	14:N:157:LEU:HD12	2.51	0.40
1:A:236:A:H2'	1:A:236:A:O5'	2.20	0.40
1:A:295:C:H2'	1:A:296:G:O4'	2.21	0.40
1:A:419:A:H1'	1:A:1921:A:C2	2.56	0.40
1:A:431:G:OP1	14:N:48:ARG:NH1	2.54	0.40
1:A:702:G:O2'	1:A:703:G:H5'	2.21	0.40
1:A:835:U:H3'	37:A:9360:HOH:O	2.21	0.40
1:A:1151:G:P	9:I:16:LYS:NZ	2.94	0.40
1:A:1877:G:C6	1:A:1878:G:C6	3.09	0.40
1:A:2073:G:C6	1:A:2607:U:C2	3.09	0.40
1:A:2107:U:O2'	1:A:2108:A:H5'	2.21	0.40
1:A:2300:A:C2	1:A:2306:U:C5	3.08	0.40
1:A:2389:U:H4'	18:R:53:HIS:CD2	2.56	0.40
3:C:100:PRO:HG2	3:C:103:VAL:CG2	2.49	0.40
3:C:179:MET:HG2	3:C:186:TRP:CG	2.56	0.40
6:F:169:THR:C	6:F:170:TYR:HD1	2.29	0.40
8:H:101:ALA:HA	37:H:5413:HOH:O	2.21	0.40
10:J:14:TYR:N	10:J:91:HIS:HE1	2.20	0.40
12:L:98:VAL:HG22	12:L:102:GLU:C	2.46	0.40
14:N:27:ARG:O	14:N:30:GLU:N	2.53	0.40
15:O:21:HIS:HB2	37:O:8532:HOH:O	2.22	0.40
16:P:22:GLY:CA	37:P:2823:HOH:O	2.69	0.40
17:Q:121:ASP:HB2	37:Q:5891:HOH:O	2.20	0.40
27:1:60:CYS:SG	27:1:62:TYR:HB2	2.61	0.40
1:A:10:U:HO2'	1:A:11:A:P	2.44	0.40
1:A:164:G:O6	1:A:165:A:C6	2.74	0.40
1:A:590:A:H2'	1:A:591:A:C5'	2.51	0.40
1:A:840:U:H2'	19:S:128:ARG:NH1	2.36	0.40
1:A:1159:G:H1	1:A:1208:C:H42	1.70	0.40
1:A:1291:A:H2	37:A:5266:HOH:O	2.05	0.40
1:A:1634:G:C3'	37:A:3866:HOH:O	2.53	0.40
1:A:1791:U:H2'	1:A:1792:C:C6	2.56	0.40
1:A:2071:C:H5'	37:A:9511:HOH:O	2.21	0.40
1:A:2780:C:C1'	7:G:143:GLN:NE2	2.83	0.40
1:A:2783:A:O2'	1:A:2784:A:H5'	2.20	0.40
1:A:2898:G:H4'	4:D:288:GLY:HA2	2.03	0.40
37:A:9744:HOH:O	13:M:41:HIS:HE1	2.04	0.40
3:C:1:GLY:HA2	3:C:197:VAL:HG23	2.03	0.40
4:D:234:ARG:NH1	37:D:8616:HOH:O	2.53	0.40
6:F:170:TYR:N	6:F:170:TYR:CD1	2.89	0.40
14:N:12:TRP:CE2	14:N:20:ILE:CD1	3.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:122:GLU:HB2	14:N:126:HIS:O	2.22	0.40
16:P:47:ARG:NH1	37:P:4564:HOH:O	2.54	0.40
17:Q:10:ALA:O	17:Q:13:VAL:HG12	2.21	0.40
17:Q:131:PHE:CE1	17:Q:137:LEU:HD13	2.56	0.40
21:U:105:ASP:OD1	21:U:107:LYS:N	2.54	0.40
24:X:101:LEU:HD23	24:X:101:LEU:HA	1.94	0.40
30:4:36:ILE:HD12	30:4:36:ILE:HA	1.95	0.40
1:A:154:C:H2'	1:A:155:C:C6	2.56	0.40
1:A:240:C:O2	1:A:240:C:H2'	2.22	0.40
1:A:638:C:H2'	1:A:639:A:C8	2.56	0.40
1:A:821:U:H2'	1:A:822:C:C6	2.49	0.40
1:A:1495:C:H1'	1:A:1573:A:H1'	2.03	0.40
1:A:1523:G:C6	1:A:1524:U:O4	2.74	0.40
1:A:2346:C:O3'	6:F:52:THR:CG2	2.69	0.40
1:A:2484:U:N3	37:A:9601:HOH:O	2.52	0.40
1:A:2729:C:H2'	1:A:2730:G:C8	2.48	0.40
1:A:2783:A:H2'	1:A:2784:A:C8	2.56	0.40
37:A:4945:HOH:O	10:J:57:ARG:HG3	2.21	0.40
3:C:153:ARG:HH11	3:C:153:ARG:CB	2.33	0.40
3:C:192:VAL:HG23	3:C:201:PHE:HB3	2.03	0.40
5:E:233:THR:HG22	5:E:234:VAL:H	1.84	0.40
7:G:119:HIS:HE1	7:G:147:ASP:OD2	2.05	0.40
8:H:21:GLU:HA	8:H:24:ARG:HE	1.85	0.40
12:L:32:ILE:O	12:L:33:SER:OG	2.39	0.40
21:U:24:ARG:HH21	21:U:39:ASN:ND2	2.20	0.40
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.83	0.40
1:A:187:A:H3'	1:A:188:C:C6	2.56	0.40
1:A:290:C:O2'	1:A:291:C:H5'	2.20	0.40
1:A:1336:U:C2	1:A:1337:A:C8	3.09	0.40
1:A:2044:G:C6	1:A:2045:G:C5	3.09	0.40
1:A:2377:U:H6	1:A:2377:U:O5'	2.04	0.40
1:A:2815:G:N7	11:K:80:LYS:NZ	2.66	0.40
1:A:2851:G:C2'	1:A:2852:A:H5'	2.52	0.40
37:A:4379:HOH:O	3:C:11:ARG:CZ	2.70	0.40
37:B:5071:HOH:O	15:O:20:TYR:HE2	1.98	0.40
3:C:36:ASP:HB2	3:C:84:VAL:N	2.37	0.40
4:D:57:GLU:HA	4:D:58:PRO:HD2	1.94	0.40
4:D:312:ARG:HD3	4:D:315:VAL:HG13	2.02	0.40
6:F:19:GLU:O	6:F:133:ASN:HB3	2.21	0.40
10:J:1:LYS:HA	10:J:2:PRO:HD3	1.72	0.40
10:J:113:ALA:N	10:J:114:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:13:GLU:O	12:L:14:LYS:C	2.64	0.40
14:N:85:ARG:CA	14:N:87:MET:HE2	2.47	0.40
27:1:81:LYS:O	27:1:82:ALA:C	2.64	0.40
27:1:81:LYS:HB2	27:1:82:ALA:H	1.76	0.40
1:A:440:C:O2'	1:A:441:A:H5'	2.21	0.40
1:A:1127:C:C5	1:A:1128:U:C4	3.09	0.40
1:A:1549:C:N3	1:A:1637:A:C2	2.89	0.40
1:A:1552:G:C2	1:A:1553:C:C2	3.10	0.40
1:A:2088:C:H1'	1:A:2841:A:C2	2.56	0.40
1:A:2379:G:H4'	1:A:2380:A:H5''	2.04	0.40
1:A:2588:G:H5''	1:A:2589:U:OP2	2.22	0.40
1:A:2782:G:O6	1:A:2790:C:H5''	2.21	0.40
37:A:5961:HOH:O	30:4:31:THR:HA	2.20	0.40
3:C:93:THR:HG23	3:C:154:ALA:O	2.22	0.40
37:D:8625:HOH:O	22:V:17:THR:HG21	2.22	0.40
7:G:149:GLU:HG3	7:G:166:VAL:O	2.21	0.40
10:J:65:ARG:NH2	10:J:66:VAL:HG22	2.37	0.40
11:K:40:ASN:OD1	11:K:106:GLY:HA2	2.22	0.40
11:K:51:GLU:O	11:K:55:GLU:HG3	2.21	0.40
11:K:70:PHE:CD2	11:K:70:PHE:O	2.74	0.40
11:K:71:TYR:CG	11:K:72:PRO:HD2	2.56	0.40
12:L:98:VAL:HG13	12:L:99:ASP:N	2.36	0.40
28:2:21:ARG:HD2	28:2:39:PHE:HB2	2.03	0.40
29:3:11:LEU:HD23	29:3:11:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	7 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	335/337 (99%)	304 (91%)	22 (7%)	9 (3%)	4	22
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	30	65
6	F	134/176 (76%)	93 (69%)	30 (22%)	11 (8%)	0	3
7	G	170/177 (96%)	159 (94%)	11 (6%)	0	100	100
8	H	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	7	32
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	131 (86%)	14 (9%)	7 (5%)	2	11
11	K	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	3	20
12	L	130/132 (98%)	119 (92%)	9 (7%)	2 (2%)	8	35
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	18	53
14	N	192/194 (99%)	173 (90%)	17 (9%)	2 (1%)	12	45
15	O	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	2	15
16	P	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	18	53
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	43
19	S	148/154 (96%)	139 (94%)	9 (6%)	0	100	100
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	14	48
22	V	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	3	18
24	X	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	9	38
25	Y	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	4	23
26	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	9	36
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	5	26
All	All	3633/4235 (86%)	3300 (91%)	271 (8%)	62 (2%)	7	32

