



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:34 PM GMT

PDB ID : 1K9M
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

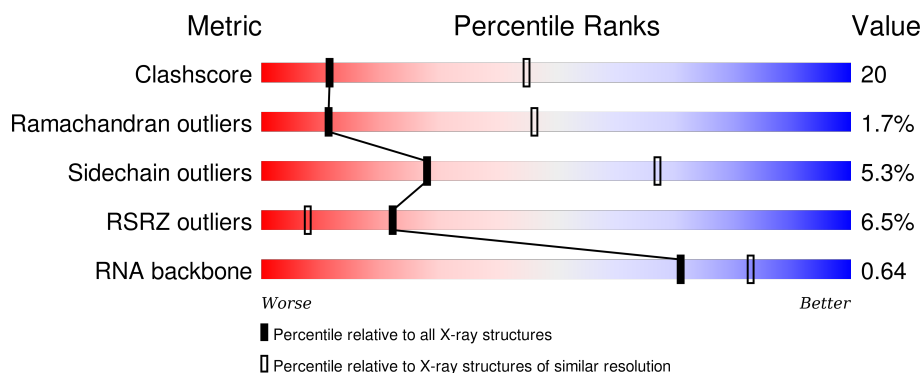
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>36%</div> <div>7%</div> <div>6%</div> </div> </div>
2	B	122	<div> <div>4%</div> <div> <div></div> <div>45%</div> <div>39%</div> <div>10%</div> <div>6%</div> </div> </div>
3	C	239	<div> <div>7%</div> <div> <div></div> <div>54%</div> <div>38%</div> <div>7%</div> <div>•</div> </div> </div>
4	D	337	<div> <div></div> <div> <div></div> <div>50%</div> <div>44%</div> <div>6%</div> </div> </div>
5	E	246	<div> <div>•</div> <div> <div></div> <div>61%</div> <div>34%</div> <div>6%</div> </div> </div>

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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
31	TYK	A	9000	-	-	-	X
32	MG	4	8078	-	-	-	X
32	MG	A	8067	-	-	-	X
33	NA	A	8303	-	-	-	X
33	NA	A	8321	-	-	-	X
33	NA	A	8323	-	-	-	X
33	NA	A	8340	-	-	-	X
33	NA	A	8350	-	-	-	X
33	NA	A	8355	-	-	-	X
33	NA	A	8356	-	-	-	X
33	NA	A	8359	-	-	-	X
33	NA	A	8362	-	-	-	X
33	NA	A	8364	-	-	-	X
33	NA	A	8365	-	-	-	X
33	NA	A	8366	-	-	-	X
33	NA	A	8371	-	-	-	X
33	NA	A	8372	-	-	-	X
33	NA	A	8373	-	-	-	X
33	NA	A	8374	-	-	-	X
33	NA	A	8376	-	-	-	X
33	NA	A	8378	-	-	-	X
33	NA	A	8382	-	-	-	X
33	NA	S	8337	-	-	-	X
33	NA	S	8386	-	-	-	X
34	CL	4	8504	-	-	-	X
34	CL	A	8505	-	-	-	X
34	CL	A	8515	-	-	-	X
34	CL	D	8519	-	-	-	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		0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O			
			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			

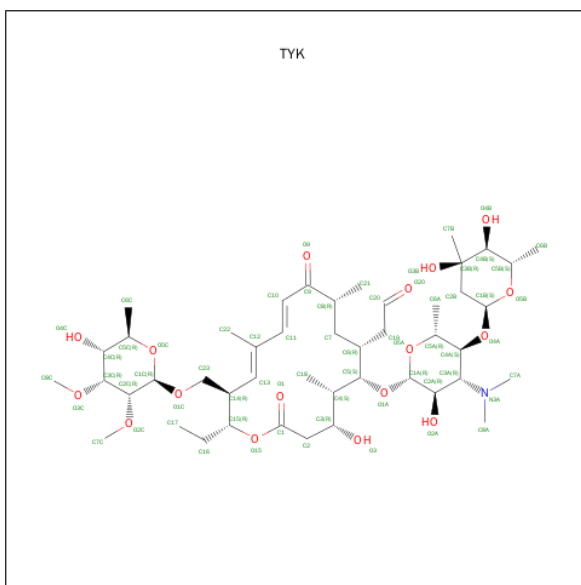
There is a discrepancy between the modelled and reference sequences:

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 (three-letter code: 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 (three-letter code: MG) (formula: Mg).

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

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	P	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	C	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	A	8	Total Cl 8 8	0	0
34	4	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Cl 1	0	0
34	S	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0
36	V	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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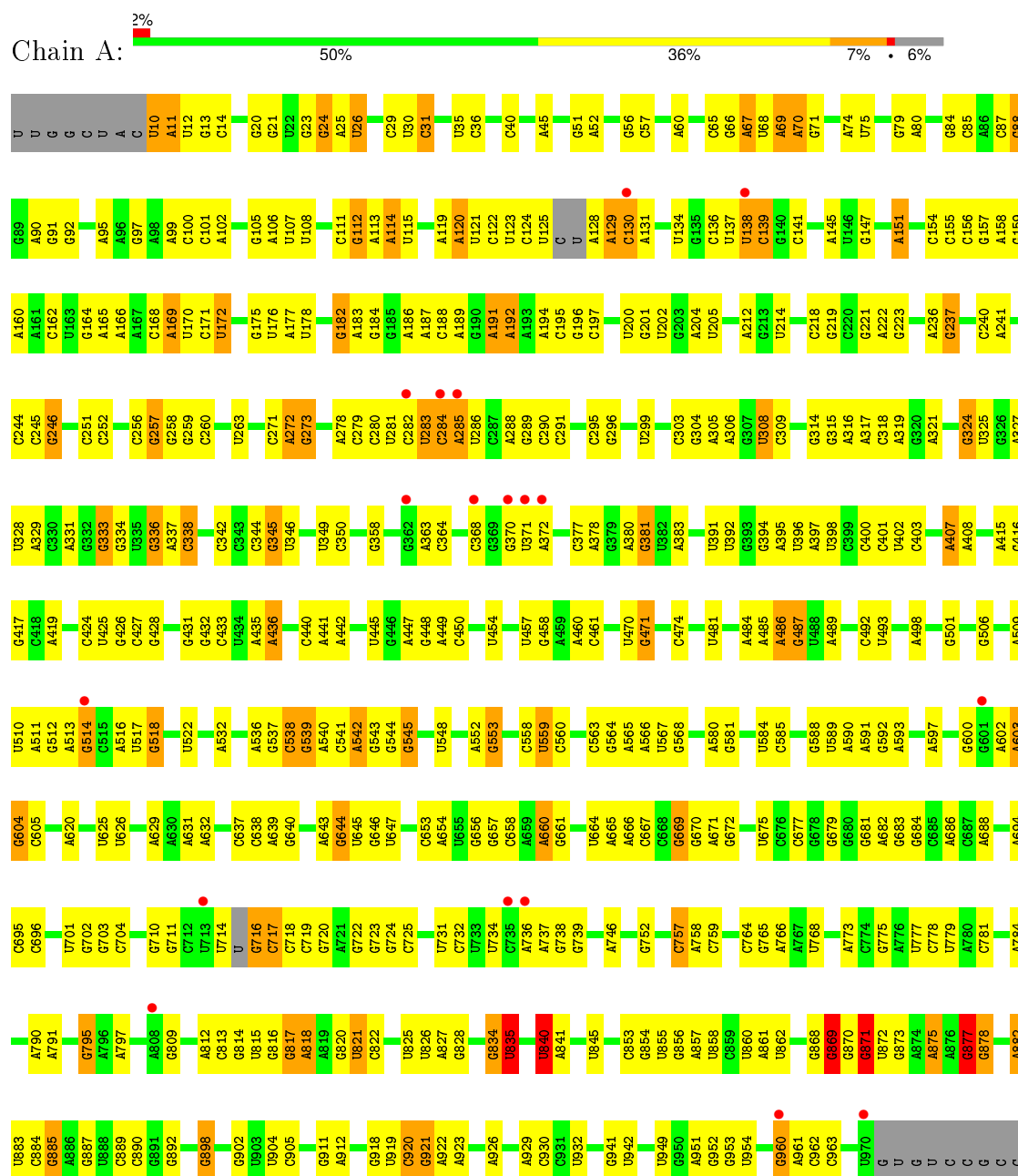
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	56	Total 56	O 56	0	0
37	3	43	Total 43	O 43	0	0
37	4	72	Total 72	O 72	0	0

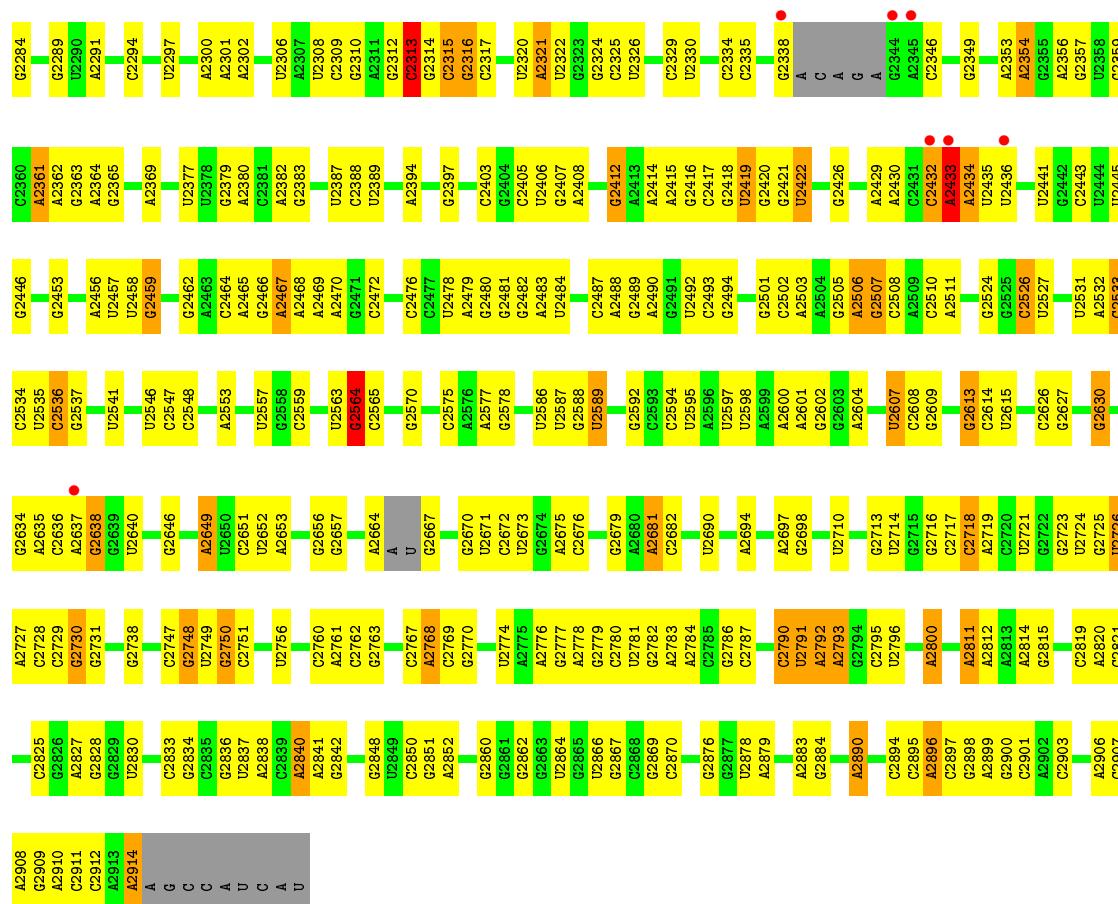
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

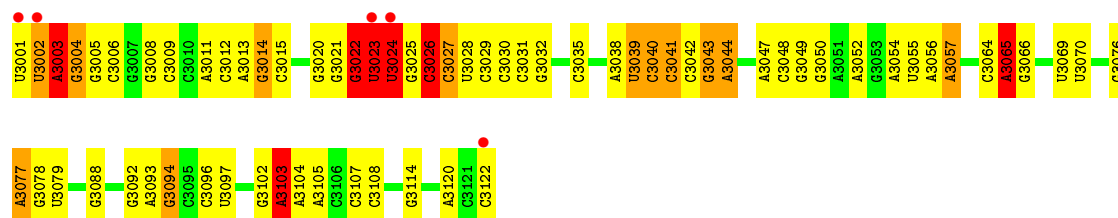
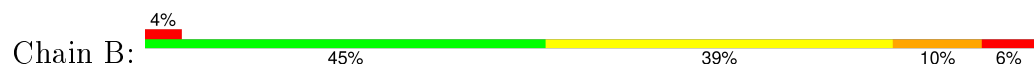
• Molecule 1: 23S rRNA



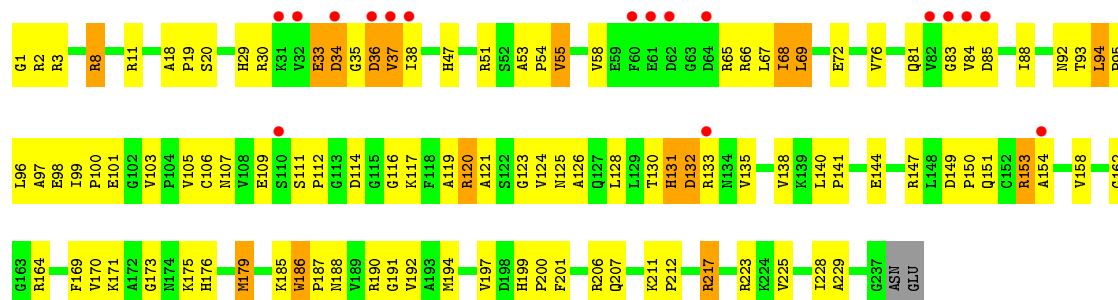
G	A2083	A1991	G1819	G1725	G1633	G1532	G1441	U1333	A1242	A1166	G1072	U
U	C2087	U1992	G1820	G1730	C1634	A1533	A1442	C1334	A1243	G1167	A1073	C
G	C2088	C1993	U1825	C1731	U1635	C1534	G1443	C1335	U1244	C1168		C
A	A2089	A1995	C1826	A1732	G1636	G1535	G1444	U1336	A1245	U1169		G
A	G2090	U1996	G1827	A1733	A1637	G1536	U1446	A1337	G1246	U1170	A1079	A
U	G2091	A1997	G1828	C1734			U1447			A1171	A1080	G
A	G2092	A1998	A1829	C1735	A1641	G1543		C1342	U1249	G1172	A1081	A
C	G2093	C1999	A1830	A1736	A1642	U1544	C1450		U1250	A1173	A1082	G
U	G2094	G2000	G1923	A1737	C1545	G1546	C1451	A1348	C1251	A1174		A
A	A2095	A1924	U1833	C1738	G1647		C1452	G1349	A1252	G1175	A1086	G
G	A2096	G1925	C1834					U1350	G1253	C1176		C
C	G2097	G1926	U1835	U1741	U1654	C1549	C1456	G1351		A1177	G1087	U
C	C2098	U2004		A1742	G1655		U1457	A1352	C1257		A1088	C
C	G2099	G2005		G1743	A1656	G1552	A1458	C1353	G1258	U1180		G
G	A2100		A1839	C1743	A1657	C1553	A1459	G1354		A1181	U1096	C
G	A2101	U2008	A1840		U1658	G1554				A1097		G
C	G2102	G2009	C1841	A1746	A1659	U1555		C1360	A1261	C1182	A1098	C
G	A2103	A2010	A1842	U1748	G1660	G1559	C1462	C1366	U1264	C1183	G1099	A
A	C2104	A2011	A1845	G1751	C1666	U	C1469		G1265	U1185		C
C	C2105	U2012	U1846	G1752	A1667	U1561	A1470	A1372	U1266	C1186	C1103	C
G	C2106	G2013	A1847	C1753	U1668	C1562	A1471	A1375	C1267	A1188	U1109	U1003
A	U2107	G2014	G1947	A1754	A1669	G1563	C1472	G1376	C1268	A1189	G1110	C1004
U	A2108	A2015	U1850		G1670	C1564	U1473	C1377	U1270	G1190		A1005
A	U2109	U2016	G1948	U1758			C1474			A1191	A1114	A1006
G	G2110		G1949					U1380	C1273	A1192	U1115	A1007
C	A2111	A2030	G1950		C1675	A1573	C1477			A1193	U1116	C1008
C	A2112	C2031	U	U1766	G1676	C1574	U1478	G1391	U1279		A1117	U1009
A	G2113	U2032	A1857	A1767	U1677	A1580		G1392		U1197	A1118	C1010
G	G2114	G2033	A	C1768	A1678		C1483	A1393	U1289	U1198	G1119	A1014
U	U2115	U2034	C	C1769	C1679	G1589	G1484	C1394	G1290	A1199	U1120	C1015
A	U2116	C2035	U1860	U1770	C1680				A1291	A1200	G1121	U1016
C	C2119	C2036	C1861	U1771	G1681	G1592	U1487	G1398	A1292	C1201	A1122	
C	U2120	C2037	C1862	C1772	A1682	C1593	U1488	A1399	U1293	A1202	A1123	G1021
C	G2121	A2038	G1863	G1773	G1683	C1594	U1489	C1400	A1294	G1203	G1127	A1022
G	C2122	G2044	A	G1774	A1684	G1595	A1494	G1401	G1295	C1204	U1128	C1023
G	A2123	G2045	G1868		A1685	U1596	C1495		A1296	U1205	U1129	G1024
C	U2127	G2046	U1874	A1778	C1686	U1597		A1407		U1206	U1130	C1025
U	G2128	G2050	G1877	A1779	C1687	A1598	U1500	U1408	G1299	A1207	U1131	U1029
A	U1966		U1878		G1688	A1599	A1501	G1409	G1300	C1208	A1132	
C	U1967	A2054	U1879	U1784	C1689	G1601	A1502		C1301	C1209	G1133	G1038
G	A1969	A2055	C1882	C1787	A1691	C1602	U1503	U1412		G1211	G1134	G1039
G	G1970	C1883	U1883	U1788	C1692	A1603	U1504	G1417	U1304	C1212	G1135	
C	A2136	G1884	G1884	C1789	G1694	G1605	U1506	U1418	C1305	C1213	U1136	C1044
C	A	U1972	A1885	C1790	C1700	A1606		U1419	U1306	G1214	U1137	G1045
C	C	A1973	A1886	U1791	A1607	A1607	G1513	C1420	A1307	A1215	G1138	
A	G1974	G1974	U1887	C1792	U1702	G1608	C1514	G1421	A1308	G1216	U1139	
C	C1975	G1975				C1609	A1515	U1422	U1309	G1217	G1140	G1053
C	U1976		U1890	C1798	A1710	G1610	U1516	C1423	U1311	U1218		U1056
G	U1977	U1977			A1711		A1522	A1424	G1312	U1219	G1151	A1057
A	U1978	A1804	C1894	A1805	C1614	C1613	G1523	G1430	G1325	C1229	G1158	A1058
U	G1979	G1805			A1712	U1524	U1524			U1234	G1159	G1059
U	U1980	C1810	G1902	C1810	A1717	A1615	G1525	G1433	A1328	G1160	A1161	C1060
C	A1981	U1903	A1904		C1721	U1625	A1526	A1434	A1329	G1162	U1062	C1061
C	C1982			A1815	U1722	A1626	A1527	A1435	U1237	G1163		
A	G1989	G1908	U1908	C1816	G1723	A1528	A1528	C1436	A1331	U1164	U1066	
A	C1990	A1909			U1724	A1630	G1529		C1332	G1165	A1067	



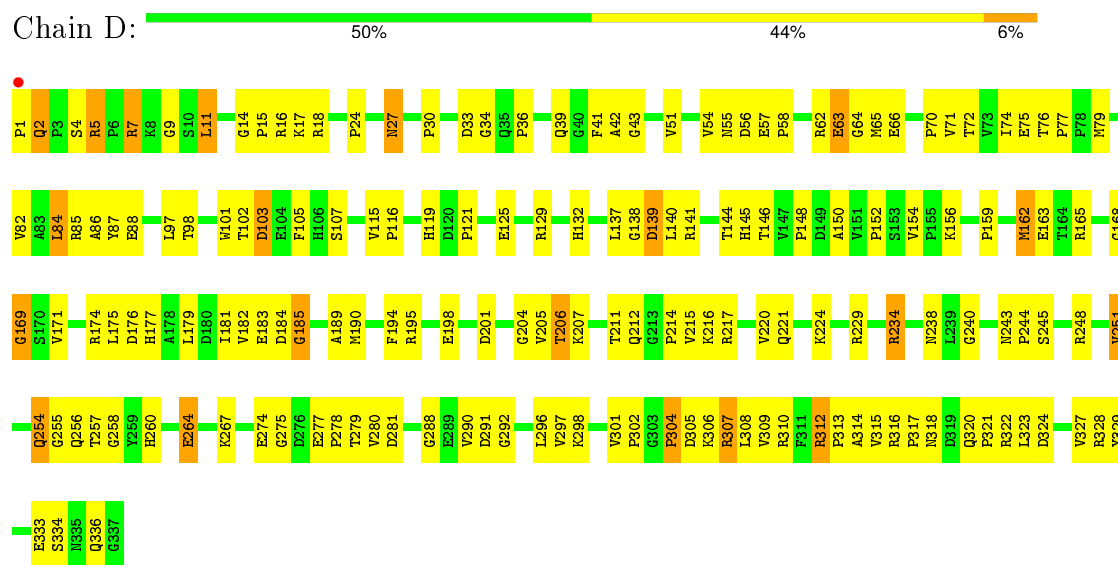
• Molecule 2: 5S RRNA



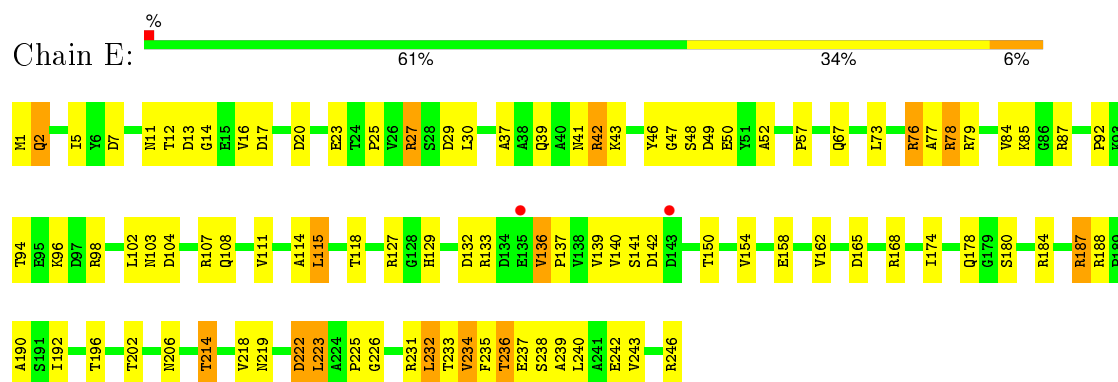
• Molecule 3: RIBOSOMAL PROTEIN L2



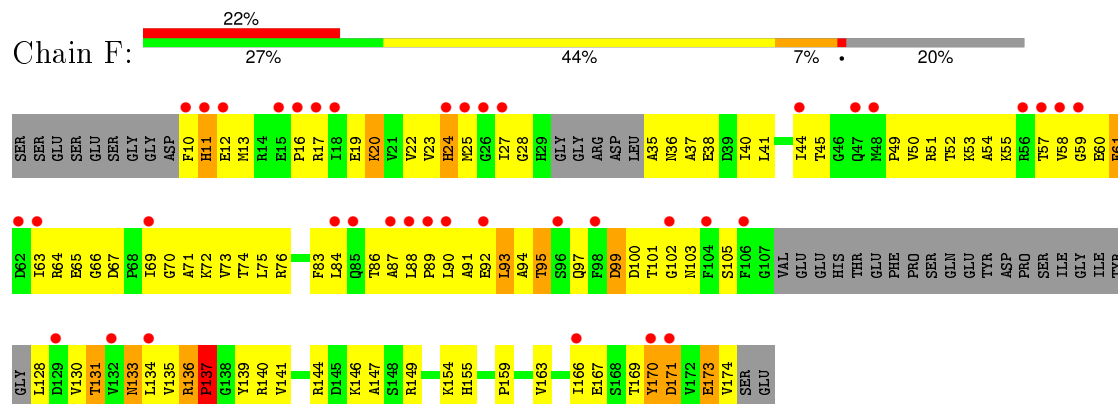
- Molecule 4: RIBOSOMAL PROTEIN L3



- Molecule 5: RIBOSOMAL PROTEIN L4

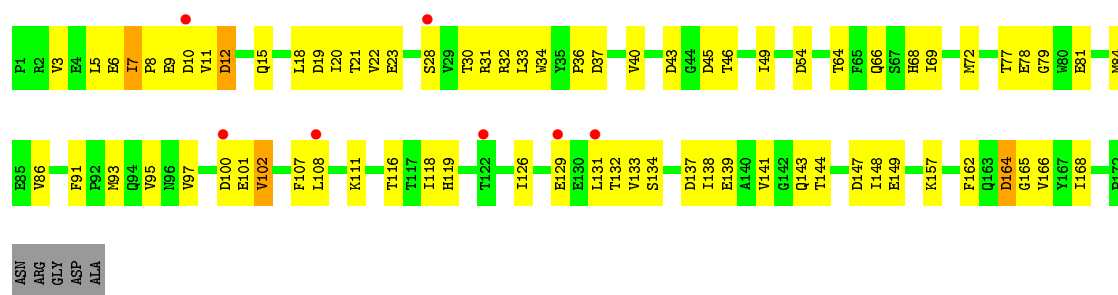


- Molecule 6: RIBOSOMAL PROTEIN L5

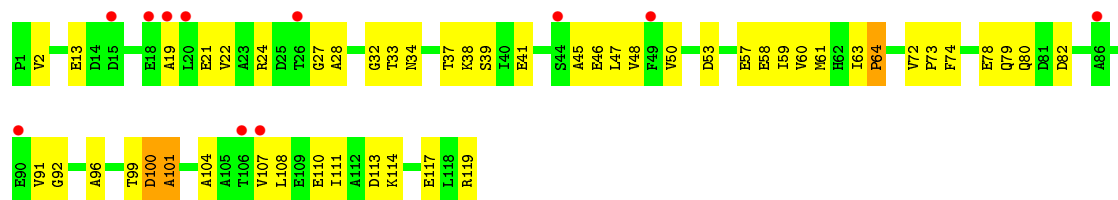


- Molecule 7: RIBOSOMAL PROTEIN L6

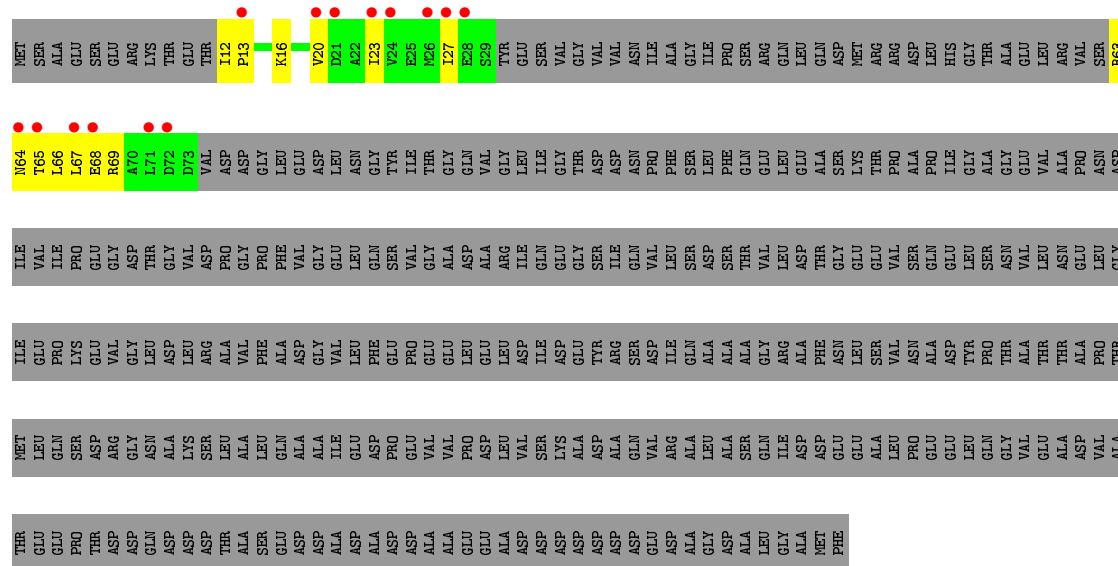




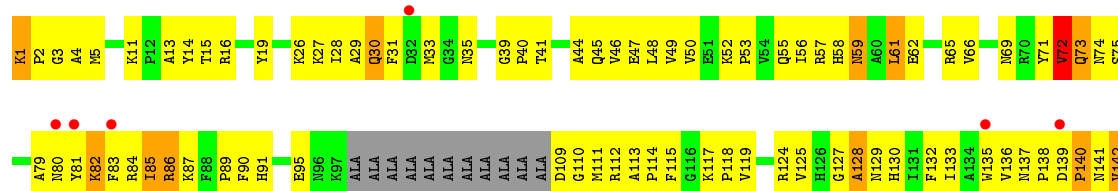
• Molecule 8: RIBOSOMAL PROTEIN L7AE



• Molecule 9: RIBOSOMAL PROTEIN L10



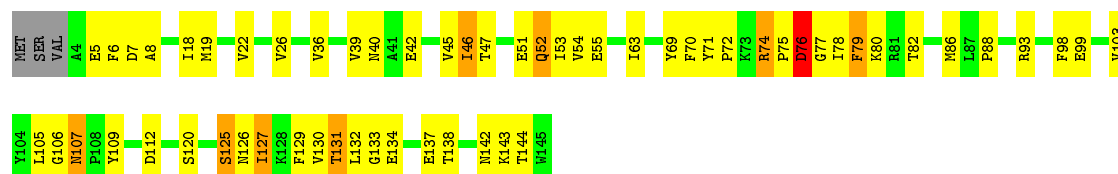
• Molecule 10: RIBOSOMAL PROTEIN L10E





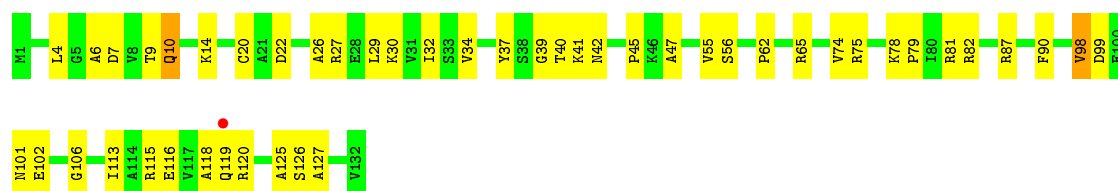
• Molecule 11: RIBOSOMAL PROTEIN L13

Chain K: 57% 34% 6% ..



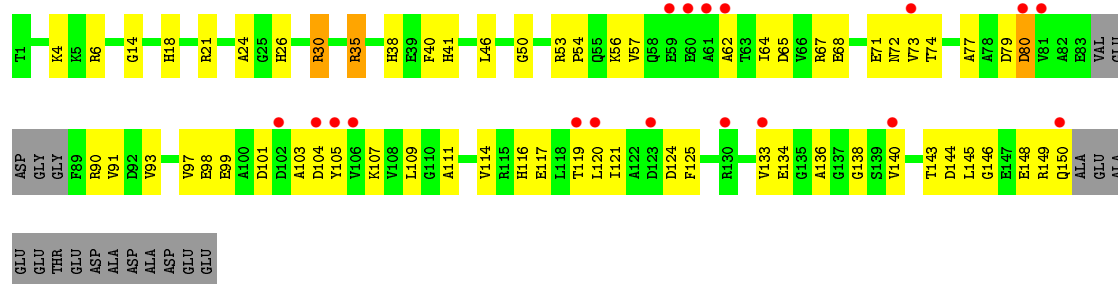
• Molecule 12: RIBOSOMAL PROTEIN L14

Chain L: 64% 34% .