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP

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Mol	Chain	Res	Type
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA
10	J	162	SER
10	J	164	ALA
13	M	80	ASP
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
23	W	43	PRO
24	X	77	ALA
3	C	34	ASP
3	C	37	VAL
4	D	34	GLY
4	D	169	GLY
4	D	184	ASP
6	F	11	HIS
6	F	20	LYS
6	F	137	PRO
11	K	5	GLU
11	K	143	LYS
12	L	119	GLN
17	Q	116	SER
30	4	57	GLY
3	C	132	ASP
6	F	16	PRO
6	F	171	ASP
8	H	64	PRO
10	J	40	PRO
10	J	138	PRO
11	K	7	ASP
14	N	140	ALA
15	O	162	ASP
15	O	181	ASP
24	X	49	ASN
27	1	81	LYS
30	4	56	PRO
3	C	119	ALA
10	J	72	VAL
11	K	76	ASP
12	L	126	SER

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Mol	Chain	Res	Type
14	N	165	SER
15	O	65	ASP
15	O	167	ASP
21	U	114	SER
25	Y	77	PHE
4	D	2	GLN
4	D	206	THR
5	E	232	LEU
6	F	60	GLU
6	F	147	ALA
6	F	170	TYR
10	J	128	ALA
18	R	54	PRO
23	W	40	PRO
4	D	107	SER
4	D	185	GLY
10	J	140	PRO
4	D	5	ARG
25	Y	70	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	168 (94%)	11 (6%)	17	49
4	D	282/282 (100%)	263 (93%)	19 (7%)	15	46
5	E	193/193 (100%)	178 (92%)	15 (8%)	11	39
6	F	117/147 (80%)	108 (92%)	9 (8%)	12	40
7	G	152/155 (98%)	148 (97%)	4 (3%)	40	72
8	H	92/92 (100%)	90 (98%)	2 (2%)	45	74
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	108 (88%)	14 (12%)	5	24
11	K	118/121 (98%)	110 (93%)	8 (7%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	106/106 (100%)	102 (96%)	4 (4%)	29	63
13	M	112/126 (89%)	109 (97%)	3 (3%)	39	71
14	N	166/166 (100%)	160 (96%)	6 (4%)	31	65
15	O	149/149 (100%)	141 (95%)	8 (5%)	20	53
16	P	93/93 (100%)	90 (97%)	3 (3%)	34	67
17	Q	113/116 (97%)	110 (97%)	3 (3%)	39	71
18	R	79/79 (100%)	75 (95%)	4 (5%)	21	55
19	S	117/121 (97%)	113 (97%)	4 (3%)	32	66
20	T	71/73 (97%)	70 (99%)	1 (1%)	59	80
21	U	105/105 (100%)	100 (95%)	5 (5%)	23	57
22	V	44/52 (85%)	43 (98%)	1 (2%)	44	74
23	W	51/56 (91%)	50 (98%)	1 (2%)	48	76
24	X	130/130 (100%)	120 (92%)	10 (8%)	12	40
25	Y	66/73 (90%)	62 (94%)	4 (6%)	17	49
26	Z	120/195 (62%)	112 (93%)	8 (7%)	15	46
27	1	56/56 (100%)	50 (89%)	6 (11%)	6	26
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	43	73
30	4	79/79 (100%)	73 (92%)	6 (8%)	12	41
All	All	3027/3441 (88%)	2867 (95%)	160 (5%)	20	54

All (160) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
4	D	7	ARG
4	D	11	LEU
4	D	27	ASN
4	D	33	ASP
4	D	63	GLU
4	D	84	LEU
4	D	97	LEU
4	D	98	THR
4	D	103	ASP
4	D	162	MET
4	D	175	LEU
4	D	195	ARG
4	D	251	VAL
4	D	254	GLN
4	D	256	GLN
4	D	264	GLU
4	D	304	PRO
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	57	PRO
5	E	67	GLN
5	E	78	ARG
5	E	94	THR
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
5	E	243	VAL
6	F	24	HIS
6	F	50	VAL
6	F	92	GLU
6	F	95	THR
6	F	99	ASP
6	F	131	THR
6	F	136	ARG
6	F	137	PRO

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Mol	Chain	Res	Type
6	F	149	ARG
7	G	7	ILE
7	G	54	ASP
7	G	86	VAL
7	G	102	VAL
8	H	12	LEU
8	H	46	GLU
10	J	1	LYS
10	J	18	GLU
10	J	30	GLN
10	J	59	ASN
10	J	61	LEU
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	85	ILE
10	J	86	ARG
10	J	93	ILE
10	J	142	VAL
10	J	150	LYS
10	J	166	ASN
11	K	46	ILE
11	K	52	GLN
11	K	74	ARG
11	K	93	ARG
11	K	120	SER
11	K	125	SER
11	K	127	ILE
11	K	131	THR
12	L	7	ASP
12	L	10	GLN
12	L	62	PRO
12	L	98	VAL
13	M	35	ARG
13	M	117	GLU
13	M	140	VAL
14	N	38	VAL
14	N	46	LEU
14	N	81	ARG
14	N	87	MET
14	N	93	ARG
14	N	164	THR

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Mol	Chain	Res	Type
15	O	17	ARG
15	O	26	LEU
15	O	43	VAL
15	O	47	LEU
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU
15	O	163	PHE
16	P	3	THR
16	P	98	LEU
16	P	111	VAL
17	Q	52	LYS
17	Q	91	LYS
17	Q	98	ILE
18	R	11	ARG
18	R	16	ASN
18	R	57	ASP
18	R	95	GLU
19	S	13	THR
19	S	39	THR
19	S	82	GLU
19	S	130	MET
20	T	10	VAL
21	U	26	THR
21	U	39	ASN
21	U	47	THR
21	U	48	VAL
21	U	96	VAL
22	V	9	CYS
23	W	43	PRO
24	X	4	LEU
24	X	26	ILE
24	X	35	VAL
24	X	52	VAL
24	X	73	LEU
24	X	120	PRO
24	X	122	ARG
24	X	142	ASP
24	X	146	ILE
24	X	154	ARG
25	Y	15	ARG
25	Y	27	ASP

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	29	HIS
3	C	47	HIS
3	C	92	ASN
3	C	127	GLN
3	C	199	HIS
4	D	27	ASN
4	D	94	GLN
4	D	145	HIS
4	D	221	GLN
4	D	238	ASN
4	D	260	HIS
4	D	318	ASN
5	E	2	GLN
5	E	39	GLN
5	E	129	HIS

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Mol	Chain	Res	Type
5	E	163	HIS
6	F	103	ASN
6	F	133	ASN
7	G	106	ASN
7	G	119	HIS
7	G	143	GLN
8	H	80	GLN
9	I	17	GLN
9	I	64	ASN
10	J	8	ASN
10	J	30	GLN
10	J	55	GLN
10	J	58	HIS
10	J	59	ASN
10	J	69	ASN
10	J	74	ASN
10	J	80	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	137	ASN
10	J	166	ASN
11	K	52	GLN
11	K	107	ASN
12	L	10	GLN
13	M	18	HIS
13	M	41	HIS
13	M	58	GLN
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	176	GLN
15	O	22	GLN
15	O	107	ASN
15	O	140	GLN
15	O	153	GLN
16	P	53	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN

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Mol	Chain	Res	Type
18	R	16	ASN
18	R	40	HIS
18	R	67	GLN
19	S	22	GLN
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN
19	S	113	HIS
19	S	117	HIS
19	S	140	GLN
20	T	25	GLN
20	T	51	GLN
20	T	53	ASN
20	T	55	GLN
21	U	39	ASN
21	U	73	HIS
22	V	39	ASN
23	W	4	HIS
23	W	60	GLN
24	X	6	GLN
24	X	28	HIS
24	X	87	HIS
24	X	110	GLN
24	X	119	HIS
24	X	125	HIS
24	X	141	HIS
25	Y	23	HIS
26	Z	133	HIS
26	Z	134	HIS
26	Z	149	GLN
26	Z	188	HIS
26	Z	189	ASN
27	1	33	HIS
28	2	8	GLN
28	2	16	HIS
28	2	28	HIS
29	3	16	ASN
29	3	18	ASN
29	3	37	HIS
29	3	41	HIS
29	3	45	ASN
30	4	30	GLN

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Mol	Chain	Res	Type
30	4	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	252 (9%)	33 (1%)
2	B	121/122 (99%)	18 (14%)	6 (4%)
All	All	2868/3044 (94%)	270 (9%)	39 (1%)

All (270) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1083	C
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1129	C
1	A	1130	U
1	A	1151	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

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Mol	Chain	Res	Type
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
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
1	A	1378	G
1	A	1407	A
1	A	1409	G
1	A	1451	C
1	A	1474	C
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

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Mol	Chain	Res	Type
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	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1943	C
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2004	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2097	G
1	A	2101	A
1	A	2102	G
1	A	2103	A
1	A	2110	G
1	A	2238	A
1	A	2258	A

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Mol	Chain	Res	Type
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2511	A
1	A	2526	C
1	A	2527	U
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G
1	A	2649	A
1	A	2650	U
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2718	C
1	A	2719	A
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C

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Mol	Chain	Res	Type
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3011	A
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3040	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 (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	716	G

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Mol	Chain	Res	Type
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	1080	C
1	A	1164	U
1	A	1237	U
1	A	1261	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1506	U
1	A	1563	G
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2102	G
1	A	2103	A
1	A	2313	C
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2791	U
2	B	3002	U
2	B	3023	U
2	B	3026	C
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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	TYK	A	9000	1	67,67,67	3.53	31 (46%)	87,97,97	2.33	26 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	TYK	A	9000	1	-	10/67/126/126	0/3/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	TYK	O1C-C1C	12.80	1.61	1.40
31	A	9000	TYK	O9-C9	10.56	1.37	1.22
31	A	9000	TYK	C22-C12	8.63	1.68	1.50
31	A	9000	TYK	C8-C9	7.34	1.62	1.51
31	A	9000	TYK	C4-C3	-6.66	1.41	1.54
31	A	9000	TYK	C7-C6	6.27	1.66	1.53
31	A	9000	TYK	C4A-C5A	5.61	1.62	1.52
31	A	9000	TYK	O4C-C4C	5.58	1.56	1.43
31	A	9000	TYK	C14-C15	5.34	1.63	1.54
31	A	9000	TYK	C6-C5	4.71	1.61	1.52
31	A	9000	TYK	C7-C8	4.60	1.65	1.54
31	A	9000	TYK	C19-C6	3.99	1.64	1.54
31	A	9000	TYK	C3C-C2C	3.53	1.59	1.52
31	A	9000	TYK	C23-C14	3.30	1.56	1.52
31	A	9000	TYK	C2-C3	-3.27	1.48	1.53
31	A	9000	TYK	C2B-C1B	3.24	1.58	1.51
31	A	9000	TYK	C1C-C2C	3.22	1.60	1.52
31	A	9000	TYK	C16-C15	3.21	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	TYK	O2C-C2C	-3.11	1.35	1.42
31	A	9000	TYK	O5A-C5A	-3.06	1.37	1.44
31	A	9000	TYK	C4C-C5C	-3.02	1.45	1.52
31	A	9000	TYK	O3-C3	2.95	1.49	1.43
31	A	9000	TYK	O20-C20	2.91	1.36	1.20
31	A	9000	TYK	C6A-C5A	-2.89	1.44	1.51
31	A	9000	TYK	O5B-C1B	2.87	1.49	1.42
31	A	9000	TYK	O3C-C3C	2.53	1.48	1.42
31	A	9000	TYK	C2A-C3A	2.46	1.57	1.53
31	A	9000	TYK	C3A-N3A	2.36	1.55	1.48
31	A	9000	TYK	C3B-C4B	2.24	1.58	1.53
31	A	9000	TYK	C18-C4	2.20	1.57	1.53
31	A	9000	TYK	C4C-C3C	-2.04	1.46	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9000	TYK	O20-C20-C19	-11.11	93.06	125.38
31	A	9000	TYK	O15-C15-C16	-6.77	96.12	106.90
31	A	9000	TYK	C6C-C5C-C4C	-6.16	101.81	113.08
31	A	9000	TYK	O1A-C5-C4	4.78	113.87	108.23
31	A	9000	TYK	C10-C11-C12	-4.55	119.50	126.23
31	A	9000	TYK	O5C-C1C-C2C	-4.51	100.72	109.49
31	A	9000	TYK	C17-C16-C15	3.87	123.49	113.23
31	A	9000	TYK	O15-C15-C14	3.86	115.97	107.60
31	A	9000	TYK	C3B-C2B-C1B	-3.13	108.95	114.77
31	A	9000	TYK	O4C-C4C-C5C	2.99	116.33	109.74
31	A	9000	TYK	C18-C4-C3	-2.98	106.34	111.09
31	A	9000	TYK	O4A-C4A-C5A	2.95	114.29	106.77
31	A	9000	TYK	O5A-C5A-C4A	2.74	114.27	109.19
31	A	9000	TYK	O5C-C5C-C6C	2.72	112.78	106.74
31	A	9000	TYK	O3B-C3B-C4B	2.68	112.25	107.52
31	A	9000	TYK	O4A-C1B-C2B	2.67	113.45	108.99
31	A	9000	TYK	O3-C3-C2	-2.53	103.35	109.45
31	A	9000	TYK	O3C-C3C-C2C	-2.40	103.38	108.93
31	A	9000	TYK	O5C-C1C-O1C	-2.22	104.79	110.04
31	A	9000	TYK	C8C-O3C-C3C	2.19	120.11	114.47
31	A	9000	TYK	O2C-C2C-C1C	2.17	117.10	110.99
31	A	9000	TYK	O15-C1-O1	2.16	128.76	123.70
31	A	9000	TYK	C2A-C3A-C4A	-2.10	107.38	110.57
31	A	9000	TYK	O1A-C1A-C2A	2.08	113.20	108.09
31	A	9000	TYK	O4C-C4C-C3C	-2.02	104.77	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9000	TYK	C1A-O1A-C5	2.01	122.73	117.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