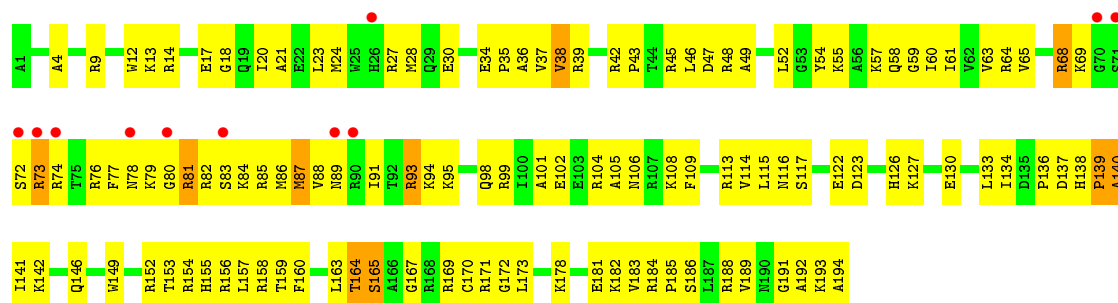
• Molecule 13: RIBOSOMAL PROTEIN L15

Chain M: 11% 50% 37% . 12%

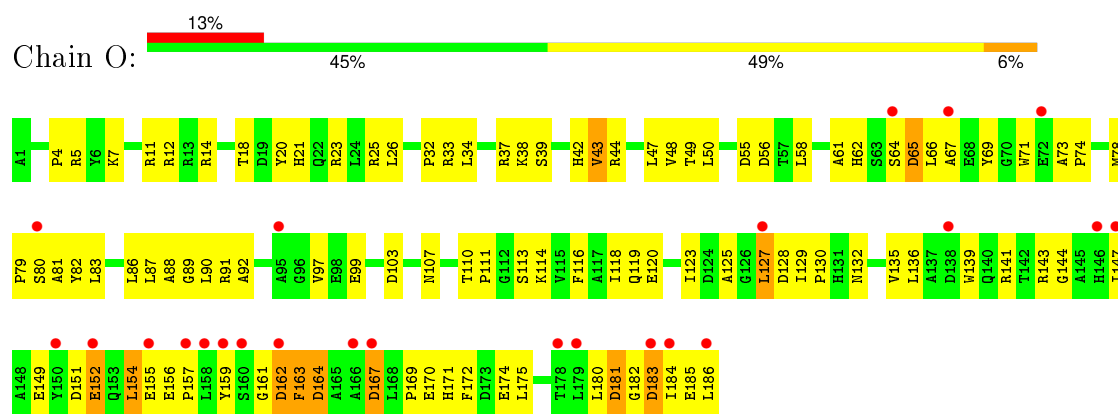


• Molecule 14: RIBOSOMAL PROTEIN L15E

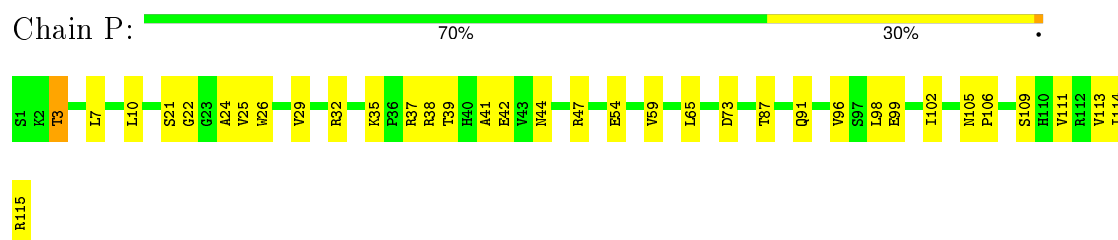
Chain N: 6% 37% 58% 5%



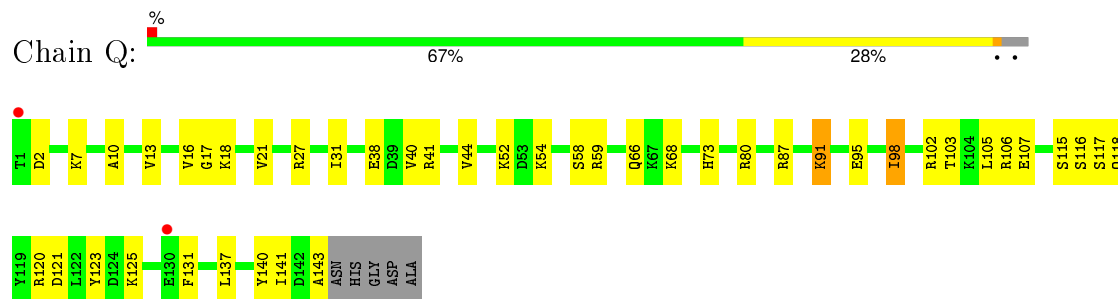
• Molecule 15: RIBOSOMAL PROTEIN L18



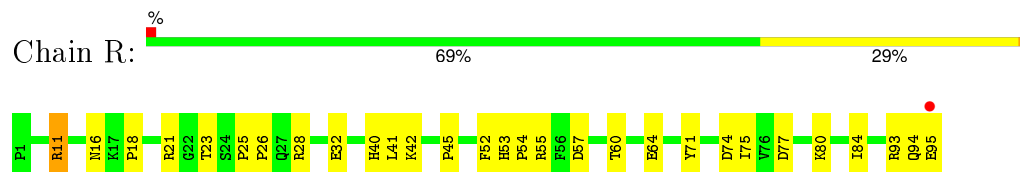
• Molecule 16: RIBOSOMAL PROTEIN L18E



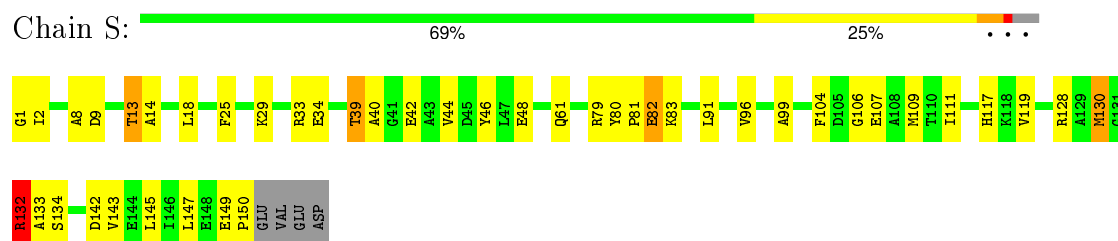
• Molecule 17: RIBOSOMAL PROTEIN L19E



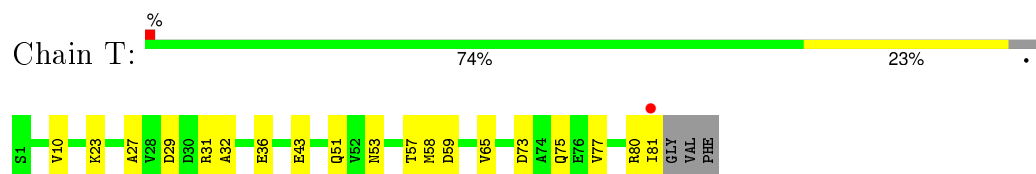
• Molecule 18: RIBOSOMAL PROTEIN L21E



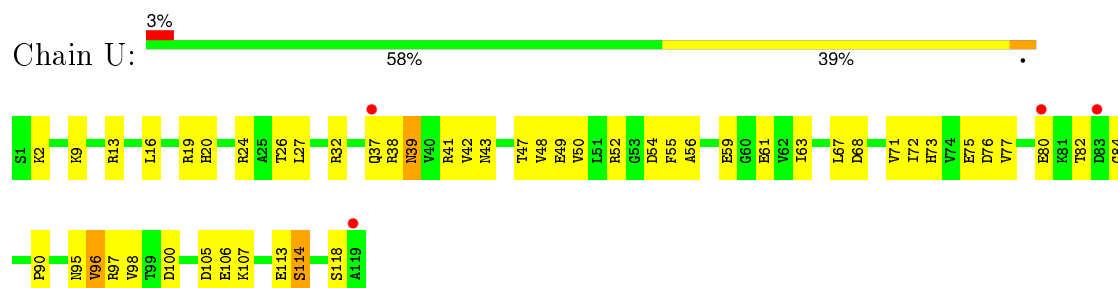
• Molecule 19: RIBOSOMAL PROTEIN L22



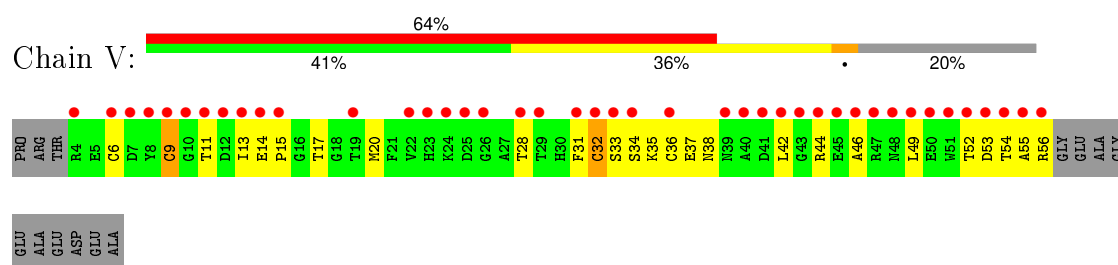
• Molecule 20: RIBOSOMAL PROTEIN L23



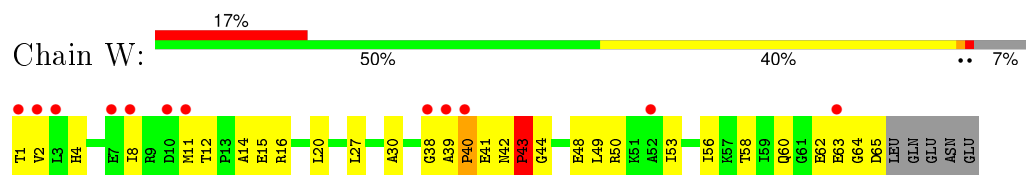
- Molecule 21: RIBOSOMAL PROTEIN L24



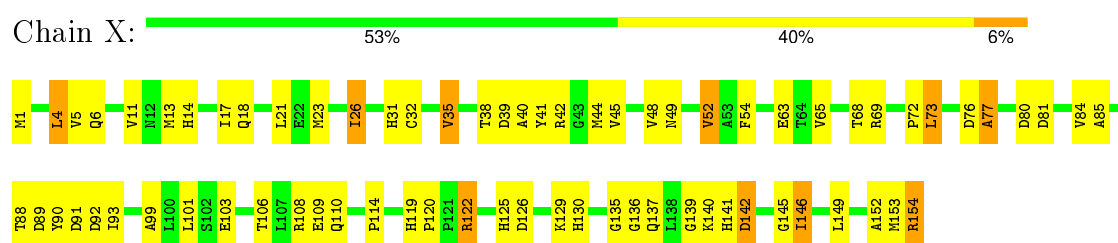
- Molecule 22: RIBOSOMAL PROTEIN L24E



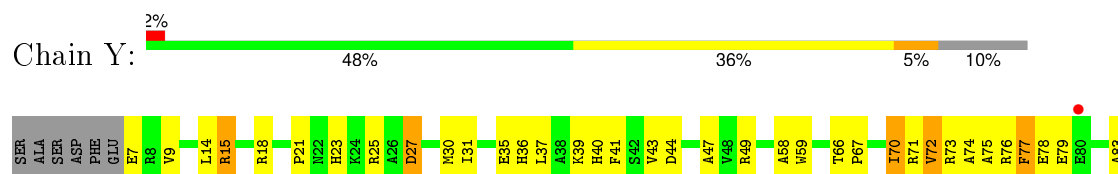
- Molecule 23: RIBOSOMAL PROTEIN L29

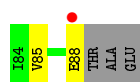


- Molecule 24: RIBOSOMAL PROTEIN L30

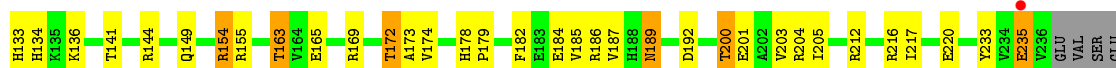
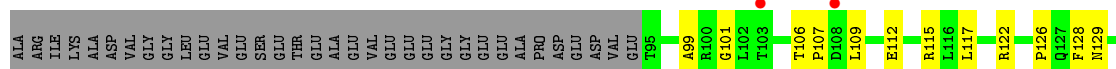


- Molecule 25: RIBOSOMAL PROTEIN L31E

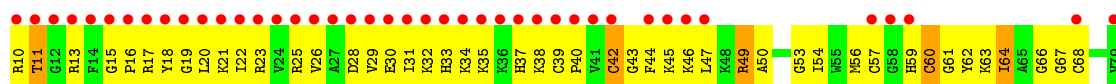




• Molecule 26: RIBOSOMAL PROTEIN L32E



• Molecule 27: RIBOSOMAL PROTEIN L37Ae



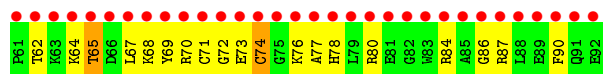
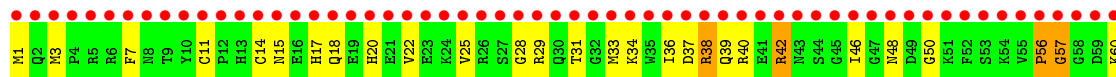
• Molecule 28: RIBOSOMAL PROTEIN L37E



• Molecule 29: RIBOSOMAL PROTEIN L39E



• Molecule 30: RIBOSOMAL PROTEIN L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 49.92 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-3.00) 92.3 (49.92-2.99)	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 1.0	Depositor
R, R_{free}	0.219 , 0.262 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 62.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 359798 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, TYK, NA, K, CL, CD

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	0.59	13/66076 (0.0%)	0.77	38/103052 (0.0%)
2	B	0.89	17/2905 (0.6%)	0.91	16/4528 (0.4%)
3	C	0.57	3/1787 (0.2%)	0.78	1/2409 (0.0%)
4	D	0.48	0/2689	0.73	0/3652
5	E	0.51	0/1883	0.74	0/2551
6	F	0.41	0/1111	0.65	0/1498
7	G	0.44	0/1382	0.63	0/1880
8	H	0.43	0/896	0.65	0/1219
9	I	0.48	0/241	0.60	0/324
10	J	0.51	0/1246	0.80	2/1686 (0.1%)
11	K	0.49	0/1135	0.68	0/1530
12	L	0.48	0/1003	0.75	0/1351
13	M	0.46	0/1126	0.74	0/1504
14	N	0.59	0/1633	0.83	2/2180 (0.1%)
15	O	0.44	0/1473	0.74	0/1999
16	P	0.50	0/873	0.73	0/1181
17	Q	0.48	0/1143	0.64	0/1521
18	R	0.49	0/748	0.76	0/1005
19	S	0.63	1/1172 (0.1%)	0.82	2/1578 (0.1%)
20	T	0.46	0/648	0.68	1/875 (0.1%)
21	U	0.44	0/957	0.72	0/1289
22	V	0.70	0/417	0.81	1/562 (0.2%)
23	W	0.41	0/502	0.62	0/675
24	X	0.49	0/1218	0.73	0/1655
25	Y	0.48	0/664	0.68	0/895
26	Z	0.47	0/1146	0.72	0/1536
27	1	0.74	0/575	0.81	0/763
28	2	0.47	0/437	0.80	0/578
29	3	0.45	0/398	0.59	0/527
30	4	0.95	0/771	0.80	0/1024
All	All	0.58	34/98255 (0.0%)	0.76	63/147027 (0.0%)

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 (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2104	C	O5'-C5'	-12.61	1.22	1.42
2	B	3023	U	C2'-O2'	12.28	1.57	1.41
1	A	2103	A	C6-N1	9.66	1.42	1.35
2	B	3025	G	O3'-P	9.21	1.72	1.61
1	A	2103	A	C5-C6	8.57	1.48	1.41
1	A	2103	A	N7-C5	8.49	1.44	1.39
2	B	3025	G	C4'-O4'	8.46	1.56	1.45
2	B	3026	C	P-O5'	-8.45	1.51	1.59
2	B	3026	C	P-OP2	-8.37	1.34	1.49
1	A	2106	C	O3'-P	-8.18	1.51	1.61
2	B	3024	U	P-OP2	-7.80	1.35	1.49
2	B	3025	G	P-OP2	-7.66	1.35	1.49
2	B	3025	G	C3'-O3'	-6.95	1.32	1.42
2	B	3023	U	O5'-C5'	6.91	1.55	1.44
1	A	2103	A	C6-N6	6.88	1.39	1.33
3	C	186	TRP	CA-CB	-6.75	1.39	1.53
2	B	3025	G	N9-C4	-6.75	1.32	1.38
1	A	1206	U	P-OP2	6.34	1.59	1.49
2	B	3025	G	C2'-O2'	6.31	1.49	1.41
19	S	132	ARG	CA-CB	-5.98	1.40	1.53
3	C	186	TRP	C-O	-5.89	1.12	1.23
1	A	2105	C	O3'-P	5.88	1.68	1.61
3	C	186	TRP	N-CA	5.76	1.57	1.46
2	B	3022	G	C5'-C4'	5.67	1.58	1.51
2	B	3025	G	C2'-C1'	5.64	1.59	1.53
1	A	2433	A	C5-C6	5.64	1.46	1.41
1	A	2099	G	C3'-O3'	5.48	1.49	1.42
2	B	3024	U	N1-C2	-5.37	1.33	1.38
1	A	2106	C	N1-C2	5.20	1.45	1.40
1	A	2104	C	O3'-P	-5.15	1.54	1.61
1	A	2103	A	N3-C4	5.15	1.38	1.34
2	B	3023	U	C3'-C2'	5.14	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3024	U	O4'-C1'	5.05	1.48	1.41
2	B	3023	U	O3'-P	-5.03	1.55	1.61

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.07	63.25	105.20
1	A	1164	U	OP2-P-O3'	-17.80	66.05	105.20
1	A	1165	G	O5'-P-OP1	-13.80	93.28	105.70
1	A	2104	C	O5'-P-OP1	-13.33	93.70	105.70
1	A	2103	A	C5'-C4'-O4'	10.96	122.25	109.10
2	B	3026	C	O5'-P-OP2	-10.22	96.50	105.70
1	A	1563	G	C2'-C3'-O3'	9.62	130.66	109.50
1	A	1942	A	C5'-C4'-C3'	8.40	129.45	116.00
1	A	1165	G	O5'-P-OP2	-8.00	98.50	105.70
1	A	1942	A	C5'-C4'-O4'	7.69	118.33	109.10
2	B	3026	C	C5'-C4'-O4'	7.20	117.74	109.10
1	A	2103	A	OP2-P-O3'	7.13	120.88	105.20
2	B	3024	U	O5'-P-OP2	7.09	119.21	110.70
22	V	36	CYS	CA-CB-SG	-6.98	101.44	114.00
1	A	1979	G	C2'-C3'-O3'	6.77	124.53	113.70
2	B	3025	G	O3'-P-O5'	6.52	116.38	104.00
2	B	3026	C	O5'-P-OP1	-6.40	99.94	105.70
1	A	2313	C	C5'-C4'-O4'	6.33	116.69	109.10
1	A	2103	A	O5'-P-OP1	-6.28	100.05	105.70
19	S	130	MET	CB-CG-SD	6.26	131.17	112.40
2	B	3103	A	C5'-C4'-O4'	6.19	116.53	109.10
1	A	1165	G	OP1-P-OP2	6.19	128.89	119.60
1	A	2103	A	O4'-C1'-N9	6.13	113.10	108.20
10	J	74	ASN	N-CA-C	-6.07	94.62	111.00
2	B	3039	U	N1-C1'-C2'	6.07	121.89	114.00
2	B	3026	C	OP1-P-OP2	5.92	128.47	119.60
1	A	2099	G	OP2-P-O3'	5.90	118.19	105.20
1	A	2106	C	N1-C1'-C2'	-5.88	105.54	112.00
1	A	2419	U	N1-C1'-C2'	5.85	121.61	114.00
2	B	3024	U	C4'-C3'-O3'	5.77	124.55	113.00
2	B	3003	A	C4'-C3'-C2'	-5.76	96.84	102.60
1	A	1504	A	C1'-O4'-C4'	-5.75	105.30	109.90
1	A	1721	C	N1-C1'-C2'	5.57	121.24	114.00
1	A	324	G	N9-C1'-C2'	-5.56	105.88	112.00
14	N	139	PRO	N-CA-C	-5.53	97.72	112.10
1	A	1819	G	C5'-C4'-C3'	5.50	124.81	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	A	C2'-C3'-O3'	5.50	122.50	113.70
1	A	2103	A	N9-C1'-C2'	-5.43	106.02	112.00
1	A	2432	C	N1-C1'-C2'	5.41	121.03	114.00
1	A	1592	G	N9-C1'-C2'	5.41	121.03	114.00
1	A	2122	C	OP2-P-O3'	5.38	117.05	105.20
1	A	871	G	C5'-C4'-O4'	-5.33	102.70	109.10
1	A	1738	C	O4'-C4'-C3'	-5.33	98.67	104.00
2	B	3026	C	O3'-P-O5'	5.33	114.13	104.00
20	T	27	ALA	N-CA-C	-5.32	96.63	111.00
2	B	3023	U	P-O5'-C5'	5.30	129.38	120.90
1	A	1842	A	N9-C1'-C2'	5.28	120.87	114.00
1	A	1971	G	O4'-C1'-N9	5.27	112.41	108.20
1	A	2726	U	N1-C1'-C2'	5.25	120.83	114.00
1	A	1062	U	N1-C1'-C2'	-5.23	106.25	112.00
14	N	73	ARG	N-CA-C	-5.23	96.89	111.00
1	A	1942	A	C1'-O4'-C4'	-5.21	105.73	109.90
2	B	3025	G	C1'-C2'-O2'	-5.20	95.01	110.60
19	S	130	MET	CG-SD-CE	5.19	108.51	100.20
1	A	1121	G	N9-C1'-C2'	-5.19	106.29	112.00
2	B	3027	C	O5'-P-OP1	-5.15	101.06	105.70
3	C	186	TRP	N-CA-C	-5.11	97.20	111.00
1	A	2034	U	N1-C1'-C2'	-5.09	106.40	112.00
1	A	2315	C	C5'-C4'-C3'	-5.06	107.90	116.00
2	B	3004	G	O5'-P-OP1	-5.05	101.16	105.70
1	A	2316	G	C5'-C4'-C3'	-5.05	107.92	116.00
2	B	3025	G	C1'-O4'-C4'	-5.03	105.88	109.90
10	J	110	GLY	N-CA-C	-5.01	100.58	113.10

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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 ⓘ

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	1175	0
2	B	2600	0	1326	79	0
3	C	1754	0	1763	134	0
4	D	2624	0	2533	189	0
5	E	1858	0	1816	121	0
6	F	1094	0	1085	137	0
7	G	1357	0	1266	76	0
8	H	885	0	854	62	0
9	I	240	0	231	20	0
10	J	1215	0	1215	160	0
11	K	1119	0	1098	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	993	0	1027	53	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	173	0
15	O	1444	0	1401	134	0
16	P	864	0	873	38	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	24	0
19	S	1149	0	1122	57	0
20	T	641	0	605	22	0
21	U	949	0	923	56	0
22	V	410	0	368	37	0
23	W	499	0	511	31	0
24	X	1195	0	1137	98	0
25	Y	654	0	653	50	0
26	Z	1130	0	1133	62	0
27	1	563	0	601	76	0
28	2	430	0	426	26	0
29	3	393	0	406	26	0
30	4	755	0	732	59	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
37	4	72	0	0	4	0
37	A	5921	0	0	271	0
37	B	142	0	0	14	0
37	C	126	0	0	20	0
37	D	146	0	0	27	0
37	E	174	0	0	34	0
37	F	51	0	0	19	0
37	G	42	0	0	9	0
37	H	26	0	0	11	0
37	I	22	0	0	5	0
37	J	79	0	0	19	0
37	K	54	0	0	5	0
37	L	60	0	0	11	0
37	M	84	0	0	18	0
37	N	127	0	0	29	0
37	O	64	0	0	18	0
37	P	42	0	0	12	0
37	Q	66	0	0	5	0
37	R	53	0	0	3	0
37	S	84	0	0	7	0
37	T	34	0	0	4	0
37	U	39	0	0	4	0
37	V	26	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3067	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 20.

All (3067) 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)
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
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.14	1.10
14:N:87:MET:CG	30:4:46:ILE:HG21	1.84	1.08
6:F:25:MET:HE2	6:F:41:LEU:HG	1.36	1.07
5:E:236:THR:HG22	5:E:239:ALA:H	1.11	1.07
1:A:871:G:H8	1:A:871:G:H5'	1.17	1.07
1:A:1134:G:H4'	10:J:151:MET:HE1	1.36	1.05
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.33	1.05
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:62:ARG:HA	4:D:65:MET:HE3	1.40	1.03
4:D:140:LEU:HA	37:D:8577:HOH:O	1.59	1.02
1:A:871:G:C8	1:A:871:G:H5'	1.94	1.02
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.40	1.01
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.46	0.97
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.47	0.97
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.47	0.97
37:A:6752:HOH:O	15:O:4:PRO:HD2	1.65	0.97
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.63	0.97
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.47	0.97
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.78	0.96
1:A:542:A:H8	1:A:542:A:H5'	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
5:E:140:VAL:HB	37:E:8456:HOH:O	1.65	0.94
4:D:86:ALA:HA	37:D:8577:HOH:O	1.67	0.94
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.50	0.93
6:F:105:SER:HB2	6:F:131:THR:HG23	1.50	0.93
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.48	0.93
1:A:1835:U:H5	1:A:1840:A:N7	1.65	0.93
1:A:1751:G:H2'	1:A:1752:G:H5''	1.51	0.93
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
12:L:10:GLN:NE2	12:L:10:GLN:H	1.68	0.91
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.51	0.91
5:E:2:GLN:HB3	37:E:8335:HOH:O	1.70	0.91
1:A:2121:G:OP2	37:A:3491:HOH:O	1.89	0.91
1:A:871:G:C5'	1:A:871:G:H8	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.34	0.90
1:A:1474:C:H5'	1:A:1474:C:H6	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
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
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.75	0.86
1:A:1166:A:H1'	1:A:1192:A:C2	2.10	0.86
1:A:1116:U:H3	1:A:1246:A:H62	1.23	0.86
1:A:1667:A:H8	1:A:1667:A:H5'	1.38	0.86
10:J:2:PRO:HB2	37:J:8367:HOH:O	1.74	0.85
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.10	0.85
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.58	0.85
10:J:162:SER:HB2	10:J:163:PRO:CD	2.04	0.85
16:P:47:ARG:HG3	16:P:47:ARG:HH11	1.41	0.85
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.76	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
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.75	0.85
1:A:2004:U:H4'	37:A:5282:HOH:O	1.76	0.85
14:N:87:MET:CB	30:4:46:ILE:HD13	2.07	0.85
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.76	0.85
1:A:645:U:OP2	13:M:4:LYS:HE2	1.77	0.85
13:M:79:ASP:HB3	37:M:8564:HOH:O	1.77	0.85
1:A:1118:A:H3'	1:A:1118:A:H8	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
29:3:41:HIS:H	29:3:45:ASN:HD22	1.24	0.84
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.41	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
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.59	0.84
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.60	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
1:A:2123:A:OP2	37:A:5264:HOH:O	1.96	0.83
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.24	0.83
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.59	0.83
5:E:246:ARG:NH1	5:E:246:ARG:HB3	1.93	0.83
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.77	0.83
26:Z:141:THR:HG23	37:Z:8589:HOH:O	1.78	0.83
14:N:172:GLY:O	14:N:183:VAL:HG11	1.79	0.83
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.61	0.83
5:E:236:THR:HG22	5:E:239:ALA:N	1.94	0.82
1:A:172:U:OP2	37:A:6192:HOH:O	1.97	0.82
1:A:346:U:H4'	37:A:6824:HOH:O	1.79	0.82
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.44	0.82
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.94	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
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
1:A:2717:C:C2'	1:A:2718:C:H5''	2.10	0.81
10:J:59:ASN:HD22	10:J:59:ASN:N	1.77	0.81
6:F:154:LYS:H	6:F:154:LYS:HD2	1.45	0.81
1:A:2533:C:H6	1:A:2533:C:H5'	1.43	0.81
22:V:9:CYS:HA	22:V:52:THR:HG23	1.60	0.81
21:U:55:PHE:HB2	37:U:6384:HOH:O	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:1:THR:HG23	23:W:2:VAL:H	1.45	0.81
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.10	0.81
1:A:1184:C:H1'	37:A:7456:HOH:O	1.81	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:H8	1:A:545:G:H5'	1.46	0.80
1:A:1118:A:C8	1:A:1118:A:H3'	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
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
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.28	0.80
37:A:7549:HOH:O	30:4:60:LYS:HG3	1.81	0.80
1:A:797:A:H4'	27:1:10:ARG:N	1.97	0.80
14:N:61:ILE:HG13	37:N:8621:HOH:O	1.80	0.80
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.64	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
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
26:Z:133:HIS:HD2	37:Z:8582:HOH:O	1.65	0.79
1:A:559:U:H6	1:A:559:U:H5'	1.47	0.79
1:A:1160:G:H5'	1:A:1161:A:C5'	2.11	0.79
10:J:26:LYS:HG2	10:J:28:ILE:H	1.47	0.79
4:D:62:ARG:CA	4:D:65:MET:HE3	2.13	0.79
1:A:1679:C:H5'	37:A:9314:HOH:O	1.83	0.79
2:B:3014:G:H8	2:B:3014:G:H5'	1.48	0.79
1:A:1160:G:C5'	1:A:1161:A:H5'	2.10	0.78
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.18	0.78
10:J:142:VAL:HG13	37:J:8383:HOH:O	1.83	0.78
37:A:5770:HOH:O	14:N:170:CYS:SG	2.41	0.78
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.13	0.78
11:K:74:ARG:HH11	11:K:74:ARG:HB3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2506:A:O2'	1:A:2507:G:H8	1.64	0.78
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.83	0.78
13:M:136:ALA:HB3	37:M:8577:HOH:O	1.83	0.78
1:A:289:G:H22	1:A:363:A:H2	1.32	0.78
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.13	0.78
5:E:246:ARG:HH11	5:E:246:ARG:HB3	1.47	0.78
16:P:32:ARG:O	16:P:32:ARG:HD3	1.83	0.78
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.65	0.78
1:A:381:G:H5''	37:A:4290:HOH:O	1.82	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
37:A:9547:HOH:O	4:D:267:LYS:HD3	1.84	0.77
1:A:1116:U:O2'	1:A:1118:A:H2	1.68	0.77
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.65	0.77
1:A:2586:U:H3	1:A:2592:G:H22	1.30	0.77
6:F:27:ILE:HG22	6:F:28:GLY:H	1.49	0.77
2:B:3069:U:OP1	15:O:4:PRO:HG3	1.85	0.77
1:A:560:C:H42	1:A:597:A:H61	1.33	0.77
1:A:506:G:H22	1:A:509:A:C5'	1.97	0.77
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.65	0.77
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.65	0.77
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.80	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
14:N:164:THR:HG23	14:N:165:SER:N	1.99	0.77
12:L:81:ARG:HB2	12:L:87:ARG:NH1	1.99	0.77
3:C:192:VAL:HB	37:C:8597:HOH:O	1.85	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
19:S:99:ALA:HB1	19:S:109:MET:CE	2.16	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
37:A:6278:HOH:O	6:F:99:ASP:HA	1.84	0.76
4:D:41:PHE:HA	4:D:79:MET:HE2	1.68	0.76
1:A:1603:A:H5'	1:A:1605:G:O4'	1.85	0.76
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.68	0.76
8:H:91:VAL:HG12	8:H:92:GLY:N	2.00	0.76
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.68	0.75
1:A:542:A:C8	1:A:542:A:H5'	2.18	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
1:A:877:G:H5'	1:A:878:G:OP1	1.86	0.75
1:A:282:C:H1'	1:A:368:C:N4	2.00	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
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: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
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.49	0.75
1:A:2054:A:N3	19:S:128:ARG:NH2	2.34	0.75
1:A:1329:A:N1	34:A:8513:CL:CL	2.56	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
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
15:O:80:SER:HB2	37:O:8535:HOH:O	1.85	0.74
37:A:9075:HOH:O	4:D:214:PRO:HD2	1.87	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
27:1:49:ARG:HD2	37:1:8427:HOH:O	1.88	0.74
1:A:960:G:H4'	37:A:7419: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
10:J:140:PRO:HB3	37:J:8383:HOH:O	1.87	0.74
1:A:1701:A:H5'	37:A:6266:HOH:O	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:148:GLU:HA	37:M:8576:HOH:O	1.87	0.74
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.20	0.74
5:E:107:ARG:HB3	5:E:107:ARG:NH1	2.03	0.73
37:A:9383:HOH:O	14:N:94:LYS:HE2	1.88	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
9:I:12:ILE:HA	37:I:4499:HOH:O	1.88	0.73
24:X:110:GLN:HA	24:X:110:GLN:NE2	2.02	0.73
1:A:1666:C:H2'	1:A:1667:A:H5'	1.69	0.73
1:A:111:C:O2'	28:2:20:ARG:HG2	1.89	0.73
19:S:39:THR:HB	19:S:42:GLU:HG3	1.70	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
3:C:53:ALA:HB3	37:C:8609:HOH:O	1.89	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
30:4:65:THR:HG23	30:4:67:LEU:HG	1.71	0.73
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:HH11	11:K:93:ARG:HB3	1.52	0.72
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	1.88	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
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.19	0.72
3:C:199:HIS:CD2	3:C:201:PHE:H	2.06	0.72
37:A:4641:HOH:O	20:T:23:LYS:HE2	1.89	0.72
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.71	0.72
4:D:179:LEU:O	4:D:183:GLU:HG2	1.88	0.72
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.19	0.72
8:H:46:GLU:O	8:H:73:PRO:HD2	1.89	0.72
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.71	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
1:A:1372:A:H3'	37:A:7173:HOH:O	1.88	0.72
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.54	0.72
1:A:1191:A:H3'	1:A:1192:A:H5''	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:12:ILE:N	9:I:13:PRO:HD3	2.04	0.72
5:E:27:ARG:HG3	5:E:29:ASP:OD1	1.88	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
24:X:154:ARG:C	37:X:4276:HOH:O	2.28	0.71
15:O:164:ASP:CG	15:O:167:ASP:HA	2.10	0.71
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.20	0.71
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.72	0.71
15:O:113:SER:HB2	37:O:8556:HOH:O	1.89	0.71
1:A:236:A:H4'	1:A:237:G:H5'	1.73	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
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.73	0.71
1:A:1701:A:H4'	1:A:1702:U:H5''	1.71	0.71
13:M:143:THR:HG22	13:M:144:ASP:N	2.05	0.71
1:A:2346:C:O2'	6:F:52:THR:HG21	1.91	0.71
26:Z:220:GLU:HG2	37:Z:8551:HOH:O	1.89	0.71
1:A:338:C:H4'	5:E:174:ILE:CD1	2.20	0.71
1:A:870:G:C2'	1:A:871:G:H5''	2.20	0.71
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.59	0.71
1:A:1329:A:H2	37:A:4657:HOH:O	1.72	0.71
29:3:41:HIS:N	29:3:45:ASN:HD22	1.88	0.71
14:N:85:ARG:NE	37:N:8519:HOH:O	2.19	0.71
6:F:97:GLN:O	6:F:97:GLN:HG2	1.89	0.71
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.73	0.71
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.72	0.71
14:N:138:HIS:ND1	14:N:139:PRO:O	2.19	0.71
2:B:3013:A:O2'	2:B:3014:G:H5''	1.91	0.71
19:S:39:THR:HG23	19:S:107:GLU:O	1.90	0.71
1:A:2420:G:O2'	1:A:2421:G:H5'	1.91	0.71
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.71	0.71
14:N:60:ILE:C	14:N:61:ILE:HD12	2.11	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
14:N:186:SER:O	14:N:189:VAL:HG12	1.90	0.71
12:L:10:GLN:N	12:L:10:GLN:HE21	1.89	0.70
2:B:3029:C:H2'	2:B:3030:C:H5'	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:47:THR:HB	21:U:100:ASP:HB3	1.72	0.70
1:A:553:G:P	26:Z:204:ARG:HH22	2.14	0.70
19:S:106:GLY:HA2	19:S:109:MET:CE	2.20	0.70
27:1:30:GLU:HA	27:1:33:HIS:CB	2.21	0.70
10:J:139:ASP:HA	37:J:8373:HOH:O	1.91	0.70
8:H:99:THR:HA	37:H:3461:HOH:O	1.91	0.70
1:A:2419:U:H5''	1:A:2420:G:H5'	1.73	0.70
24:X:80:ASP:O	24:X:84:VAL:HG23	1.90	0.70
14:N:139:PRO:O	14:N:140:ALA:HB3	1.92	0.70
1:A:1353:C:P	37:A:4652:HOH:O	2.50	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
1:A:338:C:H4'	5:E:174:ILE:HD11	1.73	0.70
7:G:11:VAL:HG12	7:G:12:ASP:N	2.07	0.70
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.56	0.70
3:C:121:ALA:O	3:C:124:VAL:HG22	1.92	0.70
1:A:1160:G:N3	37:A:5610:HOH:O	2.24	0.70
1:A:544:G:C2'	1:A:545:G:H5''	2.21	0.70
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.73	0.70
10:J:41:THR:HA	37:J:8397:HOH:O	1.91	0.70
8:H:53:ASP:OD1	8:H:80:GLN:HB2	1.92	0.70
1:A:2768:A:H2'	1:A:2769:C:O4'	1.91	0.70
6:F:25:MET:HE1	6:F:37:ALA:HB1	1.73	0.69
1:A:2748:G:H2'	37:A:7534:HOH:O	1.92	0.69
1:A:1753:C:O2	4:D:229:ARG:NH2	2.25	0.69
1:A:871:G:C5'	1:A:871:G:C8	2.65	0.69
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.22	0.69
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.74	0.69
19:S:9:ASP:O	19:S:13:THR:HB	1.92	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
1:A:214:U:H5'	37:A:6120:HOH:O	1.91	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: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
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
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.75	0.69
14:N:104:ARG:O	14:N:108:LYS:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:U:H2'	1:A:282:C:O4'	1.92	0.69
1:A:131:A:OP2	37:A:3135:HOH:O	2.10	0.69
30:4:48:ASN:ND2	30:4:50:GLY:H	1.91	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
6:F:23:VAL:HG23	6:F:23:VAL:O	1.92	0.69
5:E:139:VAL:HG13	37:E:8453:HOH: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
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
3:C:35:GLY:O	3:C:36:ASP:HB3	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
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.26	0.69
11:K:131:THR:HG22	11:K:134:GLU:H	1.55	0.69
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.75	0.69
14:N:152:ARG:HG3	37:N:8554:HOH:O	1.93	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
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:204:A:H2'	1:A:205:U:H5'	1.74	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
11:K:19:MET:CE	11:K:132:LEU:HD11	2.22	0.68
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.75	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
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.06	0.68
37:A:9116:HOH:O	14:N:82:ARG:HD2	1.93	0.68
1:A:20:G:H21	19:S:117:HIS:HD2	1.40	0.68
10:J:27:LYS:H	10:J:58:HIS:CD2	2.06	0.68
1:A:1187:U:HO2'	1:A:1189:A:H2	1.42	0.68
24:X:65:VAL:HA	24:X:68:THR:HG22	1.76	0.68
1:A:2467:A:OP1	37:A:9040:HOH:O	2.12	0.68
1:A:1919:A:H4'	37:A:4819:HOH:O	1.92	0.68
22:V:14:GLU:O	22:V:17:THR:HB	1.93	0.68
1:A:2578:G:H8	1:A:2578:G:H5'	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.09	0.68
25:Y:15:ARG:HH11	25:Y:15:ARG:HB3	1.59	0.68
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.59	0.68
1:A:1667:A:H5'	1:A:1667:A:C8	2.27	0.68
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.11	0.68
11:K:19:MET:HE2	11:K:132:LEU:HD11	1.75	0.68
16:P:87:THR:O	16:P:91:GLN:HG3	1.94	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
10:J:49:VAL:O	10:J:157:ILE:HG23	1.94	0.67
3:C:105:VAL:HG12	3:C:106:CYS:N	2.10	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
6:F:95:THR:O	6:F:97:GLN:N	2.24	0.67
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.77	0.67
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.58	0.67
23:W:56:ILE:O	23:W:60:GLN:HG3	1.95	0.67
24:X:88:THR:HG22	24:X:89:ASP:N	2.10	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
1:A:869:G:OP1	14:N:79:LYS:HE2	1.94	0.67
1:A:506:G:H22	1:A:509:A:H5'	1.59	0.67
1:A:88:G:N7	29:3:28:LYS:HD2	2.09	0.67
14:N:69:LYS:O	14:N:73:ARG:NH2	2.25	0.67
1:A:447:A:OP1	21:U:2:LYS:HG2	1.95	0.67
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.76	0.67
4:D:248:ARG:HG2	37:K:8541:HOH:O	1.94	0.67
5:E:237:GLU:HB2	37:E:8433:HOH:O	1.94	0.67
24:X:149:LEU:HG	24:X:153:MET:HE2	1.76	0.67
1:A:2420:G:H4'	37:A:4067:HOH:O	1.95	0.67
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.77	0.67
1:A:2646:G:H1'	31:A:9000:TYK:H221	1.76	0.67
1:A:711:G:H1'	37:A:7079:HOH:O	1.93	0.67
22:V:6:CYS:SG	22:V:31:PHE:HA	2.35	0.67
6:F:69:ILE:O	6:F:69:ILE:HG22	1.95	0.67
1:A:2830:U:H3'	37:A:5204:HOH:O	1.94	0.67
10:J:71:TYR:C	10:J:73:GLN:H	1.98	0.67
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:14:GLU:OE1	22:V:15:PRO:HD2	1.94	0.67
20:T:43:GLU:HB3	37:T:8343:HOH:O	1.95	0.67
1:A:450:C:OP1	5:E:184:ARG:NH2	2.22	0.67
5:E:233:THR:HG22	5:E:234:VAL:N	2.09	0.67
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.77	0.66
1:A:1909:A:N1	1:A:2128:G:H1'	2.10	0.66
30:4:7:PHE:HE2	30:4:22:VAL:HG21	1.60	0.66
1:A:1170:U:O2'	1:A:1172:G:N7	2.24	0.66
27:1:42:CYS:SG	27:1:44:PHE:N	2.60	0.66
4:D:162:MET:HE3	4:D:308:LEU:HD21	1.76	0.66
1:A:1766:U:O2	1:A:1778:A:H5'	1.95	0.66
4:D:190:MET:HE2	4:D:194:PHE:HD1	1.59	0.66
9:I:63:ARG:N	37:I:2569:HOH:O	2.28	0.66
1:A:21:G:C5'	19:S:2:ILE:HA	2.24	0.66
11:K:133:GLY:O	11:K:137:GLU:HG3	1.96	0.66
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.76	0.66
37:A:9380:HOH:O	27:1:34:LYS:HD3	1.94	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
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.31	0.66
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:4515:HOH:O	10:J:151:MET:HE2	1.95	0.66
27:1:10:ARG:HA	37:1:8414:HOH:O	1.94	0.66
1:A:1878:G:H1'	37:A:6101:HOH:O	1.96	0.66
13:M:145:LEU:O	13:M:148:GLU:HG3	1.96	0.66
5:E:214:THR:HG23	37:E:8441:HOH:O	1.94	0.66
4:D:175:LEU:HD23	4:D:175:LEU:C	2.15	0.66
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.94	0.66
1:A:664:U:OP1	37:A:3755:HOH:O	2.13	0.66
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.30	0.66
23:W:64:GLY:O	23:W:65:ASP:HB2	1.96	0.66
20:T:53:ASN:ND2	37:T:8322:HOH:O	2.28	0.66
23:W:12:THR:HG22	23:W:15:GLU:CG	2.16	0.66
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.93	0.66
26:Z:235:GLU:CD	26:Z:235:GLU:H	1.99	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
14:N:30:GLU:O	14:N:34:GLU:HG3	1.96	0.66
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.77	0.66
1:A:603:A:H5''	1:A:604:G:OP1	1.95	0.66
5:E:236:THR:CG2	5:E:239:ALA:H	2.01	0.65
1:A:820:G:OP1	27:1:17:ARG:NH2	2.23	0.65
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.96	0.65
7:G:132:THR:HB	37:G:2227:HOH:O	1.96	0.65
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.77	0.65
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.31	0.65
1:A:845:U:OP2	37:A:9197:HOH:O	2.14	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: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
5:E:236:THR:H	5:E:239:ALA:HB3	1.61	0.65
1:A:506:G:H22	1:A:509:A:H5''	1.61	0.65
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.44	0.65
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.32	0.65
37:A:9495:HOH:O	4:D:18:ARG:HD3	1.97	0.65
5:E:234:VAL:O	5:E:234:VAL:HG22	1.97	0.65
3:C:33:GLU:O	3:C:34:ASP:HB2	1.95	0.65
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.29	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
13:M:53:ARG:NH2	13:M:57:VAL:HG12	2.10	0.65
4:D:145:HIS:HD2	4:D:146:THR:O	1.79	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
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.25	0.65
1:A:2310:G:OP2	10:J:114:PRO:HD2	1.96	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
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.62	0.65
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.79	0.65
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.27	0.65
22:V:9:CYS:CA	22:V:52:THR:HG23	2.26	0.65
1:A:2421:G:H3'	1:A:2422:U:C5'	2.27	0.65
14:N:139:PRO:O	14:N:140:ALA:CB	2.45	0.65
14:N:172:GLY:C	14:N:183:VAL:HG11	2.18	0.65
1:A:2908:A:H2'	1:A:2909:G:O4'	1.97	0.65
24:X:130:HIS:O	24:X:136:GLY:HA3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:154:ARG:NE	37:N:8639:HOH:O	2.31	0.64
4:D:258:GLY:H	4:D:260:HIS:CE1	2.14	0.64
28:2:25:LYS:HE2	37:3:7213:HOH:O	1.95	0.64
5:E:236:THR:HA	37:E:8456:HOH:O	1.96	0.64
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.26	0.64
1:A:2432:C:O2'	1:A:2433:A:H5'	1.98	0.64
11:K:107:ASN:ND2	11:K:109:TYR:H	1.95	0.64
6:F:135:VAL:HG22	6:F:136:ARG:H	1.60	0.64
1:A:2637:A:H5'	37:A:9265:HOH:O	1.97	0.64
1:A:962:C:C1'	15:O:5:ARG:NH1	2.59	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
37:A:6951:HOH:O	23:W:4:HIS:HB3	1.97	0.64
1:A:2281:C:H2'	1:A:2282:U:H5'	1.80	0.64
1:A:31:C:H4'	37:A:7413:HOH:O	1.97	0.64
1:A:1700:C:OP2	37:A:6013:HOH:O	2.14	0.64
1:A:272:A:H3'	37:A:7522:HOH:O	1.97	0.64
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.12	0.64
1:A:1185:U:H2'	1:A:1186:C:C6	2.32	0.64
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.31	0.64
1:A:1123:A:C6	1:A:1238:C:H5'	2.33	0.64
11:K:99:GLU:HA	37:K:8573:HOH:O	1.97	0.64
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.30	0.64
1:A:2359:G:N7	37:A:3675:HOH:O	2.29	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
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.80	0.64
1:A:1329:A:C2	37:A:4657:HOH:O	2.49	0.64
3:C:94:LEU:HD23	3:C:94:LEU:N	2.12	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
2:B:3020:G:O2'	2:B:3021:G:H5'	1.98	0.63
1:A:188:C:H5''	14:N:163:LEU:HD21	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.80	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
4:D:162:MET:CE	4:D:308:LEU:HD21	2.27	0.63
1:A:282:C:O2'	1:A:283:U:H5'	1.99	0.63
27:1:18:TYR:HB3	27:1:22:ILE:HG21	1.79	0.63
1:A:263:U:O4'	8:H:59:ILE:HD13	1.98	0.63
1:A:157:G:OP2	37:A:9466:HOH:O	2.15	0.63
6:F:25:MET:CE	6:F:37:ALA:HB1	2.28	0.63
24:X:4:LEU:O	24:X:32:CYS:HA	1.99	0.63
1:A:1159:G:P	37:A:4264:HOH:O	2.56	0.63
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.28	0.63
1:A:272:A:H5'	1:A:273:G:OP2	1.99	0.63
15:O:58:LEU:HD12	15:O:58:LEU:N	2.14	0.63
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.13	0.63
26:Z:186:ARG:HH11	26:Z:186:ARG:HG2	1.64	0.63
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
16:P:47:ARG:NH1	16:P:47:ARG:HG3	2.12	0.63
23:W:39:ALA:C	23:W:41:GLU:H	2.02	0.63
1:A:251:C:O2'	1:A:252:C:H5'	1.99	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
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
6:F:95:THR:C	6:F:97:GLN:H	2.02	0.63
1:A:941:G:O2'	1:A:942:U:H5'	1.98	0.63
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.29	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
1:A:656:G:OP2	16:P:37:ARG:HD2	1.98	0.62
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.81	0.62
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.28	0.62
10:J:127:GLY:O	10:J:128:ALA:HB3	1.99	0.62
1:A:2094:G:H4'	4:D:245:SER:HB3	1.81	0.62
24:X:38:THR:HG22	37:X:3580:HOH:O	1.99	0.62
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.80	0.62
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
24:X:13:MET:CE	24:X:17:ILE:HG22	2.29	0.62
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.62	0.62
28:2:28:HIS:CD2	28:2:31:LYS:HG3	2.34	0.62
14:N:154:ARG:HG3	37:N:8612:HOH:O	1.99	0.62
10:J:166:ASN:N	10:J:166:ASN:HD22	1.97	0.62
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.40	0.62
5:E:12:THR:HB	37:E:8446:HOH:O	1.98	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
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.29	0.62
18:R:25:PRO:HB2	37:R:4350:HOH:O	2.00	0.62
1:A:2064:U:H5'	1:A:2652:U:H4'	1.82	0.62
6:F:101:THR:HG22	37:F:7400:HOH:O	1.99	0.62
1:A:1119:G:H8	11:K:52:GLN:NE2	1.97	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
22:V:35:LYS:NZ	37:V:6621:HOH:O	2.27	0.62
1:A:299:U:H5'	37:A:7324:HOH:O	1.99	0.62
21:U:19:ARG:HD3	21:U:67:LEU:O	2.00	0.62
27:1:46:LYS:HB2	27:1:57:CYS:SG	2.38	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
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
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.82	0.62
1:A:1187:U:O2'	1:A:1189:A:H2	1.82	0.62
1:A:2346:C:H6	1:A:2346:C:O5'	1.83	0.62
23:W:58:THR:O	23:W:62:GLU:HG3	2.00	0.62
1:A:1735:C:O2'	1:A:1736:A:H5'	1.99	0.62
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.81	0.62
1:A:960:G:N3	1:A:960:G:H2'	2.15	0.62
3:C:11:ARG:HD3	37:C:8517:HOH:O	1.99	0.62
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.65	0.61
1:A:1377:C:H5'	1:A:1377:C:H6	1.65	0.61
16:P:42:GLU:HB2	37:P:2176:HOH:O	1.97	0.61
37:A:4806:HOH:O	11:K:47:THR:HB	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:61:GLY:HA3	37:1:8425:HOH:O	1.99	0.61
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.34	0.61
15:O:154:LEU:O	15:O:155:GLU:HB3	2.00	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
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
1:A:2044:G:OP1	25:Y:23:HIS:HE1	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
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
37:A:4162:HOH:O	26:Z:186:ARG:HD2	2.00	0.61
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.81	0.61
1:A:155:C:OP2	14:N:188:ARG:NH1	2.28	0.61
5:E:133:ARG:HD2	37:E:8411:HOH:O	2.01	0.61
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.83	0.61
24:X:110:GLN:HA	24:X:110:GLN:HE21	1.62	0.61
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.31	0.61
1:A:558:C:C2'	1:A:559:U:H5''	2.31	0.61
26:Z:189:ASN:ND2	26:Z:192:ASP:H	1.97	0.61
37:A:6229:HOH:O	22:V:56:ARG:HB3	2.00	0.61
1:A:119:A:H2'	1:A:120:A:H5''	1.83	0.61
5:E:132:ASP:HB3	37:E:8365:HOH:O	2.01	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
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.99	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: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
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
2:B:3107:C:H5	37:B:3167:HOH:O	1.84	0.61
1:A:625:U:H5''	1:A:1044:C:N4	2.15	0.61
12:L:29:LEU:HB3	12:L:55:VAL:CG1	2.27	0.60
2:B:3049:G:H5''	37:B:4707:HOH:O	2.00	0.60
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.31	0.60
1:A:2324:G:H4'	1:A:2418:G:O2'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2649:A:H8	1:A:2649:A:H5'	1.66	0.60
30:4:57:GLY:HA2	37:4:8529:HOH:O	2.00	0.60
6:F:25:MET:CE	6:F:41:LEU:HG	2.23	0.60
12:L:55:VAL:HG12	12:L:56:SER:N	2.16	0.60
24:X:122:ARG:CG	24:X:122:ARG:HH11	2.13	0.60
27:1:42:CYS:SG	27:1:43:GLY:N	2.74	0.60
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.66	0.60
1:A:121:U:OP2	29:3:10:ARG:NH2	2.34	0.60
5:E:78:ARG:NH1	5:E:78:ARG:HG3	2.12	0.60
14:N:48:ARG:NH2	37:N:8561:HOH:O	2.32	0.60
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.81	0.60
29:3:18:ASN:HD21	29:3:40:ARG:H	1.49	0.60
13:M:26:HIS:HB2	37:M:8512:HOH:O	2.00	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
1:A:661:G:C5	1:A:686:A:C2	2.89	0.60
1:A:2780:C:H2'	1:A:2781:U:C6	2.37	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
3:C:191:GLY:HA2	3:C:194:MET:HE3	1.83	0.60
14:N:133:LEU:O	14:N:134:ILE:HD13	2.01	0.60
7:G:69:ILE:HA	7:G:72:MET:CE	2.32	0.60
1:A:775:G:OP1	28:2:16:HIS:HE1	1.85	0.60
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.83	0.60
5:E:115:LEU:O	5:E:118:THR:HB	2.01	0.60
5:E:16:VAL:HG12	5:E:17:ASP:N	2.16	0.60
1:A:2533:C:C6	1:A:2533:C:H5'	2.32	0.60
9:I:12:ILE:N	9:I:13:PRO:CD	2.65	0.60
1:A:204:A:C2'	1:A:205:U:H5'	2.30	0.60
37:A:4540:HOH:O	5:E:50:GLU:HG2	2.00	0.60
7:G:81:GLU:HG2	7:G:134:SER:CB	2.32	0.60
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.82	0.60
6:F:37:ALA:O	6:F:40:ILE:HG12	2.02	0.60
1:A:283:U:H5''	1:A:284:C:P	2.42	0.60
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.83	0.60
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.82	0.60
1:A:474:C:O3'	5:E:73:LEU:HD21	2.01	0.60
1:A:558:C:H5'	37:A:5233:HOH:O	2.02	0.60
1:A:2768:A:O2'	1:A:2769:C:H5'	2.02	0.60
1:A:212:A:O4'	1:A:214:U:C6	2.55	0.60
1:A:2361:A:H2'	1:A:2362:A:C8	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:136:ARG:HD2	6:F:155:HIS:O	2.01	0.60
4:D:36:PRO:HA	4:D:168:GLY:CA	2.31	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
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.31	0.60
1:A:2429:A:H2'	1:A:2430:A:C8	2.37	0.60
1:A:2748:G:H5'	37:A:7534:HOH:O	2.02	0.59
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.02	0.59
1:A:2088:C:H1'	1:A:2841:A:N1	2.17	0.59
1:A:1422:U:H2'	1:A:1423:C:C6	2.36	0.59
1:A:2851:G:O2'	1:A:2852:A:H5'	2.01	0.59
34:K:8501:CL:CL	37:K:8547:HOH:O	2.53	0.59
19:S:119:VAL:HG12	19:S:119:VAL:O	2.01	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
15:O:163:PHE:HA	37:O:8520:HOH:O	2.02	0.59
1:A:151:A:C2	1:A:442:A:C8	2.90	0.59
5:E:118:THR:O	5:E:136:VAL:HG13	2.02	0.59
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.83	0.59
4:D:79:MET:HE1	37:D:8623:HOH:O	2.02	0.59
6:F:135:VAL:HG22	6:F:136:ARG:N	2.16	0.59
23:W:44:GLY:O	23:W:48:GLU:HG2	2.01	0.59
37:A:9111:HOH:O	5:E:103:ASN:HB3	2.01	0.59
1:A:739:G:C5	37:A:7536:HOH:O	2.51	0.59
1:A:2505:G:O2'	1:A:2506:A:H5'	2.02	0.59
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.32	0.59
37:A:3960:HOH:O	21:U:82:THR:HA	2.02	0.59
1:A:951:A:C2'	1:A:952:G:H5'	2.33	0.59
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.84	0.59
14:N:74:ARG:NH2	37:N:8629:HOH:O	2.32	0.59
10:J:136:VAL:HG22	10:J:137:ASN:O	2.02	0.59
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.32	0.59
15:O:151:ASP:O	15:O:154:LEU:HB2	2.03	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
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:1819:G:H2'	1:A:1820:G:H4'	1.84	0.59
1:A:820:G:H5'	1:A:821:U:H5'	1.84	0.59
10:J:136:VAL:HG23	37:J:8345:HOH:O	2.03	0.59
2:B:3003:A:N6	2:B:3022:G:H1'	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.18	0.59
1:A:182:G:H4'	14:N:157:LEU:HD13	1.83	0.59
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.32	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
1:A:485:A:N3	1:A:487:G:H5''	2.17	0.59
3:C:188:ASN:OD1	37:C:8559:HOH:O	2.16	0.59
10:J:144:GLU:HA	10:J:144:GLU:OE1	2.03	0.59
30:4:40:ARG:HD2	37:4:8553:HOH:O	2.02	0.59
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.02	0.59
1:A:57:C:H5''	37:A:6739:HOH:O	2.02	0.59
6:F:105:SER:CB	6:F:131:THR:HG23	2.30	0.58
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.33	0.58
4:D:7:ARG:HD3	4:D:9:GLY:O	2.02	0.58
20:T:51:GLN:NE2	20:T:53:ASN:HD21	2.01	0.58
2:B:3042:C:H2'	37:B:6700:HOH:O	2.02	0.58
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.84	0.58
7:G:32:ARG:O	7:G:33:LEU:HD23	2.03	0.58
4:D:254:GLN:HG2	4:D:255:GLY:N	2.18	0.58
10:J:44:ALA:HA	10:J:163:PRO:O	2.04	0.58
1:A:559:U:C6	1:A:559:U:H5'	2.36	0.58
1:A:485:A:O2'	1:A:487:G:H5'	2.03	0.58
9:I:64:ASN:N	9:I:64:ASN:HD22	2.01	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
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.04	0.58
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.15	0.58
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.33	0.58
4:D:168:GLY:N	4:D:174:ARG:HD3	2.18	0.58
3:C:37:VAL:HG22	37:C:8601:HOH:O	2.03	0.58
6:F:50:VAL:O	6:F:71:ALA:HA	2.03	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
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.18	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
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.43	0.58
1:A:1615:A:H4'	37:A:5863:HOH:O	2.02	0.58
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.86	0.58
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.66	0.58
24:X:41:TYR:O	24:X:45:VAL:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2064:U:OP1	37:A:3324:HOH:O	2.17	0.58
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.33	0.58
8:H:58:GLU:HA	8:H:61:MET:HG3	1.86	0.58
14:N:68:ARG:O	14:N:68:ARG:HD3	2.04	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
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.86	0.58
1:A:2502:C:C2'	1:A:2503:A:H5'	2.33	0.58
1:A:157:G:H4'	14:N:95:LYS:HE3	1.85	0.58
2:B:3044:A:O4'	6:F:76:ARG:NE	2.37	0.58
1:A:2394:A:OP1	37:A:7078:HOH:O	2.17	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
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.85	0.58
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.03	0.58
1:A:2415:A:C2	15:O:25:ARG:HB3	2.39	0.58
1:A:1200:A:H4'	37:A:7328:HOH:O	2.02	0.58
13:M:73:VAL:HG23	13:M:74:THR:H	1.67	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
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.38	0.58
1:A:1333:U:H2'	1:A:1334:C:C6	2.39	0.58
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.34	0.58
1:A:2897:C:H2'	1:A:2898:G:H8	1.68	0.58
1:A:1127:C:H2'	1:A:1128:U:H5'	1.85	0.58
3:C:211:LYS:NZ	37:C:8575:HOH:O	2.37	0.58
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.36	0.58
1:A:281:U:O2'	1:A:282:C:H5'	2.04	0.58
1:A:1118:A:C8	1:A:1118:A:C3'	2.81	0.58
25:Y:25:ARG:CZ	37:Y:3861:HOH:O	2.50	0.58
26:Z:212:ARG:HD2	37:Z:8601:HOH:O	2.03	0.58
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.04	0.58
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.84	0.58
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.85	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
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.17	0.58
23:W:39:ALA:N	23:W:40:PRO:CD	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:ARG:HD2	4:D:163:GLU:OE2	2.03	0.58
5:E:84:VAL:O	5:E:85:LYS:HB2	2.04	0.58
1:A:2783:A:H3'	37:A:5208:HOH:O	2.03	0.58
10:J:75:SER:C	10:J:79:ALA:HB2	2.24	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:1825:U:O4'	1:A:1999:C:H5''	2.04	0.57
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.87	0.57
22:V:52:THR:CG2	22:V:54:THR:HB	2.34	0.57
1:A:289:G:N2	1:A:363:A:H2	1.99	0.57
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.04	0.57
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.04	0.57
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.66	0.57
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.07	0.57
4:D:14:GLY:HA2	4:D:15:PRO:C	2.25	0.57
19:S:132:ARG:CZ	37:S:8583:HOH:O	2.52	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
24:X:26:ILE:O	24:X:26:ILE:CG1	2.52	0.57
19:S:39:THR:HG22	19:S:42:GLU:H	1.69	0.57
7:G:7:ILE:HD11	7:G:11:VAL:C	2.25	0.57
1:A:182:G:H5'	37:A:5132:HOH:O	2.04	0.57
23:W:64:GLY:O	23:W:65:ASP:CB	2.52	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
6:F:27:ILE:HG22	6:F:28:GLY:N	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
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.20	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
4:D:2:GLN:CD	37:D:8618:HOH:O	2.42	0.57
1:A:513:A:N3	37:A:3635:HOH:O	2.33	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
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
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
7:G:15:GLN:HG2	7:G:19:ASP: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
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
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.40	0.57
1:A:1505:U:H6	1:A:1505:U:H5'	1.68	0.57
1:A:2729:C:O2'	1:A:2730:G:H5'	2.05	0.57
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.70	0.57
1:A:136:C:H2'	1:A:137:U:O4'	2.04	0.57
4:D:275:GLY:O	4:D:291:ASP:HA	2.05	0.57
1:A:1827:G:H2'	1:A:1828:G:C8	2.40	0.57
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.39	0.57
1:A:1192:A:O2'	1:A:1193:A:OP1	2.20	0.57
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.86	0.57
15:O:64:SER:C	15:O:66:LEU:H	2.08	0.57
6:F:25:MET:HE1	6:F:37:ALA:O	2.05	0.57
8:H:99:THR:O	8:H:99:THR:HG23	2.04	0.57
3:C:36:ASP:OD2	3:C:85:ASP:HB2	2.04	0.57
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.05	0.57
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.68	0.57
24:X:149:LEU:HG	24:X:153:MET:CE	2.35	0.57
1:A:681:G:N3	1:A:681:G:H5'	2.20	0.57
37:L:1387:HOH:O	22:V:20:MET:HE3	2.04	0.57
18:R:40:HIS:HD2	18:R:60:THR:OG1	1.88	0.57
1:A:2484:U:C2	37:A:9601:HOH:O	2.52	0.57
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.35	0.57
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.86	0.56
1:A:2466:G:H5'	37:A:3621:HOH:O	2.05	0.56
1:A:545:G:H5'	1:A:545:G:C8	2.35	0.56
2:B:3014:G:H5'	2:B:3014:G:C8	2.34	0.56
13:M:143:THR:HG22	13:M:144:ASP:H	1.70	0.56
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.18	0.56
1:A:183:A:H5'	14:N:157:LEU:HD12	1.87	0.56
28:2:25:LYS:HG2	28:2:25:LYS:O	2.04	0.56
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.34	0.56
1:A:1855:G:H8	3:C:144:GLU:OE2	1.88	0.56
4:D:280:VAL:CG1	4:D:334:SER:HA	2.35	0.56
7:G:137:ASP:O	7:G:141:VAL:HG23	2.05	0.56
37:A:3731:HOH:O	21:U:9:LYS:HD2	2.04	0.56
15:O:110:THR:HB	15:O:113:SER:OG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:125:GLU:O	4:D:129:ARG:HG3	2.05	0.56
14:N:24:MET:O	14:N:28:MET:HG3	2.05	0.56
30:4:3:MET:O	30:4:90:PHE:HA	2.04	0.56
15:O:37:ARG:NE	37:O:8533:HOH:O	2.38	0.56
22:V:52:THR:HG22	22:V:54:THR:HB	1.88	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: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
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.87	0.56
1:A:470:U:O2'	28:2:16:HIS:HD2	1.87	0.56
8:H:2:VAL:HG22	8:H:57:GLU:OE1	2.04	0.56
19:S:132:ARG:HG2	19:S:133:ALA:N	2.20	0.56
1:A:1947:G:N2	1:A:1966:U:C2	2.73	0.56
1:A:816:G:H5'	1:A:1598:A:H4'	1.86	0.56
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.87	0.56
16:P:25:VAL:HG23	16:P:26:TRP:N	2.21	0.56
1:A:1523:G:H2'	1:A:1524:U:C6	2.40	0.56
1:A:2010:A:H2'	37:A:5935:HOH:O	2.05	0.56
1:A:1189:A:H1'	1:A:1209:C:C1'	2.36	0.56
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.86	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
2:B:3002:U:H4'	2:B:3002:U:OP2	2.05	0.56
28:2:8:GLN:HE22	28:2:11:LYS:NZ	2.03	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:1151:G:OP1	9:I:63:ARG:NH1	2.39	0.56
1:A:558:C:O2'	1:A:559:U:H5''	2.06	0.56
1:A:88:G:H5'	1:A:88:G:H8	1.70	0.56
1:A:2710:U:H1'	37:A:7618:HOH:O	2.06	0.56
1:A:1234:U:N3	4:D:244:PRO:HB3	2.20	0.56
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.88	0.56
11:K:52:GLN:HG3	11:K:53:ILE:N	2.21	0.56
1:A:1205:U:H2'	1:A:1206:U:C5'	2.34	0.56
8:H:110:GLU:O	8:H:114:LYS:HG3	2.06	0.56
8:H:19:ALA:O	8:H:22:VAL:HG22	2.06	0.56
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.06	0.56
1:A:1308:A:H5'	37:A:6916:HOH:O	2.06	0.56
1:A:1162:G:H2'	37:A:6565:HOH:O	2.05	0.56
1:A:1636:G:O2'	1:A:1637:A:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:37:GLN:OE1	21:U:118:SER:HA	2.05	0.56
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.88	0.56
1:A:283:U:H5''	1:A:284:C:OP2	2.06	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
1:A:1423:C:O2'	1:A:1424:A:H5'	2.06	0.56
1:A:1025:C:H5'	24:X:23:MET:O	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
1:A:536:A:H3'	37:A:5022:HOH:O	2.05	0.56
17:Q:143:ALA:HA	37:Q:2178:HOH:O	2.06	0.56
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.87	0.56
1:A:1528:A:H2'	1:A:1529:G:O4'	2.06	0.56
1:A:1086:A:C6	24:X:11:VAL:HG11	2.40	0.56
1:A:1918:U:OP2	37:A:3996:HOH:O	2.18	0.56
11:K:74:ARG:CB	11:K:74:ARG:HH11	2.17	0.56
8:H:28:ALA:HB3	8:H:99:THR:O	2.05	0.56
2:B:3028:U:H2'	2:B:3029:C:C6	2.41	0.56
1:A:2362:A:H2'	1:A:2363:G:C8	2.40	0.56
28:2:1:THR:HB	37:2:6858:HOH:O	2.06	0.56
1:A:168:C:O2'	1:A:169:A:H5'	2.06	0.56
37:A:6687:HOH:O	26:Z:165:GLU:HB3	2.05	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.55
15:O:155:GLU:O	15:O:156:GLU:HG3	2.06	0.55
1:A:660:A:H4'	1:A:661:G:O5'	2.06	0.55
26:Z:144:ARG:CZ	37:Z:8612:HOH:O	2.53	0.55
1:A:926:A:O2'	13:M:41:HIS:HD2	1.88	0.55
14:N:35:PRO:O	37:N:8537:HOH:O	2.18	0.55
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.22	0.55
1:A:2038:A:OP2	4:D:224:LYS:NZ	2.32	0.55
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.88	0.55
2:B:3055:U:H4'	2:B:3056:A:H8	1.70	0.55
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.41	0.55
20:T:51:GLN:HE21	20:T:53:ASN:ND2	2.03	0.55
14:N:154:ARG:CD	37:N:8639:HOH:O	2.55	0.55
10:J:57:ARG:O	10:J:61:LEU:HD22	2.06	0.55
1:A:1166:A:H1'	1:A:1192:A:N1	2.20	0.55
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.36	0.55
1:A:1044:C:H5''	37:A:9022:HOH:O	2.07	0.55
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.87	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:83:PHE:HZ	10:J:146:TRP:HE1	1.51	0.55
10:J:59:ASN:ND2	10:J:59:ASN:N	2.50	0.55
24:X:21:LEU:HD13	24:X:26:ILE:HD11	1.87	0.55
9:I:12:ILE:HG22	9:I:12:ILE:O	2.06	0.55
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.42	0.55
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.27	0.55
7:G:79:GLY:HA3	37:G:7046:HOH:O	2.06	0.55
5:E:37:ALA:O	5:E:41:ASN:ND2	2.39	0.55
1:A:2301:A:H5'	1:A:2302:A:H5'	1.88	0.55
1:A:1659:A:H2'	1:A:1660:G:O4'	2.07	0.55
3:C:211:LYS:NZ	37:C:8622:HOH:O	2.39	0.55
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.42	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
10:J:149:ALA:C	10:J:151:MET:H	2.10	0.55
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.89	0.55
5:E:107:ARG:HH11	5:E:107:ARG:CB	2.19	0.55
8:H:91:VAL:CG1	8:H:92:GLY:N	2.70	0.55
4:D:7:ARG:NH1	4:D:11:LEU:HD21	2.22	0.55
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.07	0.55
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.06	0.55
13:M:104:ASP:O	13:M:105:TYR:HB3	2.05	0.55
6:F:99:ASP:HB3	6:F:103:ASN:H	1.71	0.55
24:X:88:THR:O	37:X:2374:HOH:O	2.18	0.55
1:A:1116:U:O2'	1:A:1118:A:C2	2.51	0.55
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.07	0.55
21:U:19:ARG:NH1	21:U:68:ASP:O	2.40	0.55
1:A:2649:A:C8	1:A:2649:A:H5'	2.42	0.55
37:A:4432:HOH:O	14:N:146:GLN:HG2	2.06	0.55
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.22	0.55
1:A:564:G:H1'	37:A:6293:HOH:O	2.07	0.55
1:A:158:A:O2'	1:A:159:G:H5'	2.07	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
14:N:38:VAL:C	14:N:63:VAL:HG13	2.28	0.55
4:D:248:ARG:O	4:D:251:VAL:CG1	2.55	0.55
37:L:408:HOH:O	22:V:37:GLU:HB3	2.06	0.55
4:D:305:ASP:O	4:D:306:LYS:CB	2.55	0.55
15:O:73:ALA:N	37:O:8563:HOH:O	2.40	0.55
1:A:625:U:H5'	37:A:3162:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.42	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:75:GLU:C	4:D:77:PRO:HD3	2.28	0.55
27:1:39:CYS:CB	27:1:47:LEU:HD21	2.36	0.54
13:M:114:VAL:HG11	37:M:8577:HOH:O	2.08	0.54
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.20	0.54