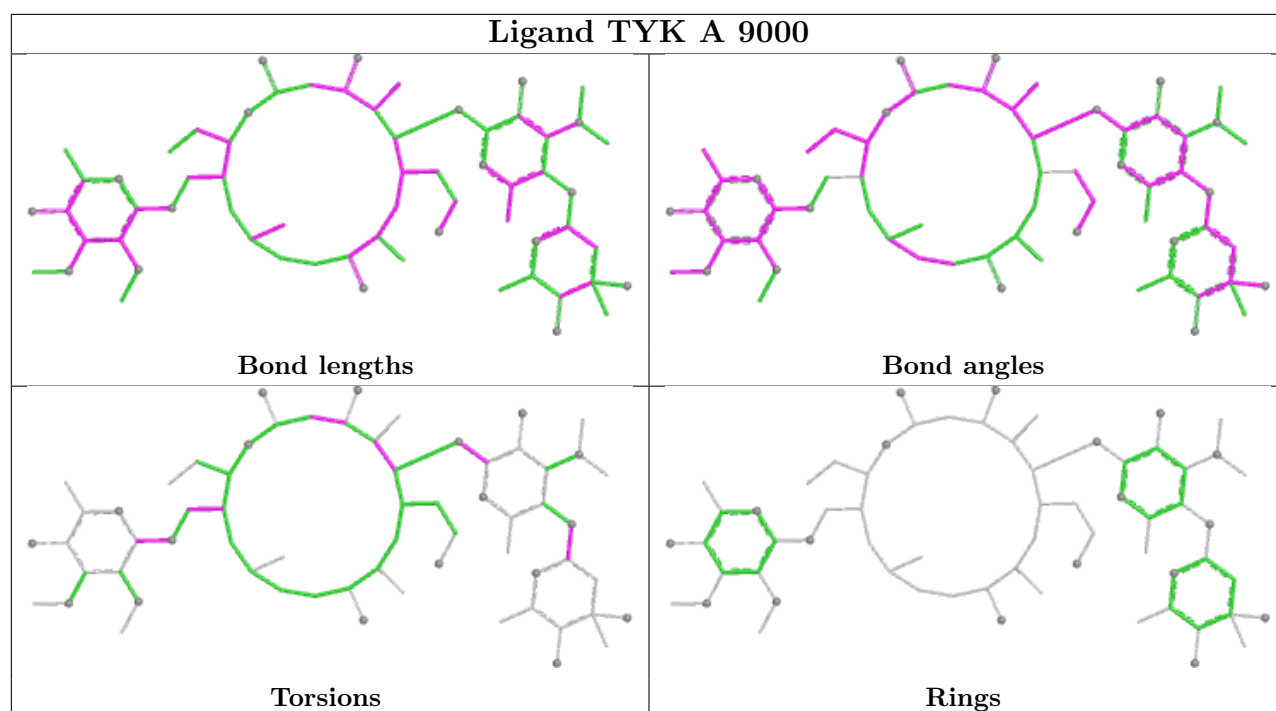
Mol	Chain	Res	Type	Atoms
31	A	9000	TYK	C2B-C1B-O4A-C4A
31	A	9000	TYK	O5C-C1C-O1C-C23
31	A	9000	TYK	O5B-C1B-O4A-C4A
31	A	9000	TYK	C2C-C1C-O1C-C23
31	A	9000	TYK	C1-C2-C3-C4
31	A	9000	TYK	C18-C4-C5-C6
31	A	9000	TYK	C13-C14-C23-O1C
31	A	9000	TYK	C3-C4-C5-C6
31	A	9000	TYK	C1-C2-C3-O3
31	A	9000	TYK	O5A-C1A-O1A-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9000	TYK	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2754/2922 (94%)	-0.05	104 (3%) 44 24	20, 47, 93, 139	0
2	B	122/122 (100%)	0.48	6 (4%) 35 18	31, 65, 95, 145	0
3	C	237/239 (99%)	0.18	4 (1%) 69 45	27, 61, 90, 109	0
4	D	337/337 (100%)	0.10	1 (0%) 90 79	20, 54, 81, 90	0
5	E	246/246 (100%)	0.00	1 (0%) 88 76	19, 49, 72, 81	0
6	F	140/176 (79%)	1.24	20 (14%) 6 3	54, 101, 118, 126	0
7	G	172/177 (97%)	0.33	3 (1%) 69 45	39, 65, 88, 94	0
8	H	119/119 (100%)	0.57	1 (0%) 82 64	56, 78, 99, 103	0
9	I	29/348 (8%)	1.84	11 (37%) 1 1	68, 91, 100, 101	0
10	J	156/167 (93%)	0.30	4 (2%) 57 34	32, 55, 79, 88	0
11	K	142/145 (97%)	-0.06	1 (0%) 84 66	32, 47, 71, 82	0
12	L	132/132 (100%)	0.10	1 (0%) 82 64	30, 53, 76, 82	0
13	M	145/164 (88%)	0.43	6 (4%) 41 23	23, 72, 105, 115	0
14	N	194/194 (100%)	0.36	14 (7%) 21 11	34, 53, 83, 88	0
15	O	186/186 (100%)	0.73	12 (6%) 25 13	41, 69, 107, 119	0
16	P	115/115 (100%)	0.23	0 100 100	38, 57, 76, 80	0
17	Q	143/148 (96%)	0.22	4 (2%) 55 32	33, 58, 73, 81	0
18	R	95/95 (100%)	-0.01	1 (1%) 78 57	33, 48, 59, 73	0
19	S	150/154 (97%)	-0.21	0 100 100	27, 42, 66, 74	0
20	T	81/84 (96%)	0.19	1 (1%) 76 55	47, 62, 80, 84	0
21	U	119/119 (100%)	0.32	3 (2%) 58 35	37, 58, 81, 91	0
22	V	53/66 (80%)	1.50	14 (26%) 1 1	81, 91, 97, 105	0
23	W	65/70 (92%)	0.53	3 (4%) 37 20	52, 77, 106, 113	0
24	X	154/154 (100%)	-0.12	1 (0%) 85 69	31, 46, 66, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	82/91 (90%)	0.23	4 (4%) 35 18	39, 55, 81, 93	0
26	Z	142/240 (59%)	-0.12	1 (0%) 84 66	25, 45, 69, 85	0
27	1	73/73 (100%)	1.90	28 (38%) 1 1	79, 92, 98, 99	0
28	2	56/56 (100%)	-0.39	0 100 100	26, 34, 41, 47	0
29	3	46/48 (95%)	0.22	1 (2%) 62 39	33, 59, 85, 97	0
30	4	92/92 (100%)	2.57	63 (68%) 0 0	90, 101, 105, 107	0
All	All	6577/7279 (90%)	0.18	313 (4%) 35 19	19, 54, 99, 145	0