4:D:7:ARG:CD	4:D:9:GLY:O	2.54	0.54
15:O:152:GLU:C	15:O:154:LEU:H	2.09	0.54
8:H:58:GLU:HA	8:H:61:MET:HE2	1.88	0.54
13:M:104:ASP:HB3	37:M:8569:HOH:O	2.07	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:371:U:H2'	1:A:372:A:H8	1.72	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
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.89	0.54
1:A:567:U:H5''	37:X:5817:HOH:O	2.07	0.54
22:V:9:CYS:HA	22:V:52:THR:CG2	2.35	0.54
1:A:484:A:N1	1:A:506:G:H4'	2.21	0.54
1:A:1741:U:O2'	1:A:2723:G:H4'	2.07	0.54
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.72	0.54
27:1:22:ILE:O	27:1:26:VAL:HG23	2.08	0.54
16:P:26:TRP:N	37:P:3062:HOH:O	2.39	0.54
1:A:710:G:OP1	16:P:24:ALA:HB3	2.07	0.54
21:U:106:GLU:HG3	37:U:4913:HOH:O	2.07	0.54
18:R:32:GLU:HA	18:R:71:TYR:OH	2.07	0.54
1:A:1477:C:O2'	1:A:1478:U:H5'	2.06	0.54
1:A:1393:A:H2'	1:A:1394:C:C6	2.43	0.54
10:J:31:PHE:HE2	10:J:87:LYS:O	1.89	0.54
25:Y:37:LEU:CD1	25:Y:85:VAL:HG21	2.28	0.54
1:A:2779:G:H21	7:G:143:GLN:NE2	2.05	0.54
8:H:104:ALA:HA	37:H:6617:HOH:O	2.08	0.54
19:S:29:LYS:HB3	37:S:8533:HOH:O	2.07	0.54
1:A:134:U:C2	1:A:145:A:C2	2.95	0.54
6:F:10:PHE:CG	6:F:11:HIS:N	2.75	0.54
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.90	0.54
10:J:154:THR:HB	10:J:155:PRO:HD3	1.89	0.54
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.42	0.54
10:J:14:TYR:N	10:J:91:HIS:CE1	2.76	0.54
1:A:558:C:H2'	1:A:559:U:C5'	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:143:THR:HG22	13:M:145:LEU:H	1.71	0.54
4:D:24:PRO:HG3	4:D:204:GLY:HA2	1.89	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
1:A:590:A:H2'	1:A:591:A:H5'	1.90	0.54
12:L:30:LYS:O	12:L:55:VAL:HG13	2.07	0.54
24:X:90:TYR:CD1	24:X:90:TYR:N	2.75	0.54
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.39	0.54
1:A:1165:G:OP1	1:A:1165:G:H3'	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
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.35	0.54
26:Z:133:HIS:CD2	37:Z:8582:HOH:O	2.50	0.54
37:A:4330:HOH:O	16:P:37:ARG:HG3	2.07	0.54
1:A:2325:C:H1'	37:A:4122:HOH:O	2.08	0.54
6:F:140:ARG:O	6:F:144:ARG:HG2	2.08	0.54
1:A:1118:A:H8	1:A:1119:G:H5''	1.72	0.54
5:E:76:ARG:HD3	37:E:8368:HOH:O	2.07	0.54
4:D:43:GLY:O	4:D:308:LEU:HD12	2.07	0.54
1:A:305:A:C5	1:A:329:A:C2	2.96	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:2672:C:H1'	37:D:8634:HOH:O	2.08	0.54
6:F:59:GLY:C	6:F:61:PHE:H	2.11	0.54
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.72	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: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
24:X:139:GLY:O	24:X:141:HIS:HD2	1.90	0.54
4:D:146:THR:O	4:D:159:PRO:HB3	2.07	0.54
1:A:431:G:P	14:N:48:ARG:HH12	2.31	0.54
1:A:221:G:H2'	1:A:222:A:C8	2.42	0.54
6:F:170:TYR:O	6:F:171:ASP:HB3	2.07	0.54
1:A:349:U:O2'	1:A:350:C:H5'	2.08	0.54
7:G:37:ASP:OD1	11:K:125:SER:HB3	2.08	0.54
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.08	0.54
14:N:79:LYS:HD2	37:N:8555:HOH:O	2.08	0.54
26:Z:186:ARG:NH1	26:Z:186:ARG:HG2	2.22	0.54
1:A:138:U:H5''	1:A:139:C:OP2	2.08	0.54
27:1:34:LYS:HE2	37:1:8424:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:71:ARG:CD	37:Y:2171:HOH:O	2.55	0.54
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.23	0.54
10:J:71:TYR:C	10:J:73:GLN:N	2.59	0.54
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.06	0.54
8:H:58:GLU:HG3	8:H:61:MET:HE1	1.89	0.54
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.43	0.54
1:A:2906:A:H5'	1:A:2907:C:O4'	2.07	0.54
4:D:82:VAL:O	4:D:82:VAL:HG12	2.07	0.54
30:4:34:LYS:HB2	30:4:37:ASP:OD2	2.07	0.54
4:D:72:THR:HB	37:D:8603:HOH:O	2.07	0.54
14:N:79:LYS:NZ	37:N:8565:HOH:O	2.41	0.54
1:A:2507:G:H2'	1:A:2510:C:H42	1.73	0.54
9:I:16:LYS:O	9:I:20:VAL:HG23	2.08	0.54
27:1:19:GLY:O	27:1:23:ARG:HG2	2.07	0.54
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.38	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
7:G:15:GLN:NE2	7:G:40:VAL:O	2.41	0.53
5:E:107:ARG:CB	5:E:107:ARG:NH1	2.70	0.53
1:A:2123:A:H5'	14:N:89:ASN:HD21	1.73	0.53
1:A:2769:C:C2'	1:A:2770:G:H5'	2.38	0.53
1:A:1168:C:H2'	1:A:1169:U:O4'	2.07	0.53
13:M:73:VAL:HG23	13:M:74:THR:N	2.23	0.53
4:D:204:GLY:HA3	37:D:8652:HOH:O	2.07	0.53
1:A:926:A:O2'	13:M:41:HIS:CD2	2.61	0.53
4:D:119:HIS:O	4:D:121:PRO:HD3	2.07	0.53
1:A:2256:G:H2'	1:A:2257:G:H5'	1.90	0.53
10:J:69:ASN:O	10:J:72:VAL:HG12	2.08	0.53
1:A:1711:A:O2'	1:A:1712:A:H5'	2.08	0.53
1:A:1559:A:H1'	37:A:5842:HOH:O	2.07	0.53
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.43	0.53
1:A:1182:C:H1'	1:A:1192:A:H8	1.73	0.53
10:J:139:ASP:N	10:J:140:PRO:CD	2.70	0.53
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.90	0.53
6:F:57:THR:HG23	6:F:63:ILE:CB	2.38	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
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:2721:U:H4'	12:L:87:ARG:HG3	1.90	0.53
1:A:1733:A:H4'	4:D:212:GLN:HA	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1887:U:OP1	27:1:21:LYS:HE3	2.09	0.53
3:C:179:MET:HG2	3:C:186:TRP:CB	2.39	0.53
1:A:2276:U:H2'	1:A:2277:U:C6	2.42	0.53
10:J:109:ASP:HB2	37:J:8348:HOH:O	2.08	0.53
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.34	0.53
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.90	0.53
14:N:186:SER:OG	14:N:189:VAL:HG12	2.09	0.53
13:M:143:THR:CG2	13:M:144:ASP:N	2.70	0.53
7:G:22:VAL:O	7:G:28:SER:HA	2.08	0.53
1:A:631:A:N3	1:A:2073:G:O2'	2.38	0.53
10:J:118:PRO:HD2	37:J:8341:HOH:O	2.09	0.53
6:F:35:ALA:N	37:F:5576:HOH:O	2.41	0.53
1:A:56:G:H5''	23:W:50:ARG:NH1	2.23	0.53
1:A:2433:A:H2'	1:A:2434:A:C8	2.43	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:1299:G:O6	13:M:6:ARG:HD3	2.08	0.53
6:F:146:LYS:NZ	15:O:107:ASN:ND2	2.54	0.53
4:D:51:VAL:HG21	4:D:327:VAL:HG13	1.90	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
1:A:1060:C:H6	1:A:1060:C:H5'	1.73	0.53
1:A:2860:G:H1'	37:A:6782:HOH:O	2.09	0.53
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.09	0.53
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.24	0.53
1:A:2349:G:OP1	6:F:20:LYS:NZ	2.34	0.53
1:A:1172:G:H1'	37:A:4947:HOH:O	2.08	0.53
13:M:57:VAL:HG12	13:M:57:VAL:O	2.09	0.53
1:A:489:A:C8	21:U:82:THR:HG22	2.44	0.53
26:Z:112:GLU:OE1	26:Z:112:GLU:HA	2.09	0.53
1:A:2256:G:H2'	1:A:2257:G:C5'	2.38	0.53
4:D:88:GLU:O	4:D:88:GLU:HG3	2.08	0.53
19:S:82:GLU:HG3	19:S:83:LYS:N	2.23	0.53
14:N:87:MET:SD	37:N:8530:HOH:O	2.59	0.53
5:E:142:ASP:OD1	5:E:236:THR:HG23	2.08	0.53
15:O:37:ARG:HD3	34:O:8507:CL:CL	2.46	0.53
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.90	0.53
1:A:1189:A:H1'	1:A:1209:C:H1'	1.91	0.53
1:A:51:G:O2'	1:A:52:A:H5'	2.08	0.53
22:V:33:SER:O	22:V:37:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:7:PHE:HE2	30:4:22:VAL:CG2	2.21	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
37:A:7662:HOH:O	26:Z:172:THR:HB	2.08	0.53
1:A:1857:A:N6	1:A:2247:C:H1'	2.24	0.53
2:B:3096:C:H2'	2:B:3097:U:C6	2.44	0.53
1:A:45:A:N6	1:A:147:G:C4	2.77	0.53
1:A:1525:G:H5'	1:A:1526:A:OP2	2.09	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
1:A:1441:G:O2'	1:A:1442:A:H5'	2.09	0.53
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.08	0.53
1:A:2321:A:O2'	1:A:2322:U:H3'	2.09	0.53
26:Z:144:ARG:NE	37:Z:8612:HOH:O	2.41	0.53
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.07	0.53
23:W:11:MET:HB3	23:W:15:GLU:HB2	1.90	0.53
10:J:163:PRO:O	10:J:164:ALA:HB2	2.09	0.53
1:A:1209:C:C2	1:A:1210:G:C8	2.97	0.53
27:1:28:ASP:O	27:1:31:ILE:HG22	2.09	0.53
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.39	0.53
6:F:86:THR:HG23	37:F:7477:HOH:O	2.09	0.53
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.91	0.53
2:B:3041:C:C6	6:F:50:VAL:HG21	2.44	0.53
1:A:113:A:OP2	1:A:114:A:H5''	2.09	0.53
1:A:21:G:H4'	19:S:2:ILE:HG22	1.90	0.53
1:A:516:A:P	37:A:5623:HOH:O	2.67	0.53
14:N:76:ARG:HG2	14:N:76:ARG:HH11	1.73	0.53
1:A:2089:A:O2'	1:A:2090:G:H5'	2.09	0.53
7:G:93:MET:HE1	7:G:165:GLY:N	2.24	0.53
1:A:256:C:H2'	1:A:257:G:O4'	2.08	0.53
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.41	0.53
3:C:18:ALA:O	3:C:20:SER:N	2.38	0.53
15:O:89:GLY:O	15:O:92:ALA:HB3	2.09	0.52
2:B:3006:C:P	15:O:37:ARG:NH1	2.82	0.52
1:A:1159:G:H21	1:A:1189:A:H8	1.55	0.52
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.73	0.52
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.90	0.52
1:A:512:G:O3'	1:A:513:A:H8	1.92	0.52
13:M:149:ARG:O	13:M:150:GLN:HB2	2.09	0.52
29:3:48:ASP:O	29:3:49:GLU:HB2	2.10	0.52
1:A:2478:U:O2'	1:A:2479:A:H5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.73	0.52
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.24	0.52
1:A:1166:A:H61	1:A:1180:U:H3	1.56	0.52
6:F:64:ARG:O	6:F:67:ASP:OD2	2.26	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:2911:C:H3'	37:A:5528:HOH:O	2.09	0.52
26:Z:144:ARG:NH2	37:Z:8612:HOH:O	2.42	0.52
4:D:74:ILE:HG13	37:D:8603:HOH:O	2.08	0.52
1:A:415:A:O2'	1:A:416:G:H5'	2.09	0.52
16:P:21:SER:OG	16:P:106:PRO:HB2	2.09	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
16:P:10:LEU:HD13	16:P:99:GLU:HG3	1.91	0.52
4:D:215:VAL:HB	4:D:234:ARG:HH12	1.75	0.52
37:A:3818:HOH:O	10:J:11:LYS:HE2	2.08	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
9:I:63:ARG:O	9:I:67:LEU:HG	2.09	0.52
1:A:2004:U:H5''	1:A:2005:G:C8	2.45	0.52
1:A:2780:C:H2'	1:A:2781:U:H6	1.73	0.52
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.91	0.52
7:G:11:VAL:CG1	7:G:12:ASP:N	2.72	0.52
37:A:6303:HOH:O	6:F:55:LYS:HB2	2.10	0.52
7:G:69:ILE:HA	7:G:72:MET:HE3	1.91	0.52
37:A:9312:HOH:O	27:1:16:PRO:HG3	2.10	0.52
5:E:242:GLU:HG3	37:E:8383:HOH:O	2.09	0.52
1:A:2604:A:H5'	37:A:5768:HOH:O	2.10	0.52
20:T:81:ILE:HG23	37:T:8335:HOH:O	2.09	0.52
15:O:119:GLN:O	15:O:123:ILE:HG13	2.09	0.52
1:A:1535:G:H2'	1:A:1536:C:C6	2.44	0.52
6:F:163:VAL:HA	37:F:6326:HOH:O	2.09	0.52
17:Q:115:SER:O	17:Q:117:SER:N	2.43	0.52
1:A:1666:C:C2'	1:A:1667:A:C5'	2.88	0.52
1:A:1450:C:C4'	1:A:1451:C:OP2	2.57	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
21:U:32:ARG:NH1	21:U:38:ARG:NH1	2.57	0.52
1:A:1829:A:H2'	1:A:1830:C:H5'	1.92	0.52
4:D:76:THR:N	4:D:77:PRO:HD3	2.25	0.52
6:F:11:HIS:O	6:F:12:GLU:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:297:VAL:HB	37:D:8603:HOH:O	2.10	0.52
1:A:1058:A:H2'	1:A:1060:C:H5''	1.90	0.52
4:D:27:ASN:H	4:D:27:ASN:HD22	1.57	0.52
1:A:2833:C:C2	1:A:2848:G:N2	2.78	0.52
1:A:834:G:H5''	1:A:835:U:O5'	2.10	0.52
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.10	0.52
1:A:1119:G:C8	11:K:52:GLN:NE2	2.78	0.52
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.40	0.52
1:A:285:A:H2'	1:A:286:U:O4'	2.09	0.52
1:A:2638:G:H5'	37:A:4902:HOH:O	2.09	0.52
1:A:2382:A:OP1	30:4:80:ARG:HG2	2.10	0.52
1:A:92:G:H4'	23:W:44:GLY:HA3	1.91	0.52
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.45	0.52
7:G:157:LYS:NZ	37:G:2401:HOH:O	2.43	0.52
1:A:160:A:C4	1:A:177:A:C2	2.98	0.52
1:A:1003:U:O2	10:J:90:PHE:CZ	2.62	0.52
4:D:41:PHE:CE1	4:D:79:MET:HG3	2.43	0.52
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.27	0.52
1:A:1269:G:H2'	1:A:1270:U:C6	2.45	0.52
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.56	0.52
19:S:39:THR:HB	19:S:42:GLU:CD	2.29	0.52
6:F:94:ALA:O	6:F:95:THR:O	2.28	0.52
1:A:1847:A:OP1	3:C:175:LYS:HG3	2.10	0.52
3:C:191:GLY:HA2	3:C:194:MET:CE	2.40	0.52
16:P:25:VAL:HG23	16:P:26:TRP:H	1.74	0.52
1:A:2795:C:O2'	1:A:2796:U:H5'	2.09	0.52
1:A:344:C:H2'	1:A:345:G:O4'	2.09	0.52
4:D:87:TYR:O	4:D:138:GLY:N	2.36	0.52
10:J:5:MET:HG3	37:J:8367:HOH:O	2.09	0.52
27:1:11:THR:HG21	27:1:23:ARG:HB2	1.91	0.52
11:K:19:MET:HE1	11:K:79:PHE:HA	1.91	0.52
8:H:2:VAL:HG11	14:N:23:LEU:HD23	1.91	0.52
1:A:2819:C:H2'	1:A:2820:A:C8	2.44	0.52
37:A:5053:HOH:O	4:D:216:LYS:HA	2.09	0.52
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.74	0.52
1:A:920:C:H5'	1:A:921:G:C4	2.45	0.52
1:A:2866:U:H4'	1:A:2867:G:H5'	1.92	0.52
1:A:1015:C:H2'	1:A:1016:U:H6	1.74	0.52
1:A:1752:G:H2'	37:A:7541:HOH:O	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:U:H5	1:A:284:C:N4	2.07	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
2:B:3107:C:C5	37:B:3167:HOH:O	2.54	0.52
1:A:454:U:O4	37:A:9155:HOH:O	2.19	0.52
1:A:394:G:H1	14:N:181:GLU:CD	2.14	0.52
14:N:164:THR:HB	37:N:8520:HOH:O	2.10	0.52
12:L:37:TYR:CD2	37:L:7169:HOH:O	2.55	0.52
1:A:1119:G:N2	1:A:1246:A:H2	2.04	0.52
1:A:1666:C:C2'	1:A:1667:A:H5'	2.38	0.52
3:C:105:VAL:CG1	3:C:106:CYS:N	2.72	0.52
1:A:2256:G:C2'	1:A:2257:G:H5'	2.40	0.52
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.45	0.52
1:A:1139:U:H2'	1:A:1140:C:C6	2.45	0.52
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.09	0.52
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.39	0.51
27:1:47:LEU:CD2	27:1:57:CYS:HB2	2.40	0.51
2:B:3029:C:C2'	2:B:3030:C:H5'	2.40	0.51
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.45	0.51
7:G:68:HIS:O	7:G:72:MET:HG3	2.10	0.51
1:A:1056:U:H2'	1:A:1057:A:O4'	2.10	0.51
1:A:2536:C:OP1	37:A:3089:HOH:O	2.19	0.51
13:M:21:ARG:N	37:M:8536:HOH:O	2.43	0.51
37:A:7212:HOH:O	14:N:13:LYS:HE2	2.10	0.51
1:A:2760:C:H5''	37:A:5303:HOH:O	2.10	0.51
1:A:1555:G:H4'	1:A:1630:A:H2	1.75	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
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.40	0.51
37:A:7009:HOH:O	3:C:211:LYS:HG2	2.09	0.51
1:A:1209:C:O2	1:A:1210:G:C8	2.63	0.51
16:P:35:LYS:HD3	37:P:3360:HOH:O	2.09	0.51
1:A:1701:A:H4'	1:A:1702:U:C5'	2.40	0.51
20:T:23:LYS:HD3	20:T:65:VAL:HG12	1.91	0.51
1:A:952:G:H4'	37:A:4002:HOH:O	2.11	0.51
19:S:132:ARG:NH2	37:S:8583:HOH:O	2.41	0.51
7:G:77:THR:OG1	7:G:78:GLU:N	2.41	0.51
10:J:150:LYS:HE2	37:J:8381:HOH:O	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:ALA:HB3	37:J:8367:HOH:O	2.11	0.51
1:A:1189:A:H1'	1:A:1209:C:O4'	2.11	0.51
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.75	0.51
3:C:192:VAL:CG1	3:C:192:VAL:O	2.58	0.51
10:J:71:TYR:O	10:J:73:GLN:N	2.43	0.51
1:A:2010:A:C2'	37:A:5935:HOH:O	2.58	0.51
21:U:20:HIS:ND1	21:U:41:ARG:NE	2.55	0.51
2:B:3092:G:H2'	2:B:3093:A:C8	2.45	0.51
23:W:16:ARG:NH2	23:W:63:GLU:HG3	2.25	0.51
15:O:157:PRO:HA	37:O:8527:HOH:O	2.09	0.51
1:A:558:C:H2'	1:A:559:U:H5''	1.92	0.51
13:M:148:GLU:HB2	37:M:8592:HOH:O	2.09	0.51
1:A:2768:A:H3'	37:A:4392:HOH:O	2.11	0.51
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.44	0.51
23:W:4:HIS:O	23:W:8:ILE:HG13	2.11	0.51
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.40	0.51
26:Z:115:ARG:NE	37:Z:8557:HOH:O	2.43	0.51
1:A:113:A:OP2	1:A:114:A:H2'	2.10	0.51
13:M:77:ALA:HB3	37:M:8535:HOH:O	2.09	0.51
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.10	0.51
14:N:137:ASP:HA	14:N:142:LYS:HE3	1.92	0.51
1:A:440:C:H2'	1:A:441:A:C8	2.45	0.51
1:A:629:A:C2	1:A:2074:A:C2	2.99	0.51
10:J:157:ILE:CG2	10:J:158:ASN:N	2.73	0.51
27:1:39:CYS:HA	27:1:47:LEU:CD1	2.38	0.51
5:E:16:VAL:HG12	5:E:17:ASP:H	1.74	0.51
1:A:1667:A:H2'	1:A:1668:U:C6	2.46	0.51
1:A:2812:A:H1'	37:A:5767:HOH:O	2.09	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:166:ASN:ND2	10:J:166:ASN:N	2.58	0.51
1:A:661:G:C4	1:A:686:A:C2	2.99	0.51
1:A:1768:C:H2'	1:A:1769:C:O4'	2.10	0.51
18:R:93:ARG:HG3	18:R:93:ARG:HH11	1.75	0.51
17:Q:131:PHE:CD1	17:Q:137:LEU:HD13	2.44	0.51
10:J:162:SER:CB	10:J:163:PRO:CD	2.79	0.51
12:L:34:VAL:HB	37:L:7169:HOH:O	2.11	0.51
1:A:51:G:N2	1:A:111:C:C2	2.78	0.51
4:D:333:GLU:HB2	22:V:14:GLU:OE2	2.11	0.51
1:A:657:G:OP1	5:E:27:ARG:NH2	2.40	0.51
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:127:GLY:O	10:J:128:ALA:CB	2.58	0.51
8:H:57:GLU:O	8:H:61:MET:HG3	2.09	0.51
6:F:11:HIS:C	6:F:13:MET:H	2.13	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
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.09	0.51
1:A:1134:G:C4'	10:J:151:MET:HE1	2.26	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
4:D:175:LEU:O	4:D:175:LEU:HD23	2.10	0.51
24:X:38:THR:HG22	24:X:39:ASP:H	1.76	0.51
1:A:1827:G:C6	1:A:1828:G:C6	2.99	0.51
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.93	0.51
1:A:1097:A:H5''	24:X:125:HIS:NE2	2.26	0.51
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.75	0.51
11:K:142:ASN:O	11:K:144:THR:N	2.44	0.51
10:J:65:ARG:HB3	37:J:8387:HOH:O	2.10	0.51
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.40	0.51
1:A:2506:A:O2'	1:A:2507:G:O5'	2.29	0.51
1:A:1625:U:H5''	37:A:5999:HOH:O	2.11	0.51
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.92	0.51
1:A:2487:C:H5	37:A:4859:HOH:O	1.94	0.51
1:A:2314:G:C2'	1:A:2315:C:H5'	2.40	0.51
1:A:2613:G:O2'	1:A:2614:C:H5'	2.11	0.51
1:A:1942:A:H3'	37:A:7334:HOH:O	2.10	0.51
27:1:30:GLU:CA	27:1:33:HIS:HB3	2.37	0.51
1:A:21:G:H5''	19:S:1:GLY:O	2.11	0.51
4:D:162:MET:HG3	4:D:310:ARG:CZ	2.41	0.51
1:A:317:A:H5''	21:U:52:ARG:HD2	1.93	0.51
8:H:59:ILE:O	8:H:59:ILE:HG22	2.10	0.51
29:3:18:ASN:ND2	29:3:40:ARG:H	2.09	0.51
1:A:795:G:N3	1:A:817:G:C2	2.79	0.51
1:A:694:A:H2'	1:A:695:C:H5'	1.92	0.51
1:A:2459:G:OP2	30:4:64:LYS:HD2	2.11	0.51
1:A:1862:C:C2'	1:A:1863:G:H5'	2.41	0.51
6:F:23:VAL:CG2	6:F:23:VAL:O	2.59	0.51
1:A:1118:A:C8	1:A:1119:G:H5''	2.45	0.51
27:1:10:ARG:HG3	27:1:11:THR:N	2.26	0.51
4:D:162:MET:CE	4:D:310:ARG:HD3	2.41	0.51
8:H:100:ASP:O	8:H:101:ALA:O	2.29	0.51
7:G:7:ILE:HD11	7:G:11:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:205:VAL:O	4:D:307:ARG:NE	2.44	0.51
28:2:15:THR:O	28:2:29:THR:HG22	2.11	0.51
16:P:26:TRP:HB2	37:P:3062:HOH:O	2.11	0.51
1:A:2326:U:H4'	1:A:2412:G:C4'	2.41	0.51
30:4:1:MET:N	30:4:87:ARG:O	2.41	0.51
3:C:173:GLY:O	3:C:176:HIS:HB3	2.10	0.51
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
10:J:35:ASN:ND2	10:J:79:ALA:O	2.44	0.50
1:A:2730:G:O2'	1:A:2731:G:H5'	2.12	0.50
22:V:20:MET:CG	22:V:28:THR:HG23	2.41	0.50
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.58	0.50
1:A:1595:G:O2'	1:A:1596:U:H5'	2.11	0.50
6:F:146:LYS:HZ1	15:O:107:ASN:HD21	1.57	0.50
11:K:45:VAL:HG22	11:K:46:ILE:N	2.25	0.50
1:A:1819:G:H5'	37:A:4684:HOH:O	2.12	0.50
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.41	0.50
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.76	0.50
16:P:25:VAL:O	16:P:29:VAL:HG23	2.10	0.50
10:J:129:ASN:N	10:J:129:ASN:HD22	2.09	0.50
1:A:2679:G:H2'	1:A:2681:A:OP2	2.11	0.50
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.92	0.50
14:N:113:ARG:HH21	14:N:156:ARG:HG2	1.73	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
5:E:133:ARG:NH2	37:E:8428:HOH:O	2.43	0.50
1:A:952:G:OP1	18:R:42:LYS:HE2	2.11	0.50
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.46	0.50
1:A:1015:C:H2'	1:A:1016:U:C6	2.46	0.50
14:N:78:ASN:ND2	37:N:8642:HOH:O	2.37	0.50
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.11	0.50
19:S:34:GLU:HG2	19:S:46:TYR:OH	2.11	0.50
13:M:30:ARG:NH2	37:M:8525:HOH:O	2.33	0.50
27:1:59:HIS:HA	37:1:8440:HOH:O	2.11	0.50
1:A:2121:G:O2'	1:A:2122:C:H5'	2.12	0.50
25:Y:25:ARG:CG	37:Y:5356:HOH:O	2.54	0.50
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.75	0.50
8:H:28:ALA:CB	8:H:99:THR:HG23	2.41	0.50
1:A:257:G:O2'	1:A:258:G:H5'	2.10	0.50
4:D:138:GLY:O	4:D:139:ASP:O	2.29	0.50
2:B:3008:G:O6	15:O:11:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:49:LEU:O	23:W:53:ILE:HG13	2.11	0.50
15:O:32:PRO:HD2	15:O:99:GLU:O	2.12	0.50
1:A:539:G:H2'	1:A:540:A:C8	2.46	0.50
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.59	0.50
14:N:61:ILE:N	14:N:61:ILE:HD12	2.26	0.50
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.17	0.50
17:Q:41:ARG:O	17:Q:44:VAL:HB	2.12	0.50
15:O:163:PHE:HA	37:O:8564:HOH:O	2.09	0.50
11:K:22:VAL:O	11:K:26:VAL:HG23	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
26:Z:122:ARG:NH2	37:Z:8536:HOH:O	2.45	0.50
16:P:44:ASN:HA	16:P:65:LEU:O	2.11	0.50
1:A:522:U:O2'	1:A:1366:C:H5'	2.12	0.50
25:Y:7:GLU:HA	25:Y:74:ALA:O	2.11	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
3:C:132:ASP:OD1	3:C:133:ARG:N	2.42	0.50
10:J:53:PRO:HG3	10:J:127:GLY:H	1.77	0.50
15:O:149:GLU:O	15:O:152:GLU:HB2	2.12	0.50
24:X:76:ASP:O	24:X:77:ALA:C	2.50	0.50
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.77	0.50
1:A:2713:G:O2'	1:A:2714:U:H5'	2.12	0.50
6:F:36:ASN:HA	37:F:7500:HOH:O	2.12	0.50
22:V:34:SER:O	22:V:38:ASN:ND2	2.45	0.50
1:A:1681:G:H5'	1:A:1682:A:H5'	1.93	0.50
1:A:653:C:H2'	1:A:654:A:C8	2.45	0.50
10:J:26:LYS:CD	10:J:28:ILE:HB	2.42	0.50
10:J:26:LYS:HD2	10:J:28:ILE:HB	1.93	0.50
1:A:820:G:C5	3:C:171:LYS:HB2	2.47	0.50
3:C:192:VAL:O	3:C:207:GLN:HG2	2.11	0.50
19:S:40:ALA:O	19:S:44:VAL:HG23	2.11	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
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.59	0.50
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.26	0.50
1:A:514:G:O5'	1:A:514:G:H8	1.95	0.50
4:D:221:GLN:HE22	12:L:42:ASN:ND2	2.09	0.50
3:C:8:ARG:NH1	37:C:8553:HOH:O	2.32	0.50
1:A:1503:U:H2'	1:A:1504:A:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:23:ILE:O	9:I:27:ILE:HG13	2.11	0.50
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.94	0.50
6:F:10:PHE:CD1	6:F:11:HIS:N	2.80	0.50
1:A:40:C:O5'	1:A:40:C:H6	1.95	0.50
1:A:703:G:O2'	1:A:704:C:H5'	2.11	0.50
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.94	0.50
24:X:88:THR:CG2	24:X:89:ASP:H	2.20	0.50
29:3:39:ARG:NH1	37:3:6391:HOH:O	2.45	0.50
24:X:5:VAL:O	24:X:52:VAL:HG22	2.11	0.50
3:C:192:VAL:O	3:C:192:VAL:HG12	2.11	0.50
37:A:9870:HOH:O	11:K:46:ILE:HA	2.12	0.50
24:X:38:THR:HG22	24:X:39:ASP:N	2.27	0.50
4:D:280:VAL:HG13	4:D:334:SER:HA	1.94	0.50
1:A:590:A:C2'	1:A:591:A:H5'	2.42	0.50
1:A:2073:G:OP2	1:A:2490:A:H5'	2.12	0.50
1:A:1783:A:O2'	1:A:1784:U:H5'	2.11	0.50
18:R:41:LEU:HB3	18:R:52:PHE:CZ	2.46	0.50
15:O:170:GLU:O	15:O:174:GLU:HG3	2.12	0.50
1:A:1669:A:H2'	1:A:1670:G:C8	2.47	0.50
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.46	0.49
5:E:236:THR:O	5:E:237:GLU:C	2.49	0.49
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.39	0.49
14:N:14:ARG:HB3	14:N:17:GLU:HG3	1.94	0.49
5:E:27:ARG:HG2	5:E:30:LEU:HG	1.92	0.49
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.25	0.49
4:D:2:GLN:HA	37:D:8618:HOH:O	2.12	0.49
1:A:949:U:O2'	18:R:40:HIS:HE1	1.95	0.49
1:A:920:C:H4'	1:A:921:G:C2	2.47	0.49
2:B:3009:C:OP2	37:B:466:HOH:O	2.19	0.49
1:A:1434:A:H2'	1:A:1436:C:C5	2.46	0.49
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.47	0.49
1:A:2769:C:O2'	1:A:2770:G:H5'	2.12	0.49
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.12	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:316:A:N3	1:A:336:G:O2'	2.43	0.49
16:P:59:VAL:HG23	16:P:111:VAL:HG23	1.94	0.49
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.26	0.49
5:E:43:LYS:NZ	37:E:8390:HOH:O	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2256:G:O2'	1:A:2257:G:H5'	2.12	0.49
1:A:1850:U:H2'	1:A:1851:G:H8	1.76	0.49
1:A:714:U:H3'	37:A:6924:HOH:O	2.12	0.49
1:A:639:A:H2'	1:A:640:G:C8	2.46	0.49
2:B:3064:C:H2'	2:B:3065:A:H5'	1.95	0.49
15:O:71:TRP:N	37:O:8538:HOH:O	2.44	0.49
1:A:1450:C:O2'	1:A:1494:A:H5'	2.13	0.49
37:B:7568:HOH:O	15:O:107:ASN:HB3	2.10	0.49
6:F:86:THR:C	6:F:89:PRO:HD2	2.32	0.49
1:A:664:U:O4	1:A:681:G:H5''	2.12	0.49
15:O:58:LEU:CD1	15:O:58:LEU:N	2.75	0.49
1:A:1500:U:P	17:Q:41:ARG:HH22	2.35	0.49
6:F:58:VAL:HG12	6:F:59:GLY:N	2.27	0.49
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.94	0.49
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.37	0.49
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.42	0.49
30:4:69:TYR:CB	30:4:78:HIS:CE1	2.95	0.49
2:B:3023:U:C4'	2:B:3024:U:OP2	2.56	0.49
1:A:1209:C:H2'	1:A:1210:G:C8	2.44	0.49
1:A:400:C:O3'	37:A:5770:HOH:O	2.20	0.49
1:A:2756:U:H3	1:A:2896:A:H2	1.58	0.49
1:A:2359:G:H3'	37:A:5667:HOH:O	2.12	0.49
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.94	0.49
1:A:2251:G:H2'	1:A:2252:A:C8	2.48	0.49
1:A:2502:C:C4'	10:J:151:MET:HG2	2.43	0.49
1:A:2265:U:H2'	1:A:2266:A:C8	2.48	0.49
1:A:2064:U:H5'	1:A:2652:U:O3'	2.13	0.49
1:A:449:A:N7	5:E:43:LYS:HG2	2.27	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:820:G:C6	3:C:171:LYS:HB2	2.48	0.49
1:A:1174:A:C5	1:A:1201:C:H4'	2.47	0.49
8:H:91:VAL:CG1	8:H:92:GLY:H	2.20	0.49
1:A:1268:C:O2'	1:A:1269:G:H5'	2.12	0.49
5:E:77:ALA:O	5:E:78:ARG:HG3	2.12	0.49
1:A:960:G:N3	1:A:960:G:C2'	2.75	0.49
1:A:2346:C:O3'	6:F:52:THR:HG23	2.11	0.49
10:J:53:PRO:HA	10:J:125:VAL:O	2.13	0.49
1:A:154:C:H2'	1:A:155:C:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2459:G:P	30:4:64:LYS:HB2	2.52	0.49
20:T:80:ARG:NH1	37:T:8344:HOH:O	2.45	0.49
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.12	0.49
1:A:2271:G:P	37:A:9418:HOH:O	2.70	0.49
1:A:195:C:H2'	1:A:196:G:H5'	1.94	0.49
25:Y:30:MET:HE3	25:Y:59:TRP:HE1	1.77	0.49
23:W:12:THR:HG23	23:W:14:ALA:H	1.76	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
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.43	0.49
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.78	0.49
14:N:77:PHE:HD2	37:N:8527:HOH:O	1.94	0.49
4:D:177:HIS:O	4:D:181:ILE:HG13	2.13	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
2:B:3031:C:H2'	2:B:3032:G:O4'	2.11	0.49
1:A:1657:A:H2'	1:A:1658:A:C8	2.47	0.49
6:F:102:GLY:O	6:F:134:LEU:HD12	2.13	0.49
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.95	0.49
7:G:7:ILE:HG22	7:G:45:ASP:O	2.13	0.49
18:R:28:ARG:HG2	37:R:4350:HOH:O	2.13	0.49
1:A:470:U:O2'	28:2:16:HIS:CD2	2.65	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:1656:A:H2'	1:A:1657:A:O4'	2.13	0.49
1:A:95:A:H5'	1:A:97:G:O4'	2.13	0.49
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.12	0.49
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.93	0.49
1:A:1218:U:H2'	1:A:1219:U:C6	2.47	0.49
1:A:1723:G:H2'	37:A:9608:HOH:O	2.13	0.49
22:V:52:THR:HG22	22:V:54:THR:N	2.28	0.49
1:A:1213:C:C2'	1:A:1214:G:H5'	2.43	0.49
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.42	0.49
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.48	0.49
30:4:31:THR:HB	30:4:33:MET:CE	2.42	0.49
14:N:77:PHE:O	14:N:77:PHE:CD1	2.65	0.49
7:G:118:ILE:HG23	7:G:144:THR:HG21	1.95	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
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:43:VAL:HG11	15:O:81:ALA:HA	1.95	0.49
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.95	0.48
4:D:140:LEU:HD23	37:D:8577:HOH:O	2.13	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
7:G:108:LEU:HD11	7:G:164:ASP:HB2	1.94	0.48
1:A:739:G:N7	37:A:7536:HOH:O	2.44	0.48
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:2894:C:O2'	1:A:2895:C:H5'	2.13	0.48
1:A:812:A:H2'	1:A:813:C:C6	2.48	0.48
25:Y:36:HIS:CE1	25:Y:40:HIS:CD2	3.01	0.48
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.42	0.48
15:O:47:LEU:HD12	15:O:92:ALA:HB1	1.94	0.48
1:A:542:A:H1'	37:A:4650:HOH:O	2.13	0.48
1:A:2269:C:C2'	1:A:2270:G:H5'	2.43	0.48
2:B:3049:G:H2'	2:B:3050:G:O4'	2.13	0.48
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.60	0.48
1:A:1189:A:O2'	1:A:1208:C:H2'	2.13	0.48
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.26	0.48
3:C:76:VAL:CG2	27:1:63:LYS:HB3	2.42	0.48
1:A:187:A:H3'	1:A:188:C:H6	1.77	0.48
1:A:2459:G:OP1	30:4:64:LYS:N	2.25	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:1197:G:N2	37:A:6214:HOH:O	2.46	0.48
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.21	0.48
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.96	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
37:A:6017:HOH:O	30:4:84:ARG:HB3	2.13	0.48
37:L:7438:HOH:O	22:V:20:MET:HE1	2.12	0.48
4:D:85:ARG:NH1	37:D:8634:HOH:O	2.46	0.48
6:F:59:GLY:O	6:F:61:PHE:N	2.36	0.48
1:A:790:A:H1'	1:A:1710:A:H2'	1.95	0.48
1:A:2630:G:O6	3:C:206:ARG:NH2	2.46	0.48
1:A:2365:G:H4'	18:R:45:PRO:O	2.13	0.48
4:D:301:VAL:HG13	4:D:302:PRO:HD2	1.95	0.48
1:A:2464:C:H5''	1:A:2465:A:OP1	2.13	0.48
14:N:36:ALA:HB1	37:N:8549:HOH:O	2.13	0.48
20:T:73:ASP:OD1	20:T:75:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1593:C:OP1	17:Q:117:SER:CB	2.62	0.48
1:A:2432:C:H4'	30:4:36:ILE:HG12	1.95	0.48
24:X:48:VAL:O	24:X:48:VAL:CG1	2.59	0.48
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.94	0.48
25:Y:71:ARG:HD3	37:Y:2171:HOH:O	2.13	0.48
4:D:4:SER:O	4:D:5:ARG:HB2	2.14	0.48
1:A:2524:G:H21	1:A:2526:C:N4	2.11	0.48
31:A:9000:TYK:H7A2	31:A:9000:TYK:O2A	2.13	0.48
1:A:120:A:H2'	1:A:120:A:N3	2.27	0.48
19:S:33:ARG:NH2	37:S:8533:HOH:O	2.37	0.48
1:A:2598:U:O2	1:A:2600:A:H8	1.96	0.48
1:A:1135:G:H5'	37:A:5905:HOH:O	2.12	0.48
24:X:26:ILE:O	24:X:26:ILE:HG13	2.11	0.48
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.42	0.48
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.43	0.48
1:A:1589:G:N2	1:A:1605:G:H1'	2.28	0.48
1:A:553:G:P	26:Z:204:ARG:NH2	2.86	0.48
1:A:1909:A:H2'	1:A:1910:A:C8	2.48	0.48
1:A:1862:C:H1'	37:A:7204:HOH:O	2.14	0.48
4:D:274:GLU:HA	4:D:292:GLY:O	2.13	0.48
1:A:1444:G:O2'	1:A:1445:G:H5'	2.13	0.48
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.13	0.48
14:N:49:ALA:HB1	14:N:54:TYR:CB	2.43	0.48
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.42	0.48
1:A:1840:A:OP1	37:A:9595:HOH:O	2.20	0.48
1:A:281:U:H3'	37:A:7191:HOH:O	2.14	0.48
3:C:51:ARG:NH2	37:C:8609:HOH:O	2.47	0.48
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.95	0.48
1:A:182:G:O2'	1:A:183:A:H5'	2.14	0.48
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.44	0.48
2:B:3042:C:O2	6:F:76:ARG:NH1	2.47	0.48
1:A:1699:C:H4'	37:A:6425:HOH:O	2.13	0.48
14:N:169:ARG:HD2	37:N:8590:HOH:O	2.14	0.48
12:L:101:ASN:O	12:L:102:GLU:HB2	2.13	0.48
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.49	0.48
1:A:2501:G:H1'	37:A:4515:HOH:O	2.13	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
1:A:2815:G:OP2	11:K:99:GLU:HG2	2.14	0.48
14:N:123:ASP:OD1	14:N:123:ASP:C	2.52	0.48
1:A:1883:U:OP1	37:A:7834:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:54:GLU:HG2	16:P:73:ASP:O	2.14	0.48
1:A:1995:G:O2'	1:A:1997:A:N7	2.46	0.48
3:C:149:ASP:OD1	3:C:151:GLN:HB2	2.14	0.48
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.43	0.48
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.74	0.48
13:M:133:VAL:HB	37:M:8563:HOH:O	2.13	0.48
37:B:4707:HOH:O	15:O:147:ILE:HB	2.14	0.48
13:M:143:THR:CG2	13:M:144:ASP:H	2.26	0.48
11:K:93:ARG:HH11	11:K:93:ARG:CB	2.22	0.48
3:C:105:VAL:HG12	3:C:106:CYS:H	1.79	0.48
4:D:54:VAL:O	4:D:55:ASN:C	2.51	0.48
1:A:716:G:H2'	1:A:717:C:O5'	2.14	0.48
1:A:241:A:C2	1:A:378:A:H4'	2.49	0.48
1:A:2133:U:H4'	1:A:2134:G:H5'	1.96	0.48
14:N:115:LEU:HD13	14:N:116:ASN:HB2	1.95	0.48
20:T:57:THR:C	20:T:59:ASP:H	2.17	0.48
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.79	0.48
1:A:1328:A:N7	1:A:1329:A:C5	2.82	0.48
10:J:39:GLY:O	10:J:41:THR:N	2.47	0.48
1:A:2361:A:H5''	37:A:9001:HOH:O	2.14	0.48
1:A:2089:A:C2'	1:A:2090:G:H5'	2.43	0.48
1:A:1976:G:O2'	1:A:1977:U:H5'	2.13	0.48
8:H:34:ASN:O	8:H:38:LYS:HG3	2.14	0.48
1:A:1183:C:N4	37:A:4370:HOH:O	2.42	0.48
1:A:2502:C:H4'	10:J:151:MET:HG2	1.96	0.48
1:A:1191:A:C3'	1:A:1192:A:H5''	2.39	0.48
1:A:559:U:H2'	1:A:560:C:O4'	2.14	0.48
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.94	0.48
15:O:171:HIS:CE1	37:O:8563:HOH:O	2.67	0.48
8:H:117:GLU:C	8:H:119:ARG:H	2.17	0.48
1:A:2326:U:H4'	1:A:2412:G:H4'	1.96	0.48
1:A:1132:A:N6	1:A:1229:C:H2'	2.29	0.48
1:A:602:A:O2'	1:A:605:C:H4'	2.14	0.48
7:G:36:PRO:HD3	11:K:127:ILE:HD12	1.96	0.48
1:A:1925:G:OP1	30:4:29:ARG:NH2	2.47	0.48
27:1:37:HIS:O	27:1:45:LYS:HA	2.13	0.47
24:X:13:MET:HE1	24:X:18:GLN:HA	1.94	0.47
6:F:174:VAL:CG1	37:F:6555:HOH:O	2.61	0.47
6:F:84:LEU:C	6:F:86:THR:H	2.17	0.47
1:A:450:C:H4'	5:E:46:TYR:CE1	2.49	0.47
24:X:76:ASP:O	24:X:77:ALA:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.49	0.47
1:A:918:G:C2	1:A:926:A:C2	3.02	0.47
1:A:371:U:H2'	1:A:372:A:C8	2.47	0.47
1:A:2050:G:H5''	19:S:80:TYR:O	2.14	0.47
24:X:142:ASP:HB3	24:X:145:GLY:H	1.78	0.47
23:W:27:LEU:O	23:W:30:ALA:N	2.47	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:1562:C:H42	1:A:2738:G:H1	1.62	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:407:A:H5'	37:A:6003:HOH:O	2.13	0.47
5:E:180:SER:HB2	37:E:8450:HOH:O	2.14	0.47
37:A:7447:HOH:O	5:E:188:ARG:HD3	2.14	0.47
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.90	0.47
14:N:87:MET:CE	37:N:8530:HOH:O	2.63	0.47
37:A:9583:HOH:O	14:N:165:SER:HB3	2.14	0.47
27:I:47:LEU:HD23	27:I:57:CYS:CB	2.44	0.47
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.96	0.47
3:C:93:THR:C	3:C:94:LEU:HD23	2.34	0.47
14:N:80:GLY:O	14:N:81:ARG:HD3	2.14	0.47
4:D:248:ARG:O	4:D:251:VAL:HG12	2.14	0.47
1:A:951:A:H2'	1:A:952:G:H5'	1.95	0.47
1:A:2284:G:H5'	37:A:9440:HOH:O	2.13	0.47
19:S:25:PHE:CE2	19:S:29:LYS:HE2	2.49	0.47
1:A:1477:C:H5'	1:A:1868:G:C5'	2.45	0.47
24:X:40:ALA:O	24:X:44:MET:HG3	2.14	0.47
12:L:40:THR:O	12:L:41:LYS:C	2.52	0.47
1:A:457:U:H5	1:A:460:A:OP2	1.97	0.47
1:A:1462:C:H2'	1:A:1463:A:C8	2.49	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
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.14	0.47
3:C:36:ASP:O	3:C:38:ILE:N	2.48	0.47
15:O:141:ARG:N	37:O:8566:HOH:O	2.47	0.47
18:R:75:ILE:HD11	18:R:84:ILE:HD11	1.96	0.47
7:G:69:ILE:HA	7:G:72:MET:HE2	1.95	0.47
1:A:1773:G:H2'	1:A:1774:G:H5'	1.96	0.47
1:A:710:G:P	16:P:24:ALA:HB3	2.55	0.47
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.96	0.47
1:A:716:G:C2'	1:A:717:C:O5'	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:7447:HOH:O	5:E:188:ARG:CD	2.62	0.47
1:A:2724:U:H2'	1:A:2725:G:O4'	2.14	0.47
17:Q:58:SER:HB3	37:Q:4744:HOH:O	2.12	0.47
24:X:137:GLN:HG3	24:X:137:GLN:O	2.15	0.47
1:A:445:U:H1'	37:A:7324:HOH:O	2.14	0.47
4:D:279:THR:CG2	4:D:280:VAL:N	2.77	0.47
1:A:2000:G:O2'	1:A:2001:G:H5'	2.15	0.47
1:A:130:C:H5'	37:A:5189:HOH:O	2.13	0.47
1:A:2353:A:H4'	1:A:2354:A:O5'	2.14	0.47
11:K:77:GLY:O	11:K:78:ILE:C	2.53	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
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.49	0.47
13:M:146:GLY:C	13:M:148:GLU:H	2.18	0.47
22:V:44:ARG:CB	37:V:3805:HOH:O	2.61	0.47
1:A:2896:A:N3	1:A:2896:A:H2'	2.30	0.47
10:J:113:ALA:N	10:J:114:PRO:CD	2.78	0.47
18:R:75:ILE:HD13	18:R:84:ILE:HD11	1.97	0.47
4:D:55:ASN:HB3	4:D:64:GLY:H	1.79	0.47
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.44	0.47
1:A:1820:G:C6	1:A:2030:A:C2	3.03	0.47
5:E:165:ASP:O	5:E:168:ARG:HB3	2.15	0.47
1:A:1850:U:H2'	1:A:1851:G:C8	2.48	0.47
1:A:764:C:H2'	1:A:765:G:O4'	2.15	0.47
5:E:20:ASP:O	5:E:23:GLU:HB2	2.15	0.47
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.44	0.47
1:A:2718:C:H6	1:A:2718:C:H5'	1.79	0.47
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.44	0.47
1:A:1116:U:H3	1:A:1246:A:N6	2.03	0.47
37:A:7413:HOH:O	21:U:9:LYS:HD2	2.14	0.47
1:A:2466:G:H8	37:A:9516:HOH:O	1.98	0.47
21:U:55:PHE:CD2	21:U:77:VAL:HG13	2.49	0.47
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.50	0.47
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.83	0.47
30:4:74:CYS:SG	30:4:76:LYS:CB	3.03	0.47
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.30	0.47
5:E:238:SER:HB3	37:E:8383:HOH:O	2.13	0.47
12:L:101:ASN:O	12:L:102:GLU:CB	2.63	0.47
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.50	0.47
21:U:80:GLU:OE2	21:U:84:GLY:HA2	2.15	0.47
1:A:125:U:H2'	37:A:3740:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:C:H2'	1:A:102:A:H8	1.80	0.47
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.14	0.47
5:E:49:ASP:HB3	5:E:52:ALA:HB2	1.96	0.47
1:A:1380:U:H5'	37:A:9211:HOH:O	2.14	0.47
30:4:17:HIS:O	30:4:18:GLN:HG3	2.15	0.47
3:C:88:ILE:O	3:C:88:ILE:HG22	2.14	0.47
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.14	0.47
1:A:1167:G:O2'	1:A:1168:C:H5'	2.15	0.47
1:A:222:A:H2'	1:A:223:G:O4'	2.14	0.47
1:A:2791:U:H1'	1:A:2792:A:H5''	1.96	0.47
1:A:1029:U:O2'	1:A:1273:C:OP1	2.30	0.47
1:A:2269:C:H2'	1:A:2270:G:H5'	1.96	0.47
1:A:1942:A:O2'	1:A:1943:C:H5'	2.15	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
9:I:12:ILE:HG13	37:I:6833:HOH:O	2.15	0.47
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.13	0.47
37:A:5383:HOH:O	3:C:164:ARG:NE	2.47	0.47
15:O:154:LEU:HG	15:O:155:GLU:H	1.80	0.47
1:A:1333:U:H2'	1:A:1334:C:H6	1.78	0.47
21:U:41:ARG:NH1	21:U:42:VAL:O	2.48	0.47
2:B:3064:C:C2'	2:B:3065:A:H5'	2.45	0.47
3:C:55:VAL:HG13	3:C:67:LEU:HD22	1.97	0.47
3:C:2:ARG:NH1	37:C:8513:HOH:O	2.29	0.47
1:A:2667:G:H1'	1:A:2914:A:N3	2.29	0.47
28:2:5:THR:HB	28:2:6:PRO:CD	2.45	0.47
25:Y:73:ARG:O	25:Y:85:VAL:HG13	2.14	0.47
24:X:122:ARG:HH22	24:X:154:ARG:C	2.19	0.47
1:A:1887:U:OP1	27:1:21:LYS:HG3	2.14	0.47
6:F:92:GLU:O	6:F:93:LEU:O	2.33	0.47
4:D:175:LEU:C	4:D:175:LEU:CD2	2.82	0.47
26:Z:106:THR:CG2	26:Z:107:PRO:HD2	2.45	0.47
1:A:1003:U:O2	10:J:90:PHE:HZ	1.98	0.47
15:O:82:TYR:C	15:O:82:TYR:CD2	2.88	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
1:A:2106:C:H2'	1:A:2107:U:C6	2.50	0.47
1:A:778:C:C4	1:A:779:U:C4	3.03	0.47
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.97	0.46
2:B:3057:A:C8	6:F:141:VAL:HG21	2.50	0.46
1:A:1592:G:O2'	1:A:1593:C:O5'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:246:ARG:NE	37:E:8426:HOH:O	2.48	0.46
1:A:2533:C:H5'	37:A:6882: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
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.97	0.46
18:R:93:ARG:HG3	18:R:93:ARG:NH1	2.31	0.46
2:B:3008:G:C6	2:B:3009:C:C4	3.03	0.46
26:Z:134:HIS:H	26:Z:134:HIS:CD2	2.33	0.46
1:A:1114:A:H2'	1:A:1115:U:H6	1.79	0.46
1:A:2453:G:H4'	13:M:50:GLY:C	2.35	0.46
1:A:675:U:O2'	5:E:42:ARG:NH1	2.48	0.46
1:A:1743:G:H1'	37:A:4863:HOH:O	2.15	0.46
21:U:27:LEU:HD23	21:U:98:VAL:HB	1.97	0.46
14:N:87:MET:HB3	30:4:46:ILE:CD1	2.32	0.46
30:4:69:TYR:O	30:4:77:ALA:HA	2.15	0.46
14:N:89:ASN:HA	37:N:8551:HOH:O	2.14	0.46
25:Y:79:GLU:OE2	37:Y:5564:HOH:O	2.21	0.46
1:A:1594:C:C2	1:A:1601:G:C2	3.03	0.46
1:A:1269:G:H2'	1:A:1270:U:H6	1.79	0.46
13:M:148:GLU:HG2	37:M:8558:HOH:O	2.14	0.46
11:K:19:MET:HE3	11:K:132:LEU:CD1	2.46	0.46
21:U:38:ARG:NH1	37:U:6217:HOH:O	2.47	0.46
1:A:1352:A:N1	5:E:48:SER:HB3	2.31	0.46
1:A:818:A:O2'	27:1:13:ARG:HD3	2.15	0.46
1:A:1996:U:O2'	1:A:1997:A:H5'	2.15	0.46
1:A:128:A:H3'	1:A:128:A:C8	2.50	0.46
16:P:105:ASN:HD21	16:P:109:SER:H	1.64	0.46
15:O:34:LEU:HA	15:O:47:LEU:CD2	2.45	0.46
1:A:1191:A:N1	1:A:1206:U:O4	2.48	0.46
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.45	0.46
1:A:111:C:H2'	1:A:112:G:O4'	2.15	0.46
28:2:29:THR:O	28:2:32:LYS:HE2	2.16	0.46
5:E:84:VAL:O	5:E:85:LYS:CB	2.63	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
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:37:ARG:HA	15:O:37:ARG:HD3	1.78	0.46
1:A:567:U:O2'	1:A:568:G:H5'	2.14	0.46
6:F:154:LYS:H	6:F:154:LYS:CD	2.22	0.46
28:2:28:HIS:O	28:2:32:LYS:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:159:G:H2'	1:A:175:G:N2	2.31	0.46
7:G:34:TRP:O	11:K:127:ILE:HD11	2.14	0.46
26:Z:109:LEU:HA	37:Z:8571:HOH:O	2.14	0.46
15:O:120:GLU:HG3	15:O:136:LEU:HD13	1.97	0.46
1:A:1079:A:N1	1:A:2068:G:O2'	2.43	0.46
2:B:3014:G:H2'	2:B:3015:C:H5'	1.98	0.46
1:A:401:C:P	37:A:5770:HOH:O	2.74	0.46
8:H:72:VAL:HA	8:H:73:PRO:HD3	1.84	0.46
4:D:146:THR:C	4:D:148:PRO:HD3	2.35	0.46
2:B:3088:G:OP1	24:X:130:HIS:NE2	2.46	0.46
15:O:154:LEU:HG	15:O:155:GLU:N	2.29	0.46
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.16	0.46
4:D:154:VAL:CG1	4:D:156:LYS:HG2	2.45	0.46
1:A:1044:C:C5'	37:A:9022:HOH:O	2.61	0.46
8:H:79:GLN:HB2	8:H:82:ASP:OD2	2.16	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
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.96	0.46
1:A:2594:C:O2'	1:A:2595:U:H5'	2.16	0.46
15:O:180:LEU:O	15:O:181:ASP:HB3	2.14	0.46
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.44	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:1086:A:N6	24:X:11:VAL:HG11	2.31	0.46
7:G:18:LEU:HD13	7:G:34:TRP:CG	2.51	0.46
5:E:111:VAL:HB	37:E:8321:HOH:O	2.15	0.46
1:A:1375:A:O2'	1:A:1376:G:H5'	2.16	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
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.98	0.46
15:O:182:GLY:N	37:O:8567:HOH:O	2.49	0.46
1:A:288:A:H2'	1:A:289:G:C8	2.51	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
7:G:64:THR:HG22	7:G:68:HIS:CD2	2.51	0.46
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.34	0.46
28:2:37:CYS:SG	28:2:39:PHE:HB2	2.55	0.46
1:A:1615:A:H5'	37:A:4155:HOH:O	2.14	0.46
10:J:81:TYR:C	10:J:81:TYR:CD1	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1989:G:O2'	1:A:1990:C:H5'	2.15	0.46
1:A:1815:A:H4'	1:A:2751:C:O4'	2.16	0.46
1:A:278:A:H2'	1:A:279:C:O4'	2.16	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
14:N:87:MET:SD	37:N:8532:HOH:O	2.61	0.46
14:N:63:VAL:O	14:N:130:GLU:HA	2.16	0.46
1:A:2506:A:H1'	37:A:6034:HOH:O	2.16	0.46
27:1:21:LYS:O	27:1:25:ARG:HG3	2.15	0.46
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.98	0.46
4:D:238:ASN:HD22	4:D:240:GLY:N	2.08	0.46
11:K:126:ASN:O	11:K:129:PHE:HE2	1.99	0.46
2:B:3044:A:H1'	6:F:76:ARG:NH2	2.30	0.46
24:X:35:VAL:HG23	24:X:41:TYR:CD2	2.51	0.46
5:E:13:ASP:N	37:E:8446:HOH:O	2.49	0.46
6:F:101:THR:O	6:F:101:THR:HG22	2.16	0.46
21:U:48:VAL:HG13	21:U:49:GLU:N	2.30	0.46
1:A:175:G:H2'	14:N:192:ALA:HB3	1.96	0.46
6:F:169:THR:O	6:F:170:TYR:HB2	2.16	0.46
13:M:72:ASN:HB2	37:M:8585:HOH:O	2.15	0.46
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.45	0.46
15:O:37:ARG:NH2	37:O:8533:HOH:O	2.49	0.46
1:A:1474:C:C5'	1:A:1474:C:H6	2.18	0.46
12:L:87:ARG:NH1	37:L:4066:HOH:O	2.48	0.46
1:A:677:C:H4'	5:E:246:ARG:NH2	2.31	0.46
1:A:544:G:H2'	1:A:545:G:C5'	2.41	0.46
1:A:1185:U:H5'	37:A:7456:HOH:O	2.16	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
1:A:259:G:H21	14:N:58:GLN:NE2	2.14	0.46
1:A:2087:C:O2'	1:A:2088:C:H5'	2.15	0.46
8:H:58:GLU:HG3	8:H:61:MET:CE	2.45	0.46
3:C:125:ASN:CB	3:C:158:VAL:HG12	2.46	0.46
25:Y:14:LEU:HD12	25:Y:67:PRO:O	2.16	0.46
1:A:2488:A:H2	37:A:7264:HOH:O	1.98	0.46
2:B:3031:C:O2'	2:B:3032:G:H5'	2.15	0.46
1:A:402:U:H2'	1:A:403:C:C6	2.50	0.46
1:A:1894:C:C2	1:A:1939:U:C4	3.03	0.46
1:A:13:G:H2'	1:A:14:C:H6	1.80	0.46
1:A:2564:G:OP2	1:A:2565:C:H5''	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1730:G:H5'	1:A:1731:C:C5	2.51	0.46
11:K:54:VAL:HG11	11:K:138:THR:HG21	1.97	0.46
15:O:50:LEU:HB2	37:O:8524:HOH:O	2.16	0.46
1:A:1754:A:N7	37:A:7857:HOH:O	2.36	0.46
14:N:74:ARG:HD3	14:N:91:ILE:HD12	1.97	0.46
1:A:2121:G:H5'	37:A:3491:HOH:O	2.16	0.46
12:L:14:LYS:NZ	12:L:32:ILE:O	2.46	0.46
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.77	0.46
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.16	0.46
6:F:84:LEU:HA	6:F:87:ALA:HB3	1.98	0.46
4:D:168:GLY:O	4:D:169:GLY:O	2.34	0.46
25:Y:21:PRO:HD3	37:Y:6179:HOH:O	2.15	0.46
14:N:155:HIS:O	14:N:158:ARG:HG2	2.15	0.46
20:T:57:THR:HG22	20:T:59:ASP:HB2	1.97	0.45
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.98	0.45
1:A:553:G:H5'	37:A:3479:HOH:O	2.15	0.45
7:G:11:VAL:HG11	7:G:22:VAL:HG13	1.97	0.45
6:F:86:THR:CG2	37:F:7477:HOH:O	2.64	0.45
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.84	0.45
9:I:64:ASN:O	9:I:68:GLU:HG3	2.15	0.45
3:C:109:GLU:HG2	3:C:116:GLY:N	2.31	0.45
1:A:1398:G:O2'	1:A:1399:A:H5'	2.16	0.45
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:646:G:H2'	1:A:647:U:C6	2.51	0.45
1:A:2435:U:P	30:4:28:GLY:HA3	2.56	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:1441:G:H1'	37:A:7762:HOH:O	2.16	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
16:P:96:VAL:HA	37:P:4258:HOH:O	2.16	0.45
1:A:2670:G:O2'	1:A:2671:U:H5'	2.17	0.45
14:N:98:GLN:NE2	14:N:117:SER:O	2.49	0.45
10:J:157:ILE:HG22	10:J:158:ASN:N	2.31	0.45
14:N:57:LYS:HE2	14:N:140:ALA:O	2.16	0.45
6:F:53:LYS:HA	6:F:67:ASP:O	2.17	0.45
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.52	0.45
4:D:316:ARG:N	4:D:317:PRO:HD3	2.32	0.45
1:A:657:G:H2'	1:A:658:C:C6	2.52	0.45
6:F:93:LEU:HG	37:F:3862:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:304:PRO:HD2	4:D:307:ARG:HD2	1.98	0.45
11:K:42:GLU:O	11:K:131:THR:HG23	2.16	0.45
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.16	0.45
4:D:215:VAL:HA	4:D:220:VAL:HG22	1.97	0.45
1:A:517:U:H2'	1:A:518:G:H5'	1.97	0.45
1:A:2719:A:C2	4:D:70:PRO:HG3	2.51	0.45
12:L:125:ALA:C	12:L:127:ALA:H	2.19	0.45
5:E:236:THR:C	37:E:8453:HOH:O	2.55	0.45
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.31	0.45
37:A:9401:HOH:O	14:N:52:LEU:HD23	2.17	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
1:A:2421:G:H4'	37:A:4751:HOH:O	2.17	0.45
1:A:319:A:H4'	1:A:338:C:C5	2.51	0.45
3:C:29:HIS:HB2	3:C:153:ARG:HH12	1.82	0.45
4:D:1:PRO:O	4:D:2:GLN:HB2	2.17	0.45
1:A:926:A:H1'	13:M:38:HIS:O	2.16	0.45
1:A:818:A:H2	27:1:13:ARG:HA	1.81	0.45
1:A:2314:G:H2'	1:A:2315:C:H5'	1.98	0.45
4:D:198:GLU:HB3	37:D:8593:HOH:O	2.16	0.45
1:A:2445:U:H2'	1:A:2446:G:C8	2.51	0.45
28:2:52:SER:HA	37:2:4248:HOH:O	2.15	0.45
1:A:2112:A:H2'	1:A:2113:G:C8	2.52	0.45
1:A:683:G:O2'	1:A:684:G:H5'	2.16	0.45
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.97	0.45
21:U:71:VAL:HG11	21:U:90:PRO:CB	2.30	0.45
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.16	0.45
5:E:85:LYS:NZ	37:E:8325:HOH:O	2.42	0.45
1:A:1292:G:HO2'	1:A:1293:U:H6	1.62	0.45
19:S:82:GLU:HG3	19:S:83:LYS:H	1.82	0.45
1:A:2271:G:N3	1:A:2271:G:H2'	2.32	0.45
1:A:1375:A:C2'	1:A:1376:G:H5'	2.46	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
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
6:F:40:ILE:HG23	37:F:5583:HOH:O	2.15	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:558:C:C2	1:A:600:G:N2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:134:ILE:O	14:N:136:PRO:HD3	2.17	0.45
4:D:280:VAL:CG1	4:D:281:ASP:N	2.80	0.45
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.49	0.45
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.31	0.45
1:A:746:A:C6	16:P:65:LEU:HD13	2.52	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
19:S:79:ARG:C	19:S:81:PRO:HD3	2.37	0.45
1:A:1391:G:C5	1:A:1435:U:C4	3.04	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
1:A:35:U:O2'	1:A:36:C:H5'	2.17	0.45
24:X:63:GLU:HG2	24:X:93:ILE:HG22	1.98	0.45
1:A:1161:A:H8	1:A:1161:A:O5'	2.00	0.45
1:A:797:A:H5'	27:1:10:ARG:HG2	1.99	0.45
1:A:1299:G:N2	37:A:4657:HOH:O	2.49	0.45
9:I:12:ILE:HB	37:I:4714:HOH:O	2.16	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
17:Q:98:ILE:O	17:Q:98:ILE:HD13	2.16	0.45
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.15	0.45
2:B:3093:A:C5	2:B:3094:G:H1'	2.52	0.45
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.45	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:164:G:H3'	37:A:3620:HOH:O	2.17	0.45
1:A:1592:G:C5	1:A:1593:C:C4	3.04	0.45
3:C:105:VAL:CG1	3:C:106:CYS:H	2.30	0.45
1:A:1878:G:O2'	1:A:1879:U:C6	2.68	0.45
1:A:2456:A:H2'	1:A:2457:U:H6	1.82	0.45
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.46	0.45
1:A:2073:G:C6	1:A:2489:G:H4'	2.52	0.45
1:A:2001:G:C2'	1:A:2002:C:H5'	2.47	0.45
1:A:738:G:H3'	37:A:7031:HOH:O	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:766:A:H5'	37:A:4624:HOH:O	2.17	0.45
1:A:2356:A:H2'	1:A:2357:G:O4'	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
2:B:3035:C:H5''	37:B:4078:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2761:A:C4	1:A:2763:G:C8	3.04	0.45
1:A:105:G:O2'	1:A:106:A:H5'	2.17	0.45
14:N:84:LYS:O	14:N:87:MET:CG	2.65	0.45
2:B:3056:A:C3'	2:B:3057:A:H5''	2.47	0.45
10:J:84:ARG:CZ	10:J:135:TRP:CH2	3.00	0.45
1:A:1010:C:H4'	15:O:4:PRO:HB2	1.99	0.45
1:A:1834:C:H2'	1:A:1840:A:H62	1.78	0.45
24:X:48:VAL:O	24:X:48:VAL:HG12	2.15	0.45
5:E:246:ARG:CB	5:E:246:ARG:HH11	2.24	0.45
37:A:3749:HOH:O	22:V:17:THR:CG2	2.64	0.45
7:G:11:VAL:HG12	7:G:12:ASP:H	1.82	0.45
1:A:2896:A:H5''	37:A:6079:HOH:O	2.16	0.45
4:D:243:ASN:HA	4:D:244:PRO:C	2.36	0.45
4:D:132:HIS:HB2	4:D:137:LEU:HD22	1.99	0.45
4:D:132:HIS:CE1	4:D:171:VAL:CG2	3.00	0.45
1:A:1687:C:O2	28:2:9:GLY:HA2	2.17	0.45
7:G:43:ASP:HA	37:G:5864:HOH:O	2.16	0.45
1:A:2032:U:O2'	1:A:2033:G:H5''	2.17	0.45
1:A:929:A:O5'	1:A:929:A:H8	2.00	0.45
1:A:565:A:OP2	1:A:592:G:N1	2.43	0.45
10:J:26:LYS:HG2	10:J:28:ILE:N	2.24	0.45
27:1:46:LYS:NZ	37:1:8440:HOH:O	2.49	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
1:A:558:C:H2'	1:A:559:U:H5'	1.99	0.45
9:I:12:ILE:HD12	37:I:692:HOH:O	2.16	0.45
24:X:14:HIS:HB2	24:X:17:ILE:HG13	1.99	0.45
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.85	0.45
1:A:251:C:H1'	14:N:58:GLN:HE22	1.81	0.45
4:D:2:GLN:NE2	37:D:8618:HOH:O	2.50	0.45
1:A:1057:A:C6	1:A:1058:A:C6	3.05	0.45
1:A:679:G:OP2	37:A:4408:HOH:O	2.20	0.45
1:A:584:U:H3'	37:A:6075:HOH:O	2.15	0.45
1:A:333:G:O2'	1:A:334:G:H5'	2.17	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.17	0.45
10:J:117:LYS:O	10:J:119:VAL:HG13	2.17	0.45
10:J:150:LYS:NZ	37:J:8381:HOH:O	2.49	0.44
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.47	0.44
23:W:42:ASN:O	23:W:44:GLY:N	2.50	0.44
2:B:3020:G:H3'	37:B:2984:HOH:O	2.17	0.44
1:A:1829:A:C2'	1:A:1830:C:H5'	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3092:G:C6	2:B:3093:A:C6	3.06	0.44
1:A:1669:A:H2	37:A:3678:HOH:O	2.00	0.44
7:G:95:VAL:O	7:G:126:ILE:HD13	2.17	0.44
1:A:883:U:H2'	1:A:883:U:O2	2.17	0.44
5:E:187:ARG:HG3	5:E:187:ARG:O	2.16	0.44
1:A:2559:C:H4'	37:A:7243:HOH:O	2.17	0.44
1:A:328:U:O4'	5:E:202:THR:HG22	2.17	0.44
1:A:1242:A:H5'	11:K:82:THR:CG2	2.38	0.44
24:X:26:ILE:HB	37:X:5420:HOH:O	2.16	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
1:A:558:C:C2'	1:A:559:U:C5'	2.95	0.44
23:W:39:ALA:C	23:W:41:GLU:N	2.70	0.44
3:C:95:PRO:HA	3:C:153:ARG:HA	2.00	0.44
1:A:2607:U:O5'	1:A:2609:G:H4'	2.16	0.44
1:A:1139:U:H2'	1:A:1140:C:H6	1.82	0.44
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.32	0.44
12:L:118:ALA:C	12:L:120:ARG:H	2.21	0.44
1:A:84:G:O2'	1:A:85:C:H5'	2.17	0.44
1:A:2546:U:OP1	37:A:3821:HOH:O	2.21	0.44
2:B:3038:A:H2	2:B:3043:G:H5''	1.83	0.44
1:A:1004:C:O2'	1:A:1005:A:H5'	2.17	0.44
1:A:2697:A:H2'	1:A:2698:G:O4'	2.16	0.44
37:N:8532:HOH:O	30:4:46:ILE:HB	2.17	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:HD3	14:N:108:LYS:N	2.32	0.44
2:B:3014:G:C2'	2:B:3015:C:H5'	2.47	0.44
1:A:282:C:H2'	1:A:283:U:O4'	2.16	0.44
3:C:36:ASP:HB2	3:C:83:GLY:HA3	2.00	0.44
1:A:88:G:C8	29:3:28:LYS:HB2	2.52	0.44
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.80	0.44
6:F:59:GLY:C	6:F:61:PHE:N	2.71	0.44
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	1.99	0.44
16:P:44:ASN:OD1	16:P:65:LEU:HB2	2.17	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
1:A:883:U:C2'	1:A:883:U:O2	2.65	0.44
1:A:1066:U:H2'	1:A:1067:A:C8	2.52	0.44
5:E:79:ARG:O	5:E:87:ARG:HG2	2.18	0.44
27:1:57:CYS:O	27:1:61:GLY:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.47	0.44
1:A:2346:C:H4'	6:F:52:THR:CG2	2.46	0.44
24:X:42:ARG:O	24:X:45:VAL:HG22	2.18	0.44
1:A:2045:G:H2'	1:A:2046:G:O4'	2.17	0.44
29:3:40:ARG:HG2	29:3:40:ARG:HH11	1.82	0.44
1:A:873:G:H2'	1:A:875:A:N7	2.32	0.44
1:A:68:U:O2'	1:A:69:A:H5''	2.17	0.44
7:G:162:PHE:N	7:G:162:PHE:CD1	2.85	0.44
1:A:492:C:O2'	1:A:493:U:H5'	2.17	0.44
1:A:1236:A:H2'	1:A:1237:U:O4'	2.16	0.44
3:C:126:ALA:HB1	3:C:138:VAL:CG1	2.47	0.44
1:A:10:U:O4	1:A:532:A:OP2	2.35	0.44
14:N:182:LYS:HB2	14:N:194:ALA:HB2	1.99	0.44
1:A:2135:A:O2'	1:A:2136:G:H5'	2.18	0.44
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.48	0.44
1:A:2338:G:H1'	6:F:105:SER:OG	2.17	0.44
10:J:114:PRO:O	10:J:115:PHE:C	2.55	0.44
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.29	0.44
1:A:902:G:N7	13:M:18:HIS:CD2	2.84	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
8:H:22:VAL:HG21	8:H:104:ALA:HB2	2.00	0.44
1:A:694:A:C2'	1:A:695:C:H5'	2.47	0.44
1:A:67:A:H5''	1:A:69:A:C8	2.53	0.44
1:A:2334:C:O2'	1:A:2335:C:H5'	2.18	0.44
1:A:245:C:C2'	1:A:246:G:H5'	2.48	0.44
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.18	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
23:W:1:THR:HG23	23:W:2:VAL:N	2.23	0.44
4:D:240:GLY:HA3	37:D:8654:HOH:O	2.17	0.44
1:A:1081:A:C6	1:A:1082:A:N1	2.85	0.44
2:B:3107:C:H2'	2:B:3108:C:C6	2.52	0.44
21:U:75:GLU:O	21:U:76:ASP:HB2	2.18	0.44
1:A:245:C:H2'	1:A:246:G:H5'	1.98	0.44
25:Y:27:ASP:N	25:Y:27:ASP:OD2	2.51	0.44
17:Q:27:ARG:O	17:Q:31:ILE:HG13	2.18	0.44
24:X:126:ASP:HB3	24:X:135:GLY:O	2.18	0.44
5:E:235:PHE:CE2	5:E:243:VAL:HG21	2.48	0.44
12:L:55:VAL:CG1	12:L:56:SER:N	2.80	0.44
24:X:65:VAL:HA	24:X:68:THR:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:A:H2'	1:A:205:U:C5'	2.45	0.44
1:A:2289:G:H21	1:A:2291:A:H2	1.63	0.44
1:A:1127:C:C2'	1:A:1128:U:H5'	2.48	0.44
10:J:72:VAL:CG1	10:J:81:TYR:CZ	3.01	0.44
16:P:99:GLU:CG	37:P:6044:HOH:O	2.66	0.44
1:A:449:A:C8	5:E:43:LYS:HG2	2.52	0.44
1:A:1409:G:H5'	37:A:3700:HOH:O	2.17	0.44
5:E:25:PRO:HD2	37:E:8431:HOH:O	2.15	0.44
1:A:1969:A:N7	1:A:1970:G:C6	2.85	0.44
1:A:2727:A:H2'	1:A:2728:C:H5'	1.99	0.44
1:A:1515:A:H2'	1:A:1516:C:C6	2.53	0.44
10:J:31:PHE:CD2	10:J:85:ILE:HG23	2.53	0.44
6:F:103:ASN:ND2	6:F:134:LEU:H	2.16	0.44
1:A:2506:A:C1'	37:A:6034:HOH:O	2.65	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
1:A:259:G:O2'	1:A:260:C:H5'	2.18	0.44
1:A:2055:A:H5'	19:S:134:SER:HB2	2.00	0.44
19:S:132:ARG:NH1	37:S:8559:HOH:O	2.51	0.44
1:A:538:C:H5''	1:A:539:G:C8	2.53	0.44
21:U:26:THR:HA	21:U:39:ASN:HB3	1.99	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: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
10:J:31:PHE:HD2	10:J:85:ILE:O	2.01	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
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:435:A:O2'	1:A:436:A:H5'	2.18	0.44
1:A:2482:G:O2'	1:A:2535:U:OP2	2.29	0.44
1:A:861:A:H2'	1:A:862:U:C6	2.52	0.44
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.18	0.44
1:A:870:G:C3'	1:A:871:G:H5''	2.48	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
14:N:57:LYS:HB3	14:N:60:ILE:HD12	2.00	0.43
1:A:1666:C:H2'	1:A:1667:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:G:C2	1:A:111:C:C2	3.06	0.43
1:A:1169:U:C5	1:A:1170:U:C4	3.06	0.43
14:N:106:ASN:ND2	34:N:8518:CL:CL	2.88	0.43
1:A:445:U:C1'	37:A:7324:HOH:O	2.66	0.43
1:A:2408:A:H4'	30:4:15:ASN:O	2.17	0.43
6:F:58:VAL:CG1	6:F:59:GLY:N	2.80	0.43
1:A:244:C:H6	1:A:244:C:O5'	2.00	0.43
1:A:2724:U:O4	1:A:2725:G:N1	2.51	0.43
17:Q:27:ARG:HA	37:Q:3969:HOH:O	2.18	0.43
14:N:184:ARG:NH1	14:N:184:ARG:HB2	2.33	0.43
16:P:41:ALA:HA	37:P:5104:HOH:O	2.18	0.43
13:M:65:ASP:HA	13:M:109:LEU:O	2.17	0.43
17:Q:115:SER:C	17:Q:117:SER:H	2.21	0.43
20:T:57:THR:CG2	20:T:58:MET:N	2.81	0.43
1:A:1173:A:H4'	1:A:1174:A:C8	2.53	0.43
8:H:99:THR:O	8:H:100:ASP:HB2	2.17	0.43
6:F:95:THR:C	6:F:97:GLN:N	2.67	0.43
5:E:162:VAL:O	5:E:162:VAL:HG12	2.18	0.43
1:A:2265:U:H2'	1:A:2266:A:H8	1.84	0.43
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.46	0.43
1:A:244:C:OP2	8:H:38:LYS:HE3	2.18	0.43
1:A:13:G:H2'	1:A:14:C:C6	2.53	0.43
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.49	0.43
1:A:69:A:H5'	1:A:69:A:H8	1.83	0.43
1:A:1419:U:O2	1:A:1419:U:H3'	2.18	0.43
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.47	0.43
13:M:98:GLU:O	13:M:99:GLU:CB	2.66	0.43
1:A:892:G:H5''	28:2:54:ALA:HB2	2.00	0.43
1:A:1096:U:H5''	1:A:1258:G:O6	2.18	0.43
1:A:912:A:C4	1:A:1294:A:C2	3.06	0.43
15:O:37:ARG:CD	34:O:8507:CL:CL	3.03	0.43
10:J:57:ARG:C	10:J:59:ASN:N	2.70	0.43
4:D:190:MET:CE	4:D:194:PHE:CD1	2.94	0.43
4:D:144:THR:HG22	4:D:145:HIS:N	2.33	0.43
25:Y:43:VAL:HG12	25:Y:47:ALA:HB3	2.00	0.43
17:Q:143:ALA:HA	37:Q:5521:HOH:O	2.17	0.43
14:N:76:ARG:HG2	14:N:76:ARG:NH1	2.34	0.43
1:A:1097:A:H5''	24:X:125:HIS:CE1	2.53	0.43
4:D:103:ASP:HB2	37:D:8590:HOH:O	2.17	0.43
1:A:1215:A:O3'	1:A:1216:G:C4'	2.66	0.43
37:A:6175:HOH:O	29:3:44:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2119:C:O2'	1:A:2120:U:H5'	2.18	0.43
19:S:96:VAL:HG13	19:S:106:GLY:HA3	2.00	0.43
37:B:4707:HOH:O	15:O:147:ILE:HD12	2.18	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
19:S:39:THR:CB	19:S:42:GLU:HG3	2.42	0.43
2:B:3047:A:C2	2:B:3048:C:C2	3.06	0.43
37:A:7395:HOH:O	21:U:2:LYS:HE2	2.17	0.43
21:U:48:VAL:HG22	21:U:97:ARG:O	2.19	0.43
1:A:329:A:OP2	5:E:206:ASN:HB2	2.18	0.43
1:A:2092:G:H2'	1:A:2613:G:OP1	2.18	0.43
1:A:538:C:OP2	26:Z:134:HIS:HE1	2.01	0.43
14:N:169:ARG:NH1	37:N:8572:HOH:O	2.52	0.43
1:A:580:A:N1	1:A:1253:C:O2'	2.47	0.43
11:K:6:PHE:O	11:K:8:ALA:N	2.51	0.43
15:O:67:ALA:HA	15:O:71:TRP:H	1.83	0.43
15:O:37:ARG:CZ	37:O:8533:HOH:O	2.67	0.43
1:A:566:A:H2'	1:A:567:U:O4'	2.18	0.43
3:C:211:LYS:CB	3:C:212:PRO:HD2	2.36	0.43
1:A:1666:C:O2'	1:A:1667:A:C5'	2.62	0.43
15:O:91:ARG:HG3	15:O:186:LEU:HD23	2.01	0.43
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.65	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
15:O:116:PHE:HB2	37:O:8556:HOH:O	2.19	0.43
1:A:2468:A:N6	30:4:50:GLY:O	2.52	0.43
17:Q:13:VAL:CG2	17:Q:41:ARG:HG2	2.46	0.43
15:O:184:ILE:HG22	15:O:185:GLU:N	2.33	0.43
13:M:101:ASP:C	13:M:103:ALA:H	2.21	0.43
1:A:1783:A:C2'	1:A:1784:U:H5'	2.48	0.43
1:A:101:C:H2'	1:A:102:A:C8	2.53	0.43
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.36	0.43
1:A:1257:C:H2'	1:A:1258:G:O4'	2.18	0.43
1:A:65:C:O2'	1:A:66:G:H5'	2.18	0.43
13:M:93:VAL:HG12	13:M:97:VAL:HG23	2.01	0.43
1:A:1609:C:H2'	1:A:1610:G:H8	1.82	0.43
2:B:3104:A:O2'	2:B:3105:A:H5'	2.19	0.43
1:A:2095:A:C2	1:A:2651:C:C2	3.06	0.43
5:E:114:ALA:HB1	5:E:223:LEU:HB3	2.01	0.43
14:N:35:PRO:HD2	14:N:38:VAL:HG21	2.01	0.43
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:110:GLN:CA	24:X:110:GLN:HE21	2.27	0.43
1:A:1164:U:O4'	1:A:1165:G:OP1	2.35	0.43
1:A:2054:A:H2	19:S:128:ARG:HH22	1.62	0.43
15:O:114:LYS:O	15:O:118:ILE:HG13	2.18	0.43
1:A:2346:C:H4'	6:F:52:THR:HG22	2.01	0.43
11:K:39:VAL:CG1	11:K:107:ASN:HB2	2.49	0.43
1:A:2911:C:H2'	1:A:2912:C:C6	2.54	0.43
3:C:170:VAL:HG13	27:1:22:ILE:CG2	2.48	0.43
1:A:643:A:N1	1:A:902:G:O2'	2.45	0.43
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
14:N:191:GLY:O	14:N:192:ALA:HB3	2.17	0.43
2:B:3092:G:H22	10:J:52:LYS:NZ	2.16	0.43
20:T:73:ASP:O	20:T:77:VAL:HG23	2.19	0.43
1:A:2598:U:O2	1:A:2600:A:C8	2.72	0.43
14:N:49:ALA:C	14:N:54:TYR:HB3	2.38	0.43
1:A:734:U:O2'	1:A:737:A:N6	2.51	0.43
1:A:2900:G:H2'	1:A:2901:C:O4'	2.19	0.43
1:A:2036:C:OP1	37:A:6682:HOH:O	2.21	0.43
27:1:46:LYS:HB3	37:1:8438:HOH:O	2.17	0.43
15:O:67:ALA:C	15:O:69:TYR:H	2.22	0.43
1:A:820:G:H5'	1:A:821:U:C5'	2.49	0.43
14:N:138:HIS:C	14:N:139:PRO:O	2.50	0.43
27:1:50:ALA:HB3	27:1:54:ILE:HG22	2.00	0.43
26:Z:187:VAL:CG1	26:Z:205:ILE:HA	2.47	0.43
4:D:162:MET:HG3	4:D:310:ARG:NH1	2.33	0.43
5:E:129:HIS:CE1	5:E:232:LEU:H	2.37	0.43
1:A:1332:C:O2'	1:A:1333:U:H5'	2.19	0.43
1:A:2898:G:O2'	1:A:2899:A:H5'	2.18	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
3:C:8:ARG:HG2	37:C:8553:HOH:O	2.17	0.43
5:E:39:GLN:O	5:E:43:LYS:HD3	2.19	0.43
1:A:929:A:C8	1:A:930:C:C5	3.07	0.43
13:M:91:VAL:O	13:M:91:VAL:HG13	2.18	0.43
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.53	0.43
18:R:53:HIS:O	18:R:55:ARG:N	2.52	0.43
13:M:35:ARG:O	13:M:40:PHE:HA	2.18	0.43
14:N:42:ARG:HA	14:N:43:PRO:HD3	1.79	0.43
3:C:211:LYS:HD3	37:C:8613:HOH:O	2.18	0.43
20:T:58:MET:SD	29:3:8:LYS:HE3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:15:THR:HG22	10:J:91:HIS:HA	1.99	0.43
2:B:3078:G:N2	2:B:3103:A:OP2	2.48	0.43
3:C:94:LEU:CD2	3:C:94:LEU:N	2.82	0.43
7:G:7:ILE:HA	7:G:8:PRO:HD3	1.82	0.43
1:A:2837:U:H2'	37:A:6820:HOH:O	2.19	0.43
25:Y:15:ARG:NH1	25:Y:15:ARG:HB3	2.29	0.43
3:C:169:PHE:O	3:C:170:VAL:HB	2.18	0.43
15:O:161:GLY:O	15:O:162:ASP:C	2.56	0.43
7:G:49:ILE:HD11	7:G:69:ILE:HD12	2.00	0.43
1:A:489:A:C8	21:U:82:THR:CG2	3.02	0.43
1:A:1308:A:O4'	5:E:226:GLY:HA3	2.19	0.43
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.81	0.43
12:L:118:ALA:O	12:L:120:ARG:N	2.52	0.43
1:A:2416:G:H2'	1:A:2417:C:C6	2.54	0.43
17:Q:2:ASP:C	17:Q:2:ASP:OD1	2.56	0.43
1:A:1992:U:H2'	1:A:1994:A:OP2	2.19	0.43
1:A:757:C:H2'	1:A:758:A:C8	2.54	0.43
1:A:392:U:H4'	14:N:193:LYS:HB3	2.01	0.43
10:J:50:VAL:HA	10:J:157:ILE:HG12	2.00	0.43
5:E:115:LEU:HD12	5:E:115:LEU:HA	1.83	0.43
15:O:71:TRP:CE3	15:O:175:LEU:CD2	2.97	0.43
14:N:37:VAL:HG21	14:N:108:LYS:HG3	2.01	0.43
1:A:2781:U:C2'	1:A:2782:G:H5'	2.49	0.43
15:O:113:SER:C	37:O:8556:HOH:O	2.58	0.43
1:A:553:G:O2'	26:Z:179:PRO:HG3	2.19	0.43
8:H:80:GLN:HB3	37:H:2563:HOH:O	2.19	0.43
15:O:66:LEU:HA	15:O:66:LEU:HD12	1.92	0.43
1:A:221:G:OP2	13:M:46:LEU:HB3	2.19	0.43
1:A:2681:A:N6	1:A:2714:U:H4'	2.33	0.43
1:A:69:A:H2'	1:A:70:A:OP2	2.18	0.43
1:A:2626:C:H2'	1:A:2627:G:C8	2.54	0.43
1:A:321:A:H1'	37:A:7016:HOH:O	2.19	0.43
37:E:8360:HOH:O	16:P:3:THR:HG21	2.19	0.43
1:A:1301:C:O2'	1:A:1331:A:H4'	2.19	0.43
15:O:129:ILE:HA	15:O:130:PRO:HD3	1.93	0.43
1:A:1176:C:H1'	37:A:3901:HOH:O	2.18	0.43
1:A:1921:A:C6	1:A:1922:A:C2	3.07	0.43
2:B:3057:A:H5'	2:B:3057:A:N3	2.33	0.43
1:A:542:A:C8	1:A:542:A:C5'	2.98	0.43
3:C:223:ARG:NH1	37:C:8518:HOH:O	2.50	0.43
4:D:41:PHE:N	37:D:8647:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:30:GLU:O	27:1:33:HIS:HB3	2.18	0.43
3:C:101:GLU:HG2	3:C:131:HIS:ND1	2.34	0.43
4:D:11:LEU:HA	37:D:8614:HOH:O	2.18	0.43
2:B:3039:U:H3'	2:B:3040:C:H5''	2.00	0.43
8:H:113:ASP:O	8:H:117:GLU:HG3	2.19	0.43
14:N:47:ASP:CG	14:N:48:ARG:N	2.73	0.43
1:A:1543:G:N1	1:A:1641:A:OP2	2.40	0.43
4:D:279:THR:HG22	4:D:280:VAL:N	2.33	0.43
3:C:217:ARG:HH11	3:C:217:ARG:CG	2.30	0.43
13:M:30:ARG:NH1	37:M:8511:HOH:O	2.42	0.43
10:J:95:GLU:HB3	10:J:119:VAL:HG11	2.01	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:192:A:N6	1:A:194:A:C2	2.87	0.43
18:R:77:ASP:N	18:R:80:LYS:O	2.52	0.43
24:X:90:TYR:N	37:X:6679:HOH:O	2.52	0.42
20:T:57:THR:CG2	20:T:59:ASP:HB2	2.49	0.42
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.18	0.42
24:X:6:GLN:HA	24:X:52:VAL:HG23	2.00	0.42
10:J:136:VAL:HG22	10:J:137:ASN:N	2.34	0.42
2:B:3078:G:O2'	2:B:3079:U:P	2.77	0.42
22:V:49:LEU:O	22:V:55:ALA:CB	2.67	0.42
1:A:2656:G:C2'	1:A:2657:G:H5'	2.48	0.42
5:E:14:GLY:N	37:E:8446:HOH:O	2.52	0.42
1:A:818:A:C2	27:1:13:ARG:HA	2.54	0.42
14:N:77:PHE:CE2	14:N:86:MET:HG2	2.53	0.42
1:A:1137:G:H1'	37:A:3851:HOH:O	2.19	0.42
6:F:17:ARG:NH2	37:F:3723:HOH:O	2.40	0.42
1:A:1513:C:O2'	1:A:1514:C:H5'	2.18	0.42
1:A:100:C:H4'	21:U:16:LEU:HB2	2.01	0.42
23:W:12:THR:O	23:W:15:GLU:N	2.51	0.42
2:B:3006:C:P	15:O:37:ARG:HH11	2.42	0.42
5:E:98:ARG:NH1	37:E:8358:HOH:O	2.45	0.42
11:K:107:ASN:HD22	11:K:107:ASN:C	2.22	0.42
4:D:254:GLN:HG2	4:D:255:GLY:H	1.83	0.42
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.97	0.42
30:4:31:THR:HB	30:4:33:MET:HE2	2.00	0.42
4:D:129:ARG:NH2	4:D:176:ASP:OD1	2.51	0.42
1:A:1947:G:N2	1:A:1966:U:O2	2.51	0.42
3:C:55:VAL:CG1	3:C:67:LEU:HD22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:K:88:PRO:HA	34:K:8502:CL:CL	2.55	0.42
1:A:1746:A:N3	1:A:1748:U:C4	2.87	0.42
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.49	0.42
24:X:122:ARG:HG3	24:X:152:ALA:O	2.20	0.42
7:G:20:ILE:O	7:G:30:THR:HA	2.19	0.42
1:A:1733:A:C6	1:A:1734:C:C2	3.07	0.42
1:A:1701:A:H5''	1:A:1702:U:H3'	2.01	0.42
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.81	0.42
1:A:1123:A:C2	1:A:1129:C:H4'	2.54	0.42
3:C:81:GLN:CB	3:C:92:ASN:ND2	2.81	0.42
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.48	0.42
2:B:3003:A:H2'	37:B:2430:HOH:O	2.19	0.42
1:A:1773:G:C2'	1:A:1774:G:H5'	2.49	0.42
1:A:2833:C:O2	1:A:2848:G:C2	2.72	0.42
14:N:137:ASP:C	14:N:142:LYS:HE3	2.40	0.42
1:A:407:A:C2	1:A:408:A:C4	3.07	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
4:D:84:LEU:HD13	4:D:84:LEU:O	2.19	0.42
1:A:1532:G:C6	1:A:1533:A:C6	3.08	0.42
1:A:29:C:O2'	1:A:30:U:H5'	2.19	0.42
14:N:18:GLY:O	14:N:21:ALA:HB3	2.20	0.42
10:J:150:LYS:HA	10:J:153:VAL:CG2	2.49	0.42
15:O:67:ALA:C	15:O:69:TYR:N	2.73	0.42
17:Q:115:SER:C	17:Q:117:SER:N	2.73	0.42
1:A:2432:C:C4'	37:A:9716:HOH:O	2.60	0.42
25:Y:25:ARG:CD	37:Y:3861:HOH:O	2.47	0.42
7:G:137:ASP:OD1	7:G:139:GLU:HB2	2.19	0.42
21:U:38:ARG:HG3	21:U:38:ARG:HH11	1.83	0.42
1:A:2656:G:O2'	1:A:2657:G:H5'	2.18	0.42
1:A:2637:A:C4'	37:A:4335:HOH:O	2.67	0.42
3:C:170:VAL:HG13	27:1:22:ILE:HG21	2.01	0.42
28:2:19:CYS:SG	28:2:21:ARG:N	2.93	0.42
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.55	0.42
1:A:1862:C:O2'	1:A:1863:G:H5'	2.20	0.42
1:A:1804:A:H2'	1:A:1805:G:H8	1.84	0.42
1:A:585:C:H6	37:A:6075:HOH:O	2.01	0.42
1:A:23:G:C6	1:A:24:G:N1	2.88	0.42
1:A:2405:C:H5'	37:A:6578:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1573:A:H2'	1:A:1574:C:O4'	2.19	0.42
15:O:47:LEU:HA	15:O:47:LEU:HD23	1.79	0.42
1:A:2121:G:C2'	1:A:2122:C:H5'	2.50	0.42
1:A:1751:G:C3'	1:A:1752:G:H5''	2.49	0.42
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.82	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
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
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.49	0.42
1:A:1863:G:OP2	37:A:3122:HOH:O	2.22	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:1506:U:H5'	1:A:1506:U:H6	1.85	0.42
1:A:1459:A:OP2	37:A:9229:HOH:O	2.22	0.42
1:A:911:G:H5'	1:A:932:U:OP1	2.19	0.42
1:A:80:A:H3'	21:U:43:ASN:OD1	2.18	0.42
10:J:47:GLU:HG2	10:J:133:ILE:HD12	2.00	0.42
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.53	0.42
24:X:122:ARG:CZ	37:X:5817:HOH:O	2.67	0.42
1:A:1166:A:N3	1:A:1166:A:H2'	2.34	0.42
1:A:2812:A:C2	1:A:2814:A:N6	2.75	0.42
6:F:64:ARG:HD3	6:F:67:ASP:HB3	2.02	0.42
15:O:38:LYS:HB2	15:O:38:LYS:HE3	1.71	0.42
4:D:16:ARG:NE	37:D:8553:HOH:O	2.19	0.42
4:D:168:GLY:H	4:D:174:ARG:HD3	1.83	0.42
26:Z:112:GLU:OE1	26:Z:115:ARG:NH1	2.52	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:736:A:H2'	1:A:737:A:O4'	2.19	0.42
1:A:666:A:H2'	1:A:667:C:O4'	2.20	0.42
1:A:69:A:C2'	1:A:70:A:OP2	2.68	0.42
1:A:492:C:C2'	1:A:493:U:H5'	2.49	0.42
2:B:3012:C:H5'	2:B:3070:U:O4'	2.20	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
6:F:24:HIS:HB2	6:F:72:LYS:CB	2.50	0.42
12:L:37:TYR:CE2	12:L:45:PRO:HA	2.55	0.42
15:O:86:LEU:O	15:O:90:LEU:HG	2.18	0.42
14:N:186:SER:OG	14:N:189:VAL:CG1	2.67	0.42
10:J:55:GLN:HE21	10:J:124:ARG:NE	2.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:39:THR:O	19:S:40:ALA:C	2.58	0.42
7:G:11:VAL:HG13	7:G:23:GLU:O	2.18	0.42
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.19	0.42
30:4:7:PHE:CE2	30:4:22:VAL:CG2	3.00	0.42
1:A:2909:G:H2'	1:A:2910:A:H8	1.84	0.42
1:A:1123:A:N6	1:A:1238:C:H5'	2.33	0.42
1:A:710:G:N2	1:A:719:C:C2	2.88	0.42
1:A:2833:C:C2	1:A:2848:G:C2	3.08	0.42
4:D:277:GLU:N	4:D:278:PRO:HD2	2.34	0.42
1:A:581:G:H5'	37:A:7679:HOH:O	2.20	0.42
1:A:1211:G:O2'	1:A:1212:C:H5'	2.19	0.42
26:Z:101:GLY:HA3	37:Z:8561:HOH:O	2.20	0.42
24:X:88:THR:HG23	24:X:110:GLN:HB3	2.02	0.42
1:A:2432:C:C2'	1:A:2433:A:H5'	2.50	0.42
5:E:107:ARG:HB3	5:E:107:ARG:CZ	2.48	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
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:1886:A:H4'	37:1:8405:HOH:O	2.19	0.42
2:B:3078:G:N2	2:B:3102:G:H2'	2.34	0.42
17:Q:120:ARG:NH2	17:Q:123:TYR:HD2	2.12	0.42
6:F:173:GLU:HG3	6:F:174:VAL:N	2.35	0.42
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.31	0.42
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.55	0.42
1:A:2883:A:H2'	1:A:2884:G:O4'	2.20	0.42
6:F:10:PHE:CE1	6:F:11:HIS:HB3	2.54	0.42
4:D:101:TRP:HB2	4:D:119:HIS:CD2	2.55	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
37:A:4546:HOH:O	14:N:83:SER:HA	2.19	0.42
3:C:123:GLY:HA3	3:C:162:GLY:HA2	2.01	0.42
1:A:1934:A:C8	1:A:1935:C:C5	3.07	0.42
1:A:752:G:O6	37:A:4299:HOH:O	2.22	0.42
5:E:141:SER:HA	37:E:8381:HOH:O	2.19	0.42
12:L:14:LYS:CB	12:L:45:PRO:HG2	2.45	0.42
37:A:3731:HOH:O	21:U:9:LYS:HD3	2.18	0.42
1:A:1185:U:O4'	37:A:7456:HOH:O	2.21	0.42
3:C:69:LEU:CD2	3:C:120:ARG:HB3	2.44	0.42
1:A:1299:G:N7	13:M:6:ARG:NH1	2.67	0.42
13:M:145:LEU:O	13:M:145:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:27:ARG:CG	5:E:29:ASP:OD1	2.63	0.42
2:B:3030:C:OP1	6:F:137:PRO:O	2.37	0.42
22:V:49:LEU:CD1	37:V:3805:HOH:O	2.68	0.42
4:D:16:ARG:NH1	37:D:8614:HOH:O	2.53	0.42
4:D:248:ARG:NH2	37:D:8522:HOH:O	2.52	0.42
2:B:3040:C:N4	6:F:51:ARG:HB2	2.34	0.42
1:A:2897:C:O2'	1:A:2898:G:H5'	2.20	0.42
1:A:2012:U:H2'	1:A:2013:G:OP1	2.19	0.42
4:D:215:VAL:HB	4:D:234:ARG:NH1	2.34	0.42
1:A:1692:C:H1'	37:A:9450:HOH:O	2.19	0.42
1:A:1400:C:O2'	1:A:1401:G:H5'	2.20	0.42
1:A:2531:U:O2'	1:A:2532:A:H5'	2.19	0.42
1:A:218:C:P	30:4:39:GLN:HE21	2.42	0.42
1:A:25:A:C2'	1:A:26:U:H5'	2.50	0.42
1:A:724:G:O2'	1:A:725:C:H5'	2.20	0.42
1:A:1483:C:O2'	1:A:1484:G:H5'	2.20	0.42
27:1:47:LEU:HA	27:1:56:MET:O	2.20	0.42
12:L:9:THR:O	12:L:10:GLN:C	2.56	0.42
7:G:81:GLU:HA	7:G:133:VAL:O	2.19	0.42
1:A:841:A:OP2	19:S:128:ARG:HD2	2.20	0.42
7:G:23:GLU:HG2	7:G:28:SER:HB2	2.01	0.42
10:J:111:MET:O	10:J:114:PRO:HD3	2.20	0.42
8:H:33:THR:HG21	8:H:59:ILE:O	2.19	0.42
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.48	0.42
12:L:6:ALA:HB3	12:L:116:GLU:HG2	2.01	0.42
30:4:62:THR:HG23	30:4:86:GLY:HA2	2.02	0.42
9:I:64:ASN:N	9:I:64:ASN:ND2	2.67	0.42
37:A:7050:HOH:O	19:S:33:ARG:HD3	2.20	0.42
1:A:2415:A:C2	15:O:25:ARG:CB	3.03	0.42
1:A:1773:G:O2'	27:1:15:GLY:HA2	2.20	0.42
1:A:818:A:H5"	37:A:6570:HOH:O	2.20	0.42
12:L:118:ALA:HA	12:L:125:ALA:HB2	2.02	0.42
3:C:111:SER:O	3:C:112:PRO:C	2.58	0.42
1:A:889:C:H2'	1:A:890:C:C6	2.55	0.42
2:B:3026:C:O2'	2:B:3027:C:H5'	2.20	0.42
15:O:39:SER:HB3	15:O:42:HIS:H	1.85	0.42
1:A:827:A:H2'	1:A:828:G:O4'	2.19	0.42
7:G:5:LEU:HD21	7:G:66:GLN:HG3	2.02	0.42
3:C:88:ILE:CD1	3:C:100:PRO:HD3	2.39	0.41
15:O:38:LYS:HE2	15:O:107:ASN:ND2	2.34	0.41
13:M:148:GLU:CG	37:M:8558:HOH:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:ARG:HB2	37:C:8609:HOH:O	2.19	0.41
6:F:57:THR:HA	6:F:63:ILE:HA	2.01	0.41
13:M:54:PRO:HG2	13:M:57:VAL:HG21	2.01	0.41
4:D:17:LYS:O	4:D:260:HIS:HD2	2.03	0.41
2:B:3039:U:HO2'	2:B:3042:C:H5	1.58	0.41
24:X:38:THR:O	24:X:42:ARG:HB2	2.20	0.41
1:A:2379:G:N7	1:A:2408:A:N1	2.67	0.41
1:A:2044:G:OP1	25:Y:23:HIS:CE1	2.69	0.41
1:A:2443:C:O3'	13:M:56:LYS:HE3	2.20	0.41
10:J:154:THR:HB	10:J:155:PRO:CD	2.50	0.41
30:4:87:ARG:HD2	37:4:8528:HOH:O	2.21	0.41
1:A:201:G:N1	1:A:202:U:C4	2.88	0.41
14:N:98:GLN:O	14:N:101:ALA:HB3	2.19	0.41
13:M:98:GLU:O	13:M:99:GLU:HB2	2.20	0.41
1:A:1098:A:H2'	1:A:1099:G:O4'	2.20	0.41
1:A:825:U:H5''	1:A:826:U:OP1	2.20	0.41
1:A:1469:C:N3	1:A:1472:C:OP2	2.53	0.41
12:L:78:LYS:HA	12:L:79:PRO:HD3	1.85	0.41
1:A:2869:G:H2'	1:A:2870:C:C6	2.55	0.41
6:F:23:VAL:HG12	6:F:130:VAL:HG22	2.01	0.41
25:Y:74:ALA:HB2	25:Y:85:VAL:HG13	2.01	0.41
4:D:307:ARG:HG3	4:D:307:ARG:NH1	2.35	0.41
1:A:315:G:C6	1:A:316:A:C6	3.08	0.41
3:C:186:TRP:CG	3:C:187:PRO:HA	2.55	0.41
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.74	0.41
37:A:5662:HOH:O	15:O:21:HIS:HE1	2.04	0.41
7:G:138:ILE:HG22	37:G:5404:HOH:O	2.19	0.41
5:E:102:LEU:HD12	37:E:8315:HOH:O	2.20	0.41
1:A:593:A:N7	37:A:4369:HOH:O	2.52	0.41
19:S:104:PHE:HB2	19:S:109:MET:HE1	2.01	0.41
19:S:99:ALA:CB	19:S:109:MET:HE1	2.25	0.41
10:J:56:ILE:HG21	10:J:61:LEU:HD13	2.02	0.41
4:D:41:PHE:HB3	4:D:190:MET:HE1	2.02	0.41
16:P:39:THR:HB	37:P:3360:HOH:O	2.19	0.41
24:X:13:MET:O	24:X:14:HIS:C	2.58	0.41
23:W:38:GLY:C	23:W:40:PRO:HD2	2.41	0.41
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.50	0.41
29:3:40:ARG:NH1	29:3:40:ARG:HG2	2.35	0.41
21:U:96:VAL:HG13	21:U:97:ARG:N	2.36	0.41
1:A:1014:A:H2'	1:A:1015:C:H5'	2.02	0.41
25:Y:30:MET:CE	25:Y:58:ALA:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:MET:HE1	7:G:148:ILE:HD12	2.01	0.41
1:A:517:U:C2'	1:A:518:G:H5'	2.50	0.41
1:A:99:A:H3'	1:A:100:C:C6	2.56	0.41
13:M:64:ILE:O	13:M:64:ILE:HG23	2.19	0.41
19:S:149:GLU:HA	19:S:150:PRO:HD3	1.92	0.41
12:L:98:VAL:HG13	12:L:99:ASP:O	2.21	0.41
16:P:113:VAL:O	16:P:114:ILE:HD13	2.20	0.41
15:O:132:ASN:O	15:O:135:VAL:HG12	2.20	0.41
1:A:2470:A:O2'	37:A:6532:HOH:O	2.20	0.41
1:A:637:C:OP1	26:Z:136:LYS:NZ	2.43	0.41
4:D:150:ALA:O	4:D:152:PRO:HD3	2.20	0.41
23:W:12:THR:HG23	23:W:14:ALA:N	2.36	0.41
6:F:44:ILE:HG12	6:F:83:PHE:CE1	2.52	0.41
10:J:26:LYS:HE3	10:J:28:ILE:HB	2.02	0.41
1:A:1943:C:O4'	3:C:212:PRO:HA	2.19	0.41
14:N:173:LEU:HA	14:N:183:VAL:HG11	2.03	0.41
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.50	0.41
1:A:711:G:C2	1:A:718:C:C2	3.08	0.41
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.55	0.41
1:A:1846:U:H2'	1:A:1847:A:C4	2.56	0.41
12:L:4:LEU:HD22	12:L:116:GLU:HB3	2.02	0.41
37:A:4806:HOH:O	11:K:47:THR:CB	2.64	0.41
1:A:380:A:H5''	14:N:48:ARG:NH2	2.35	0.41
21:U:48:VAL:HG22	21:U:97:ARG:C	2.40	0.41
1:A:159:G:H2'	1:A:175:G:H22	1.85	0.41
1:A:454:U:C2	37:A:9027:HOH:O	2.57	0.41
22:V:38:ASN:O	22:V:42:LEU:HG	2.20	0.41
3:C:135:VAL:N	37:C:8600:HOH:O	2.52	0.41
1:A:492:C:C2	1:A:501:G:N2	2.88	0.41
1:A:377:C:H5	37:A:3286:HOH:O	2.03	0.41
19:S:61:GLN:NE2	37:S:8540:HOH:O	2.54	0.41
10:J:86:ARG:HG2	10:J:86:ARG:H	1.63	0.41
2:B:3057:A:H8	6:F:141:VAL:HG21	1.85	0.41
10:J:84:ARG:NH2	10:J:135:TRP:CH2	2.82	0.41
24:X:110:GLN:CA	24:X:110:GLN:NE2	2.69	0.41
25:Y:9:VAL:HG22	25:Y:88:GLU:OE2	2.20	0.41
10:J:112:ARG:O	10:J:113:ALA:C	2.58	0.41
23:W:42:ASN:N	23:W:43:PRO:HD3	2.35	0.41
17:Q:13:VAL:HG11	17:Q:40:VAL:HG12	2.03	0.41
1:A:695:C:H2'	1:A:696:C:C6	2.55	0.41
1:A:654:A:OP2	16:P:38:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2488:A:H1'	37:A:9092:HOH:O	2.20	0.41
1:A:79:G:H22	1:A:97:G:H1'	1.85	0.41
1:A:1132:A:H2'	1:A:1133:A:C8	2.55	0.41
1:A:1969:A:O2'	1:A:1970:G:H5'	2.20	0.41
1:A:1609:C:H2'	1:A:1610:G:C8	2.56	0.41
1:A:1992:U:C2	1:A:1994:A:OP2	2.74	0.41
5:E:154:VAL:O	5:E:158:GLU:HG3	2.20	0.41
21:U:113:GLU:O	21:U:114:SER:C	2.58	0.41
1:A:1305:C:O2'	1:A:1306:U:H5'	2.19	0.41
1:A:2836:G:C6	1:A:2838:A:C2	3.08	0.41
1:A:123:U:H2'	1:A:124:C:C6	2.56	0.41
1:A:2767:C:OP1	4:D:318:ASN:ND2	2.53	0.41
24:X:122:ARG:NH1	24:X:152:ALA:O	2.54	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
3:C:51:ARG:CZ	37:C:8609:HOH:O	2.68	0.41
6:F:52:THR:N	6:F:70:GLY:O	2.53	0.41
4:D:7:ARG:CG	4:D:7:ARG:HH11	2.25	0.41
4:D:7:ARG:CG	4:D:7:ARG:NH1	2.81	0.41
19:S:119:VAL:CG1	19:S:119:VAL:O	2.68	0.41
37:A:9678:HOH:O	4:D:254:GLN:HG3	2.19	0.41
15:O:64:SER:C	15:O:66:LEU:N	2.74	0.41
1:A:168:C:H6	1:A:168:C:O5'	2.03	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:790:A:H1'	1:A:1710:A:O2'	2.21	0.41
1:A:682:A:H2'	1:A:683:G:O4'	2.21	0.41
21:U:16:LEU:HA	21:U:16:LEU:HD23	1.85	0.41
10:J:82:LYS:NZ	10:J:82:LYS:CB	2.84	0.41
1:A:644:G:H5'	1:A:644:G:N3	2.35	0.41
24:X:73:LEU:HD12	24:X:73:LEU:HA	1.90	0.41
4:D:105:PHE:CD1	4:D:115:VAL:HG11	2.56	0.41
5:E:196:THR:HG23	37:E:8400:HOH:O	2.20	0.41
1:A:2570:G:H5''	37:A:4885:HOH:O	2.20	0.41
16:P:98:LEU:O	16:P:102:ILE:HG13	2.20	0.41
1:A:107:U:H2'	1:A:108:U:H5'	2.02	0.41
14:N:74:ARG:O	14:N:88:VAL:HG13	2.20	0.41
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.50	0.41
10:J:30:GLN:H	10:J:65:ARG:NH1	2.18	0.41
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.51	0.41
1:A:2434:A:O3'	30:4:28:GLY:CA	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:312:ARG:HG2	4:D:313:PRO:N	2.33	0.41
4:D:162:MET:HE1	4:D:308:LEU:HD21	2.01	0.41
3:C:53:ALA:HB1	3:C:54:PRO:HD2	2.02	0.41
1:A:1909:A:HO2'	1:A:2266:A:HO2'	1.67	0.41
28:2:10:LYS:CB	37:2:2979:HOH:O	2.68	0.41
15:O:74:PRO:HG2	15:O:159:TYR:CZ	2.56	0.41
1:A:470:U:H2'	1:A:471:G:O4'	2.21	0.41
21:U:48:VAL:CG1	21:U:96:VAL:HG13	2.51	0.41
8:H:34:ASN:HA	14:N:4:ALA:HB2	2.03	0.41
37:A:5876:HOH:O	3:C:185:LYS:HE2	2.20	0.41
25:Y:70:ILE:HG23	25:Y:70:ILE:O	2.20	0.41
12:L:90:PHE:CD1	12:L:90:PHE:N	2.89	0.41
4:D:189:ALA:HB1	37:D:8564:HOH:O	2.20	0.41
1:A:90:A:H2'	1:A:91:G:O4'	2.21	0.41
7:G:9:GLU:HG3	7:G:10:ASP:N	2.36	0.41
37:A:9657:HOH:O	26:Z:163:THR:HG23	2.21	0.41
1:A:1789:G:O6	17:Q:73:HIS:HE1	2.04	0.41
1:A:1188:A:C5	1:A:1189:A:C2	3.09	0.41
7:G:11:VAL:HG11	7:G:22:VAL:CG1	2.51	0.41
3:C:130:THR:HG22	3:C:131:HIS:O	2.20	0.41
1:A:2896:A:OP1	25:Y:15:ARG:NH1	2.54	0.41
1:A:2363:G:O2'	18:R:11:ARG:HG3	2.21	0.41
1:A:2094:G:H4'	4:D:245:SER:CB	2.50	0.41
1:A:396:U:H5'	30:4:42:ARG:NH1	2.35	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:177:A:H2'	1:A:178:U:O4'	2.21	0.41
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.53	0.41
1:A:2274:A:N3	14:N:86:MET:CE	2.84	0.41
1:A:2397:G:C5	1:A:2465:A:C6	3.09	0.41
1:A:331:A:H1'	37:A:4765:HOH:O	2.19	0.41
1:A:1951:G:N2	37:A:6241:HOH:O	2.52	0.41
1:A:904:U:O2	1:A:1354:G:H3'	2.20	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
21:U:71:VAL:CG1	21:U:72:ILE:N	2.83	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
1:A:1840:A:H4'	1:A:1841:C:O5'	2.21	0.41
4:D:321:PRO:HG3	37:D:8597:HOH:O	2.20	0.41
24:X:21:LEU:HB3	24:X:26:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:86:LEU:HD12	15:O:125:ALA:CB	2.42	0.41
1:A:2072:G:C6	1:A:2533:C:H1'	2.56	0.41
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.21	0.41
8:H:32:GLY:N	37:H:3111:HOH:O	2.53	0.41
6:F:64:ARG:HG2	6:F:66:GLY:O	2.21	0.41
2:B:3014:G:H2'	2:B:3015:C:C5'	2.51	0.41
15:O:110:THR:HA	15:O:111:PRO:HD3	1.95	0.41
1:A:553:G:O4'	1:A:1325:G:H5'	2.20	0.41
1:A:1684:A:O2'	1:A:1685:A:H5''	2.21	0.41
4:D:55:ASN:HB3	4:D:64:GLY:N	2.35	0.41
15:O:73:ALA:HB1	15:O:74:PRO:HD2	2.02	0.41
30:4:74:CYS:SG	30:4:76:LYS:HD2	2.61	0.41
1:A:485:A:H4'	1:A:486:A:OP1	2.21	0.41
1:A:1352:A:P	5:E:92:PRO:HG3	2.61	0.41
4:D:279:THR:OG1	4:D:290:VAL:HB	2.21	0.41
1:A:2012:U:C2'	1:A:2013:G:OP1	2.69	0.41
1:A:1882:C:O2'	1:A:2012:U:OP2	2.31	0.41
1:A:314:G:N2	1:A:316:A:H3'	2.36	0.41
3:C:55:VAL:HG11	3:C:67:LEU:HD13	2.02	0.41
1:A:2453:G:H3'	37:A:5897:HOH:O	2.20	0.41
1:A:1815:A:H2'	1:A:1816:C:O4'	2.21	0.41
5:E:25:PRO:HG2	37:E:8322:HOH:O	2.20	0.41
1:A:860:U:H2'	1:A:861:A:C8	2.56	0.41
4:D:185:GLY:HA2	37:D:8633:HOH:O	2.21	0.41
1:A:74:A:H2'	1:A:75:U:C6	2.56	0.41
2:B:3004:G:O2'	15:O:44:ARG:NH2	2.54	0.41
1:A:814:G:H8	37:A:7194:HOH:O	2.02	0.41
3:C:30:ARG:HB3	3:C:30:ARG:HE	1.68	0.41
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
3:C:114:ASP:HB2	3:C:117:LYS:HE2	2.02	0.41
1:A:1545:C:H2'	1:A:1546:G:O4'	2.21	0.41
1:A:1103:C:O2'	11:K:86:MET:HB3	2.21	0.41
3:C:19:PRO:HD3	37:C:8604:HOH:O	2.21	0.41
6:F:25:MET:SD	6:F:40:ILE:HD11	2.61	0.41
7:G:149:GLU:OE1	7:G:168:ILE:HG12	2.21	0.41
1:A:2781:U:H2'	1:A:2782:G:H5'	2.03	0.41
24:X:5:VAL:O	24:X:52:VAL:CG2	2.69	0.41
5:E:78:ARG:HH11	5:E:78:ARG:CG	2.27	0.41
22:V:14:GLU:OE1	22:V:15:PRO:CD	2.65	0.41
3:C:83:GLY:O	3:C:94:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.36	0.41
8:H:59:ILE:O	8:H:59:ILE:CG2	2.69	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:1234:U:C4	4:D:244:PRO:HB3	2.56	0.41
1:A:2325:C:H2'	1:A:2326:U:C6	2.56	0.41
1:A:746:A:N6	16:P:65:LEU:HD13	2.36	0.41
1:A:1444:G:O2'	1:A:1502:A:N1	2.46	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
15:O:50:LEU:HA	15:O:50:LEU:HD12	1.80	0.41
1:A:932:U:O2'	1:A:1296:A:H1'	2.21	0.41
1:A:1304:U:H2'	1:A:1305:C:C6	2.56	0.41
1:A:2793:A:H2'	37:A:4464:HOH:O	2.19	0.41
4:D:102:THR:HG23	4:D:182:VAL:CG1	2.51	0.41
37:A:3140:HOH:O	14:N:87:MET:HE3	2.21	0.40
14:N:27:ARG:O	14:N:30:GLU:N	2.53	0.40
3:C:100:PRO:HG2	3:C:103:VAL:CG2	2.49	0.40
1:A:1151:G:P	9:I:16:LYS:NZ	2.94	0.40
10:J:14:TYR:N	10:J:91:HIS:HE1	2.20	0.40
8:H:101:ALA:HA	37:H:5413:HOH:O	2.21	0.40
1:A:236:A:H2'	1:A:236:A:O5'	2.20	0.40
6:F:173:GLU:O	6:F:174:VAL:C	2.59	0.40
1:A:183:A:C5'	14:N:157:LEU:HD12	2.51	0.40
1:A:1877:G:C6	1:A:1878:G:C6	3.09	0.40
1:A:119:A:C2	1:A:122:C:C4	3.09	0.40
1:A:431:G:OP1	14:N:48:ARG:NH1	2.54	0.40
14:N:59:GLY:C	14:N:141:ILE:HD11	2.41	0.40
27:1:60:CYS:SG	27:1:62:TYR:HB2	2.61	0.40
1:A:2300:A:C2	1:A:2306:U:C5	3.08	0.40
3:C:179:MET:HG2	3:C:186:TRP:CG	2.56	0.40
1:A:2073:G:C6	1:A:2607:U:C2	3.09	0.40
1:A:835:U:H3'	37:A:9360:HOH:O	2.21	0.40
1:A:702:G:O2'	1:A:703:G:H5'	2.21	0.40
1:A:2107:U:O2'	1:A:2108:A:H5'	2.21	0.40
15:O:21:HIS:HB2	37:O:8532:HOH:O	2.22	0.40
1:A:2389:U:H4'	18:R:53:HIS:CD2	2.56	0.40
1:A:419:A:H1'	1:A:1921:A:C2	2.56	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
1:A:295:C:H2'	1:A:296:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:4:36:ILE:HA	30:4:36:ILE:HD12	1.95	0.40
1:A:1634:G:C3'	37:A:3866:HOH:O	2.53	0.40
16:P:47:ARG:NH1	37:P:4564:HOH:O	2.54	0.40
1:A:2780:C:C1'	7:G:143:GLN:NE2	2.83	0.40
1:A:1159:G:H1	1:A:1208:C:H42	1.70	0.40
1:A:840:U:H2'	19:S:128:ARG:NH1	2.36	0.40
14:N:12:TRP:CE2	14:N:20:ILE:CD1	3.02	0.40
17:Q:10:ALA:O	17:Q:13:VAL:HG12	2.21	0.40
1:A:2898:G:H4'	4:D:288:GLY:HA2	2.03	0.40
1:A:2783:A:O2'	1:A:2784:A:H5'	2.20	0.40
37:A:9744:HOH:O	13:M:41:HIS:HE1	2.04	0.40
14:N:122:GLU:HB2	14:N:126:HIS:O	2.22	0.40
1:A:590:A:H2'	1:A:591:A:C5'	2.51	0.40
6:F:170:TYR:N	6:F:170:TYR:CD1	2.89	0.40
4:D:234:ARG:NH1	37:D:8616:HOH:O	2.53	0.40
10:J:11:LYS:NZ	37:J:8336:HOH:O	2.45	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
1:A:164:G:O6	1:A:165:A:C6	2.74	0.40
1:A:10:U:HO2'	1:A:11:A:P	2.44	0.40
24:X:101:LEU:HD23	24:X:101:LEU:HA	1.94	0.40
1:A:2071:C:H5'	37:A:9511:HOH:O	2.21	0.40
3:C:1:GLY:HA2	3:C:197:VAL:HG23	2.03	0.40
1:A:1791:U:H2'	1:A:1792:C:C6	2.56	0.40
1:A:1291:A:H2	37:A:5266:HOH:O	2.05	0.40
1:A:821:U:H2'	1:A:822:C:C6	2.49	0.40
37:A:4945:HOH:O	10:J:57:ARG:HG3	2.21	0.40
1:A:1494:A:O2'	1:A:1505:U:O2	2.24	0.40
3:C:192:VAL:HG23	3:C:201:PHE:HB3	2.03	0.40
1:A:2346:C:O3'	6:F:52:THR:CG2	2.69	0.40
5:E:233:THR:HG22	5:E:234:VAL:H	1.84	0.40
1:A:2729:C:H2'	1:A:2730:G:C8	2.48	0.40
3:C:153:ARG:CB	3:C:153:ARG:HH11	2.33	0.40
1:A:154:C:H2'	1:A:155:C:C6	2.56	0.40
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.83	0.40
1:A:240:C:O2	1:A:240:C:H2'	2.22	0.40
1:A:2783:A:H2'	1:A:2784:A:C8	2.56	0.40
1:A:2484:U:N3	37:A:9601:HOH:O	2.52	0.40
1:A:1523:G:C6	1:A:1524:U:O4	2.74	0.40
21:U:24:ARG:HH21	21:U:39:ASN:ND2	2.20	0.40
1:A:638:C:H2'	1:A:639:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:C:H1'	1:A:1573:A:H1'	2.03	0.40
7:G:119:HIS:HE1	7:G:147:ASP:OD2	2.05	0.40
6:F:128:LEU:C	6:F:128:LEU:HD23	2.42	0.40
8:H:21:GLU:HA	8:H:24:ARG:HE	1.85	0.40
10:J:1:LYS:HA	10:J:2:PRO:HD3	1.72	0.40
6:F:19:GLU:O	6:F:133:ASN:HB3	2.21	0.40
4:D:312:ARG:HD3	4:D:315:VAL:HG13	2.02	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
10:J:113:ALA:N	10:J:114:PRO:HD3	2.36	0.40
1:A:2815:G:N7	11:K:80:LYS:NZ	2.66	0.40
1:A:187:A:H3'	1:A:188:C:C6	2.56	0.40
37:A:4379:HOH:O	3:C:11:ARG:CZ	2.70	0.40
1:A:2044:G:C6	1:A:2045:G:C5	3.09	0.40
1:A:2851:G:C2'	1:A:2852:A:H5'	2.52	0.40
3:C:228:ILE:O	3:C:229:ALA:C	2.60	0.40
1:A:1815:A:HO2'	1:A:2750:G:HO2'	1.65	0.40
13:M:65:ASP:CG	13:M:111:ALA:HB3	2.41	0.40
1:A:2377:U:O5'	1:A:2377:U:H6	2.04	0.40
4:D:57:GLU:HA	4:D:58:PRO:HD2	1.94	0.40
1:A:1336:U:C2	1:A:1337:A:C8	3.09	0.40
27:1:81:LYS:HB2	27:1:82:ALA:H	1.76	0.40
1:A:290:C:O2'	1:A:291:C:H5'	2.20	0.40
30:4:71:CYS:SG	30:4:72:GLY:N	2.94	0.40
10:J:65:ARG:NH2	10:J:66:VAL:HG22	2.37	0.40
7:G:149:GLU:HG3	7:G:166:VAL:O	2.21	0.40
1:A:2782:G:O6	1:A:2790:C:H5''	2.21	0.40
37:D:8625:HOH:O	22:V:17:THR:HG21	2.22	0.40
3:C:93:THR:HG23	3:C:154:ALA:O	2.22	0.40
11:K:70:PHE:CD2	11:K:70:PHE:O	2.74	0.40
11:K:40:ASN:OD1	11:K:106:GLY:HA2	2.22	0.40
1:A:2379:G:H4'	1:A:2380:A:H5''	2.04	0.40
1:A:2088:C:H1'	1:A:2841:A:C2	2.56	0.40
28:2:21:ARG:HD2	28:2:39:PHE:HB2	2.03	0.40
1:A:1127:C:C5	1:A:1128:U:C4	3.09	0.40
1:A:2588:G:H5''	1:A:2589:U:OP2	2.22	0.40
37:A:5961:HOH:O	30:4:31:THR:HA	2.20	0.40
1:A:1549:C:N3	1:A:1637:A:C2	2.89	0.40
17:Q:141:ILE:C	17:Q:143:ALA:H	2.25	0.40
1:A:440:C:O2'	1:A:441:A:H5'	2.21	0.40
12:L:98:VAL:HG13	12:L:99:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:11:LEU:HD23	29:3:11:LEU:HA	1.87	0.40
11:K:51:GLU:O	11:K:55:GLU:HG3	2.21	0.40
11:K:71:TYR:CG	11:K:72:PRO:HD2	2.56	0.40
1:A:1552:G:C2	1:A:1553:C:C2	3.10	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%)	11	46
4	D	335/337 (99%)	304 (91%)	22 (7%)	9 (3%)	6	32
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	39	80
6	F	134/176 (76%)	93 (69%)	30 (22%)	11 (8%)	1	5
7	G	170/177 (96%)	159 (94%)	11 (6%)	0	100	100
8	H	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	11	46
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	131 (86%)	14 (9%)	7 (5%)	3	18
11	K	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	6	29
12	L	130/132 (98%)	119 (92%)	9 (7%)	2 (2%)	13	50
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	26	70
14	N	192/194 (99%)	173 (90%)	17 (9%)	2 (1%)	19	61
15	O	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	4	22
16	P	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	26	70
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	17	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	64
22	V	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	27
24	X	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	15	53
25	Y	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	7	34
26	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	14	51
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%)	8	38
All	All	3633/4235 (86%)	3300 (91%)	271 (8%)	62 (2%)	11	46