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1173	A	6.9
1	A	2433	A	6.8
14	N	80	GLY	6.5
1	A	1175	G	6.0
23	W	1	THR	5.8
14	N	89	ASN	5.8
1	A	2432	C	5.6
30	4	60	LYS	5.5
30	4	12	PRO	5.3
1	A	1160	G	5.1
1	A	1168	C	5.1
1	A	1176	C	5.1
27	1	40	PRO	5.1
27	1	22	ILE	5.1
1	A	1184	C	5.0
4	D	1	PRO	4.8
6	F	10	PHE	4.8
27	1	26	VAL	4.7
30	4	48	ASN	4.6
30	4	33	MET	4.5
30	4	79	LEU	4.5
14	N	70	GLY	4.3
1	A	735	C	4.3
1	A	1190	G	4.2
30	4	7	PHE	4.2
27	1	41	VAL	4.2
30	4	77	ALA	4.1
30	4	85	ALA	4.1
1	A	1188	A	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	2436	U	4.0
30	4	88	LEU	4.0
1	A	1166	A	4.0
1	A	1198	U	4.0
1	A	1167	G	4.0
30	4	83	TRP	4.0
15	O	186	LEU	3.9
30	4	61	PRO	3.9
1	A	1193	A	3.9
30	4	43	ASN	3.9
30	4	36	ILE	3.9
6	F	138	GLY	3.8
1	A	736	A	3.8
15	O	162	ASP	3.8
9	I	24	VAL	3.8
27	1	20	LEU	3.8
1	A	1171	A	3.7
1	A	1192	A	3.7
30	4	17	HIS	3.7
1	A	1204	C	3.7
1	A	1165	G	3.7
1	A	1925	G	3.7
30	4	47	GLY	3.7
9	I	71	LEU	3.7
18	R	95	GLU	3.6
1	A	1169	U	3.6
30	4	52	PHE	3.6
30	4	84	ARG	3.6
9	I	26	MET	3.6
30	4	51	LYS	3.6
1	A	2345	A	3.5
27	1	12	GLY	3.5
30	4	54	LYS	3.5
27	1	16	PRO	3.5
1	A	1172	G	3.5
30	4	35	TRP	3.5
30	4	67	LEU	3.5
1	A	1187	U	3.5
2	B	3001	U	3.5
1	A	1174	A	3.4
1	A	1161	A	3.4
1	A	1197	G	3.4

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Mol	Chain	Res	Type	RSRZ
21	U	119	ALA	3.4
1	A	10	U	3.4
14	N	71	SER	3.4
1	A	1162	G	3.4
10	J	167	ALA	3.4
30	4	1	MET	3.4
30	4	62	THR	3.4
30	4	53	SER	3.3
17	Q	1	THR	3.3
27	1	11	THR	3.2
5	E	135	GLU	3.2
30	4	42	ARG	3.2
30	4	13	HIS	3.2
2	B	3024	U	3.2
1	A	1203	G	3.2
27	1	24	VAL	3.2
27	1	44	PHE	3.2
1	A	1205	U	3.2
1	A	1177	A	3.2
1	A	2344	G	3.2
14	N	83	SER	3.2
1	A	1180	U	3.1
1	A	1964	U	3.1
2	B	3002	U	3.1
27	1	39	CYS	3.1
1	A	1924	A	3.1
6	F	104	PHE	3.1
6	F	63	ILE	3.1
30	4	14	CYS	3.1
15	O	147	ILE	3.1
26	Z	108	ASP	3.1
14	N	72	SER	3.1
6	F	171	ASP	3.1
1	A	1163	G	3.0
2	B	3025	G	3.0
1	A	734	U	3.0
27	1	18	TYR	3.0
30	4	34	LYS	3.0
21	U	1	SER	3.0
7	G	10	ASP	3.0
27	1	35	LYS	3.0
1	A	1199	A	3.0

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Mol	Chain	Res	Type	RSRZ
22	V	42	LEU	3.0
1	A	1186	C	3.0
22	V	39	ASN	3.0
9	I	29	SER	2.9
30	4	55	VAL	2.9
30	4	11	CYS	2.9
27	1	17	ARG	2.9
25	Y	88	GLU	2.9
30	4	69	TYR	2.9
1	A	1195	G	2.9
15	O	154	LEU	2.9
1	A	282	C	2.9
1	A	1183	C	2.9
30	4	22	VAL	2.9
6	F	26	GLY	2.9
30	4	46	ILE	2.9
30	4	8	ASN	2.9
30	4	9	THR	2.9
30	4	31	THR	2.9
30	4	56	PRO	2.9
27	1	13	ARG	2.9
1	A	2249	G	2.9
22	V	49	LEU	2.9
30	4	78	HIS	2.8
22	V	55	ALA	2.8
27	1	29	VAL	2.8
1	A	1202	A	2.8
1	A	1214	G	2.8
2	B	3023	U	2.8
6	F	58	VAL	2.8
1	A	1179	C	2.8
30	4	76	LYS	2.8
6	F	131	THR	2.8
1	A	737	A	2.8
10	J	32	ASP	2.7
15	O	167	ASP	2.7
22	V	40	ALA	2.7
17	Q	116	SER	2.7
30	4	10	TYR	2.7
22	V	13	ILE	2.7
30	4	82	GLY	2.7
1	A	1159	G	2.7