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
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

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Mol	Chain	Res	Type
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
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%)	166 (93%)	13 (7%)	17	52
4	D	282/282 (100%)	265 (94%)	17 (6%)	24	62
5	E	193/193 (100%)	176 (91%)	17 (9%)	12	42
6	F	117/147 (80%)	108 (92%)	9 (8%)	16	50
7	G	152/155 (98%)	147 (97%)	5 (3%)	45	82
8	H	92/92 (100%)	91 (99%)	1 (1%)	80	94
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	110 (90%)	12 (10%)	10	36
11	K	118/121 (98%)	107 (91%)	11 (9%)	11	39
12	L	106/106 (100%)	103 (97%)	3 (3%)	51	84
13	M	112/126 (89%)	108 (96%)	4 (4%)	42	79
14	N	166/166 (100%)	158 (95%)	8 (5%)	31	71
15	O	149/149 (100%)	143 (96%)	6 (4%)	38	77
16	P	93/93 (100%)	92 (99%)	1 (1%)	80	94
17	Q	113/116 (97%)	110 (97%)	3 (3%)	52	85
18	R	79/79 (100%)	75 (95%)	4 (5%)	29	69
19	S	117/121 (97%)	112 (96%)	5 (4%)	35	75
20	T	71/73 (97%)	70 (99%)	1 (1%)	74	93
21	U	105/105 (100%)	102 (97%)	3 (3%)	50	84
22	V	44/52 (85%)	42 (96%)	2 (4%)	34	74
23	W	51/56 (91%)	50 (98%)	1 (2%)	63	89
24	X	130/130 (100%)	121 (93%)	9 (7%)	19	56
25	Y	66/73 (90%)	62 (94%)	4 (6%)	23	61
26	Z	120/195 (62%)	113 (94%)	7 (6%)	25	63
27	1	56/56 (100%)	50 (89%)	6 (11%)	8	31
28	2	46/46 (100%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	3	42/44 (96%)	41 (98%)	1 (2%)	57 87
30	4	79/79 (100%)	73 (92%)	6 (8%)	16 51
All	All	3027/3441 (88%)	2868 (95%)	159 (5%)	28 67