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Mol	Chain	Res	Type	RSRZ
9	I	27	ILE	2.7
1	A	1206	U	2.7
6	F	22	VAL	2.7
13	M	81	VAL	2.7
30	4	2	GLN	2.7
15	O	78	MET	2.7
1	A	1279	U	2.7
9	I	20	VAL	2.7
1	A	2434	A	2.6
30	4	25	VAL	2.6
30	4	68	LYS	2.6
1	A	1207	A	2.6
9	I	15	TRP	2.6
14	N	88	VAL	2.6
30	4	32	GLY	2.6
27	1	47	LEU	2.6
14	N	82	ARG	2.6
30	4	64	LYS	2.6
1	A	2338	G	2.6
14	N	1	ALA	2.6
22	V	46	ALA	2.6
30	4	39	GLN	2.5
1	A	1194	A	2.5
13	M	82	ALA	2.5
6	F	132	VAL	2.5
6	F	69	ILE	2.5
1	A	1908	G	2.5
2	B	3022	G	2.5
30	4	38	ARG	2.5
27	1	34	LYS	2.5
1	A	1181	A	2.5
3	C	37	VAL	2.5
25	Y	87	ALA	2.5
1	A	1182	C	2.5
13	M	148	GLU	2.5
27	1	32	LYS	2.5
30	4	71	CYS	2.4
1	A	1191	A	2.4
24	X	38	THR	2.4
1	A	138	U	2.4
27	1	21	LYS	2.4
22	V	25	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1178	G	2.4
1	A	1917	G	2.4
6	F	44	ILE	2.4
9	I	23	ILE	2.4
27	1	31	ILE	2.4
30	4	18	GLN	2.4
6	F	49	PRO	2.4
1	A	960	G	2.4
30	4	4	PRO	2.4
27	1	33	HIS	2.4
30	4	3	MET	2.4
30	4	90	PHE	2.4
1	A	1189	A	2.4
1	A	2321	A	2.4
22	V	34	SER	2.4
30	4	44	SER	2.4
6	F	21	VAL	2.4
9	I	13	PRO	2.4
1	A	1212	C	2.3
9	I	64	ASN	2.3
1	A	2257	G	2.3
1	A	806	A	2.3
3	C	31	LYS	2.3
15	O	165	ALA	2.3
1	A	1185	U	2.3
15	O	168	LEU	2.3
27	1	14	PHE	2.3
6	F	73	VAL	2.3
30	4	65	THR	2.3
1	A	2511	A	2.3
1	A	1164	U	2.3
1	A	1170	U	2.3
25	Y	82	GLU	2.3
23	W	39	ALA	2.3
27	1	27	ALA	2.3
15	O	179	LEU	2.3
1	A	1525	G	2.3
30	4	24	LYS	2.3
13	M	83	GLU	2.3
14	N	81	ARG	2.3
25	Y	80	GLU	2.3
1	A	970	U	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1915	U	2.3
1	A	1916	C	2.3
10	J	41	THR	2.3
22	V	19	THR	2.3
30	4	63	LYS	2.3
11	K	32	ASP	2.3
13	M	102	ASP	2.3
1	A	362	G	2.2
27	1	64	ILE	2.2
1	A	1152	A	2.2
14	N	63	VAL	2.2
30	4	49	ASP	2.2
9	I	22	ALA	2.2
1	A	1951	G	2.2
6	F	170	TYR	2.2
1	A	808	A	2.2
6	F	47	GLN	2.2
1	A	1208	C	2.2
23	W	37	GLY	2.2
30	4	57	GLY	2.2
1	A	1158	G	2.2
15	O	158	LEU	2.2
6	F	107	GLY	2.2
15	O	148	ALA	2.2
27	1	50	ALA	2.2
22	V	51	TRP	2.2
27	1	10	ARG	2.2
29	3	35	ARG	2.2
20	T	81	ILE	2.1
17	Q	110	ASP	2.1
1	A	2827	A	2.1
1	A	1926	G	2.1
3	C	32	VAL	2.1
30	4	59	ASP	2.1
14	N	79	LYS	2.1
12	L	119	GLN	2.1
30	4	91	GLN	2.1
1	A	2637	A	2.1
17	Q	58	SER	2.1
14	N	78	ASN	2.1
1	A	1634	G	2.1
1	A	1948	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2250	G	2.1
1	A	2251	G	2.1
1	A	2256	G	2.1
1	A	2337	G	2.1
1	A	287	C	2.1
1	A	1156	C	2.1
22	V	52	THR	2.1
7	G	81	GLU	2.1
14	N	77	PHE	2.1
3	C	64	ASP	2.1
22	V	6	CYS	2.1
1	A	999	C	2.1
1	A	1157	C	2.1
10	J	164	ALA	2.1
1	A	2435	U	2.0
13	M	73	VAL	2.0
30	4	27	SER	2.0
30	4	15	ASN	2.0
1	A	1626	A	2.0
6	F	61	PHE	2.0
8	H	90	GLU	2.0
1	A	1524	U	2.0
1	A	1561	U	2.0
15	O	146	HIS	2.0
7	G	45	ASP	2.0
22	V	31	PHE	2.0
27	1	15	GLY	2.0
1	A	128	A	2.0
21	U	115	GLU	2.0
6	F	27	ILE	2.0
1	A	1196	C	2.0
1	A	1914	C	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
34	CL	4	8504	1/1	0.17	0.21	112,112,112,112	0
33	NA	S	8337	1/1	0.53	0.14	34,34,34,34	0
33	NA	T	8312	1/1	0.59	0.13	69,69,69,69	0
33	NA	A	8326	1/1	0.59	0.28	56,56,56,56	0
32	MG	A	8050	1/1	0.66	0.13	77,77,77,77	0
33	NA	A	8384	1/1	0.69	0.30	106,106,106,106	0
32	MG	A	8104	1/1	0.73	0.14	51,51,51,51	0
33	NA	B	8383	1/1	0.76	0.17	54,54,54,54	0
32	MG	A	8067	1/1	0.76	0.20	49,49,49,49	0
33	NA	A	8356	1/1	0.77	0.36	57,57,57,57	0
33	NA	S	8386	1/1	0.77	0.28	75,75,75,75	0
33	NA	A	8377	1/1	0.78	0.46	77,77,77,77	0
33	NA	E	8304	1/1	0.78	0.10	32,32,32,32	0
33	NA	B	8351	1/1	0.78	0.14	58,58,58,58	0
33	NA	A	8382	1/1	0.79	0.22	41,41,41,41	0
32	MG	A	8070	1/1	0.80	0.35	70,70,70,70	0
33	NA	A	8362	1/1	0.81	0.28	63,63,63,63	0
33	NA	A	8366	1/1	0.81	0.12	43,43,43,43	0
32	MG	A	8066	1/1	0.81	0.10	70,70,70,70	0
32	MG	D	8055	1/1	0.81	0.12	84,84,84,84	0
33	NA	A	8311	1/1	0.82	0.14	50,50,50,50	0
33	NA	A	8368	1/1	0.82	0.23	43,43,43,43	0
33	NA	A	8323	1/1	0.83	0.17	38,38,38,38	0
33	NA	A	8385	1/1	0.83	0.14	28,28,28,28	0
32	MG	A	8116	1/1	0.83	0.12	80,80,80,80	0
33	NA	A	8357	1/1	0.84	0.15	53,53,53,53	0
33	NA	J	8322	1/1	0.84	0.25	56,56,56,56	0
32	MG	A	8112	1/1	0.84	0.12	58,58,58,58	0
33	NA	A	8303	1/1	0.84	0.25	53,53,53,53	0
33	NA	A	8327	1/1	0.84	0.13	28,28,28,28	0
32	MG	A	8045	1/1	0.84	0.10	61,61,61,61	0
33	NA	A	8319	1/1	0.85	0.09	39,39,39,39	0
33	NA	A	8363	1/1	0.85	0.19	49,49,49,49	0
32	MG	A	8024	1/1	0.85	0.27	99,99,99,99	0
32	MG	A	8087	1/1	0.85	0.10	52,52,52,52	0
36	CD	4	8404	1/1	0.85	0.30	148,148,148,148	0
36	CD	P	8405	1/1	0.86	0.17	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CD	V	8401	1/1	0.86	0.20	142,142,142,142	0
32	MG	A	8081	1/1	0.86	0.12	64,64,64,64	0
33	NA	A	8330	1/1	0.87	0.10	46,46,46,46	0
33	NA	A	8364	1/1	0.87	0.13	39,39,39,39	0
32	MG	A	8102	1/1	0.87	0.52	82,82,82,82	0
34	CL	A	8517	1/1	0.87	0.09	49,49,49,49	0
33	NA	A	8367	1/1	0.87	0.14	37,37,37,37	0
32	MG	1	8105	1/1	0.87	0.08	42,42,42,42	0
33	NA	A	8371	1/1	0.87	0.16	31,31,31,31	0
33	NA	A	8302	1/1	0.87	0.13	24,24,24,24	0
33	NA	A	8361	1/1	0.88	0.11	48,48,48,48	0
33	NA	A	8321	1/1	0.88	0.19	45,45,45,45	0
33	NA	A	8373	1/1	0.88	0.07	37,37,37,37	0
33	NA	A	8374	1/1	0.88	0.14	41,41,41,41	0
33	NA	A	8341	1/1	0.88	0.07	17,17,17,17	0
34	CL	A	8512	1/1	0.89	0.10	32,32,32,32	0
34	CL	A	8515	1/1	0.89	0.21	97,97,97,97	0
33	NA	A	8365	1/1	0.89	0.15	41,41,41,41	0
34	CL	A	8522	1/1	0.89	0.40	80,80,80,80	0
34	CL	K	8516	1/1	0.89	0.12	40,40,40,40	0
33	NA	A	8331	1/1	0.89	0.13	46,46,46,46	0
33	NA	A	8310	1/1	0.89	0.10	31,31,31,31	0
33	NA	A	8350	1/1	0.89	0.11	24,24,24,24	0
33	NA	A	8379	1/1	0.89	0.11	32,32,32,32	0
32	MG	A	8090	1/1	0.90	0.16	11,11,11,11	0
33	NA	A	8378	1/1	0.90	0.15	30,30,30,30	0
32	MG	A	8117	1/1	0.90	0.06	19,19,19,19	0
34	CL	A	8513	1/1	0.90	0.12	64,64,64,64	0
33	NA	A	8332	1/1	0.90	0.08	34,34,34,34	0
33	NA	A	8333	1/1	0.90	0.12	26,26,26,26	0
32	MG	A	8092	1/1	0.90	0.12	83,83,83,83	0
32	MG	A	8023	1/1	0.90	0.08	42,42,42,42	0
33	NA	A	8355	1/1	0.90	0.22	55,55,55,55	0