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	C	8	ARG
3	C	33	GLU
3	C	36	ASP
3	C	55	VAL
3	C	68	ILE
3	C	69	LEU
3	C	94	LEU
3	C	120	ARG
3	C	131	HIS
3	C	153	ARG
3	C	179	MET
3	C	217	ARG
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	234	ARG
4	D	251	VAL
4	D	254	GLN
4	D	264	GLU
4	D	304	PRO
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	27	ARG
5	E	42	ARG
5	E	57	PRO

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Mol	Chain	Res	Type
5	E	67	GLN
5	E	76	ARG
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
6	F	24	HIS
6	F	61	PHE
6	F	99	ASP
6	F	100	ASP
6	F	131	THR
6	F	133	ASN
6	F	136	ARG
6	F	137	PRO
6	F	149	ARG
7	G	7	ILE
7	G	12	ASP
7	G	54	ASP
7	G	102	VAL
7	G	164	ASP
8	H	100	ASP
10	J	1	LYS
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	142	VAL
10	J	150	LYS
10	J	166	ASN
11	K	46	ILE
11	K	52	GLN

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Mol	Chain	Res	Type
11	K	74	ARG
11	K	76	ASP
11	K	79	PHE
11	K	107	ASN
11	K	112	ASP
11	K	120	SER
11	K	125	SER
11	K	127	ILE
11	K	131	THR
12	L	7	ASP
12	L	10	GLN
12	L	98	VAL
13	M	30	ARG
13	M	35	ARG
13	M	80	ASP
13	M	117	GLU
14	N	38	VAL
14	N	46	LEU
14	N	68	ARG
14	N	81	ARG
14	N	87	MET
14	N	93	ARG
14	N	99	ARG
14	N	164	THR
15	O	26	LEU
15	O	43	VAL
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU
15	O	163	PHE
16	P	3	THR
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

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Mol	Chain	Res	Type
19	S	132	ARG
20	T	10	VAL
21	U	39	ASN
21	U	73	HIS
21	U	96	VAL
22	V	9	CYS
22	V	32	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	122	ARG
24	X	142	ASP
24	X	146	ILE
24	X	154	ARG
25	Y	15	ARG
25	Y	27	ASP
25	Y	49	ARG
25	Y	72	VAL
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	32	LYS
27	1	42	CYS
27	1	49	ARG
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such

sidechains are listed below:

Mol	Chain	Res	Type
3	C	29	HIS
3	C	47	HIS
3	C	92	ASN
3	C	125	ASN
3	C	127	GLN
3	C	199	HIS
4	D	27	ASN
4	D	145	HIS
4	D	191	ASN
4	D	221	GLN
4	D	238	ASN
4	D	260	HIS
4	D	332	ASN
5	E	2	GLN
5	E	39	GLN
5	E	129	HIS
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	35	ASN
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

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Mol	Chain	Res	Type
13	M	41	HIS
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	176	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
18	R	16	ASN
18	R	40	HIS
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN
19	S	113	HIS
19	S	117	HIS
19	S	122	GLN
19	S	123	GLN
20	T	53	ASN
21	U	39	ASN
22	V	38	ASN
22	V	39	ASN
23	W	60	GLN
24	X	14	HIS
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	189	ASN
27	1	33	HIS
28	2	8	GLN

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	244 (8%)	33 (1%)
2	B	121/122 (99%)	16 (13%)	6 (4%)
All	All	2868/3044 (94%)	260 (9%)	39 (1%)

All (260) 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

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Mol	Chain	Res	Type
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C
1	A	487	G
1	A	498	A
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	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

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Mol	Chain	Res	Type
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
1	A	882	A
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	920	C
1	A	921	G
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

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Mol	Chain	Res	Type
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1216	G
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	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

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Mol	Chain	Res	Type
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1737	A
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	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

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Mol	Chain	Res	Type
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	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	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	2664	A
1	A	2681	A
1	A	2682	C
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G

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Mol	Chain	Res	Type
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	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
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G

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Mol	Chain	Res	Type
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	TYK	A	9000	1	66,67,67	3.30	29 (43%)	73,97,97	2.36	23 (31%)

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	-	0/67/126/126	0/3/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	TYK	C4-C3	-6.43	1.41	1.54
31	A	9000	TYK	C4C-C5C	-3.40	1.45	1.52
31	A	9000	TYK	C2-C3	-3.20	1.48	1.53
31	A	9000	TYK	C6A-C5A	-2.86	1.44	1.51
31	A	9000	TYK	O5A-C5A	-2.85	1.37	1.44
31	A	9000	TYK	O2C-C2C	-2.78	1.35	1.42
31	A	9000	TYK	C4C-C3C	-2.02	1.46	1.52
31	A	9000	TYK	C2A-C3A	2.25	1.57	1.53
31	A	9000	TYK	O3C-C3C	2.26	1.48	1.42
31	A	9000	TYK	O20-C20	2.58	1.36	1.19
31	A	9000	TYK	O3-C3	2.74	1.49	1.43
31	A	9000	TYK	O5B-C1B	2.84	1.49	1.42
31	A	9000	TYK	C16-C15	2.99	1.63	1.52
31	A	9000	TYK	C1C-C2C	2.99	1.60	1.52
31	A	9000	TYK	C23-C14	3.04	1.56	1.52
31	A	9000	TYK	C3B-C4B	3.04	1.58	1.53
31	A	9000	TYK	C2B-C1B	3.13	1.58	1.51
31	A	9000	TYK	C3C-C2C	3.40	1.59	1.52
31	A	9000	TYK	C3A-N3A	3.45	1.55	1.48
31	A	9000	TYK	C19-C6	3.46	1.64	1.54
31	A	9000	TYK	C7-C8	4.03	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	TYK	C6-C5	4.83	1.61	1.52
31	A	9000	TYK	C4A-C5A	5.25	1.62	1.52
31	A	9000	TYK	C14-C15	5.38	1.63	1.54
31	A	9000	TYK	O4C-C4C	5.76	1.56	1.43
31	A	9000	TYK	C7-C6	6.04	1.66	1.53
31	A	9000	TYK	C22-C12	8.14	1.68	1.50
31	A	9000	TYK	O9-C9	10.34	1.37	1.22
31	A	9000	TYK	O1C-C1C	11.83	1.61	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9000	TYK	O20-C20-C19	-8.82	93.06	125.24
31	A	9000	TYK	O15-C15-C16	-6.16	96.12	106.59
31	A	9000	TYK	C6C-C5C-C4C	-5.73	101.81	113.08
31	A	9000	TYK	C15-C14-C13	-5.59	98.98	110.69
31	A	9000	TYK	C10-C11-C12	-4.41	119.50	126.22
31	A	9000	TYK	O5C-C1C-C2C	-4.34	100.72	109.47
31	A	9000	TYK	C3B-C2B-C1B	-3.30	108.95	114.88
31	A	9000	TYK	C18-C4-C3	-3.10	106.34	111.22
31	A	9000	TYK	C19-C6-C5	-3.00	104.94	111.77
31	A	9000	TYK	O3-C3-C2	-2.55	103.35	109.50
31	A	9000	TYK	O3C-C3C-C2C	-2.23	103.38	108.94
31	A	9000	TYK	O5C-C1C-O1C	-2.19	104.79	110.05
31	A	9000	TYK	O4C-C4C-C3C	-2.16	104.77	109.87
31	A	9000	TYK	C2A-C3A-C4A	-2.12	107.38	110.46
31	A	9000	TYK	O2C-C2C-C1C	2.06	117.10	111.01
31	A	9000	TYK	O1A-C1A-C2A	2.10	113.20	108.10
31	A	9000	TYK	O5A-C5A-C4A	2.68	114.27	109.13
31	A	9000	TYK	O4A-C1B-C2B	2.70	113.45	108.99
31	A	9000	TYK	O4C-C4C-C5C	2.77	116.33	109.84
31	A	9000	TYK	O5C-C5C-C6C	2.81	112.78	106.64
31	A	9000	TYK	O4A-C4A-C5A	2.84	114.29	106.83
31	A	9000	TYK	C17-C16-C15	3.35	123.49	113.14
31	A	9000	TYK	O1A-C5-C4	4.51	113.87	108.19

There are no chirality outliers.

There are no torsion outliers.