32	MG	A	8085	1/1	0.90	0.13	79,79,79,79	0
32	MG	A	8046	1/1	0.90	0.10	62,62,62,62	0
33	NA	A	8307	1/1	0.90	0.08	20,20,20,20	0
32	MG	A	8022	1/1	0.91	0.11	39,39,39,39	0
33	NA	A	8305	1/1	0.91	0.10	33,33,33,33	0
32	MG	A	8106	1/1	0.91	0.09	62,62,62,62	0
32	MG	A	8100	1/1	0.91	0.08	48,48,48,48	0
34	CL	N	8518	1/1	0.91	0.11	38,38,38,38	0
32	MG	A	8040	1/1	0.91	0.17	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	K	A	8602	1/1	0.91	0.13	56,56,56,56	0
34	CL	A	8505	1/1	0.91	0.14	83,83,83,83	0
33	NA	A	8352	1/1	0.91	0.18	37,37,37,37	0
33	NA	A	8313	1/1	0.91	0.09	64,64,64,64	0
33	NA	A	8301	1/1	0.92	0.06	20,20,20,20	0
33	NA	A	8369	1/1	0.92	0.21	53,53,53,53	0
35	K	A	8603	1/1	0.92	0.07	76,76,76,76	0
32	MG	A	8079	1/1	0.92	0.06	24,24,24,24	0
33	NA	M	8380	1/1	0.92	0.09	49,49,49,49	0
32	MG	A	8118	1/1	0.92	0.18	31,31,31,31	0
34	CL	K	8521	1/1	0.93	0.08	50,50,50,50	0
34	CL	M	8510	1/1	0.93	0.10	75,75,75,75	0
33	NA	A	8338	1/1	0.93	0.08	59,59,59,59	0
34	CL	R	8511	1/1	0.93	0.12	57,57,57,57	0
33	NA	A	8360	1/1	0.93	0.14	38,38,38,38	0
31	TYK	A	9000	64/64	0.93	0.11	33,43,48,51	0
33	NA	A	8306	1/1	0.93	0.11	36,36,36,36	0
32	MG	A	8041	1/1	0.93	0.09	62,62,62,62	0
32	MG	A	8084	1/1	0.93	0.09	40,40,40,40	0
36	CD	1	8403	1/1	0.93	0.14	139,139,139,139	0
32	MG	A	8042	1/1	0.93	0.10	31,31,31,31	0
32	MG	4	8078	1/1	0.94	0.11	91,91,91,91	0
33	NA	A	8353	1/1	0.94	0.04	16,16,16,16	0
32	MG	A	8099	1/1	0.94	0.09	46,46,46,46	0
32	MG	A	8001	1/1	0.94	0.08	38,38,38,38	0
35	K	A	8601	1/1	0.94	0.06	62,62,62,62	0
32	MG	A	8064	1/1	0.94	0.12	18,18,18,18	0
32	MG	A	8049	1/1	0.94	0.06	62,62,62,62	0
32	MG	A	8093	1/1	0.94	0.09	38,38,38,38	0
33	NA	A	8324	1/1	0.94	0.35	42,42,42,42	0
33	NA	A	8349	1/1	0.94	0.10	33,33,33,33	0
32	MG	A	8111	1/1	0.94	0.06	54,54,54,54	0
33	NA	A	8317	1/1	0.95	0.05	9,9,9,9	0
34	CL	A	8503	1/1	0.95	0.09	55,55,55,55	0
32	MG	A	8103	1/1	0.95	0.11	69,69,69,69	0
32	MG	A	8059	1/1	0.95	0.06	33,33,33,33	0
32	MG	A	8082	1/1	0.95	0.09	59,59,59,59	0
34	CL	A	8514	1/1	0.95	0.08	51,51,51,51	0
33	NA	A	8375	1/1	0.95	0.15	53,53,53,53	0
33	NA	A	8376	1/1	0.95	0.22	80,80,80,80	0
32	MG	A	8108	1/1	0.95	0.16	73,73,73,73	0
34	CL	C	8509	1/1	0.95	0.12	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	CL	D	8519	1/1	0.95	0.20	59,59,59,59	0
34	CL	K	8501	1/1	0.95	0.06	58,58,58,58	0
34	CL	K	8502	1/1	0.95	0.08	56,56,56,56	0
32	MG	A	8072	1/1	0.95	0.11	88,88,88,88	0
32	MG	A	8097	1/1	0.95	0.11	37,37,37,37	0
33	NA	A	8359	1/1	0.95	0.11	52,52,52,52	0
33	NA	A	8329	1/1	0.95	0.08	33,33,33,33	0
32	MG	A	8076	1/1	0.95	0.08	61,61,61,61	0
34	CL	Z	8520	1/1	0.95	0.11	30,30,30,30	0
32	MG	A	8053	1/1	0.95	0.06	52,52,52,52	0
32	MG	A	8101	1/1	0.95	0.11	38,38,38,38	0
32	MG	A	8089	1/1	0.95	0.06	64,64,64,64	0
33	NA	J	8309	1/1	0.95	0.12	25,25,25,25	0
32	MG	U	8073	1/1	0.95	0.04	38,38,38,38	0
33	NA	A	8339	1/1	0.95	0.09	22,22,22,22	0
33	NA	A	8340	1/1	0.95	0.11	31,31,31,31	0
33	NA	A	8314	1/1	0.95	0.15	45,45,45,45	0
32	MG	A	8048	1/1	0.96	0.05	47,47,47,47	0
33	NA	A	8318	1/1	0.96	0.12	37,37,37,37	0
32	MG	A	8071	1/1	0.96	0.07	84,84,84,84	0
32	MG	A	8094	1/1	0.96	0.07	60,60,60,60	0
34	CL	O	8507	1/1	0.96	0.07	54,54,54,54	0
33	NA	A	8354	1/1	0.96	0.06	40,40,40,40	0
32	MG	A	8096	1/1	0.96	0.07	54,54,54,54	0
33	NA	A	8334	1/1	0.96	0.07	26,26,26,26	0
33	NA	A	8370	1/1	0.96	0.20	55,55,55,55	0
32	MG	L	8069	1/1	0.96	0.06	72,72,72,72	0
33	NA	A	8325	1/1	0.96	0.08	47,47,47,47	0
32	MG	A	8091	1/1	0.96	0.04	45,45,45,45	0
33	NA	A	8316	1/1	0.96	0.08	31,31,31,31	0
33	NA	N	8347	1/1	0.96	0.04	24,24,24,24	0
33	NA	A	8344	1/1	0.96	0.04	16,16,16,16	0
33	NA	A	8342	1/1	0.97	0.07	39,39,39,39	0
33	NA	A	8320	1/1	0.97	0.07	32,32,32,32	0
32	MG	A	8114	1/1	0.97	0.14	82,82,82,82	0
33	NA	A	8372	1/1	0.97	0.14	53,53,53,53	0
34	CL	P	8508	1/1	0.97	0.06	83,83,83,83	0
32	MG	A	8075	1/1	0.97	0.06	38,38,38,38	0
33	NA	A	8315	1/1	0.97	0.12	27,27,27,27	0
32	MG	A	8044	1/1	0.97	0.09	44,44,44,44	0
32	MG	A	8088	1/1	0.97	0.07	28,28,28,28	0
33	NA	K	8346	1/1	0.97	0.04	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	B	8095	1/1	0.97	0.07	68,68,68,68	0
33	NA	A	8328	1/1	0.97	0.05	24,24,24,24	0
33	NA	R	8348	1/1	0.97	0.04	15,15,15,15	0
32	MG	A	8113	1/1	0.97	0.06	40,40,40,40	0
33	NA	A	8381	1/1	0.97	0.05	33,33,33,33	0
32	MG	A	8062	1/1	0.98	0.04	46,46,46,46	0
32	MG	A	8063	1/1	0.98	0.10	73,73,73,73	0
32	MG	A	8002	1/1	0.98	0.05	42,42,42,42	0
32	MG	A	8043	1/1	0.98	0.07	58,58,58,58	0
32	MG	A	8115	1/1	0.98	0.03	46,46,46,46	0
32	MG	A	8003	1/1	0.98	0.04	19,19,19,19	0
32	MG	A	8007	1/1	0.98	0.06	24,24,24,24	0
32	MG	A	8025	1/1	0.98	0.03	54,54,54,54	0
32	MG	A	8119	1/1	0.98	0.07	30,30,30,30	0
32	MG	A	8028	1/1	0.98	0.05	43,43,43,43	0
32	MG	C	8065	1/1	0.98	0.03	52,52,52,52	0
32	MG	A	8037	1/1	0.98	0.04	45,45,45,45	0
32	MG	A	8098	1/1	0.98	0.12	43,43,43,43	0
32	MG	A	8039	1/1	0.98	0.06	54,54,54,54	0
32	MG	Z	8109	1/1	0.98	0.04	39,39,39,39	0
32	MG	A	8051	1/1	0.98	0.04	66,66,66,66	0
32	MG	A	8052	1/1	0.98	0.07	36,36,36,36	0
32	MG	A	8012	1/1	0.98	0.04	34,34,34,34	0
32	MG	A	8083	1/1	0.98	0.06	47,47,47,47	0
32	MG	A	8057	1/1	0.98	0.06	34,34,34,34	0
32	MG	A	8018	1/1	0.98	0.03	32,32,32,32	0
32	MG	A	8061	1/1	0.98	0.05	35,35,35,35	0
32	MG	A	8110	1/1	0.98	0.09	23,23,23,23	0
33	NA	A	8335	1/1	0.98	0.06	45,45,45,45	0
33	NA	A	8336	1/1	0.98	0.04	46,46,46,46	0
33	NA	A	8308	1/1	0.98	0.09	50,50,50,50	0
32	MG	A	8029	1/1	0.99	0.04	51,51,51,51	0
32	MG	A	8077	1/1	0.99	0.02	28,28,28,28	0
32	MG	A	8107	1/1	0.99	0.05	51,51,51,51	0
32	MG	A	8030	1/1	0.99	0.02	29,29,29,29	0
32	MG	A	8031	1/1	0.99	0.06	14,14,14,14	0
32	MG	A	8032	1/1	0.99	0.06	29,29,29,29	0
32	MG	A	8033	1/1	0.99	0.02	22,22,22,22	0
33	NA	A	8343	1/1	0.99	0.02	11,11,11,11	0
32	MG	A	8034	1/1	0.99	0.03	32,32,32,32	0
32	MG	A	8054	1/1	0.99	0.03	50,50,50,50	0
32	MG	A	8086	1/1	0.99	0.05	40,40,40,40	0

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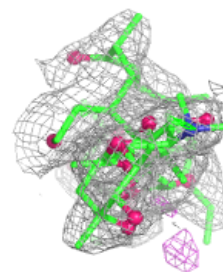
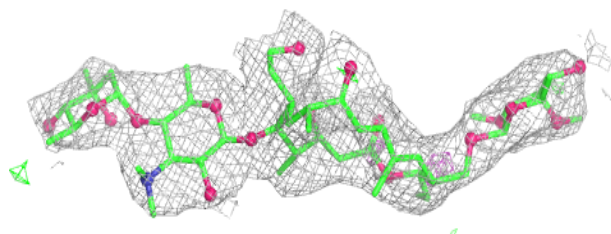
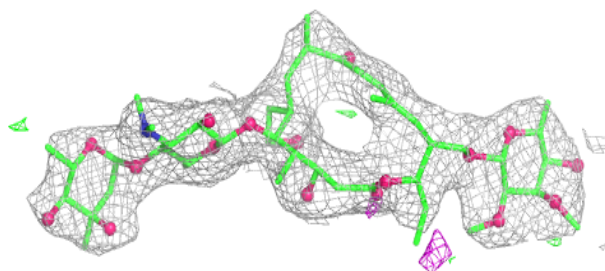
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8035	1/1	0.99	0.03	48,48,48,48	0
32	MG	A	8058	1/1	0.99	0.04	34,34,34,34	0
32	MG	A	8010	1/1	0.99	0.04	29,29,29,29	0
32	MG	A	8060	1/1	0.99	0.03	48,48,48,48	0
32	MG	A	8038	1/1	0.99	0.05	14,14,14,14	0
32	MG	A	8019	1/1	0.99	0.04	27,27,27,27	0
33	NA	C	8345	1/1	0.99	0.03	34,34,34,34	0
32	MG	A	8021	1/1	0.99	0.03	27,27,27,27	0
34	CL	S	8506	1/1	0.99	0.07	42,42,42,42	0
32	MG	A	8005	1/1	0.99	0.03	47,47,47,47	0
32	MG	A	8013	1/1	0.99	0.03	42,42,42,42	0
32	MG	A	8014	1/1	0.99	0.06	13,13,13,13	0
32	MG	A	8068	1/1	0.99	0.04	40,40,40,40	0
32	MG	A	8015	1/1	0.99	0.03	46,46,46,46	0
32	MG	A	8027	1/1	0.99	0.03	51,51,51,51	0
32	MG	A	8016	1/1	0.99	0.02	43,43,43,43	0
32	MG	A	8074	1/1	0.99	0.06	12,12,12,12	0
36	CD	2	8402	1/1	0.99	0.03	52,52,52,52	0
32	MG	A	8047	1/1	0.99	0.07	45,45,45,45	0
32	MG	A	8017	1/1	1.00	0.03	28,28,28,28	0
32	MG	A	8004	1/1	1.00	0.02	35,35,35,35	0
32	MG	A	8026	1/1	1.00	0.01	15,15,15,15	0
32	MG	A	8008	1/1	1.00	0.03	41,41,41,41	0
32	MG	A	8036	1/1	1.00	0.03	41,41,41,41	0
32	MG	A	8080	1/1	1.00	0.03	35,35,35,35	0
32	MG	A	8056	1/1	1.00	0.03	41,41,41,41	0
32	MG	A	8020	1/1	1.00	0.05	34,34,34,34	0
32	MG	A	8009	1/1	1.00	0.05	19,19,19,19	0
32	MG	A	8006	1/1	1.00	0.04	48,48,48,48	0
32	MG	A	8011	1/1	1.00	0.02	25,25,25,25	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 TYK A 9000:

$2mF_o-DF_c$ (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.