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.02	67 (2%) 62 32	20, 47, 93, 139	0
2	B	122/122 (100%)	0.26	5 (4%) 41 16	31, 65, 95, 145	0
3	C	237/239 (99%)	0.20	17 (7%) 18 7	27, 61, 90, 109	0
4	D	337/337 (100%)	-0.07	1 (0%) 94 84	20, 54, 81, 90	0
5	E	246/246 (100%)	-0.15	2 (0%) 87 67	19, 49, 72, 81	0
6	F	140/176 (79%)	1.47	39 (27%) 1 0	54, 101, 118, 126	0
7	G	172/177 (97%)	0.57	7 (4%) 41 16	39, 65, 88, 94	0
8	H	119/119 (100%)	0.80	11 (9%) 11 4	56, 78, 99, 103	0
9	I	29/348 (8%)	2.07	14 (48%) 0 0	68, 91, 100, 101	0
10	J	156/167 (93%)	0.21	7 (4%) 37 15	32, 55, 79, 88	0
11	K	142/145 (97%)	-0.12	0 100 100	32, 47, 71, 82	0
12	L	132/132 (100%)	-0.01	1 (0%) 87 67	30, 53, 76, 82	0
13	M	145/164 (88%)	0.57	18 (12%) 5 2	23, 72, 105, 115	0
14	N	194/194 (100%)	0.12	11 (5%) 27 10	34, 53, 83, 88	0
15	O	186/186 (100%)	0.70	24 (12%) 5 2	41, 69, 107, 119	0
16	P	115/115 (100%)	-0.06	0 100 100	38, 57, 76, 80	0
17	Q	143/148 (96%)	0.06	2 (1%) 78 51	33, 58, 73, 81	0
18	R	95/95 (100%)	-0.20	1 (1%) 82 58	33, 48, 59, 73	0
19	S	150/154 (97%)	-0.13	0 100 100	27, 42, 66, 74	0
20	T	81/84 (96%)	0.13	1 (1%) 81 55	47, 62, 80, 84	0
21	U	119/119 (100%)	0.38	4 (3%) 49 21	37, 58, 81, 91	0
22	V	53/66 (80%)	3.16	42 (79%) 0 0	81, 91, 97, 105	0
23	W	65/70 (92%)	1.13	12 (18%) 2 1	52, 77, 106, 113	0
24	X	154/154 (100%)	-0.31	0 100 100	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%)	0.30	2 (2%) 62 32	39, 55, 81, 93	0
26	Z	142/240 (59%)	-0.01	3 (2%) 67 36	25, 45, 69, 85	0
27	1	73/73 (100%)	3.06	43 (58%) 0 0	79, 92, 98, 99	0
28	2	56/56 (100%)	-0.50	0 100 100	26, 34, 41, 47	0
29	3	46/48 (95%)	0.14	2 (4%) 39 16	33, 59, 85, 97	0
30	4	92/92 (100%)	6.12	92 (100%) 0 0	90, 101, 105, 107	0
All	All	6577/7279 (90%)	0.25	428 (6%) 22 8	19, 54, 99, 145	0

All (428) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	14.2
30	4	62	THR	13.6
30	4	82	GLY	12.6
27	1	11	THR	11.4
30	4	38	ARG	11.3
30	4	83	TRP	11.3
30	4	11	CYS	10.5
30	4	33	MET	10.4
30	4	1	MET	9.6
30	4	35	TRP	9.6
30	4	56	PRO	9.6
30	4	2	GLN	9.5
30	4	59	ASP	9.3
30	4	91	GLN	9.1
30	4	84	ARG	8.9
30	4	65	THR	8.6
30	4	14	CYS	8.5
30	4	8	ASN	8.4
30	4	32	GLY	8.4
30	4	41	GLU	8.2
23	W	1	THR	8.1
14	N	71	SER	8.1
30	4	85	ALA	8.0
27	1	12	GLY	8.0
27	1	15	GLY	7.9
30	4	34	LYS	7.9
27	1	22	ILE	7.7
30	4	47	GLY	7.5
27	1	26	VAL	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	1173	A	7.4
30	4	86	GLY	7.4
22	V	40	ALA	7.4
30	4	31	THR	7.4
30	4	71	CYS	7.2
30	4	60	LYS	7.2
30	4	4	PRO	7.1
30	4	42	ARG	7.0
27	1	16	PRO	6.9
22	V	55	ALA	6.9
30	4	9	THR	6.9
30	4	3	MET	6.8
30	4	40	ARG	6.7
30	4	43	ASN	6.6
30	4	88	LEU	6.5
30	4	57	GLY	6.5
30	4	74	CYS	6.5
30	4	53	SER	6.4
15	O	186	LEU	6.3
30	4	81	GLU	6.2
30	4	61	PRO	6.1
9	I	24	VAL	6.1
27	1	44	PHE	6.0
30	4	18	GLN	6.0
27	1	23	ARG	5.9
30	4	78	HIS	5.9
22	V	51	TRP	5.9
27	1	30	GLU	5.9
30	4	48	ASN	5.9
30	4	22	VAL	5.8
30	4	27	SER	5.8
30	4	58	GLY	5.8
6	F	57	THR	5.8
27	1	39	CYS	5.7
30	4	77	ALA	5.7
9	I	27	ILE	5.7
21	U	119	ALA	5.7
30	4	75	GLY	5.7
22	V	9	CYS	5.7
22	V	54	THR	5.6
30	4	20	HIS	5.6
1	A	1198	U	5.6

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Mol	Chain	Res	Type	RSRZ
30	4	25	VAL	5.6
6	F	10	PHE	5.6
22	V	53	ASP	5.5
30	4	36	ILE	5.5
27	1	20	LEU	5.4
30	4	76	LYS	5.3
15	O	162	ASP	5.3
6	F	88	LEU	5.2
30	4	68	LYS	5.2
22	V	52	THR	5.2
27	1	21	LYS	5.2
30	4	10	TYR	5.2
27	1	24	VAL	5.2
30	4	67	LEU	5.1
27	1	19	GLY	5.1
27	1	17	ARG	5.1
30	4	39	GLN	5.0
9	I	23	ILE	5.0
14	N	89	ASN	5.0
30	4	55	VAL	5.0
1	A	1172	G	4.9
30	4	44	SER	4.9
22	V	41	ASP	4.9
22	V	33	SER	4.9
15	O	157	PRO	4.8
30	4	17	HIS	4.8
14	N	70	GLY	4.8
27	1	13	ARG	4.8
1	A	1175	G	4.7
1	A	735	C	4.7
30	4	21	GLU	4.7
27	1	34	LYS	4.7
22	V	39	ASN	4.6
22	V	50	GLU	4.6
30	4	15	ASN	4.6
30	4	5	ARG	4.6
30	4	72	GLY	4.6
30	4	24	LYS	4.6
30	4	19	GLU	4.6
30	4	13	HIS	4.6
30	4	16	GLU	4.6
30	4	7	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
30	4	45	GLY	4.6
30	4	63	LYS	4.5
30	4	51	LYS	4.5
30	4	87	ARG	4.5
1	A	1168	C	4.4
22	V	12	ASP	4.4
1	A	1199	A	4.4
30	4	80	ARG	4.4
2	B	3001	U	4.4
27	1	35	LYS	4.4
27	1	45	LYS	4.4
1	A	285	A	4.3
8	H	90	GLU	4.3
30	4	12	PRO	4.3
30	4	30	GLN	4.3
15	O	160	SER	4.3
27	1	10	ARG	4.3
27	1	40	PRO	4.3
30	4	89	GLU	4.2
6	F	26	GLY	4.2
30	4	92	GLU	4.2
27	1	28	ASP	4.2
27	1	18	TYR	4.2
1	A	1171	A	4.2
22	V	6	CYS	4.2
30	4	6	ARG	4.2
15	O	147	ILE	4.1
27	1	31	ILE	4.1
22	V	32	CYS	4.1
27	1	33	HIS	4.1
26	Z	108	ASP	4.1
30	4	49	ASP	4.1
22	V	11	THR	4.1
1	A	1192	A	4.1
3	C	85	ASP	4.0
23	W	39	ALA	4.0
30	4	46	ILE	4.0
1	A	1177	A	4.0
15	O	179	LEU	4.0
15	O	150	TYR	3.9
6	F	96	SER	3.9
8	H	86	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1948	G	3.9
27	1	25	ARG	3.9
15	O	184	ILE	3.8
3	C	37	VAL	3.8
27	1	42	CYS	3.8
30	4	52	PHE	3.8
27	1	29	VAL	3.8
6	F	58	VAL	3.8
15	O	159	TYR	3.8
6	F	102	GLY	3.8
22	V	4	ARG	3.7
3	C	62	ASP	3.7
27	1	59	HIS	3.7
30	4	69	TYR	3.7
3	C	64	ASP	3.7
13	M	104	ASP	3.7
22	V	29	THR	3.6
1	A	1951	G	3.6
27	1	41	VAL	3.6
9	I	26	MET	3.6
22	V	49	LEU	3.6
27	1	58	GLY	3.5
6	F	18	ILE	3.5
8	H	106	THR	3.5
1	A	1169	U	3.5
30	4	23	GLU	3.5
22	V	10	GLY	3.5
30	4	64	LYS	3.5
13	M	102	ASP	3.5
15	O	158	LEU	3.5
1	A	1188	A	3.5
7	G	10	ASP	3.4
27	1	27	ALA	3.4
1	A	1204	C	3.4
8	H	15	ASP	3.4
6	F	16	PRO	3.4
22	V	48	ASN	3.4
30	4	26	ARG	3.4
1	A	1949	G	3.4
1	A	1167	G	3.4
1	A	960	G	3.3
22	V	19	THR	3.3

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Mol	Chain	Res	Type	RSRZ
27	1	14	PHE	3.3
1	A	1279	U	3.3
27	1	36	LYS	3.3
1	A	1190	G	3.2
6	F	84	LEU	3.2
30	4	66	ASP	3.2
1	A	1525	G	3.2
30	4	54	LYS	3.2
1	A	1205	U	3.2
3	C	82	VAL	3.2
6	F	56	ARG	3.2
17	Q	1	THR	3.2
22	V	47	ARG	3.2
4	D	1	PRO	3.2
8	H	107	VAL	3.2
1	A	2345	A	3.1
27	1	37	HIS	3.1
23	W	40	PRO	3.1
1	A	2344	G	3.1
3	C	36	ASP	3.1
1	A	713	U	3.1
22	V	43	GLY	3.1
8	H	19	ALA	3.1
6	F	11	HIS	3.1
22	V	25	ASP	3.1
6	F	63	ILE	3.0
14	N	72	SER	3.0
30	4	79	LEU	3.0
1	A	2433	A	3.0
27	1	80	MET	3.0
6	F	69	ILE	3.0
13	M	80	ASP	3.0
1	A	1197	G	3.0
10	J	83	PHE	3.0
9	I	68	GLU	3.0
9	I	20	VAL	2.9
18	R	95	GLU	2.9
27	1	46	LYS	2.9
23	W	8	ILE	2.9
6	F	104	PHE	2.9
30	4	29	ARG	2.9
1	A	284	C	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	3024	U	2.9
6	F	62	ASP	2.9
22	V	46	ALA	2.9
14	N	74	ARG	2.9
8	H	20	LEU	2.9
22	V	8	TYR	2.9
25	Y	80	GLU	2.9
22	V	34	SER	2.9
23	W	2	VAL	2.9
27	1	47	LEU	2.9
13	M	105	TYR	2.9
14	N	90	ARG	2.9
29	3	35	ARG	2.9
8	H	44	SER	2.8
20	T	81	ILE	2.8
9	I	72	ASP	2.8
13	M	73	VAL	2.8
22	V	28	THR	2.8
1	A	2004	U	2.8
6	F	15	GLU	2.8
6	F	171	ASP	2.8
15	O	67	ALA	2.8
9	I	71	LEU	2.8
27	1	57	CYS	2.8
1	A	1950	G	2.8
5	E	135	GLU	2.8
15	O	155	GLU	2.8
15	O	167	ASP	2.8
23	W	38	GLY	2.8
9	I	28	GLU	2.8
15	O	152	GLU	2.8
13	M	123	ASP	2.7
27	1	68	CYS	2.7
14	N	78	ASN	2.7
23	W	7	GLU	2.7
6	F	89	PRO	2.7
6	F	24	HIS	2.7
15	O	146	HIS	2.7
1	A	1182	C	2.7
30	4	90	PHE	2.7
1	A	1166	A	2.7
22	V	15	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	90	LEU	2.7
7	G	100	ASP	2.7
22	V	56	ARG	2.7
1	A	1180	U	2.7
1	A	1200	A	2.6
30	4	28	GLY	2.6
3	C	32	VAL	2.6
1	A	2637	A	2.6
10	J	32	ASP	2.6
1	A	2436	U	2.6
1	A	1203	G	2.6
13	M	106	VAL	2.6
22	V	13	ILE	2.6
2	B	3002	U	2.6
6	F	59	GLY	2.6
30	4	70	ARG	2.6
23	W	52	ALA	2.6
6	F	98	PHE	2.6
15	O	138	ASP	2.5
6	F	132	VAL	2.5
30	4	73	GLU	2.5
1	A	736	A	2.5
13	M	59	GLU	2.5
6	F	134	LEU	2.5
6	F	129	ASP	2.5
30	4	50	GLY	2.5
27	1	38	LYS	2.5
13	M	140	VAL	2.5
1	A	1181	A	2.5
22	V	45	GLU	2.5
9	I	67	LEU	2.5
22	V	42	LEU	2.5
22	V	7	ASP	2.5
22	V	23	HIS	2.5
1	A	1174	A	2.5
1	A	1193	A	2.5
6	F	170	TYR	2.5
1	A	368	C	2.5
23	W	10	ASP	2.5
12	L	119	GLN	2.4
1	A	1176	C	2.4
6	F	87	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
13	M	81	VAL	2.4
26	Z	235	GLU	2.4
22	V	36	CYS	2.4
1	A	371	U	2.4
10	J	135	TRP	2.4
14	N	80	GLY	2.4
6	F	48	MET	2.4
13	M	60	GLU	2.4
1	A	2237	G	2.3
8	H	49	PHE	2.3
1	A	1522	A	2.3
3	C	34	ASP	2.3
15	O	183	ASP	2.3
15	O	127	LEU	2.3
23	W	11	MET	2.3
1	A	282	C	2.3
27	1	32	LYS	2.3
8	H	18	GLU	2.3
1	A	970	U	2.3
6	F	17	ARG	2.3
7	G	122	THR	2.3
1	A	130	C	2.3
1	A	1913	C	2.3
3	C	83	GLY	2.3
21	U	37	GLN	2.3
6	F	106	PHE	2.3
9	I	13	PRO	2.2
9	I	65	THR	2.2
1	A	370	G	2.2
1	A	601	G	2.2
13	M	120	LEU	2.2
23	W	3	LEU	2.2
3	C	110	SER	2.2
7	G	28	SER	2.2
7	G	108	LEU	2.2
13	M	130	ARG	2.2
1	A	2432	C	2.2
3	C	38	ILE	2.2
17	Q	130	GLU	2.2
22	V	14	GLU	2.2
1	A	2338	G	2.2
6	F	27	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	3023	U	2.2
1	A	2249	G	2.2
2	B	3122	C	2.2
9	I	21	ASP	2.2
22	V	24	LYS	2.2
22	V	26	GLY	2.2
6	F	92	GLU	2.2
3	C	61	GLU	2.2
13	M	150	GLN	2.2
15	O	80	SER	2.2
15	O	166	ALA	2.2
3	C	60	PHE	2.2
7	G	131	LEU	2.2
13	M	62	ALA	2.2
10	J	80	ASN	2.1
6	F	85	GLN	2.1
25	Y	88	GLU	2.1
1	A	372	A	2.1
14	N	83	SER	2.1
26	Z	103	THR	2.1
1	A	1162	G	2.1
1	A	1201	C	2.1
10	J	146	TRP	2.1
13	M	61	ALA	2.1
15	O	95	ALA	2.1
13	M	133	VAL	2.1
1	A	514	G	2.1
3	C	84	VAL	2.1
6	F	44	ILE	2.1
22	V	44	ARG	2.1
1	A	138	U	2.1
10	J	81	TYR	2.1
14	N	26	HIS	2.1
3	C	154	ALA	2.1
1	A	1158	G	2.1
9	I	64	ASN	2.1
1	A	1165	G	2.1
1	A	1184	C	2.1
3	C	133	ARG	2.1
6	F	12	GLU	2.1
6	F	25	MET	2.1
15	O	64	SER	2.1

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Mol	Chain	Res	Type	RSRZ
22	V	22	VAL	2.1
6	F	47	GLN	2.1
3	C	31	LYS	2.1
15	O	72	GLU	2.1
1	A	808	A	2.0
29	3	36	ASN	2.0
6	F	166	ILE	2.0
14	N	73	ARG	2.0
10	J	139	ASP	2.0
21	U	83	ASP	2.0
13	M	119	THR	2.0
23	W	63	GLU	2.0
27	1	79	VAL	2.0
1	A	362	G	2.0
5	E	143	ASP	2.0
1	A	1925	G	2.0
21	U	80	GLU	2.0
8	H	26	THR	2.0
22	V	31	PHE	2.0
7	G	129	GLU	2.0
15	O	178	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	NA	A	8356	1/1	0.78	0.73	68.78	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	A	8362	1/1	0.85	0.32	23.74	63,63,63,63	0
34	CL	A	8515	1/1	0.91	0.49	23.11	97,97,97,97	0
33	NA	A	8323	1/1	0.88	0.31	15.37	38,38,38,38	0
34	CL	A	8505	1/1	0.78	0.54	12.56	83,83,83,83	0
33	NA	A	8321	1/1	0.87	0.28	12.04	45,45,45,45	0
33	NA	A	8376	1/1	0.89	0.33	10.80	80,80,80,80	0
33	NA	A	8340	1/1	0.93	0.37	10.77	31,31,31,31	0
33	NA	A	8382	1/1	0.81	0.29	10.44	41,41,41,41	0
33	NA	S	8386	1/1	0.64	0.54	10.34	75,75,75,75	0
33	NA	A	8355	1/1	0.91	0.65	9.50	55,55,55,55	0
33	NA	A	8372	1/1	0.89	0.48	9.43	53,53,53,53	0
33	NA	A	8359	1/1	0.93	0.43	9.42	52,52,52,52	0
33	NA	A	8303	1/1	0.84	0.26	8.44	53,53,53,53	0
34	CL	D	8519	1/1	0.96	0.47	8.29	59,59,59,59	0
33	NA	A	8371	1/1	0.87	0.21	7.22	31,31,31,31	0
33	NA	A	8364	1/1	0.87	0.23	6.76	39,39,39,39	0
33	NA	A	8374	1/1	0.90	0.30	6.68	41,41,41,41	0
33	NA	A	8373	1/1	0.77	0.48	6.45	37,37,37,37	0
33	NA	A	8350	1/1	0.93	0.21	6.08	24,24,24,24	0
33	NA	A	8378	1/1	0.92	0.28	6.04	30,30,30,30	0
32	MG	A	8067	1/1	0.94	0.26	6.04	49,49,49,49	0
33	NA	A	8365	1/1	0.91	0.33	4.01	41,41,41,41	0
31	TYK	A	9000	64/64	0.94	0.22	3.39	33,43,48,51	0
33	NA	S	8337	1/1	0.47	0.34	3.34	34,34,34,34	0
33	NA	A	8366	1/1	0.88	0.29	2.97	43,43,43,43	0
34	CL	4	8504	1/1	0.47	1.21	2.36	112,112,112,112	0
32	MG	A	8044	1/1	0.95	0.17	1.73	44,44,44,44	0
33	NA	M	8380	1/1	0.93	0.26	1.64	49,49,49,49	0
33	NA	A	8331	1/1	0.91	0.18	1.57	46,46,46,46	0
32	MG	A	8013	1/1	0.99	0.18	1.34	42,42,42,42	0
34	CL	K	8521	1/1	0.95	0.21	1.32	50,50,50,50	0
33	NA	A	8326	1/1	0.80	0.26	1.08	56,56,56,56	0
33	NA	A	8335	1/1	0.97	0.18	1.07	45,45,45,45	0
34	CL	M	8510	1/1	0.86	0.32	0.99	75,75,75,75	0
33	NA	A	8325	1/1	0.95	0.15	0.75	47,47,47,47	0
33	NA	A	8368	1/1	0.91	0.17	0.74	43,43,43,43	0
33	NA	A	8379	1/1	0.96	0.15	0.59	32,32,32,32	0
34	CL	P	8508	1/1	0.96	0.22	0.39	83,83,83,83	0
33	NA	A	8332	1/1	0.79	0.18	0.31	34,34,34,34	0
33	NA	A	8339	1/1	0.97	0.16	0.00	22,22,22,22	0
32	MG	A	8064	1/1	0.92	0.15	-0.04	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	B	8383	1/1	0.81	0.20	-0.15	54,54,54,54	0
32	MG	A	8112	1/1	0.74	0.18	-0.16	58,58,58,58	0
33	NA	A	8327	1/1	0.93	0.15	-0.32	28,28,28,28	0
33	NA	A	8333	1/1	0.92	0.16	-0.42	26,26,26,26	0
32	MG	4	8078	1/1	0.92	0.42	-0.65	91,91,91,91	0
32	MG	A	8057	1/1	0.95	0.18	-0.67	34,34,34,34	0
32	MG	1	8105	1/1	0.96	0.17	-0.70	42,42,42,42	0
35	K	A	8602	1/1	0.89	0.13	-0.75	56,56,56,56	0
33	NA	J	8309	1/1	0.98	0.13	-0.76	25,25,25,25	0
33	NA	A	8314	1/1	0.96	0.14	-0.80	45,45,45,45	0
33	NA	A	8361	1/1	0.96	0.13	-0.80	48,48,48,48	0
32	MG	D	8055	1/1	0.85	0.16	-0.89	84,84,84,84	0
33	NA	A	8324	1/1	0.92	0.12	-1.06	42,42,42,42	0
33	NA	A	8338	1/1	0.93	0.12	-1.16	59,59,59,59	0
32	MG	A	8086	1/1	0.98	0.10	-1.30	40,40,40,40	0
34	CL	A	8512	1/1	0.94	0.15	-1.33	32,32,32,32	0
32	MG	Z	8109	1/1	0.92	0.14	-1.54	39,39,39,39	0
32	MG	A	8107	1/1	0.97	0.06	-1.79	51,51,51,51	0
32	MG	A	8074	1/1	0.98	0.07	-1.81	12,12,12,12	0
32	MG	U	8073	1/1	0.94	0.12	-1.84	38,38,38,38	0
36	CD	V	8401	1/1	0.68	0.40	-1.86	142,142,142,142	0
36	CD	1	8403	1/1	0.93	0.21	-1.90	139,139,139,139	0
34	CL	N	8518	1/1	0.94	0.17	-1.93	38,38,38,38	0
33	NA	A	8317	1/1	0.96	0.11	-2.19	9,9,9,9	0
33	NA	A	8305	1/1	0.92	0.13	-2.20	33,33,33,33	0
32	MG	A	8003	1/1	0.97	0.12	-2.30	19,19,19,19	0
33	NA	K	8346	1/1	0.96	0.11	-2.32	17,17,17,17	0
35	K	A	8601	1/1	0.94	0.12	-2.44	62,62,62,62	0
36	CD	2	8402	1/1	0.98	0.08	-2.47	52,52,52,52	0
32	MG	A	8062	1/1	0.94	0.11	-2.58	46,46,46,46	0
33	NA	A	8381	1/1	0.98	0.09	-2.64	33,33,33,33	0
32	MG	A	8002	1/1	0.96	0.12	-2.74	42,42,42,42	0
33	NA	A	8320	1/1	0.95	0.11	-2.89	32,32,32,32	0
33	NA	A	8353	1/1	0.99	0.09	-2.99	16,16,16,16	0
32	MG	A	8008	1/1	0.98	0.08	-3.10	41,41,41,41	0
32	MG	C	8065	1/1	0.97	0.07	-3.11	52,52,52,52	0
32	MG	A	8071	1/1	0.81	0.11	-3.16	84,84,84,84	0
32	MG	A	8110	1/1	0.95	0.11	-3.24	23,23,23,23	0
32	MG	A	8058	1/1	0.98	0.11	-3.58	34,34,34,34	0
32	MG	A	8018	1/1	0.94	0.08	-3.66	32,32,32,32	0
32	MG	A	8033	1/1	0.98	0.09	-3.91	22,22,22,22	0
33	NA	N	8347	1/1	0.95	0.11	-3.96	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	8053	1/1	0.92	0.10	-3.98	52,52,52,52	0
32	MG	A	8108	1/1	0.93	0.11	-3.99	73,73,73,73	0
33	NA	C	8345	1/1	0.98	0.10	-4.05	34,34,34,34	0
33	NA	A	8343	1/1	0.94	0.08	-4.08	11,11,11,11	0
32	MG	A	8015	1/1	0.98	0.08	-4.11	46,46,46,46	0
33	NA	R	8348	1/1	0.98	0.06	-4.17	15,15,15,15	0
32	MG	A	8001	1/1	0.82	0.11	-4.21	38,38,38,38	0
32	MG	A	8056	1/1	0.98	0.07	-4.44	41,41,41,41	0
32	MG	A	8004	1/1	0.97	0.11	-4.61	35,35,35,35	0
33	NA	A	8344	1/1	0.96	0.07	-4.65	16,16,16,16	0
32	MG	A	8012	1/1	0.99	0.11	-4.73	34,34,34,34	0
32	MG	A	8096	1/1	0.95	0.10	-5.02	54,54,54,54	0
32	MG	A	8039	1/1	0.97	0.09	-5.07	54,54,54,54	0
32	MG	A	8059	1/1	0.90	0.09	-5.10	33,33,33,33	0
32	MG	A	8088	1/1	0.93	0.08	-5.24	28,28,28,28	0
32	MG	A	8032	1/1	0.97	0.10	-5.42	29,29,29,29	0
32	MG	A	8017	1/1	0.98	0.05	-5.68	28,28,28,28	0
32	MG	A	8035	1/1	0.98	0.06	-5.99	48,48,48,48	0
32	MG	A	8038	1/1	0.98	0.05	-6.90	14,14,14,14	0
32	MG	A	8084	1/1	0.94	0.09	-7.17	40,40,40,40	0
32	MG	A	8052	1/1	0.96	0.05	-7.23	36,36,36,36	0
32	MG	A	8020	1/1	0.99	0.05	-7.27	34,34,34,34	0
32	MG	A	8060	1/1	0.97	0.10	-7.27	48,48,48,48	0
32	MG	A	8080	1/1	0.99	0.06	-7.48	35,35,35,35	0
32	MG	A	8028	1/1	0.97	0.07	-7.56	43,43,43,43	0
32	MG	A	8006	1/1	0.95	0.06	-7.94	48,48,48,48	0
32	MG	A	8010	1/1	0.99	0.07	-8.28	29,29,29,29	0
32	MG	A	8077	1/1	0.97	0.09	-8.31	28,28,28,28	0
32	MG	A	8054	1/1	0.97	0.08	-8.87	50,50,50,50	0
32	MG	A	8019	1/1	1.00	0.05	-9.13	27,27,27,27	0
32	MG	A	8027	1/1	0.92	0.06	-9.19	51,51,51,51	0
32	MG	A	8007	1/1	0.96	0.06	-12.51	24,24,24,24	0
32	MG	A	8014	1/1	0.98	0.05	-13.61	13,13,13,13	0
34	CL	S	8506	1/1	0.97	0.14	-	42,42,42,42	0
32	MG	A	8049	1/1	0.94	0.16	-	62,62,62,62	0
32	MG	A	8092	1/1	0.92	0.17	-	83,83,83,83	0
32	MG	A	8022	1/1	0.94	0.19	-	39,39,39,39	0
32	MG	A	8111	1/1	0.95	0.06	-	54,54,54,54	0
32	MG	A	8117	1/1	0.99	0.15	-	19,19,19,19	0
36	CD	4	8404	1/1	0.73	0.51	-	148,148,148,148	0
33	NA	A	8306	1/1	0.96	0.37	-	36,36,36,36	0
33	NA	A	8363	1/1	0.93	0.19	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	CL	A	8522	1/1	0.88	0.75	-	80,80,80,80	0
32	MG	A	8048	1/1	0.95	0.15	-	47,47,47,47	0
32	MG	A	8063	1/1	0.98	0.08	-	73,73,73,73	0
32	MG	A	8093	1/1	0.95	0.12	-	38,38,38,38	0
34	CL	K	8501	1/1	0.98	0.20	-	58,58,58,58	0
33	NA	A	8307	1/1	0.91	0.10	-	20,20,20,20	0
32	MG	A	8040	1/1	0.93	0.11	-	84,84,84,84	0
32	MG	A	8026	1/1	0.99	0.05	-	15,15,15,15	0
33	NA	B	8351	1/1	0.77	0.18	-	58,58,58,58	0
32	MG	A	8030	1/1	0.99	0.09	-	29,29,29,29	0
32	MG	A	8085	1/1	0.94	0.12	-	79,79,79,79	0
33	NA	A	8301	1/1	0.88	0.16	-	20,20,20,20	0
32	MG	A	8029	1/1	0.98	0.12	-	51,51,51,51	0
33	NA	A	8302	1/1	0.92	0.16	-	24,24,24,24	0
33	NA	E	8304	1/1	0.61	0.16	-	32,32,32,32	0
32	MG	A	8021	1/1	0.97	0.08	-	27,27,27,27	0
32	MG	A	8089	1/1	0.94	0.10	-	64,64,64,64	0
32	MG	A	8099	1/1	0.97	0.10	-	46,46,46,46	0
33	NA	A	8367	1/1	0.94	0.15	-	37,37,37,37	0
34	CL	A	8513	1/1	0.89	0.19	-	64,64,64,64	0
32	MG	A	8091	1/1	0.98	0.07	-	45,45,45,45	0
32	MG	A	8082	1/1	0.90	0.23	-	59,59,59,59	0
32	MG	A	8076	1/1	0.97	0.12	-	61,61,61,61	0
33	NA	A	8334	1/1	0.95	0.05	-	26,26,26,26	0
32	MG	A	8114	1/1	0.94	0.23	-	82,82,82,82	0
32	MG	A	8009	1/1	0.99	0.04	-	19,19,19,19	0
33	NA	A	8342	1/1	0.92	0.17	-	39,39,39,39	0
32	MG	A	8103	1/1	0.93	0.20	-	69,69,69,69	0
33	NA	A	8328	1/1	0.96	0.14	-	24,24,24,24	0
32	MG	A	8090	1/1	0.87	0.21	-	11,11,11,11	0
34	CL	R	8511	1/1	0.92	0.13	-	57,57,57,57	0
33	NA	A	8354	1/1	0.85	0.20	-	40,40,40,40	0
34	CL	K	8516	1/1	0.93	0.19	-	40,40,40,40	0
32	MG	A	8023	1/1	0.86	0.10	-	42,42,42,42	0
32	MG	A	8100	1/1	0.90	0.15	-	48,48,48,48	0
34	CL	K	8502	1/1	0.90	0.12	-	56,56,56,56	0
32	MG	A	8051	1/1	0.97	0.07	-	66,66,66,66	0
32	MG	A	8016	1/1	0.97	0.08	-	43,43,43,43	0
33	NA	A	8313	1/1	0.97	0.17	-	64,64,64,64	0
33	NA	A	8319	1/1	0.94	0.14	-	39,39,39,39	0
32	MG	A	8068	1/1	0.97	0.12	-	40,40,40,40	0
32	MG	L	8069	1/1	0.97	0.10	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	A	8330	1/1	0.91	0.18	-	46,46,46,46	0
33	NA	A	8316	1/1	0.96	0.12	-	31,31,31,31	0
33	NA	A	8357	1/1	0.78	0.10	-	53,53,53,53	0
32	MG	A	8098	1/1	0.99	0.20	-	43,43,43,43	0
32	MG	A	8043	1/1	0.97	0.06	-	58,58,58,58	0
32	MG	A	8115	1/1	0.91	0.10	-	46,46,46,46	0
32	MG	A	8024	1/1	0.88	0.56	-	99,99,99,99	0
32	MG	A	8031	1/1	0.96	0.04	-	14,14,14,14	0
33	NA	A	8385	1/1	0.95	0.25	-	28,28,28,28	0
32	MG	A	8081	1/1	0.85	0.18	-	64,64,64,64	0
35	K	A	8603	1/1	0.91	0.43	-	76,76,76,76	0
33	NA	A	8375	1/1	0.94	0.25	-	53,53,53,53	0
33	NA	A	8384	1/1	0.27	1.12	-	106,106,106,106	0
32	MG	A	8036	1/1	0.99	0.06	-	41,41,41,41	0
32	MG	A	8011	1/1	0.97	0.07	-	25,25,25,25	0
32	MG	A	8070	1/1	0.82	0.81	-	70,70,70,70	0
32	MG	A	8066	1/1	0.90	0.07	-	70,70,70,70	0
32	MG	A	8083	1/1	0.98	0.07	-	47,47,47,47	0
33	NA	A	8318	1/1	0.96	0.14	-	37,37,37,37	0
32	MG	A	8050	1/1	0.81	0.22	-	77,77,77,77	0
32	MG	A	8118	1/1	0.84	0.33	-	31,31,31,31	0
32	MG	A	8101	1/1	0.85	0.16	-	38,38,38,38	0
33	NA	A	8377	1/1	0.84	0.32	-	77,77,77,77	0
32	MG	A	8119	1/1	0.96	0.10	-	30,30,30,30	0
36	CD	P	8405	1/1	0.72	0.19	-	154,154,154,154	0
32	MG	A	8042	1/1	0.96	0.13	-	31,31,31,31	0
32	MG	A	8005	1/1	0.98	0.14	-	47,47,47,47	0
33	NA	A	8329	1/1	0.97	0.09	-	33,33,33,33	0
32	MG	A	8072	1/1	0.96	0.15	-	88,88,88,88	0
33	NA	A	8341	1/1	0.88	0.10	-	17,17,17,17	0
34	CL	A	8514	1/1	0.96	0.12	-	51,51,51,51	0
32	MG	A	8097	1/1	0.96	0.23	-	37,37,37,37	0
32	MG	A	8094	1/1	0.98	0.05	-	60,60,60,60	0
32	MG	A	8104	1/1	0.75	0.38	-	51,51,51,51	0
32	MG	A	8106	1/1	0.93	0.13	-	62,62,62,62	0
33	NA	A	8369	1/1	0.85	0.23	-	53,53,53,53	0
33	NA	A	8308	1/1	0.91	0.12	-	50,50,50,50	0
33	NA	A	8311	1/1	0.87	0.22	-	50,50,50,50	0
32	MG	A	8079	1/1	0.96	0.09	-	24,24,24,24	0
32	MG	B	8095	1/1	0.89	0.06	-	68,68,68,68	0
33	NA	J	8322	1/1	0.64	0.45	-	56,56,56,56	0
33	NA	A	8360	1/1	0.96	0.55	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	CL	A	8517	1/1	0.93	0.24	-	49,49,49,49	0
33	NA	T	8312	1/1	0.70	0.76	-	69,69,69,69	0
34	CL	O	8507	1/1	0.95	0.14	-	54,54,54,54	0
32	MG	A	8045	1/1	0.91	0.12	-	61,61,61,61	0
32	MG	A	8061	1/1	0.91	0.06	-	35,35,35,35	0
32	MG	A	8037	1/1	0.98	0.12	-	45,45,45,45	0
33	NA	A	8315	1/1	0.99	0.11	-	27,27,27,27	0
32	MG	A	8025	1/1	0.97	0.09	-	54,54,54,54	0
32	MG	A	8046	1/1	0.89	0.07	-	62,62,62,62	0
32	MG	A	8113	1/1	0.94	0.13	-	40,40,40,40	0
32	MG	A	8041	1/1	0.91	0.36	-	62,62,62,62	0
34	CL	C	8509	1/1	0.97	0.34	-	74,74,74,74	0
32	MG	A	8116	1/1	0.88	0.20	-	80,80,80,80	0
32	MG	A	8087	1/1	0.86	0.18	-	52,52,52,52	0
32	MG	A	8034	1/1	0.98	0.05	-	32,32,32,32	0
33	NA	A	8349	1/1	0.97	0.29	-	33,33,33,33	0
32	MG	A	8102	1/1	0.95	0.84	-	82,82,82,82	0
33	NA	A	8310	1/1	0.84	0.21	-	31,31,31,31	0
33	NA	A	8336	1/1	0.92	0.15	-	46,46,46,46	0
34	CL	Z	8520	1/1	0.91	0.14	-	30,30,30,30	0
32	MG	A	8075	1/1	0.94	0.11	-	38,38,38,38	0
34	CL	A	8503	1/1	0.86	0.27	-	55,55,55,55	0
33	NA	A	8352	1/1	0.93	0.47	-	37,37,37,37	0
32	MG	A	8047	1/1	0.98	0.14	-	45,45,45,45	0
33	NA	A	8370	1/1	0.88	0.37	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.